Department of Energy
Washington, DC 20585

June 29, 2004

The Honorable John T. Conway
Chairman
Defense Nuclear Facilities Safety Board
625 Indiana Avenue, NW, Suite 700
Washington, D.C. 20004-2941

Dear Mr. Chairman:

In September 2003, the Department reported interim completion of Commitment 4.2.1.4 in the Department's Implementation Plan for Software Quality Assurance (SQA) in response to Board Recommendation 2002-1. This commitment required the Department to issue code-specific guidance reports on the use of safety analysis toolbox codes identifying applicable regimes in accident analysis, default inputs, and special conditions for use. The September 2003 correspondence also indicated that the guidance reports may be updated based on the results of the gap analysis performed for Commitment 4.2.1.3.

The Department completed additional code developer and peer reviews to further improve their accuracy and issued the final gap analysis reports, which I provided to you on May 12, 2004. The code-specific guidance reports for the MACCS2, ALOHA, EPICODE, MELCOR, GENII, and CFAST toolbox codes have now been updated to reflect the final gap analysis conducted for each toolbox code and are attached.

Now that we have completed these reports, the Central Registry processes and procedures are being developed in conjunction with DOE Order 414.1C, *Quality Assurance*, and DOE Guide 414.1-4, *Implementation Guide for Use with Supplemental Safety Software Quality Requirements of DOE Order 414.1*. Questions concerning this commitment may be directed to Chip Lagdon at (301) 903-4218 or me at (301) 903-8008.

Sincerely,

Frank B. Russo
Deputy Assistant Secretary
for Corporate Performance Assessment

Attachments

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SEPARATION

PAGE

MACCS2 Computer Code Application Guidance for Documented Safety Analysis

Final Report

U.S. Department of Energy
Office of Environment, Safety and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

June 2004

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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the MACCS2 computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the MACCS2 documentation provided by the code developer. MACCS2 is one of six computer codes designated by the DOE Office of Environmental, Safety and Health as a toolbox code for safety analysis.

Suggestions for corrections or improvements to this document should be addressed to –

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1. Entire Document	1. Final Draft for Review	1. Original Issue
2. Entire Report	2. Final Report –June 1, 2004	2. Incorporated comments from reviewers.

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MACCS2 Computer Code Application Guidance for Support of Documented Safety Analysis

EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The DOE response to the Recommendation, *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, commits to a number of actions to improve Software Quality Assurance (SQA) in safety analysis and design software. The development and maintenance of a collection, or "toolbox," of high-use, SQA-compliant safety analysis codes is one of the major commitments. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications. The MELCOR Accident Consequence Code System (MACCS) code and its successor MACC2, developed and maintained by Sandia National Laboratories (SNL), are designated as toolbox codes.

The MACCS2 code is likely to require completion of quality assurance improvement measures before meeting current SQA standards. In the interim period before these changes are completed, MACCS2 is still considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available user's manual information.

The MACCS/MACCS2 guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

This report is supplemental to, and does not supersede, the existing suite of MACCS2 documentation available from the SNL software developer. While not ensuring correct application of MACCS2 in every DOE consequence analysis context, use of the information contained here will minimize potential user errors and further standardize the use of MACCS2 in appropriate DSA regimes of applicability.

1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and in the variability of guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its Recommendation to DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the Board's concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include:

(i) identification of a set of accident analysis software that is widely used in the DOE Complex, and
(ii) issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regime in accident analysis, default inputs, and special conditions for use.

Safety analysis software was designated for the DOE "toolbox" by the DOE Office of Environment, Safety and Health (DOE/EH) in March 2003 (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications*, (DOE, 2002b) (See http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf), and includes the MELCOR Accident Consequence Code System (MACCS) code and its successor MACCS2.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in the body of this report. This code-specific document will be maintained and updated until a minimum qualification SQA condition is achieved.

The contents of this report are applicable in the interim period until measures are completed to bring MACCS2 into compliance with defined SQA standards. The primary objective of the guidance report is to provide information on the use of MACCS2 for supporting DOE safety basis accident analysis. Specifically, the report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Overcoming known vulnerabilities and avoiding code errors
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications
- Default input value recommendations for site-independent parameters, and
- Citations of currently available SQA documentation.

This report is intended to complement existing MACCS2 user's documentation. Nevertheless, the full suite of MACCS and MACCS2 reports should be requested and utilized by the DOE safety analyst to best apply the capability of this software. Current MACCS and MACCS2 documentation is broader in the coverage of the full range of capabilities of MACCS2, and the spectrum of inputs needed depending upon the application, but lack targeted guidance for particular applications such as DOE DSA accident analyses. Furthermore, the goal of the MACCS2 guidance document is to identify limitations and vulnerabilities not found elsewhere.

MACCS/MACCS2 Guidance Document

The MACCS/MACCS2 guidance document is written using the following set of sections. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830. More information follows on the scope and purpose of this document. The next major section is a summary description of MACCS/MACCS2. A third section discusses applicable regimes for using MACCS/MACCS2 in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, succeeds this section. Following this discussion are sections on special conditions for use of the software and software limitations. Several sample cases are then provided, followed by acronyms and definitions, references, and appendices.

1.1 Background: Overview Of Toolbox Software In Context Of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software, will be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements and demonstrate that the code is

being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as "toolbox" codes. Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

The MACCS/MACCS2 guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

1.3 Purpose

The MACCS and MACCS2 codes are part of the designated group of software to be placed in the DOE Safety Analysis Toolbox. Prior to being brought under configuration management in the toolbox, MACCS2 and other designated software will be part of a SQA review. In the interim before this review process is completed, MACCS2 can be still be applied for safety analysis purposes as long as the safety analyst understands the strengths and limitations of the software and is cognizant of the information provided in this report and documentation provided by the code developer. If it is decided that upgrades are warranted, MACCS2 will be brought under configuration control only after this process is completed. At this point, MACCS2 use will be encouraged over that of its predecessor.

Use of the information contained herein will not ensure appropriate use of MACCS2 in all analytical contexts. However, it should minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

It is recognized that other computer codes besides MACCS/MACCS2 exist that perform similar type of atmospheric dispersion and radiological consequence calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for some accident analysis applications that involve releases of radiological material. The relative merits of using a different computer program or using a hand calculation for a given application is a judgment that must be made by the analyst on a case-by-case basis. The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program. As part of this program, the radiological dispersion and consequence assessment (RDCA) Working Group (WG) was established to address issues and evaluate methodologies in the RDCA domain. The RDCA WG (also referred to as WG 5) issued a report that identifies and evaluates methodologies and computer codes to support RDCA applications (O'Kula, 1998).

The RDCA WG 5 report identified the MACCS/MACCS2 computer codes as recommended software with generally broad suitability to safety basis documentation applications. In addition to code recommendations, the report also provides a broad set of recommended "best practices" for modeling radiological releases to the atmosphere.

This report builds upon the WG 5 work to provide guidance and recommendations that are targeted to the use of the MACCS/MACCS2 for atmospheric dispersion and radiological consequence calculations in the context of DSA-type applications. Specifically, the guidance is best suited for:

- Consequence analysis calculations
- Mitigated and unmitigated hazard analysis
- Bounding analysis for final hazard categorization, and
- Confirmatory calculations for evaluating mitigative and preventive safety controls.

2.0 SUMMARY DESCRIPTION OF THE MACCS2 CODE

This section provides a summary form description of the MACCS2 code. It assumes an understanding of the principles of source term development from postulated accident conditions, the interface with dispersion conditions in the atmosphere, and the overall assessment of radiological dose to receptors. These concepts are discussed in Appendix A to DOE Standard 3009-94 (DOE, 2000).

Users requiring additional background information on dispersion and consequence analysis before reviewing input file preparation are referred to Appendix A in this document, "Overview of Atmospheric Dispersion and Consequence Analysis".

2.1 MACCS/MACCS2 Summary Description

MACCS2 (Chanin, 1998) is a Gaussian plume model for calculation of radiological atmospheric dispersion and consequences. MACCS2 is IBM PC compatible, and is written in FORTRAN 77 and 90. The code is under development at Sandia National Laboratories (SNL) and is an update to MACCS.[1] Since the issuance of DOE-STD-3009-94 for nuclear facility accident analysis, MACCS2 has been used for DOE applications primarily as a tool for deterministic consequence analysis. This information is used to support decision-making on control selection in nuclear facilities, specifically identification of safety structures, systems, and components (SSCs).

MACCS2 predicts dispersion of radionuclides by the use of multiple, straight-line Gaussian plumes. The direction, duration, sensible heat, and initial radionuclide concentration may be varied from plume to plume. Crosswind dispersion is treated by a multi-step function and both wet and dry depositions features can be modeled as independent processes. For DSA applications, the MACCS2 user can apply either the stratified random sampling mode or the Latin Hypercube Sampling (LHS) mode to process one year of site-specific meteorological data, with the former approach encouraged for current applications. Based on the meteorological sampling of site-specific data, and application of user-specified dose and/or health effects models, complementary cumulative distribution functions (CCDFs) are calculated for various measures of consequence. The average, median, 95th, and 99.5th percentile consequences are provided in the output.

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[1] The United States Nuclear Regulatory Commission (NRC) sponsored the development of the MACCS code (Chanin, 1990; Jow, 1990; Rollstin, 1990; and Chanin, 1993) as a successor to the CRAC2 code for the performance of commercial nuclear industry probabilistic safety assessments (PSAs). The MACCS code was used in the NUREG-1150 PSA study (NRC, 1990a) in the early 1990's. Prior to the code being released to the public, the MACCS code was independently verified by Idaho National Engineering and Environmental Laboratory (Dobbe, 1990). After verification, the NRC released MACCS, Version 1.5.11 for use by the public. Examples of MACCS applied in this period include commercial reactor PSAs (both U.S. and international), as well as non-reactor nuclear facilities (primarily U.S.).

The major enhancements in the MACCS2 code over its MACCS predecessor are in the number of nuclides included in the dose conversion factor database, the number of daughters in the decay chain, the emergency response model, the food pathway model, and the inclusion of consequences from meteorological data in a sector as opposed to the whole site.

Other features that have been added to MACCS2 as well as those retained from MACCS are noted in Section 2.2. Table 2-1 contains summary information on MACCS2, based on the software package available from the Radiation Safety Information Computational Center (RSICC). The same version will be transmitted directly from the SNL developer upon authorization from the Nuclear Regulatory Commission.

The basis for the report is Version 1.12 of MACCS2. In March 2004, Version 1.13.1 was released to RSICC, however, nearly all of the report is applicable to the newer version. A set of user notes for Version 1.13.1 is attached to this report as Appendix F.

Table 2-1. Summary Description of MACCS2 Software

Type	Specific Information
Code Name	MACCS2 - MELCOR Accident Consequence Code System for the Calculation of the Health and Economic Consequences of Accidental Atmospheric Radiological Releases
Developing Organization and Sponsor	Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (primary) and U.S. Department of Energy (minor)
Version of the Code	Version 1.12
Auxiliary Codes	AUXILIARY CODES: DOSFAC2:NRC dose conversion factor (DCF) preprocessor. FGRDCF: DCF preprocessor based on the DCF databases of Federal Guidance Reports 11 and 12 from ORNL (DLC-172). IDCF2: DCF preprocessor based on the IDCF code developed at the Idaho National Engineering Laboratory. COMIDA2: Food pathway preprocessor based on the COMIDA (PSR-343) food pathway preprocessor developed at the Idaho National Engineering Laboratory. Note: MELMACCS (MACCS input generator from MELCOR runs) and CHAIN (Radionuclide progeny) are auxiliary codes, and not available from RSICC. CHAIN was developed by Keith Eckerman at ORNL.
Software Platform/Portability	FORTRAN 77/90, PC based some system dependencies
Coding and Computer	Fortran 77, PC based 80486 or Pentium processor (C00652/PC486/00).
Technical Support	Nathan Bixler Sandia National Laboratories P.O. Box 5800 Albuquerque, NM 87185-0748 (505) 845-3144 nbixler@sandia.gov;
Code Procurement	Radiation Safety Information Computational Center (RSICC)[2] Oak Ridge National Laboratory Post Office Box 2008 Bethel Valley Road Oak Ridge, Tennessee 37831-6171 Phone: 865-574-6176; Fax: 865-241-4046 Email: pdc@ornl.gov; Internet: http://www-rsicc.ornl.gov/rsicc.html Contact Nathan Bixler (above) or Jocelyn Mitchell @ NRC for authorization Phone: 301-415-5289 Email: jam@nrc.gov

[2] Recommended procurement route is through N. Bixler/J. Mitchell (see below). Except where noted, items shown here are valid when MACCS2 is obtained through RSICC.

Table 2-1. Summary Description of MACCS2 Software (Continued)

Code Package	CCC-652; Included are the references cited below and the Fortran source code, executables and data, which are distributed on 1 CD in self-extracting compressed DOS files.
Contributors	Sandia National Laboratories, Albuquerque, New Mexico, Oak Ridge National Laboratory, Oak Ridge, Tennessee, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID
Documentation Supplied with Code Transmittal	1. D. Chanin and M. L. Young, "Code Manual for MACCS2, User's Guide," NUREG/CR-6613, Vol. 1, SAND97-0594 (May 1998), Sandia National Laboratories, Albuquerque, NM. 2. D. Chanin and M. L. Young, "Code Manual for MACCS2, Preprocessor Codes COMIDA2, FGRDCF, IDCF2," NUREG/CR-6613, Vol. 2, SAND97-0594 (May 1998), Sandia National Laboratories, Albuquerque, NM. 3. M. L. Young and D. Chanin, "DOSFAC2 User's Guide," NUREG/CR-6547, SAND97-2776 (December 1997). 4. H-N. Jow, J. L. Sprung, J. A. Rollstin, L. T. Ritchie, D. I. Chanin, "MELCOR Accident Consequence Code System (MACCS), Model Description," NUREG/CR-4691, SAND86-1562, Vol. 2 (February 1990). 5. J. Gregory, "Software Defect Notifications" (May 1998). 6. M. L. Young, "READMAC2.txt" (April 1997).
Nature of Problem	MACCS2 simulates the impact of accidental atmospheric releases of radiological materials on the surrounding environment. This package is a major enhancement of the previous CCC-546/MACCS 1.5.11 package. The principal phenomena considered in MACCS are atmospheric transport, mitigative actions based on dose projection, dose accumulation by a number of pathways including food and water ingestion, early and latent health effects, and economic costs. MACCS can be used for a variety of applications including probabilistic risk assessment (PRA) of nuclear power plants and other nuclear facilities, sensitivity studies to gain a better understanding of the parameters important to PRA, and cost benefit analysis.
Method of Solution	MACCS2 contains simple models with convenient analytical solutions. A MACCS2 calculation consists of three phases: input processing and validation, phenomenological modeling and output processing. The phenomenological models are based mostly on empirical data, and the solutions they entail are usually analytical in nature and computationally straightforward. The modeling phase is subdivided into three modules. ATMOS treats atmospheric transport and dispersion of material and its deposition from the air utilizing a Gaussian plume model with Pasquill-Gifford dispersion parameters. EARLY models consequences of the accident to the surrounding area during an emergency action period. CHRONC considers the long term impact in the period subsequent to the emergency action period. Detailed meteorological, population, and economic and health data are required depending upon the type of analyses to be performed and output required. Model parameters can be provided by the user via input facilitating the analysis of consequence uncertainties due to uncertainties in the model parameters.

Table 2-1. Summary Description of MACCS2 Software (Continued)

Restrictions or Limitations	MACCS2 and MACCS do not comply fully with Appendix A, DOE-STD-3009-94 (NRC Regulatory Guide 1.145 Position 3) methodology for determination of direction-independent 95th percentile dose to the offsite individual. It may be used to conservatively evaluate the 95th percentile direction-independent dose to receptors equidistant to the source. 7. The atmospheric model included in the code does not model the impact of terrain effects on atmospheric dispersion, nor can it accept more than one weather spatial location. Like all Gaussian models, MACCS2 is not well suited for modeling dispersion close to the source (less than 100 meters from the source) or long-range dispersion (beyond 15 to 20 miles from the source).[3] Momentum effects of highly energetic releases can be approximated. The economic model included in the code models only the economic cost of mitigative actions.
Run Time	One source term for one meteorological sequence requires less than one second on a Pentium 2 or 3 GHZ. Running two source terms and sampling a year of weather data (Sample Problem A) requires approximately times on the order of seconds to minutes, depending on the complexity of the problem.
Computer Hardware Requirements	IBM-compatible 486/DX or Pentium PC with 8 MB of RAM The MACCS2 package files require approximately the following disk space when decompressed: MAC2ZIPA.EXE 6 MB MAC2ZIPB.EXE 4 MB FGR_DCF.EXE 2 MB COMIDA2A.EXE 3 MB IDCF_2.EXE 2 MB DOSFAC_2.EXE 4 MB COMIDA2B.EXE 3 MB. Approximately 30 MB of hard disk space is required to load the complete MACCS2 package. Approximately 11 MB of hard disk space is required to load MACCS2 without the preprocessors included in the MACCS2 package.
Computer Software Requirements	The MACCS2 software was developed in a DOS environment. Lahey F77L-EM/32 Version 5.2 compiler was used to create the executables included in the code transmittal package from RSICC, which run successfully in a DOS window of Windows 3.1, Windows 95, Windows NT, and Windows 2000. The programs can also be compiled for those PC operating systems with the Microsoft Powerstation FORTRAN 1.0a compiler. The distributed executables will not run under Windows XP. However, upon request, the code developer will supply executables for Windows XP that were compiled using Compaq FORTRAN 95.

[3] Typical PRA calculations often apply a 1000-mile radius basis.

Table 2-1. Summary Description of MACCS2 Software (Continued)

Other Versions Available	MACCS 1.5.11.1 (PC486); MACCS 1.5.11.0 (IBM RISC); Version 1.13.1 was released in March 2004 to RSICC for distribution. See Appendix F for "readme" text file notes.

2.2 OVERVIEW OF MACCS/MACCS2 FOR REGULATORY APPLICATIONS

For regulatory applications, the MACCS/MACCS2 codes are used to calculate the fifty-year Total Effective Dose Equivalent (TEDE) to specified stationary receptors from hypothetical atmospheric releases of radioactivity. The radiological dose is reported in DSA applications. The TEDE is calculated for both onsite and offsite receptors using standard uptake assumptions and dose conversion database values. Sensitivity studies may also be performed with MACCS/MACCS2 models to show the relative benefits of evacuation, sheltering, interdiction, and the effects of various shielding assumptions, although these models are generally not invoked in standard DSA applications.

The MACCS/MACCS2 codes predict dispersion of radionuclides by the use of multiple, straight-line Gaussian plumes. The direction, duration, sensible heat, and initial radionuclide concentration may be varied from plume to plume. Crosswind dispersion is treated by a multi-step function approximating the Gaussian, and both wet and dry depositions features can be modeled as independent processes. Meteorological variability can be treated in MACCS/MACCS2 with a stratified random sampling algorithm. Based on the sampled distribution, and application of user-specified dose and/or health effects models, complementary cumulative distribution functions (CCDFs) are calculated for various measures of consequence. The 50^{th} (median), 90^{th}, 95^{th}, 99^{th}, and 99.5^{th} percentile doses are provided in the output as well as the mean and peak values.

Dose conversion factors (DCFs) relate environmental concentrations and intakes to resultant human doses for specific exposure pathways, organs, and radionuclides. Doses arise from both internal and external exposures. The internal exposures consist of inhalation (from the plume and from resuspension) and ingestion. The external exposures are from cloudshine, groundshine, skin deposition, and direct (prompt) radiation from a criticality.

A total of 825 radionuclides and models for decay chains are included in MACCS2. MACCS2 models decay chains up to six generations taking into consideration half-lives, decay products, and branching ratios for those decay products. MACCS, in contrast, models a smaller number of decay chains and is limited to simple parent-daughter decay (i.e., two-member chains).

The MACCS2[4] code makes use of an input file that contains Inhalation DCFs (IDCFs) as well as DCFs for ingestion and dose coefficients for cloudshine and groundshine. Typically inhalation is the dominant pathway for dose, and recommended sources for the IDCFs are given in Section 4 of this report.

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[4] The remainder of this report will cite "MACCS2" to imply both MACCS2 and MACCS. If there is a difference, it will be explicitly specified as "MACCS2" or "MACCS".

The major enhancements in the MACCS2 code include more user options on initializing the geometry and size of the plume and in specifying the system of dispersion parameters through a look-up table. Other output types that are also capable of being output with MACCS2 are:

- the output of the atmospheric dispersion data in a complementary cumulative distribution function (CCDF)
- the sector independent peak dose for any organ, and the
- sector-dependent peak dose for any organ.

3.0 APPLICABLE REGIMES

The objective of this section is to present a discussion of MACCS2 applicability from two perspectives: (1) in terms of its overall function as a key step in accident analysis; and (2) noting the phenomenological regimes in which it provides an approximate model of dispersion in the environment and the resulting radiological exposure to downwind individuals (receptors).

3.1 Overall Application in Safety Analysis

The Department of Energy (DOE) evaluates and approves the operation of its nuclear facilities via the safety analysis process outlined in DOE Rule, 10 CFR 830 – Subpart B and DOE-STD-3009-94 (CFR, 2001; DOE, 2002a). This safety analysis process requires the development of a Documented Safety Analysis per the Rule language and includes two key types of analyses: (1) hazard analysis and (2) accident analysis.

Hazard analysis is the cornerstone of the DOE safety analysis process and is largely a qualitative process by which

- the hazards in the facility are identified,
- a spectrum of accidents are postulated for each hazard,
- a qualitative evaluation of accident likelihood and consequence is made, and
- all preventive and mitigative systems or controls are identified along with a qualitative measure of their importance.

The final product of the hazard analysis gives rise to a list of which systems or controls are important to safety and therefore are designated as safety-significant. This designation will lead to a formal commitment on the part of the facility contractor to maintain the safety function of these systems through technical safety requirements (TSRs).

Accident analysis is a follow-on activity to the hazard analysis. The focus of the DBAs is public exposure, and therefore, a quantitative calculation of dose to the maximally exposed offsite individual (MOI) is made for each DBA. The purpose of the dose calculations is to determine if some of the safety-significant systems identified in the hazard analysis should have their safety designation raised to safety-class. The standard approach for the accident analysis is outlined below in terms of the source term and the radiological dispersion and consequence analysis phases.

3.1.1 Source Term Analysis

The radiological consequences are typically established using the methods discussed in the DOE-HDBK-3010-94 (DOE, 1994a). Since the dose from the inhalation pathway will usually dominate the overall dose from most non-reactor facilities, the source term may be quantified using from the five-factor formula:

$$ST = MAR \cdot DR \cdot ARF \cdot RF \cdot LPF \qquad \text{(Equation 3-1)}$$

where:

- Source term (ST) is the total quantity of respirable material released to the atmosphere during the postulated accident condition.
- Material-at-Risk (MAR) is the total quantity of radionuclides (in grams or curies of activity for each radionuclide) available to be acted on by a given physical stress.
- Damage Ratio (DR) is the fraction of the MAR actually impacted by the accident-generated conditions.
- Airborne Release Fraction (ARF) is the fraction of a radioactive material suspended in air as an aerosol and thus available for transport due to a physical stress from a specific accident condition.
- Respirable Fraction (RF) is the fraction of airborne radionuclides as particles that can be transported through air and inhaled into the human respiratory system and is commonly assumed to include particles 10-μm Aerodynamic Equivalent Diameter (AED) and less.
- Leakpath Factor (LPF) is the fraction of the radionuclides in the aerosol transported through some confinement deposition system (e.g., facility rooms, ductwork) or filtration mechanism (e.g., HEPA or sand filters).

For most accident analyses the MAR is best defined as the maximum inventory that is permitted within the room, area or facility. While it is permissible to exclude material forms that are considered to be unaffected by an accident condition from the MAR, experience suggests that for these forms the DR is usually best set to zero for the release mechanism. The overall result using either approach is the same, but by assigning DR values to each combination of inventory form and release mechanism, there is the expectation that each credited form (e.g., a shipping package that is certified to withstand the postulated fire severity) is also reviewed against secondary events (e.g., building collapse initiated by a fire) and therefore, less likely to be overlooked.

The ARF and RF values presented in DOE-HDBK-3010-94 are derived from discrete experiments that typically evaluated a single release mechanism. For example, in a severe fire there may be many mechanisms occurring simultaneously. Powdered metals might be subject to entrainment by fire-induced air currents, falling because of equipment (glove box) collapse, and impact because of objects falling into the exposed fire. In addition, multiple occurrences could occur for specific mechanisms (e.g., impact of falling object on a stable powder). Aqueous solutions could be subject to boiling within the storage tank, spillage because of a tank collapse, and rapid evaporation plus splashing as the liquid sits in a diked area during the same postulated fire. Solid metals can be subject melting, dripping and burning during the same event. To accommodate multiple-mechanism events, it is common to consider the ARF and RF values for each mechanism in the source term estimate.

Just as with the (ARF·RF) term, there can be multiple LPF terms applied to a single material form (e.g., room leakage, ventilation system deposition, filtration system effectiveness). Thus, their cumulative effect must be accounted for. There can be interdependence between the LPF and DR in some applications. If a shipping package is considered to leak during a fire, the leakpath effect as the material exits the packaging can be accounted for as an LPF or a DR. Based on experience, it is recommended that source term reductions related to localized conditions such as at shipping packages, and glove boxes be accounted for in the DR term. This approach allows the source term contribution from individual rooms to be readily compared. It also simplifies comparisons between the room source term and the building source term.

Based on the above discussion, Equation (1) can be generally reformatted as:

$$ST_{jk} = \sum_{i=1}^{n_i} \left\{ MAR_{ij} \cdot DR_{ijk} \cdot \left[(ARF \cdot RF)_{ijk} \cdot \left(\sum_{m=1}^{n_m} LPF_m \right)_{ijk} \right] \right\} \qquad \text{(Equation 3-2)}$$

where:

- i is the MAR component in a specific form
- j is the MAR component by radionuclide species (e.g., ^{238}Pu, ^{239}Pu)
- k is the release mechanism
- m is the filtration or deposition stage
- n is the number of parameters for the form, type, mechanism or stage based on the subscript.

Thus, the source term is usually expressed in terms of an isotopic activity distribution for each release mechanism. Source term components that are associated with the same release duration can be combined, but source term components that have different release mechanisms should be kept separate to account for time-dependent variance in atmospheric dispersion for consequence assessment.

Note that the DR, but not the MAR, is shown in Equation (2) as a function of the release mechanism (k subscript), based upon the recommendation above on how to best handle the interplay between the MAR and the DR. Frequently, the DR, ARF, RF, and LPF terms are specified independently of the type, and the j subscript can be dropped from these terms as applicable.

3.1.2 Dispersion and Consequence Analysis

Once the source term is established, the consequences to the receptors can be estimated. For fires scenarios at facilities with relatively short distances to the site boundary, the receptor at the site boundary may be exposed to lower concentrations as a result of plume buoyancy that can cause lofting of the plume above the receptor. Under these circumstances, higher receptor

exposures can be expected downwind of the site boundary as the effects of increasing downwind plume growth progressively makes plume rise effect less significant. The touchdown point refers to the location of maximum receptor concentration. Thus, the maximally exposed individual for a lofted plume is not at the site boundary, but rather at the touchdown point. Rather than evaluating for this point, it can be more cost effective to estimate the fire consequences as a ground level release with the maximally exposed individual at the site boundary. While the results will be higher than the plume-buoyancy credited analysis, the increase may not be significant when compared to the uncertainties in the analysis and the analysis complexity.

Typically the off-site radiological consequences are expressed as the total effective dose equivalent (TEDE) to the receptor at the highest exposure conditions. For most accident types this is at or near the site boundary. The TEDE includes the 50-year committed effective dose equivalent (CEDE) from inhalation both during plume passage and later from resuspension, the cloudshine effective dose equivalent (EDE), the groundshine EDE, and the skin absorption EDE. This TEDE calculation does not include the ingestion CEDE from consumption of contaminated water and foodstuffs. The inhalation CEDE is usually the dominant contributor and its relationship to the source term is highlighted below.

The basic equation for the radiological consequences to an individual receptor (i.e., stationary at a specific downwind location) from the inhalation pathway during plume passage is:

$$\text{Receptor Inhalation CEDE} = BR \cdot \sum_{k=1}^{n_k} \left\{ \left(\frac{\chi}{Q} \right)_k \cdot \sum_{j=1}^{n_j} \left[ST_{jk} \cdot C_j \cdot IDCF_j \right] \right\} \qquad \text{(Equation 3-3)}$$

where: j, k, n are as defined in Equation 3-3 above

BR is the breathing rate of the individual exposed to the plume of released radiological material, with typical units of m^3/s.

C_j is the specific activity of isotope j, with typical units of Ci/kg if ST is in mass units (kg), a value of unity if ST is in conventional activity units (Ci).

$IDCF_j$ is the inhalation dose conversion factor for unit activity uptake of isotope j, with typical units of [rem/Ci] or [Sv/Bq].

$(\chi/Q)_k$ is the downwind dilution factor from atmospheric dispersion, which represents the time-integrated concentration at a specific downwind location that is normalized by the quantity released to the atmosphere, with typical units of s/m^3.

When the ST value is input into the MACCS2 code, the MACCS2 output provides the TEDE values at the requested receptor locations that will include the contribution from the plume-passage inhalation CEDE as well as the contributions from resuspension inhalation CEDE, cloudshine EDE, groundshine EDE, and skin absorption EDE.

The sequence of steps that are outlined above represents the recommended approach for calculating receptor consequences. Sometimes for matters of convenience, other approaches besides direct input of the ST value into the MACCS code are used to calculate consequences. Two of these are described below. An advantage that both these approaches share is that they allow for MACCS consequence calculations to be performed independently of the source term calculations, which is a consideration when faced with a demanding schedule.

Recall that the DR, ARF, RF, and LPF terms are frequently specified independently of the type, and the j subscript can be dropped from these terms in Equation (2). Sometimes under these circumstances, an analyst uses a normalized MAR that equals the MAR divided by the total inventory mass or total inventory volume and inputs the normalized MAR into the MACCS calculation. Under these circumstances, the consequence calculations of MACCS yield normalized TEDE values that represent the receptor TEDE per unit quantity of mass or volume of respirable material that is released to the atmosphere for each release mechanism. The product of these TEDEs with the corresponding source term mass or volume (ST quantity as defined by Equation (3-4) below) will yield the receptor dose for each of the release mechanisms.

$$(\text{ST quantity})_k = \sum_{i=1}^{n_i} \left\{ (\text{inventory mass or volume})_i \cdot DR_{ik} \cdot \left[(ARF \cdot RF)_{ik} \cdot \left(\sum_{m=1}^{n_m} LPF_m \right)_{ik} \right] \right\}$$

(Equation 3-4)

and

$$\text{Receptor TEDE} = \sum_{k=1}^{n_k} \{ (\text{ST quantity})_k \cdot (\text{normalized TEDE})_k \}$$

(Equation 3-5)

Another approach that is sometimes employed is to individually input unit activity values of the inventory into the MACCS code for each release mechanism to yield unit-activity TEDEs. Recall, that the release duration that is associated with each release mechanism is a variable that factors into the χ/Q value that is calculated by MACCS. So, unit-activity TEDEs must be calculated individually for the various time durations that represent the various release mechanisms. With the unit-activity approach, the following equation is used to determine the receptor consequences.

$$\text{Receptor TEDE} = \sum_{j=1}^{n_j} \sum_{k=1}^{n_k} \{ ST_{jk} \cdot (\text{unit TEDE})_{jk} \}$$

(Equation 3-6)

3.1.3 Computer Codes for Accident Analysis

The safety analyst may use hand calculations or computer codes to calculate source term and dispersion values. The computer codes chosen by the safety analyst fall into several categories. The categories of codes are

- radiological atmospheric dispersion codes,
- chemical atmospheric dispersion codes,
- fire modeling codes, and
- leak-path analysis codes.

The analyst typically applies one or more of these types of codes to calculate parameters such as DR, LPF, and χ/Q, or to integrate over groups of these parameters. The effect of the quality of these codes on the overall safety analysis process can be evaluated qualitatively by examining the role that these parameters play in the overall safety process.

Qualitative Effect of the Codes on Safety Analysis

The gross effect of the use of computer codes can be evaluated by examining their effect on the final MOI dose values calculated as part of the accident analysis. The values chosen or calculated for each parameter in the dose equation are near the conservative tail of any distribution that would be assigned to the individual parameter. Therefore, when each parameter is multiplied using the five-factor formula to obtain the dose, the conservatism in the calculation grows. If applied consistently in each phase of the process and in a reasonably bounding manner, this large conservatism in the calculation has always provided the DOE safety analysis process with sufficient margin when the doses are used to make decisions regarding safety. Even if a single value in the dose calculation were off by an order of magnitude, the resulting value would still not approach the mean value of dose if a cumulative distribution of dose also were calculated.

MACCS2 is used to calculate the appropriate dilution factor and ultimately quantify the radiological dose. Their net effect on safety then is related to their input in selecting safety-class systems, structures, and components (SSCs).

MACCS2 and other atmospheric dispersion and radiological consequence codes are used in analyzing atmospheric dispersion and the subsequent radiological consequence of accidental releases of radioactivity from postulated accident conditions. Codes of this type of are used primarily to calculate the appropriate dilution factor for atmospheric transport of puffs or plumes and ultimately quantify the radiological dose that is received by the maximally exposed offsite individual (MOI). The 95^{th} percentile of the distribution of doses to the MOI is the comparison point for assessment against the evaluation guideline (EG). Consequently, the importance of

these class of accident analysis codes on safety is related to their contribution in selecting safety-class systems, structures, and components (SSCs).[5]

Appendix A to DOE-STD-3009-94 prescribes the statistical method to be used to calculate the MOI dose, which is based on the method described in Position 3 of the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983). Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based doses calculated for a postulated release to downwind receptors at the site boundary that would result in a dose that is exceeded 5% of the time. Appendix A to DOE-STD-3009-94 allows for variations in distance to the site boundary as a function of distance to be taken into consideration. Assuming the minimum distance to the site boundary applies in all directions is a conservative implementation that is easily supported by MACCS2 and that essentially makes the calculations sector independent.

[5] The selection of safety-class SSCs is an important decision, but the decision to make an SSC safety-significant is made initially in the hazard analysis. Thus, the quality of the dose value will not affect the SSC being made a safety-significant SSC and having TSR coverage, only the designation of safety-class, and therefore, possibly the pedigree of the SSC.

3.2 Phenomenological Regimes of Applicability

The MACCS2 class of atmospheric dispersion codes is based on the Gaussian model of dispersion. As such, these types of computer model are best suited for specific types of conditions. The chief phenomenological regimes that should be considered before applying MACCS2 include:

- Temporal regime – The use of these codes is best suited for "short" duration plumes, ranging from approximately several minutes to several days.

- Spatial regime - The class of code also does not model dispersion close to the source (less than 100 meters from the source), especially where the influence of structures or other obstacles is still significant. Dispersion influenced by several, collocated facilities, within several hundred meters of each other should be modeled with care. Similarly, the MACCS2 class of codes should be applied with caution at distances greater than ten to fifteen miles, especially if meteorological conditions are likely to be different from those at the source of the release. Long-range projections of dose conditions are better calculated with mesoscale, regional models that are able to account for multiple weather observations. Nevertheless, some applications may require fifty-mile or greater radius analysis to meet requirements, e.g. Environmental Impact Statements (EISs) or Probabilistic Safety Assessments (PSAs).

- Terrain variability – Gaussian models are inherently flat-earth models, and perform best over regions of transport where there is minimal variation in terrain. Because of this, there is inherent conservatism (and simplicity) if the environs have a significant nearby buildings, tall vegetation, or grade variations not taken into account in the dispersion parameterization.

- Energetic releases – MACCS2 does not account for momentum-driven releases or those originating from detonation type events without appreciable post-processing of boundary and initial conditions. Using the latter approach, Steele (1998) has demonstrated a MACCS2-based, segmented methodology for a detonation source term that was found to compare well with observations.

- Thermal buoyancy - In plumes arising from fire-related source terms, the user should exercise caution with the models such as MACCS2 that use the Briggs algorithm. The Briggs approach for accounting for sensible energy in a plume is valid for "open-field" releases (not impacted by buildings and other obstacles), or if used in combination with building wake effects. Appendix C provides a limited sensitivity study of the effects of buoyancy and building wake effects on plume dispersion.

- Dose conversion factor applicability – The user should ensure that the dose conversion factors used in MACCS2 are applicable to the radionuclides in the source term and the physicochemical characteristics. For example, plutonium nitrates and oxides have different time scales for dosimetric effects in the body. Thus, the appropriate lung

absorption type should be used in the dose conversion factor file used in the MACCS2 run.

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4.0 INPUTS AND RECOMMENDATIONS

4.1 MACCS/MACCS2 CODE STRUCTURE

MACCS and MACCS2 are executed in a three-step method on the personal computer. Air and ground concentrations, plume size, and timing information for all plume segments as a function of downwind distance are calculated in the first step **ATMOS**. The next step is **EARLY**; this calculation accounts for consequences due to exposure to radiation in the emergency phase (first 7 days) of the accident. The last step is **CHRONC**. Its purpose is to calculate consequences due to exposure to radiation subsequent to the emergency phase of the postulated accident and for computing decontamination and other economic impacts incurred because of the accident. The complete three-step execution of MACCS and MACCS2, including input and output files, is shown in Figures 4-1 and 4-2, respectively. For support of a DSA, post-emergency doses are not of interest, thus the CHRONC module is not executed. In addition, a uniform population density is assumed, eliminating the need for a separate population input file.

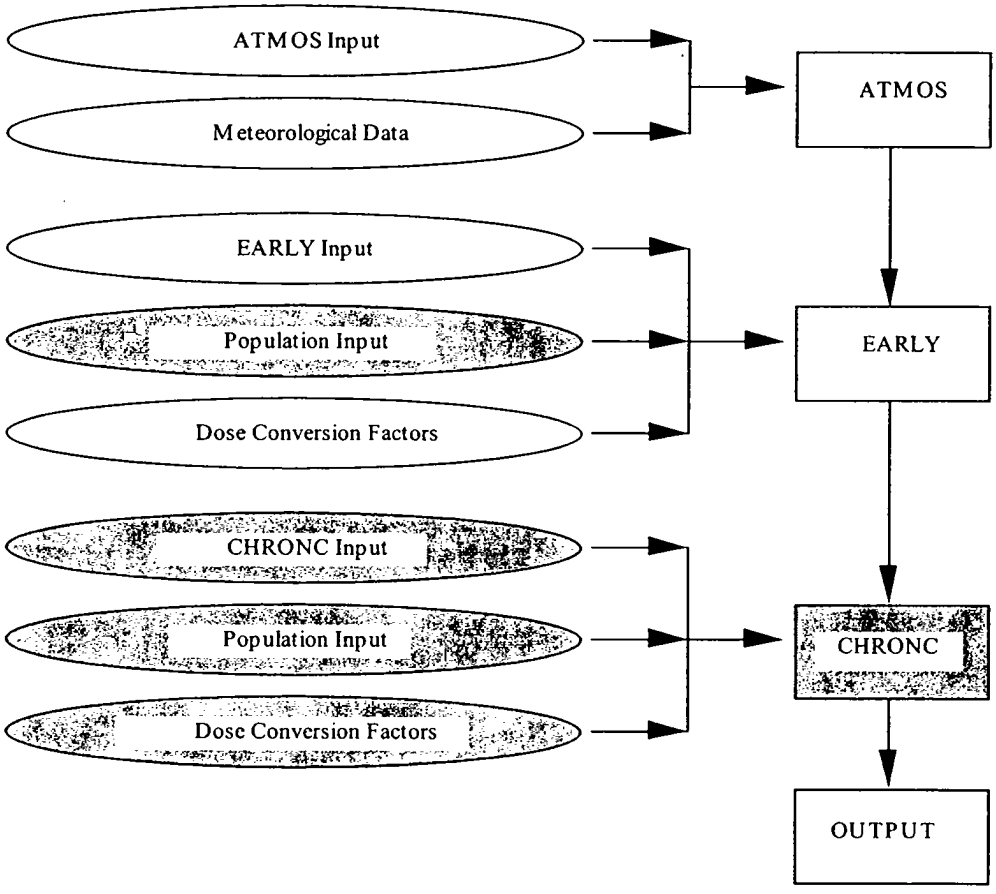

Figure 4-1. Flow Chart of the MACCS Three-Step Execution and Input Files

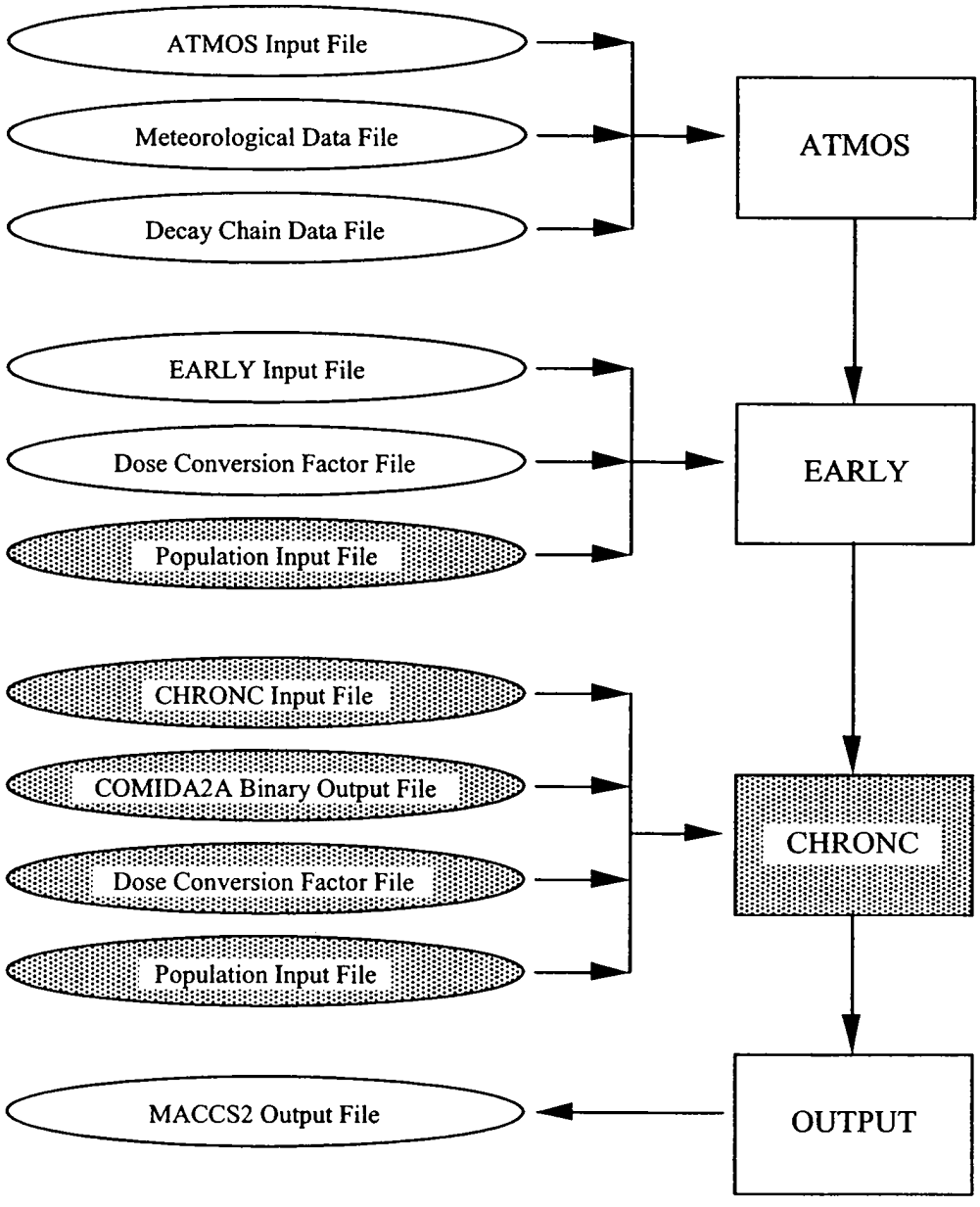

Figure 4-2. Flow Chart of the MACCS2 Three-Step Execution and Input Files

4.2 GENERAL CODE INPUT AND OUTPUT ASSUMPTIONS

For input into Safety Basis documents, the MACCS2 code is executed through the EARLY module. In the following section, standard MACCS2 ATMOS and EARLY module input files are discussed line by line. The particular input file commented upon here is used because it is the sample file supplied with the software package from the RSICC software center. In the lines that follow, the phrase, "These values should not be changed" or "This value should not be changed" is a recommendation to the user to not make any changes to the corresponding line of input in the RSICC-supplied file.

The reader with limited experience in applying radiological dispersion and consequence software to accident analysis should review one or more standard guides in this field prior to executing MACCS2. While many documents and texts are available for this purpose, several recommended references are Hanna (1982), NCRP (1996), and NRC (1998). Appendix A summarizes key methods and data for radiological dispersion and consequence analysis.

Only a limited number of input parameters need be changed for a specific MACCS execution. Of those parameters that are changed for a specific MACCS2 case, most will be related to the source term being released or more specifically the radionuclide inventory being released. When defining the radionuclide inventory for MACCS2 input, one must consider the activity of the inventory, under what conditions the material is being released (i.e. filtered or unfiltered conditions), and the material type being released. The material type influences the selection of CEDE inhalation dose conversion factors (IDCFs).

For documented safety analysis purposes, the consequences of interest are the centerline Total Effective Dose Equivalent (TEDE) incurred by the Maximally Exposed Offsite Individual (MOI) evaluated at the 95th quantile dose level. The MOI TEDE will be most easily evaluated with MACCS2 at the closest site boundary without regard to sector (i.e., sector independent). Although this method is not fully compliant with NRC Regulatory Guide 1.145, the calculated dose at the closest offsite boundary without regard to sector can be shown to be conservative relative to that calculated with regard to sector.[6] For compliance with the specific NRC Regulatory Guide 1.145 positions with regard to sector-dependent doses, post-processing of MACCS2 code output must be performed.

The sector-independent MOI TEDE output is requested in the EARLY input file through the Type 6 Number data block that in general provides the centerline dose at distance for various pathways. As discussed in the detailed coverage of the inputs that follows, the label "TOT LIF" is used to specify the total dose from all direct exposure pathways. MACCS2 automatically

---

[6] Each consequence analysis should evaluate the validity of this statement based on the location of the facility, the release height and the DOE reservation boundary. For example, for most Savannah River Site facilities, the degree of conservatism is approximately 8% - 10% (O'Kula, 2000).

provides the mean, 50th percentile, 90th percentile, 95th percentile, 99th percentile, 99.5th percentile, and peak values. The user may also request a table showing the complementary cumulative distribution function (CCDF) in terms of consequence and probability pairs.

An edited sample case run with MACCS2, containing an echo of the input, is shown in Section 7. The case illustrates the MACCS2 calculation of a unit release of plutonium (^{239}Pu) for four different conditions: ground-level release, ground-level release with sensible heat, ground-level release with building wake effects, and ground-level release with sensible heat and building wake effects. The example also provides an illustration of a sensitivity study where relatively few parameters are being changed.

This section of the report provides guidance for specifying inputs when using the MACCS2 computer code. Appendix D provides parallel guidance for specifying inputs when using the earlier version of the code, namely, MACCS 1.5.11.1.

4.3 GENERAL NOTES ON MACCS2 INPUT FILES

For MACCS2 the following conventions must be followed:

- All values not in quotes must be in UPPER case, except for the specification of the radionuclide names. MACCS2 radionuclide names are specified using uppercase letters for the first letter in the radionuclide symbol and lowercase for the second letter. In addition, the "m" metastable designation is also lower case.
- Quote marks should be single straight quote marks (i.e. 'input value') not smart quotes marks (i.e. ‘input value’).
- MACCS2 dose conversion factor files require fixed-format, and it is strongly recommended that input data files be converted to Word or Word Perfect files to display non-compliant spacing (insufficient or extra spaces) and tabs. The user can then convert back to the appropriate format prior to MACCS2 execution.
- Input files, although not fixed format, are easier to set up in Word or Word Perfect to eliminate unintentional tabs.

The MACCS2 naming convention for input parameters is as follows:

- Characters one and two indicate the specific data block
- Characters three to eight indicate the variable name (Occasionally in new MACCS2 variable names, characters one to nine are used to indicated the variable name and the data block nomenclature is dropped.)
- Characters nine to eleven indicate the line of data being entered (there must always be eleven characters in the input parameter name).

The MACCS2 naming convention for user requested output is as follows:

- Characters one to five indicate the output type
- Characters six to eleven indicate either the number of requested input or the specific output requested

The discussion in the remainder of this section is based on the MACCS2 User's Manual (Chanin, 1998).

4.4 ATMOS INPUT FILE

This section of the document addresses input file variables that may be changed for execution of MACCS2 for safety basis document applications. Also discussed are site-specific parameter inputs that are selected by the user for a specific location.

For each section of input, page-specific references to the MACCS2 User's Guide, NUREG/CR-6613 (Chanin, 1998), are provided. These references are signified by blocked text, e.g. NUREG/CR-6613, Vol. 1 – page x-y, and will allow the reader to reference the appropriate section in the User's Guide should additional explanation be needed.

The particular ATMOS input file discussed in the following is used as a beginning baseline. It is one of the sample files (e.g., IN1A.INP) supplied with the MACCS2 software compact disc from RSICC. If a variable is not explicitly mentioned, it is not necessary to change its value in the file.

Run Identification Data Block (RI)

Variable ATNAM1 (ATMOS input file identifier line)

NUREG/CR-6613, Vol. 1 – page 5-3 Line within MACCS2 IN1A.INP sample file:

```
RIATNAM1001  'IN1A.INP, SURRY, SAMPLE PROBLEM A, ATMOS INPUT'
```

For a specific application:
Change to a descriptive title for this execution of MACCS2, observing the appropriate alphanumeric character length convention.

Geometry Data Block (GE)

Variables NUMRAD and SPAEND specify the number of radial grid endpoints and locations of radial grid endpoints. For DSA applications, the radial grid endpoints are the inner and outer radii for a ring drawn around the release location. The individual dose will be calculated at the mid-point of the ring. Figure 4-3 illustrates a portion of the 35-ring grid modified from the original 26-ring grid.

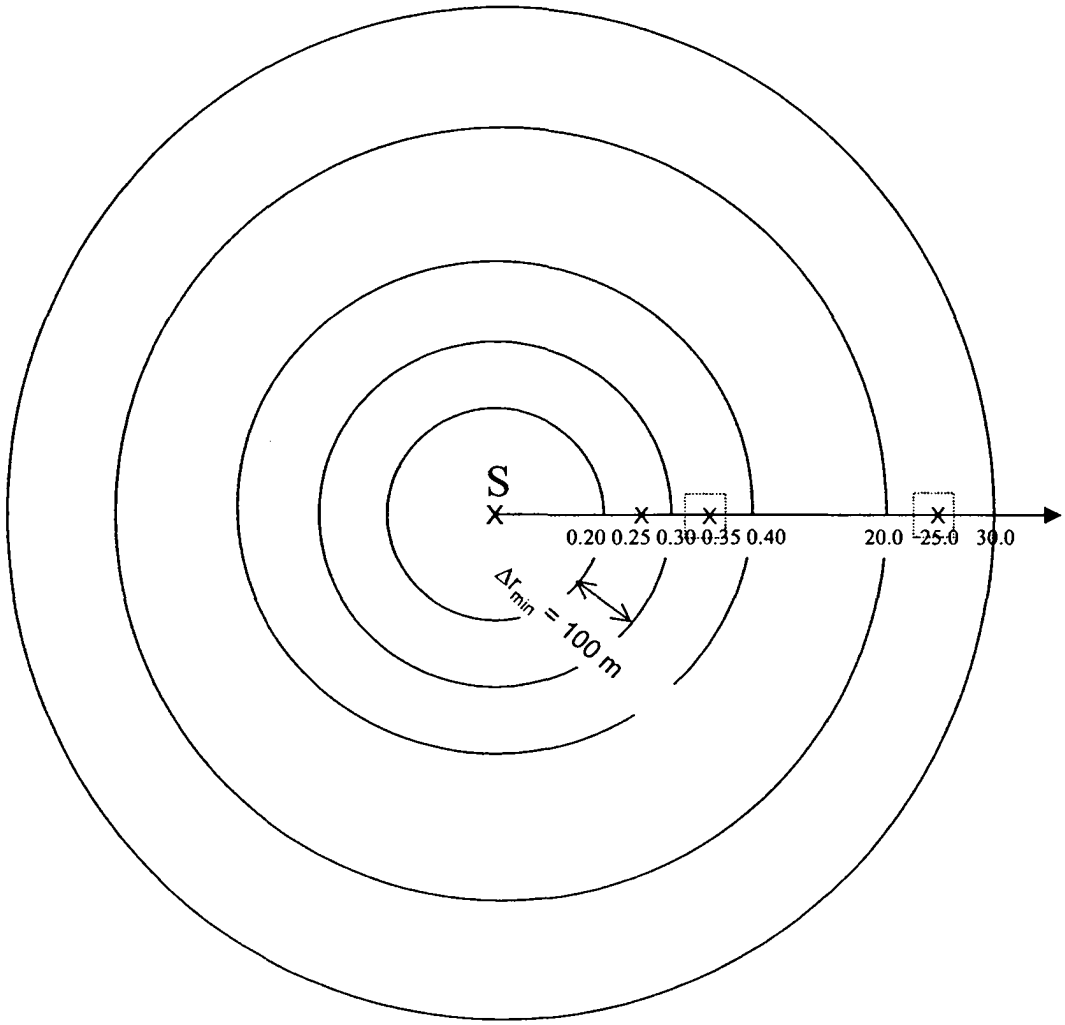

Figure 4-3. Radial grid endpoints for polar grid showing source term release point (S), several radial rings, and several receptor locations (X). Not to scale.

NUREG/CR-6613, Vol. 1 – pages 5-3 to 5-4

Lines within the MACCS2 IN1A.INP sample file supplied with MACCS2 code:

```
GENUMRAD001   26
*
GESPAEND001      .16       .52      1.21      1.61      2.13
GESPAEND002     3.22      4.02      4.83      5.63      8.05
GESPAEND003    11.27     16.09     20.92     25.75     32.19
GESPAEND004    40.23     48.28     64.37     80.47    112.65
GESPAEND005   160.93    241.14    321.87    563.27    804.67
GESPAEND006  1609.34
```

For a specific application:

If population data are being entered, the polar grid supplied with the MACCS2 code is adequate. However, distances past 80.5 km (50 miles) should be eliminated. Receptor locations closer than 100 m should not be attempted unless

the dispersion parameter data set used is based on the appropriate measurements.[7] Chanin and Young (1998) discourage application of MACCS2 for distances less than 0.5 km, based on reference to the field measurements and Gaussian model applicability in the wake of large buildings. However, it should be recognized that at least one body of tracer gas experiments that are widely used as a basis for dispersion parameters, viz., the Prairie Grass experiments (Haugen, 1959), actually recorded experimental data as close as 60 m from the point of release extending to 1 km distant. Nonetheless, the MACCS2 user should exercise caution in discretization of polar grids for the region of transport and the receptors of interest. Two or more cases may need to be executed depending on receptor location.

If a consequence at a single receptor point is required, the following, or similar lines, may be used:

```
GENUMRAD001   35
*
GESPAEND001    0.20   0.30   0.40   0.50   0.60   0.70   0.80
GESPAEND002    0.90   1.00   1.50   2.00   2.50   3.00   3.50
GESPAEND003    4.00   4.50   5.00   5.50   6.00   6.50   7.00
GESPAEND004    7.50   8.00   8.50   9.00   9.50  10.00  10.50
GESPAEND005   11.00  11.50  12.00  12.50  15.00  20.00  30.00
```

If the location of interest is not a midpoint of two of these endpoints, the two closest to the location may be changed.

Note:

If meteorological data is sampled based on binning of like conditions, values must be included here that are within 10% of the rain interval endpoints that are specified through the RNDSTS variable of the M4 data block.

For MACCS2, the endpoints must be at least 100 meters apart.

Radionuclide Data Block (IS)

Variable NUMISO (Number of radionuclides)

NUREG/CR-6613, Vol. 1 – page 5-4

Line within MACCS2 IN1A.INP sample file:

```
ISNUMISO001 60
```

[7] See Eimutis (1972), for example, for dispersion parameterization at close-in distances (< 100 m).

For a specific application:

This is the number of radionuclides being released. This number must be 150 or less. If the number of radionuclides is greater than 150, either the inventory must be divided into groups with a maximum of 150 radionuclides, or only those radionuclides that contribute to the overall TEDE should be retained. A useful cut-off for considering a group of radionuclides is whether the dose consequence contributed by one or more radionuclide is ≤ 0.1%. Below this value the radionuclides in question can be ignored because they contribute insignificantly to the dose.

Variable WETDEP and DRYDEP (Wet and dry deposition flags for each group by DEPFLA)

NUREG/CR-6613, Vol. 1 – pages 5-5 to 5-6

Line within MACCS2 IN1A.INP sample file shows whether wet and dry deposition will be modeled by group designation:

```
ISDEPFLA001     .FALSE.    .FALSE.
ISDEPFLA002     .TRUE.     .TRUE.
ISDEPFLA003     .TRUE.     .TRUE.
ISDEPFLA004     .TRUE.     .TRUE.
ISDEPFLA005     .TRUE.     .TRUE.
ISDEPFLA006     .TRUE.     .TRUE.
ISDEPFLA007     .TRUE.     .TRUE.
ISDEPFLA008     .TRUE.     .TRUE.
ISDEPFLA009     .TRUE.     .TRUE.
```

For a specific application:

For the noble gases group, both values should be set to ".FALSE." For the other groups, the first value should always be ".FALSE." indicating no wet deposition. When dry deposition is used, the second value should be set to ".TRUE."

Variable MAXGRP (Number of chemical groups)

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Line within MACCS2 IN1A.INP sample file:

```
ISMAXGRP001 9
```

For a specific application:

This is simply the total number of groups determined above with a minimum value of 1 (all radionuclides are modeled in the same manner) and a maximum value of 10. For nonreactor nuclear facilities, this value is typically three or fewer. An example is group 1 – filtered radionuclides, group 2 – tritiated water vapor, and group 3 – unfiltered radionuclides.

Greater resolution in the number of groups was historically based on reactor inventory physical-chemical types, and was used to establish timing for release as well as atmospheric transport behavior. A categorization for handling nonreactor inventories of radionuclides is found in Appendix E.

Variable NUCNAM, and IGROUP (Radionuclide name and chemical group as input by OTPGRP.

NUREG/CR-6613, Vol. 1 – pages 5-7 to 5-8

Note: The values of the parent radionuclide and half-life are input through an auxiliary input file)

Line within MACCS2 IN1A.INP sample file:

```
ISOTPGRP001     Co-58        6
ISOTPGRP002     Co-60        6
ISOTPGRP003     Kr-85        1
  .
  .
  .
ISOTPGRP060     Cm-244       7
```

For a specific application:

The selection of the chemical groups is based on similar release fractions and plume removal mechanisms (i.e. wet and dry deposition). For example, both noble gases and tritiated water vapor have a release fraction of 1.0, but the noble gases are not subjected to either removal mechanism while tritiated water vapor can be removed by both wet and dry deposition mechanisms. Thus, noble gases would be in one chemical group, and tritiated water vapor would be in another.

Variable NUMSTB and NAMSTB (Number of pseudo-stable radionuclides and the pseudo-stable radionuclides)

NUREG/CR-6613, Vol. 1 – page 5-7

Line within MACCS2 IN1A.INP sample file:

```
ISNUMSTB001      27
*
ISNAMSTB001     I-129     (daughter of Te-129 and Te-129m)
ISNAMSTB002     Xe-131m   (daughter of I-131)
ISNAMSTB003     Xe-133m   (daughter of I-133)
  .
  .
  .
ISNAMSTB027     Pm-147    (daughter of Nd-147)
```

For a specific application:

Pseudo-stable radionuclides will most often be defined as the first radioactive daughter of the radionuclides in the source term. The pseudo-stable radionuclide is used to shorten chains when the activity of the daughter products would not

contribute significantly to the consequence associated with the whole source term. For example, in a seven-day decay period following the release of ^{239}Pu, only 5.5 x 10^{-5}% of the ^{239}Pu (greater than 24,000 y half-life) has decayed to ^{235}U. Thus, the calculation of consequences from the daughters of ^{239}Pu is not beneficial, as they will not contribute significantly to the total consequence.

Note: Radionuclides listed as pseudo-stable should not be included in the source term radionuclide list. Half-life information for many radionuclides treated in nuclear facility accident analysis is listed in Appendix E.

Wet Deposition Data Block (WD)

NUREG/CR-6613, Vol. 1 – pages 5-5 to 5-6

In typical DSA applications, the data entered in this block is not used in the calculation because the WET DEPOSITION flag is 'FALSE'.

Dry Deposition Data Block (DD)

Variable NPSGRP (Number of dry deposition velocity groups)

NUREG/CR-6613, Vol. 1 – pages 5-9 to 5-10

Line within MACCS2 IN1A.INP sample file:

```
DDNPSGRP001    3
```

For general application:

Set this value to the maximum number of dry deposition velocities groups to be used in a majority of site analyses. A common use of this input parameter for accident analysis purposes assigns a value of three (3) (one group will be for releases passing through a filtration system, another for tritiated water vapor, and a final for releases directly into the environment).

Variable VDEPOS (Dry deposition velocities)

NUREG/CR-6613, Vol. 1 – page 5-10

Line within MACCS2 IN1A.INP sample file:

```
DDVDEPOS001    0.01    (VALUE SELECTED BY S. ACHARYA, NRC)
```

For general application:

Typically, the line will be:

```
DDVDEPOS001    0.001  0.005  0.010
```

The dry deposition velocity of 0.001 m/s is appropriate for filtered releases into the atmosphere. The 0.001 m/s deposition velocity is consistent with a particle with an aerodynamic equivalent diameter (AED) of 0.2 to 0.4 microns (Sehmel, 1978). The dry deposition velocity of 0.005 m/s is an approximate value for tritiated water vapor (Murphy, 1993). The dry deposition velocity of 0.01 m/s is appropriate for unfiltered releases directly into the environment and corresponds to particles with an AED between 2 to 5 microns (Sehmel, 1978).

Dispersion Data Block (DP)

Variable YSCALE (Scaling factor for sigma y)

NUREG/CR-6613, Vol. 1 – page 5-14

Line within MACCS2 IN1A.INP sample file:

```
DPYSCALE001    1.
```

For a specific application:

Normally this value should not be changed. This value may be changed to calculate a dose from a release of up to 100 hours (the upper valid range of the model). The longer release duration correction factor is calculated by dividing the new duration in seconds by 180 seconds and raising the quotient to the 0.25 power. The release duration (variable PLUDUR in the RD data block) must be set equal to 180 seconds. If the user changes the 180-second basis, e.g. use of a new dispersion set with a ten-minute basis, then this must be reflected in the calculation.

Variable ZSCALE (Scaling factor for sigma z)

NUREG/CR-6613, Vol. 1 – page 5-18

Line within MACCS2 IN1A.INP sample file:

```
DPZSCALE001    1.27
```

For general application:

The calculation of this variable is discussed in Appendix A of this document under surface roughness, and is calculated as $(z_{new}/z_{ref})^{0.2}$, where the quotient of the new and reference surface roughness length is raised to the power of 0.2 Thus, the scaling factor as a function of surface roughness length , which

approximately equals one-tenth of the height of surface feature obstacles (Hanna, 2002), is

Obstacle Height	30 cm	100 cm	10 m
Surface Roughness Length	3 cm	10 cm	100 cm
σ_z correction	1.	1.27	2.02

The surface roughness parameter is intended to be a macroscopic average for the region-of-transport and should be consistent for the environment surrounding facility in question, taking both upwind and downwind distances into account.

Variables CYSIGA, CYSIGB, CZSIGA, and CZSIGB (Linear and Exponential Terms for sigma y (σ_y) and sigma z (σ_z)), specifies the dispersion parameter coefficients used.

NUREG/CR-6613, Vol. 1 – pages 5-10 to 5-12

Chanin and Young (1998)[8] and the MACCS2 sample problem data give two parameterizations based on the Tadmor-Gur curve fits: one for 0.5–5.0 km, the second for 5.0–10.0 km. These two parameterizations were obtained from Dobbins (1979). The data below is intended for use in the range of 0.5–5.0 km, and is then followed by Tadmor-Gur dispersion parameters for the range of 5 km – 50 km. As shown here, the sample input below is for a calculation applying the shorter range inputs, i.e., the longer ranger parameters are commented out (* in first column)

```
* DISPERSION PARAMETER DATA BLOCK, LOADED BY INPDIS, STORED IN /DISPY/, /DISPZ/
*
* SIGMA = A * X ** B
*
* Tadmor and Gur Parameterization for Distance Range 0.5 to 5.0 km
* as taken from Atmospheric Motion and Air Pollution (Dobbins 1979).
*
* P-G CLASS:     A          B          C          D          E          F
DPCYSIGA001   0.3658     0.2751     0.2089     0.1474     0.1046     0.0722
DPCYSIGB001   0.9031     0.9031     0.9031     0.9031     0.9031     0.9031
DPCZSIGA001   2.5E-4     1.9E-3     0.2        0.3        0.4        0.2
DPCZSIGB001   2.125      1.6021     0.8543     0.6532     0.6021     0.6020
*
* Tadmor and Gur Parameterization for Distance Range 5 to 50 km
* as taken from Atmospheric Motion and Air Pollution (Dobbins 1979).
*
* P-G CLASS:     A          B          C          D          E          F
*DPCYSIGA001  0.3658     0.2751     0.2089     0.1474     0.1046     0.0722
*DPCYSIGB001  0.9031     0.9031     0.9031     0.9031     0.9031     0.9031
*DPCZSIGA001  0.5742     0.5742     0.5742     0.9605     2.1250     2.1820
*DPCZSIGB001  0.7160     0.7160     0.7160     0.5409     0.3979     0.3310
*
```

[8] Also discussed in NRC (1990b).

However, if an individual location has a site-specific set of linear and exponential terms for sigma y (σ_y) and sigma z (σ_z), then those values can be applied. Another possibility is using an alternative parameterization such as the Eimutis (1972) data presented in Table A-3 (x< 100 m; 100 < x < 1000 m; x > 1000 m). Use of the Eimutis data would require off-line generation of sigma-y and sigma-z values with a spreadsheet and insertion of data into the ATMOS input file using the Table Lookup option to specify the dispersion as a function of distance. See the Dispersion Parameters section of Appendix A for additional information. In MACCS2, dispersion coefficients are specified through either the curve-fit constant inputs as shown above or through tabular values as shown next. If the tabular values are used, the lines shown above for CYSIGA, CYSIGB, CZSIGA and CZSIGB are commented out.

Variable NUM_DIST, A-STB/DIS, B-STB/DIS, C-STB/DIS, D-STB/DIS, E-STB/DIS, and F-STB/DIS (Number of distances in dispersion look-up table and stability class data for each class, beginning with A-stability and proceeding through stability class F.)[9] The first value is the variable string name, the next is distance (m), the third is the horizontal dispersion parameter value, and the fourth is the vertical dispersion parameter value.

NUREG/CR-6613, Vol. 1 – pages 5-12 to 5-13

Line within MACCS2 IN1A.INP sample file:

```
NUM_DIST001   50
A-STB/DIS01        1.000E+00     3.6580E-01     2.5000E-04  Tadmor/Gur (0.5-5 km)
A-STB/DIS02        1.400E+00     4.9569E-01     5.1105E-04  Tadmor/Gur (0.5-5 km)
A-STB/DIS03        2.000E+00     6.8408E-01     1.0905E-03  Tadmor/Gur (0.5-5 km)
  .
  .
  .
F-STB/DIS50        1.000E+07     1.5144E+05     3.2736E+03  Tadmor/Gur (0.5-5 km)
```

For a specific application:

These values should be set once and then not changed. Some sites and facility locations may have experimental data applicable over the region of transport. If this is the case, then fits to those data (sigma y and sigma z values) can be used. Alternatively, if experimental data are not available, then default data can be applied.

[9] If the curve fits documented above are to be used for sigma y and sigma z, the NUM_DIST variable is set to zero and the lines for A-STB/DIS, B-STB/DIS, C-STB/DIS, D-STB/DIS, E-STB/DIS, and F-STB/DIS are commented out.

Plume Meander Data Block (PM)

Variable TIMBAS (Time base for the parameterization of the plume meander adjustment factor (seconds).)

NUREG/CR-6613, Vol. 1 – pages 5-18 to 5-19

Line within MACCS2 IN1A.INP sample file:

```
PMTIMBAS001    600.   (10 MINUTES)
```

For general application:

This value should be set once and not changed.

The recommended basis for this parameter is taken from the Project Prairie Grass field data measurements, and has been documented as three minutes (180 s) (NRC, 1990b).

If another set of dispersion coefficients is being used, the value should be consistent with the time-basis of those experiments.

Plume Rise Data Block (PR)

NUREG/CR-6613, Vol. 1 – pages 5-20 to 5-21

Variable SCLCRW (Linear scaling factor on the critical wind speed used in determining if buoyant plumes will be trapped in building wake).

```
PRSCLCRW001   1.
```

Variable SCLADP (Linear scaling factor on the plume rise formula for unstable and neutral conditions (classes A – D)).

```
SCALING FACTOR FOR THE A-D STABILITY PLUME RISE FORMULA
(USED BY FUNCTION PLMRIS)
PRSCLADP001   1.
```

Variable SCLADP (Linear scaling factor on the plume rise formula for stable conditions (classes E and F)).

```
SCALING FACTOR FOR THE E-F STABILITY PLUME RISE FORMULA
(USED BY FUNCTION PLMRIS)
PRSCLEFP001   1.
```

Wake Effects Data Block (WE)

Note: The building size may not be credited if a stack release is being modeled.

NUREG/CR-6613, Vol. 1 – pages 5-21 to 5-23

Variable SIGYINT (Initial sigma y value (σ_{y0}))
Line within MACCS2 IN1A.INP sample file:

```
SIGYINIT001  9.302  9.302 (initial sigma-y, calculated for 40 meter wide bldg.)
```

For a specific application:
Normally this value should be set equal to its minimum value of 0.1 for each plume released. Thus no credit is taken for the size of the building wake. If the building is credited, the initial sigma y value should be calculated by dividing the average width of the building by 4.3 (Chanin and Young, 1998).

Variable SIGZINT (Initial sigma z value (σ_{z0}))
Line within MACCS2 IN1A.INP sample file:

```
SIGZINIT001  23.26  23.26 (initial sigma-z, calculated for 50 meter high bldg.)
```

For a specific application:
Normally this value should be set equal to its minimum value of 0.1 for each plume released. Thus no credit is taken for the size of the building wake. If the building is credited, the initial sigma y value should be calculated by dividing the height of the building by 2.15 (Chanin and Young, 1998).

Variable BUILDH (Height of the building)
Line within MACCS2 IN1A.INP sample file:

```
WEBUILDH001   50.0  50.0  (Surry)
```

For a specific application:
Normally this value should be set equal to its minimum value of 1.0. The value is now solely used in MACCS2 to evaluate whether a buoyant plume is entrained in the turbulent wake of the facility.[10] Use of the minimum value ensures that buoyant plumes are not entrained in the building wake.

Release Description Data Block (RD)

NOTE: All values in this data block may be modified using a change case.

---

[10] In previous versions of MACCS, the building height input was also used to establish the initial value of σ_{z0} for the plume

NUREG/CR-6613, Vol. 1 – pages 5-23 to 5-29

Variable ATNAM2 (Source term identifier)

NUREG/CR-6613, Vol. 1 – page 5-24

Line within MACCS2 IN1A.INP sample file:

```
RDATNAM2001 'SECOND DRAFT 1150, WORST CASE SOURCE TERM FOR EARLY FATALITIES'
```

For a specific application:

Change the entire character string to identify the source term.

Note: A unique identifier must be used for each case

Variable NUMREL (Number of plume segments being released)

NUREG/CR-6613, Vol. 1 – page 5-24

Line within MACCS2 IN1A.INP sample file:

```
RDNUMREL001          2
```

For a specific application:

Change to the number (≤ 4) of plume segments defined in the source term. If more than four plume segments are defined, the activity of consecutive source terms may be added together if they have the same (or similar) release duration, release height, and sensible heat rate. The release duration of the combined plume segments is then the same as for the individual plume segments.

Note:

For MACCS2 applications only, if FOUR plume segments are used then change cases should NOT be used for additional source terms as the results associated with the subsequent source terms will be wrong, due to a coding error that will corrected by Sandia National Laboratories (see Appendix B). For now, it is highly recommended that only one or two plume segments be used for DSA cases applying MACCS2. The subject coding error, however, is not present in MACCS. It is highly recommended that one to two plume segments only be used for DSA cases applying MACCS2 Version 1.12. Note: This error has been corrected in version 1.13.1 of MACCS2.

Variable REFTIM (Representative time point for each plume)

NUREG/CR-6613, Vol. 1 – page 5-25

Line within MACCS2 IN1A.INP sample file:

```
RDREFTIM001       0.00       0.50
```

For a specific application:

The representative time point for each plume should be zero (0.00).

Variable PLHEAT (Sensible heat rate of each plume segment in Watts)

NUREG/CR-6613, Vol. 1 – page 5-25

Line within MACCS2 IN1A.INP sample file for two plume segments showing 3.7 MW in the first plume segment and 0.17 MW in the second plume segment:

```
RDPLHEAT001     3.7E+6     1.7E5
```

For a specific application:

If the sensible heat rate is credited and the release mechanism is an explosion, the energy of the event can be divided by sixty seconds, as a conservative reduction. This will underpredict the sensible heat rate of the event by at least an order of magnitude as explosions are normally much less than one minute in duration. Note: An alternative approach for modeling detonations with MACCS2, and a comparison to test data is documented by C. Steele, DOE/LAAO (Steele, 1998).

For most accident analysis fire types, the MACCS2 sensible energy option should be applied only for well-defined fires. Credit only sensible heat fraction for the thermal buoyancy effect, and apply conservative spatial factors to account for area-type fires. Assume shortest duration consistent with fire sequence definition.

Variable PLHITE (Release height of each plume segment)

NUREG/CR-6613, Vol. 1 – page 5-26

Line within MACCS2 IN1A.INP sample file:

```
RDPLHITE001       0.         0.
```

For a specific application:

If the release height is not defined in the given source term, this value should be set equal to zero meters for each plume segment. If the release is elevated and the release height is not at least 2.5 times the tallest collocated building height, the release height is set equal to zero.

Variable PLUDUR (Plume duration of each plume segment)

NUREG/CR-6613, Vol. 1 – page 5-26

Line within MACCS2 IN1A.INP sample file:

```
RDPLUDUR001      1800.    22000.
```

For a specific application:

If the release duration is not defined in the given source term, this value should be set equal to 180 seconds (or the value of TIMBAS defined in the expansion factor data block) for each plume segment. The value range on this parameter is the TIMBAS value (180 seconds) to 36000 seconds (10 hours). Release duration of longer than 10 hours are calculated by setting the duration of the plume segment to TIMBAS and applying the appropriate YSCALE factor. Note that in contrast to MACCS, where multiple plume segments were not allowed to overlap each other in time, MACCS2 allows the specification of overlapping plumes. This MACCS2 feature was intended to support explosive releases (e.g., Steele, 1998) as well as multiple release points from a single accident.

Variable PDELAY (Start time of each plume segment)

NUREG/CR-6613, Vol. 1 – page 5-26

Line within MACCS2 IN1A.INP sample file:

```
RDPDELAY001      3700.    10000.
```

For a specific application:

Specifies the start time of each plume segment in seconds from the time of accident initiation. Note that in contrast to MACCS, where multiple plume segments were not allowed to overlap each other in time, MACCS2 allows the specification of overlapping plumes

Variable PSDIST (Dry deposition velocity bin distribution), and is the fractional distribution among the defined particle size (deposition velocity) groups.

NUREG/CR-6613, Vol. 1 – page 5-27

Line within MACCS2 IN1A.INP sample file:

```
RDPSDIST001      1.
RDPSDIST002      1.
RDPSDIST003      1.
RDPSDIST004      1.
RDPSDIST005      1.
RDPSDIST006      1.
```

```
RDPSDIST007      1.
RDPSDIST008      1.
RDPSDIST009      1.
```

For a specific application:

A dry deposition velocity distribution must be specified for each chemical group even if dry deposition is turned off for that group. The dry deposition bins were defined in variable VDEPOS. As discussed previously, a dry deposition velocity of 0.001 m/s is appropriate for filtered releases. Similarly, a dry deposition velocity of 0.005 m/s is an approximate value for tritiated water vapor. A dry deposition velocity of 0.01 m/s is appropriate for unfiltered releases into the environment.

Variable CORINV (Inventory available for release into the environment)

NUREG/CR-6613, Vol. 1 – page 5-27

Line within MACCS2 IN1A.INP sample file:

```
RDCORINV001      Co-58          3.223E+16
RDCORINV002      Co-60          2.465E+16
RDCORINV003      Kr-85          2.475E+16
   .
   .
   .
RDCORINV060      Cm-244         2.596E+15
```

For a specific application:

Enter the radionuclides and their associated inventories for the specific application. The radionuclides here do not need to be entered in the same order as provided in the default listing.

Variable CORSCA (Inventory scaling factor)

NUREG/CR-6613, Vol. 1 – page 5-28

Line within MACCS2 IN1A.INP sample file:

```
RDCORSCA001    0.715  *  SURRY
```

For a specific application:

In nonreactor applications, this value is most often used to scale the inventory units of curies to the MACCS required value of becquerel (Bq). However, the value may be used to scale the inventory to meet any need.

Variable RELFRC (Fraction of inventory released in each plume segment)

NUREG/CR-6613, Vol. 1 – pages 5-28 – 5-29

Line within MACCS2 IN1A.INP sample file:

```
RDRELFRC001 1.0E+0 6.8E-1 6.4E-1 1.7E-1 4.2E-3 2.3E-3 1.6E-4 4.0E-4 6.3E-3
RDRELFRC002 4.3E-3 9.5E-3 2.4E-3 1.4E-1 6.8E-2 4.7E-4 6.8E-3 7.1E-3 5.4E-2
```

For a specific application:

A value must be specified for each chemical group and plume segments. The fraction of release is applied uniformly in to all radionuclides within a chemical group.

Variable APLFRC (Indicates whether the inventory of a daughter radionuclide is to be released with the release faction of the parent or the daughter)

NUREG/CR-6613, Vol. 1 – page 5-28

Line within MACCS2 IN1A.INP sample file:

```
RDAPLFRC001    PARENT       (apply rel fracs the same as prior versions)
```

For a specific application:

When the execution is being modeled to simulate a MACCS execution, this value should be set equal to "PARENT". In all other cases, the value should be set equal to "PROGENY". The PROGENY option was added in MACCS2 as a modeling improvement, but the choice between options will only affect results when daughter ingrowth between the time of the accident and the time of release is of significant duration (as is possible in a reactor accident), combined with daughter release fractions different from those of the parent nuclide).

Output Control Data Block (OC)

NUREG/CR-6613, Vol. 1 – pages 5-29 –5-31

Variable ENDAT1 (Flag for Ending Code Execution)

NUREG/CR-6613, Vol. 1 – page 5-29

Line within MACCS2 IN1A.INP sample file:

```
OCENDAT1001  .FALSE. (SET THIS VALUE TO .TRUE. TO SKIP EARLY AND CHRONC)
```

For a specific application:

Normally this value should not be changed. If the dilution factor (χ/Q) is the only consequence measure of interest, the execution should be stopped with ATMOS by setting the value to TRUE.

Variable IDEBUG (Debug Flag)

NUREG/CR-6613, Vol. 1 – pages 5-29 – 5-30

Line within MACCS2 IN1A.INP sample file:

```
OCIDEBUG001  0
```

For a specific application:

Normally this value should not be changed. However, the user may find it helpful to set the debug to a higher value – 1 or 2 for atmospheric transport results and 3 for hourly meteorological data for each trial. It is therefore useful for comparing MACCS2 results with hand calculations using the equations in the code documentation, or alternative code results. A value of 1 will print out tables of centerline dose versus distance for each weather trial. Higher values of IDEBUG are of less value, and will generate extremely large output files when weather sampling is used.

Variable NUCOUT (Radionuclide to be listed on the dispersion listings)

NUREG/CR-6613, Vol. 1 – page 5-31

Line within MACCS2 IN1A.INP sample file:

```
*OCNUCOUT001  CS-137
```

For a specific application:

Normally this value should not be changed. However, when either intermediate results or MACCS2 atmospheric results are desired, this value should be set equal to the dominant radionuclide, or any particular nuclide used for supporting hand calculations.

Variable NUM0 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 5-40 –5-41

Line within MACCS2 IN1A.INP sample file:

```
TYPE0NUMBER      2
```

For a specific application:

Normally this value should be set equal to zero (0). However, when general atmospheric results or the dilution factor only is desired, this value should be set equal to the number of desired results

Variable INDREL and INDRAD (Plume segment index and spatial endpoint index for results)

NUREG/CR-6613, Vol. 1 – pages 5-41 - 42

Line within MACCS2 IN1A.INP sample file:

```
TYPE0OUT001      1        9
TYPE0OUT002      1       10          XCCDF
```

For a specific application:

Normally these lines should be commented out. However, when general atmospheric results or the dilution factor only is desired, these values will be changed to reflect the desired results. Additional lines may be needed.

Meteorological Sampling Data Block (M1)

Variable METCOD (Meteorological sampling specification)

NUREG/CR-6613, Vol. 1 – pages 5-31 to 5-32

Line within MACCS2 IN1A.INP sample file:

```
* METEOROLOGICAL SAMPLING DATA BLOCK
*
* METEOROLOGICAL SAMPLING OPTION CODE:
*
* METCOD = 1, USER SPECIFIED DAY AND HOUR IN THE YEAR (FROM MET FILE),
*          2, WEATHER CATEGORY BIN SAMPLING,
*          3, 120 HOURS OF WEATHER SPECIFIED ON THE ATMOS USER INPUT FILE,
*          4, CONSTANT MET (BOUNDARY WEATHER USED FROM THE START),
*          5, STRATIFIED RANDOM SAMPLES FOR EACH DAY OF THE YEAR.
*
M1METCOD001   5
```

For a specific application:

For DSA applications, stratified random sampling (METCOD=5) is recommended. Older studies may still use weather category bin sampling (METCOD=2), and this can be used as an alternative if the appropriate random seed (see discussion on IRSEED) is used.

Boundary Weather Data Block (M2)

Note: The values in this data block must always be defined. When constant meteorological conditions are chosen (METCOD = 4), the input values represent the constant meteorological conditions. In all other cases, they represent the meteorological data

for the final grid region, if the plume has not traversed the entire grid in 120 hours. Older PRA studies used this value for larger grids (as large as 1000-mile radius) to conservatively account for remaining non-noble gas radioactivity in the plume before the plume "moves off" the grid.

Variable LIMSPA (Index of last radial endpoint for measured meteorological data)

NUREG/CR-6613, Vol. 1 – pages 5-32 – 5-33

Line within MACCS2 IN1A.INP sample file:

```
M2LIMSPA001  25
```

For a specific application:

This value should be set equal to the index of the last spatial interval

Variable BNDMXH (Boundary weather mixing layer height)

NUREG/CR-6613, Vol. 1 – page 5-33

Line within MACCS2 IN1A.INP sample file:

```
M2BNDMXH001  1000.  (METERS)
```

For a specific application:

This value should be set equal to the appropriate mixing height for the selected stability class.

Variable IBDSTB (Boundary weather stability class)

Line within MACCS2 IN1A.INP sample file:

NUREG/CR-6613, Vol. 1 – page 5-33

```
M2IBDSTB001  4      (D-STABILITY)
```

For a specific application:

This value should be set equal to the numeric index of the desired stability class.

Variable BNDRAN (Boundary weather rain rate)

NUREG/CR-6613, Vol. 1 – page 5-33

Line within MACCS2 IN1A.INP sample file:

```
M2BNRAND001  0.      (MILLIMETERS/HOUR)
```

Variable BNDWND (Boundary weather windspeed)

NUREG/CR-6613, Vol. 1 – page 5-34
Line within MACCS2 IN1A.INP sample file:

```
M2BNDWND001  5.      (M/S)
```

For a specific application:
This value should be set equal to the desired wind speed.

Fixed Start Time Data Block (M3)

The values in this data block must be defined if METCOD does not equal 2 or 5. Input values for ISTRHR and ISTRDY have no effect on dose calculations by the EARLY module when METCOD=2 or =5 weather sampling is utilized. However, these parameters can be used to examine in detail a single weather sequence from an annual weather file for purposes of verification, in combination with setting the ATMOS variable IPRINT to a value of 1 or higher.

Variable ISTRDY (Index of start day from meteorological data file)

NUREG/CR-6613, Vol. 1 – page 5-34
Line within MACCS2 IN1A.INP sample file:

```
M3ISTRDY001  157     (START TIME FOR PEAK ECONOMIC COST OF SAMPLE PROBLEM A)
```

For a specific application:
This line should not be changed.

Variable ISTRHR (Index of start hour from meteorological data file)

NUREG/CR-6613, Vol. 1 – page 5-34
Line within MACCS2 IN1A.INP sample file:

```
M3ISTRHR001  10      (START TIME FOR PEAK ECONOMIC COST OF SAMPLE PROBLEM A)
```

For a specific application:

This line should not be changed unless it is being used to select a particular weather start time using METCOD=1 per discussion of ISTRDY above..

Meteorological Bin Sampling Data Block (M4)

Variable NSMPLS (Number of samples per bin)

NUREG/CR-6613, Vol. 1 – page 5-37

Line within MACCS2 IN1A.INP sample file:

```
M4NSMPLS001   4   (THIS NUMBER SHOULD BE SET TO 4 FOR RISK ASSESSMENT)
```

For a specific application:

This parameter defines the number of weather sequences to be chosen from each of the individual weather category bins with METCOD=2 (weather category bin sampling) or from each day of the year with METCOD=5 (random stratified sampling). The user's manual advises that this input should be at least 4 when METCOD=2 and a divisor of 24 (i.e., 1, 2, 3, 4, 6, 8, 12 or 24) when METCOD=5. It is suggested that this value should be set equal to a maximum value of 24 for METCOD=5. With METCOD=5, setting the number of samples to 24 will result in MACCS sampling every hour of the year.

Variable IRSEED (Random Number Generator Seed)

NUREG/CR-6613, Vol. 1 – page 5-38

Line within MACCS2 IN1A.INP sample file:

```
M4IRSEED001   79
```

For a specific application:

This value should be selected based on evaluating choices of IRSEED ($1 \leq$ IRSEED ≤ 256) with the site meteorological file, and a set of representative source terms. It is also suggested that runs comparing this option with METCOD=5 be performed to ensure that a random seed number is selected leading to bounding consequences is chosen. From the set of resulting consequence values, the seed resulting in the sufficiently bounding consequences can be chosen.

See pages 5-39 and 5-40 of NUREG/CR-6613 for special inputs required for "User-Supplied Weather Sequence Data" and "CCDFs of Atmospheric Results", respectively.

4.5 EARLY INPUT FILE

Similar to the approach taken in Section 4.4 for ATMOS, the particular EARLY input file discussed here is used a starting point input file and can be changed as needed for particular case. It is one of the sample files (e.g., IN2A.INP) supplied with the MACCS2 software compact disc from RSICC. As was the case with the ATMOS file, if a variable is not explicitly mentioned, it is not necessary to change its value.

For each section of input, MACCS2 page-specific references are provided. These will allow the safety analyst to review original reports from the SNL code developer to check on a specific variable.

Dose Conversion Factor File

Review pages 6-4 through 6-5 of NUREG/CR-6613, Volume 1, for options on the particular dose conversion factor file used in a given MACCS2 run.

Miscellaneous Data Block (MI)

NUREG/CR-6613, Vol. 1 – pages 6-6 to 6-9

Variable EANAM1 (EARLY input file identifier line)

Line within MACCS2 IN2A.INP sample file:

```
MIEANAM1001  ' IN2A.INP, MODIFIED 6/92, SURRY, SAMPLE PROBLEM A, EARLY INPUT'
```

For a specific application:
Change to a descriptive title for this execution of MACCS2. It will be included in the output listing.

Variable IPLUME (Dispersion model option code)
Line within MACCS2 IN2A.INP sample file:

```
MIIPLUME001  2
```

This integer value specifies the dispersion model option to be applied in the code.
Choices are: 1 – Straight-line dispersion model; 2 – Wind shift with rotation; and 3 – Wind shift without rotation.

This value should be set to 1 for DSA applications, and not changed.[11]

Variable IPRINT (Debug Flag)
Line within MACCS2 IN2A.INP sample file:

```
MIIPRINT001  0
```

For a specific application:
Normally this value should not be changed. However, the novice user will find it helpful to set the debug to a value of 1 or higher and compare the MACCS2 results with hand calculations using the equations in the code documentation.

Variable RISCAT (Logical flag for consequences by contribution to mean)
Line within MACCS2 IN2A.INP sample file:

```
MIRISCAT001   .FALSE.
```

For a specific application:
Normally this value should not be changed. However, the novice user will find it helpful to set the value to ".TRUE." and compare the MACCS2 results with hand calculations using the equations in the code documentation.

Variable OVRRID (Logical flag for overriding the code calculated windrose)
Line within MACCS2 IN2A.INP sample file:

```
MIOVRRID001  .FALSE.  (USE THE WIND ROSE CALCULATED FOR EACH WEATHER BIN)
```

For a specific application:
Normally this value should not be changed. However, if this value should be set equal to ".TRUE.", then the user-calculated windrose is input using the WINROS parameter that is described next.

Variable WINROS (probabilities of the wind blowing from the site into each of the 16 compass sectors (rotating clockwise from N to NNW when OVRRID parameter is set equal to ".TRUE.")

For a specific application:

---

[11] The only exception would be if there was a need to calculate the 99.5% direction-dependent MOI measure defined in NRC Reg. Guide 1.145. In such cases, the use of METCOD=5 in combination with IPLUME=3 and the EARLY module's Type B results, the 99.5% result for dose at an (r, theta (θ)) location at the sixteen site boundary locations can be compared to the 99.5% direction-dependent measure used by the NRC in Reg. Guide 1.145.

Normally this parameter is not used in DSA applications.

Variable DCF_FILE (Name and location of the dose conversion factor file)

NUREG/CR-6613, Vol. 1 – page 6-5

Line within MACCS2 IN2A.INP sample file:

```
DCF_FILE001 'DOSDATA.INP'  (DCF file of MACCS 1.5.11.1)
```

For a specific application:

This value should be set once to the name and location of the dose conversion factor file and then not changed. For safety basis documents, the dose conversion factors from external radiation should be based on FGR 12, while those from internal radiation can be based on FGR 11. ICRP 68 (Worker) and 72 (General Public) are the newer recommendations for the inhalation dose conversion factors (IDCFs) from the International Commission on Radiological Protection (ICRP, 2001). Good practice would be to obtain authorization from the local or cognizant DOE office on the specific DCF set applied in DSA calculations.

Population Distribution Data Block (PD)

NUREG/CR-6613, Vol. 1 – pages 6-9 to 6-10

Variable POPFLG (Flag indicating whether a population file of uniform population is being used)

Line within MACCS2 IN2A.INP sample file:

```
PDPOPFLG001  FILE
```

For a specific application:

This value should be changed once to "UNIFORM" and then not changed unless a Site Data File with a polar-grid population is being utilized. A Site Data File is not needed for MOI calculations in a DSA, but it would be needed to calculate the conventional 50-mile collective dose typically calculated for an environmental impact assessment.

Variable IBEGIN (Index of radial endpoint where the population begins)

Line within MACCS2 IN2A.INP sample file:

```
*PDIBEGIN001  1   (SPATIAL INTERVAL AT WHICH POPULATION BEGINS)
```

For a specific application:
This line should be changed once by removing the comment indicator (the asterisk) from the beginning of the line.

Variable POPDEN (Uniform population density of the region)
Line within MACCS2 IN2A.INP sample file:

```
*PDPOPDEN001   50. (POPULATION DENSITY (PEOPLE PER SQUARE KILOMETER))
```

For a specific application:
This line should be changed once by removing the comment indicator (the asterisk) from the beginning of the line, and the value changed to zero (0.). After the line has been changed once, it will not need to be changed again.

Organ Definition Data Block (OD)

NUREG/CR-6613, Vol. 1 – pages 6-10 to 6-12

Variable NUMORG (Number of organs to be considered)
Line within MACCS2 IN2A.INP sample file:

```
ODNUMORG001    10
```

For a specific application:
If the user wishes to apply the dose conversion file generated from the FGRDCF code (Young, 1998) and supplied with the MACCS2 code, the above line may be commented out. See below for additional discussion.

Variable ORGDEF (List of organ names and flag to specify whether or not the organ is to be considered in the calculations)
Line within MACCS2 IN2A.INP sample file:

```
*
*              ORGNAM          ORGFLG
*
MIORGDEF001   'A-SKIN'         .TRUE.
MIORGDEF002   'A-RED MARR'     .TRUE.
MIORGDEF003   'A-LUNGS'        .TRUE.
MIORGDEF004   'A-THYROIDH'     .TRUE.
MIORGDEF005   'A-STOMACH'      .TRUE.
MIORGDEF006   'A-LOWER LI'     .FALSE.   (does not contribute to early fatalities)
MIORGDEF007   'L-EDEWBODY'     .TRUE.
MIORGDEF008   'L-RED MARR'     .TRUE.
MIORGDEF009   'L-BONE SUR'     .TRUE.
MIORGDEF010   'L-BREAST'       .TRUE.
MIORGDEF011   'L-LUNGS'        .TRUE.
MIORGDEF012   'L-THYROID'      .TRUE.
```

```
MIORGDEF013  'L-LOWER LI'     .TRUE.
MIORGDEF014  'L-BLAD WAL'     .TRUE.
MIORGDEF015  'L-LIVER'        .FALSE.
MIORGDEF016  'L-THYROIDH'     .TRUE.
```

For a specific application:

Again, if the user wishes to apply the dose conversion file that is generated from the FGRDCF code (Young, 1998) and supplied with the MACCS2 code, the above lines may be commented out. The FGRDCF-based dose conversion file provides inhalation and ingestion DCFs from FGR 11 and cloudshine and groundshine dose coefficients from FGR 12. Recall that FGR 11 inhalation DCFs are based on weighting factors from ICRP 26 (ICRP, 1977) and organ/tissue models documented in ICRP 30 and 48 (ICRP, 1979a to 1982c, and ICRP, 1986). With the local or cognizant DOE office's approval, the inhalation and ingestion DCFs can be replaced with those from ICRP 68 or 72.

NOTE: The dose conversion file that is created by the FGRDCF code creates a two-line header with the letter string "FGRDCF" embedded within the first header line. MACCS2 checks for the letter string "FGRDCF" within the first seven letters of the first header line and if found, assumes that the dose conversion file was generated from the FGRDCF code and sets the lists of available organs to be consistent with the FGRDCF code and with FGR 11 and 12. Note that MACCS2 adds a prefix of "L-" to the organ names that is used to indicate a 50-year committed dose. Specifically, the list of organs is as follows:

- L-GONADS
- L-BREAST
- L-LUNGS
- L-RED MARR
- L-BONE SUR
- L-THYROID
- L-REMAINDER
- L-EFFECTIVE
- L-SKIN(FGR)

Note: Because the FGRDCF does not utilize ICRP 68 or 72, a FGRDCF Dose Conversion File for MACCS2 would require editing to incorporate the newer values. If only the newer ICRP-defined Effective Dose (H_t) is being reported, then only the values for L-EFFECTIVE would require revision. However, the remaining data for the other organs would need to be left in the file; MACCS2 would not utilize doses for the other organs unless requested in the EARLY Input File.

NUREG/CR-6613, Vol. 1 – pages 6-12 to 6-14

Variable CSFACT (Cloudshine shielding factor)
Line within MACCS2 IN2A.INP sample file:

```
SECSFACT001      1.     0.75    0.6   *  SURRY SHELTERING VALUE
```

For a specific application:

The cloudshine shielding factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable PROTIN (Inhalation protection factor)
Line within MACCS2 IN2A.INP sample file:

```
SEPROTIN001      1.     0.41      0.33  * VALUES FOR NORMAL ACTIVITY AND
```

For a specific application:

The inhalation protection factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable SKPFAC (Skin absorption protection factor)
Line within MACCS2 IN2A.INP sample file:

```
SESKPFAC001  1.0      0.41     0.33    * VALUES FOR NORMAL ACTIVITY AND
```

For a specific application:

The skin absorption protection factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable GSHFAC (Groundshine shielding factor)
Line within MACCS2 IN2A.INP sample file:

```
SEGSHFAC001      0.5    0.33    0.2   * VALUE FOR NORMAL ACTIVITY SELECTED BY
```

For a specific application:

The groundshine shielding factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable BRRATE (Breathing rate)
Line within MACCS2 IN2A.INP sample file:

```
SEBRRATE001  2.66E-4  2.66E-4  2.66E-4
```

For a specific application:

The breathing rate for all three activity levels should be set equal to 3.33E-04 m^3/s (DOE, 1998), as discussed in Appendix A. Note that the basis for DOE-STD-1027-92 hazard categorization is slighter higher at 3.47E-04 m^3/s.

Variable RESCON (Resuspension inhalation model concentration coefficient)
Line within MACCS2 IN2A.INP sample file:

```
SERESCON001   1.E-4      (RESUSPENSION IS TURNED ON)
```

For a specific application:

This value should be set once and not changed. Per DOE-STD-3009-94 Appendix A, resuspension does not need to be included in the DSA calculations of TEDE. If resuspension is to be turned off, set the value equal to zero (0.). If resuspension is to be applied, this value does not need to be changed because it was chosen to conservatively reflect resuspension due to human activities such as evacuation and relocation; it is set much higher than would be appropriate for undisturbed land.

Evacuation Zone Data Block (EZ)

NUREG/CR-6613, Vol. 1 – pages 6-14 to 6-29

Variable LASMOV (Index of last radial ring involved in the evacuation)
Line within MACCS2 IN2A.INP sample file:

```
EZLASMOV001      15     (EVACUEES DISAPPEAR AFTER TRAVELING TO 20 MILES)
```

For a specific application:

This value should be set once to zero (0) and then not changed.

Shelter and Relocation Data Block (SR)

Variable ENDEMP (Duration of the emergency phase)

NUREG/CR-6613, Vol. 1 – page 6-27

Line within MACCS2 IN2A.INP sample file:

```
SRENDEMP001  604800.   (ONE WEEK)
```

For a specific application:

This is the value of the emergency phase period in units of seconds, should be set once to 86400. (24 hours), and is the minimum time value allowed by MACCS2. The maximum period is 7 days (604800. seconds). Note that the 24-hour period represents conservative implementation of the prescribed exposure duration of 2 hours (or 8 hours for slow-developing release scenarios) discussed in DOE-STD-3009-94, Appendix A.

Variable TIMHOT (Time for hot-spot relocation)
Line within MACCS2 IN2A.INP sample file:

```
SRTIMHOT001  43200.    (ONE-HALF DAY)
```

For a specific application:

This value should be set once to 86400 (24 hours) and then not changed.

Early Fatality Data Block (EF)

NUREG/CR-6613, Vol. 1 – pages 6-29 to 6-33

Variable NUMEFA (Number of early fatality effects)
Line within MACCS2 IN2A.INP sample file:

```
EFNUMEFA001   3
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Early Injury Data Block (EI)

NUREG/CR-6613, Vol. 1 – pages 6-33 to 6-35

Variable NUMEIN (Number of early injury effects)
Line within MACCS2 IN2A.INP sample file:

```
EINUMEIN001   7
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Latent Cancer Data Block (LC)

NUREG/CR-6613, Vol. 1 – pages 6-35 to 6-40

Variable NUMACA (Number of acute exposure cancer effects)
Line within MACCS2 IN2A.INP sample file:

```
LCNUMACA001    7
```

For a specific application:

Normally, this value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed. If cancer risks are requested by DOE, the use of ICRP 60 (1991) 60 risk factors are recommended, presented in Chanin and Young (1998) as shown below:

```
* NUMBER OF ACUTE EXPOSURE CANCER EFFECTS

LCNUMACA001    1

*

* THRESHOLD DOSE FOR APPLYING THE DOSE DEPENDENT REDUCTION FACTOR

LCDDTHRE001    0.0  (LOWEST DOSE FOR WHICH DDREFA WILL BE APPLIED)

* DOSE THRESHOLD FOR LINEAR DOSE RESPONSE (Sv)

* LCACTHRE001    0.0  (LINEAR-QUADRATIC MODEL IS NOT BEING USED)

*            ACNAME       ORGNAM  ACSUSC  DOSEFA DOSEFB  CFRISK  CIRISK  DDREFA

LCANCERS001 'ICRP 60'  'L-EFFECTIVE' 1.0   1.0    0.0    5.0E-2  7.3E-2   1.0
```

Type One Output - Health Effects Data Block (T1)

Variable NUM1 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – page 6-43

Line within MACCS2 IN2A.INP sample file:

```
TYPE1NUMBER    27
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Two Output – Early Fatality Radius Data Block (T2)

Variable NUM2 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – page 6-45

Line within MACCS2 IN2A.INP sample file:

```
TYPE2NUMBER  1
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Three Output – Population Exceed Dose Threshold Data Block (T3)

Variable NUM3 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – page 6-46

Line within MACCS2 IN2A.INP sample file:

```
TYPE3NUMBER  3
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Four Output – Average Individual Risk Data Block (T4

NUREG/CR-6613, Vol. 1 – page 6-47 to 6-48

Variable NUM4 (Number of requested outputs)
Line within MACCS2 IN2A.INP sample file:

```
TYPE4NUMBER   5
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Five Output – Population Dose Data Block (T5)

Variable NUM5 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 6-48 to 6-49

Line within MACCS2 IN2A.INP sample file:

```
TYPE5NUMBER      3
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Six Output – Centerline Dose at Distance Data Block (T6)

Variable NUM6 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 6-49 to 6-52

Line within MACCS2 IN2A.INP sample file:

```
TYPE6NUMBER      0
```

The output of interest for DSA applications is the Type Number 6 output, which signifies centerline doses at a distance. Refer to the sample cases illustrated in Section 7 for obtaining this result at specified distances.

Variable ORGNAM, PATHNM, I1DIS6, and I2DIS6 (Organ name, pathway name, inner spatial interval, and outer spatial interval as input by OUT)
Line within MACCS2 IN2A.INP sample file:

```
*TYPE6OUT001  'RED MARR'    'TOT ACU'      1        19      (0-50 MILES)
*TYPE6OUT002  'LUNGS'       'TOT ACU'      1        19      (0-50 MILES)
*TYPE6OUT003  'EDEWBODY'    'TOT LIF'      1        26      (0-1000 MILES)
```

For a specific application:

The comment indicator (the asterisk) should be removed from the output definition. The organ name should be change to "L-EFFECTIVE". The pathway name should be changed to "TOT LIF". The inner and outer spatial intervals (radii) should be set equal to the ring encompassing the receptor location. For example, if it is desired to output the fifty-year TEDE doses for the 250-m and 350-m receptors (rings 1 and 2) in Figure 4-3, the user would enter

```
TYPE6OUT001  'L-EFFECTIVE'    'TOT LIF'      1        1       (250 m RING ONE)
TYPE6OUT002  'L-EFFECTIVE'    'TOT LIF'      2        2       (350 m RING TWO)
```

If the release is elevated or heated and the MOI is located within several kilometers of the release location, the MOI may not be located at the closest site boundary but at the point of the dominant plume's touchdown. In this case, the inner and outer spatial intervals should be reset to encompass the location of the plume touchdown.

Type Seven Output – Centerline Risk vs. Distance Data Block (T7)

Variable NUM7 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 6-52 to 6-54
Line within MACCS2 IN2A.INP sample file:

```
TYPE7NUMBER      0
```

For a specific application:

This value should not be changed.

Type Eight Output – Population Weighted Risk Data Block (T8)

Variable NUM8 (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 6-54 to 6-55

Line within MACCS2 IN2A.INP sample file:

```
TYPE8NUMBER    2
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type A Output – Peak Dose at a Distance Data Block (TA)

Variable NUMA (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 6-56 to 6-57

Line within MACCS2 IN2A.INP sample file:

```
TYPE8NUMBER    1
```

For a specific application:

Normally, this value should be set once to zero (0.) and the rest of the lines within the block should be commented out and then not changed.

Type B Output – Peak Dose at a Distance and Sector Data Block (TB)

Variable NUMA (Number of requested outputs)

NUREG/CR-6613, Vol. 1 – pages 6-57 to 6-58

Line within MACCS2 IN2A.INP sample file:

```
TYPEBNUMBER    0
```

Normally, this value should be set at zero (0). The exception would be if the 99.5^{th} percentile direction-dependent dose was being evaluated. In this case, IPLUME is set equal to three (3).

4.6 DOSE CONVERSION FACTOR FILE

For safety basis documentation, the FGRDCF code (Young, 1998) supplied with the MACCS2 code may be used to create a dose conversion factor file for either MACCS2 or MACCS execution. To be consistent with latest available guidance from internationally recognized guidance bodies, the inhalation and ingestion dose conversion factors should be replaced with those from ICRP 68 or 72. As noted previously, however, until use of the newer ICRP values is approved at the DOE Headquarter level, the use of the newer DCF files should be based on the local or cognizant DOE office's approval..

Note that if the source term includes tritium oxide, its 50-year committed inhalation dose conversion factor should be increased by 50% to include the effects of skin absorption as directed by International Commission on Radiological Protection (ICRP) in Publication 30 (ICRP, 1978).

The omission of the skin absorption dose in the FGRDCF output file is made apparent by the fact that tritium dose conversion factors for inhalation and ingestion are identical as shown below.

```
H-3

...

EFFECTIVE  3.310E-19 0.000E+00 0.000E+00 0.000E+00-1.000E+00 1.730E-11 1.730E-11
```

According to ICRP-68/72 (2002), tritium oxide ingestion and inhalation dose conversion factors are given as identical values for both inhalation and ingestion. The newer data compendium gives values of 1.8E–11 Sv/Bq for both inhalation and ingestion to members of the public.

4.7 Radiological Dispersion and Consequence Analysis Recommendation

Recommendations on inputs for MACCS2 modeling radiological dispersion and consequences and their bases, discussed at length in Appendix A, are summarized in Table 4-1. In most cases, the standard practices and recommendations are site-independent.

Table 4-1. Standard Practices and Assumptions Recommended for DSA Dispersion and Consequence Analysis

MODEL/ATTRIBUTE	Recommendation/Basis
Model Basis	Gaussian plume or puff model; DOE-STD-3009-94, CN2, Appendix A
Receptor Distances & Meteorology	• MOI: Evaluate using or conservative to 95th percentile methodology per DOE-STD-3009-94, CN2, Appendix A and NRC Regulatory Guide 1.145; • Evaluate at touchdown point for elevated or sensible energy-buoyant releases
Default Meteorological Conditions	• Prescriptive: F and low windspeed (1 - 1.5 m/s) for offsite; • D and intermediate windspeed (~4.5 m/s) for onsite receptors;
Dispersion Parameters	• >100 meters from source: Site tracer gas parameterization; Pasquill-Gifford; Tadmor-Gur (Dobbins, 1979); Briggs (Hanna, 1982) • < 100 meters, use Eimutis and Konicek (1972), or other as justified
Mixing Layer Height	Apply local site/laboratory recommendations for seasonal and time-of-day estimates for the mixing layer height.
Surface Roughness	Adjust σ_z based on site features with AMS (1977) model
Release Duration	Should be consistent with accident analysis, and set of applicable dispersion parameters (σ_y). Scale to longer release duration by applying Gifford, or similar model. As a default conservatism, apply dispersion parameter set equal to or less than release duration.
Exposure	Two hours: DOE-STD-3009-94, CN2, App. A; RG 1.145 (to MOI) Sequences that take longer to develop; No longer than eight hours; DOE-STD-3009-94, CN2, App. A
Deposition	Dry deposition: Assume the deposition velocity is 1 cm/s for all unfiltered, non-tritium, non-noble gas species. If filtration is assumed in the scenario, apply the 0.1 cm/s deposition velocity. Tritium species deplete from airborne plumes as a function of the site environment. Recommendations have been documented indicating a range of 0.04 cm/s to 0.05 cm/s for tritium gas (HT), and 0.4 cm/s to 0.8 cm/s for tritiated water vapor (HTO). Wet deposition: Not used.
Dose Conversion Factors	1. ICRP-60 for biokinetic model and ICRP-68/72 for dose coefficients 2. ICRP-26 for metabolic model; ICRP 30/48-based:DOE/EH-0070 and 0071; or Federal Guidance Reports 11 and 12
Pathways	Primary: Inhalation; DOE-STD-3009-94, CN2, Appendix A Secondary: Cloudshine, Groundshine (Important only for criticality source terms in non-reactor applications);

Table 4-1. Standard Practices and Assumptions Recommended for DSA Dispersion and Consequence Analysis (continued)

Breathing Rate	3.33E-04 m^3/s; DOE (1998); 3.47E-04 m^3/s; DOE-STD-1027-92.
Dose Commitment	50-year, per definition of TEDE in DOE-STD-3009-94, CN2, Appendix A
Evaluation Criterion	Offsite/MOI Evaluation Guideline - 25 rem; DOE-STD-3009-94, CN2, Appendix A
Terrain	Flat Earth acceptable for most near-field and MOI estimates; Terrain realistic for other site areas and offsite calculations (valley, land/water interface, and/or mountainous terrain)
Sensible heat in plume	1. The conservative assumption is to not credit plume rise due to fire or explosive release, apply a short duration, and assume ground-level release. 2. If the fire is "well-defined" and the release of sensible heat (and radionuclides) and the certainty of release from one location (i.e. approximates point source) is high, then current model in MACCS2 is adequate. 3. If the fire being modeled is out-of-facility, without intervening structures, and the sensible heat fraction is known, then for: (a.) pool fires – MACCS2 model should not be applied as is, but some initial plume conditions can be adjusted to estimate the thermal buoyancy effect; (b.) spatially localized fire – MACCS2 model is adequate. 4. For primarily indoor fires, the fraction of heat radiated to walls and ceilings may be uncertain, and interpretation of the results from a MACCS2 model would be uncertain. 5. For all fire scenarios, the analyst is strongly urged to review Appendix A and refer to documents being cited,, including Hills (1998), where the Mills (1987) fire model was implemented in MACCS2.
Protective Actions	None; Conservatively assume no shielding by any structure or cut-off of ventilation (sheltering), or movement to avoid plume (evacuation). While these actions can be evaluated with MACCS2 for sensitivity studies to plan dose mitigation strategies, the DSA applications should not credit these avoidance measures.
Meteorological Sampling	Stratified Random Sampling – draw samples from each time interval (~day) of the year. Twenty-four samples are recommended for MACCS2 if METCOD=5. At least one year of representative, qualified, hourly data;. Alternatively, Latin Hypercube Sampling of meteorological bins (categories of stability, wind speed); four or more samples are recommended if METCOD=2 in MACCS2
Meteorological Data	At least one year of representative, qualified, hourly data; Two to five years is recommended (Regulatory Guide 1.23; and Regulatory Guide 1.194 (NRC, 2003))

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5.0 SPECIAL CONDITIONS FOR USE

MACCS2 is public domain software that is the current code in a series designed for the purpose of calculating consequences for probabilistic safety analysis of nuclear facilities. Even though MACCS2 was not developed specifically for deterministic safety analysis applications, it is widely used throughout the DOE complex for this purpose and has been designated for the DOE Safety Software Toolbox to support 10 CFR 830 documents. This document serves as a guide for implementation of the MACCS2 code for the purpose of modeling source term and consequence phenomenology supporting safety basis documentation. The user, however, must still demonstrate that MACCS2 is being used within its domain of applicability and that site/laboratory SQA procedures governing use of safety analysis software are being followed. Use in accident analysis applications is conditional based on the following:

1. MACCS2 is being used as a tool in decision-making in the selection of safety structures, systems, and components, and as such its output is applied in safety analysis only after appropriate technical review;

2. The user is knowledgeable on MACCS2 limitations, and specifies inputs that are reasonably conservative level and consistent for the application;

3. The analytic applications are appropriate for MACCS2 and do not apply the code outside of the domain for which it is intended.

The MACCS2 code and its predecessor, MACCS, have additional capabilities that generally are not used in standard DSA applications. For example, food ingestion doses can be calculated, but these results are not part of the DOE 3009 Appendix A requirement for safety basis dose calculations. Also, MACCS2 has models to calculate population doses and show the relative benefits of evacuation and sheltering (as well as interdiction when food ingestion is considered), but results of this type also are not needed for safety basis dose calculations.

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6.0 SOFTWARE LIMITATIONS

Radiological dispersion and consequence computer software that is based on the Gaussian plume model is generally limited to certain domains of applicability. Initially, this section will highlight the general regime for which the Gaussian model provides a reasonable estimate of the behavior of radioactive releases into the atmosphere. Next, code specific issues shall be discussed for both MACCS and MACCS2.

Table 6-1 lists several of the primary limitations of the Gaussian model with respect to its use in accident analysis.

Table 6-1. Limitations of Gaussian Plume Model in MACCS2 and MACCS

Topic	Applicable Regime	Basis	Source or Reference
Distance from Source	100 m < x < 10 km – 20 km	Dispersion parameterization	(Haugen, 1959); Other accounts of Prairie Grass experiments;
Sensible Energy	Well-defined (e.g., sensible heat, timing, certainty of radiological release with combustibles) releases	Point-wise (stack) or pool-type (area) release	Briggs (1975); Mills (1987)
Release Duration	Approximately three minutes to ten hours	Dependent on basis dispersion parameters	NUREG/CR-4551; Tadmor (1969); Gifford (1975)
Terrain Sensitivity	Flat-earth to "gently rolling"	Adjust dispersion parameter set to region of interest with AMS model; Complicated terrain over the region of transport may require Lagrangian particle or other models	AMS (1977); (Hanna, 1982); Hanna (2002); Others
Building wake effects	Within approximately ten x characteristic building dimension lengths	See discussion beginning page A-29 of this report.	Turner (1970)

6.1 Code-Specific Issues

This section summarizes MACCS (6.1.1) and MACCS2 (6.1.2) software limitations in terms of past occurrences of errors and defects in various versions of the code. The last section (6.2) summarizes the gap analysis, i.e., evaluation of MACCS2 against defined software standards.

6.1.1 Issues Associated with MACCS

During the use of MACCS 1.5.11 by different organizations for various reactor and non-reactor applications,[12] errors were discovered in the code. These errors prompted the issuance of a maintenance version of the MACCS code (i.e. version 1.5.11.1). The changes in the original MACCS source code were independently verified (Chanin, 1993) before the new source code (MACCS, Version 1.5.11.1) was released in 1993. In addition to the correction of errors in the original MACCS code, the MACCS, Version 1.5.11.1 distribution package included executables for several operating systems in addition to the original VAX/VMS system.

Although the aforementioned changes had a small impact on the results, the maintenance version of MACCS has an additional cancer fatality model. The older model is a linear quadratic equation based on BEIR III cancer model. The newer model is a discontinuous linear equation, based on review of the BEIR V cancer models in a report (LMF-132) prepared by the Lovelace Inhalation and Toxicology Research Institute (ITRI) (Chanin, 1993). This cancer model was the only one for cancer estimates distributed with MACCS. The discontinuity between 1) low doses at low dose rates and 2) higher doses or high dose rates remained in the post-BEIR-V cancer risk model of ICRP 60 (1991). MACCS2 includes data for the use of both older and newer cancer models, but the use of the more recent ICRP 60 cancer risk model is recommended for DOE applications.

Since the issuance of the maintenance version of MACCS, several errors have been catalogued. The errors and additional enhancements have been corrected in MACCS2 (RSICC, 1997). Table 6-2 lists enhancements and corrections. It should be pointed out that except in one case, i.e., groundshine from criticality source terms (item #5), there is no impact to dose calculations performed in support of DSA from these modifications.

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[12] - The MACCS code is used for PSA studies and facility licensing throughout the United States and abroad by both commercial and government organizations

Table 6-2. Code Modifications to MACCS2 and Impact to DSA Calculation (See Pages 3-9 through 3-16 of RSICC (1997))

Error/Enhancement	Action	Impact to DSA MOI Dose Analysis
1. Dose-Dependent Reduction Factor Implementation Error	Corrected EARLY module for error to cancer risk estimates. Did not affect chronic, cancer risk calculations.	Cancer risks are not calculated for DSAs – No Impact
2. Number of People Exceeding Dose Threshold - Incorrect calculations when ten results are requested for the number of people exceeding a dose threshold - Inability to Report Small Values of Dose Threshold	- Subject coding error has been corrected in MACCS2 - MACCS2 has automatic switch to exponential format (from fixed) to allow reporting of dose thresholds < 0.0005 Sv (50 mrem)	This type of result is not calculated for DSAs – No Impact
3. Incomplete Implementation of the Intermediate Phase - health effects and collective doses - lack of interaction between intermediate phase relocation and farm interdiction	Corrections made in MACCS2 only: - Corrected dose data stored for intermediate phase - Mitigative actions are based upon intermediate phase results.	Intermediate and long-term phases are not calculated for DSAs – No Impact
4. Summation of Early and Intermediate Phase Costs	MACCS2 improved to report emergency and intermediate phase costs due to evacuation and relocation separately	Evacuation and relocation costs are not considered in DSAs – No Impact
5. Dose Calculations for Groundshine Following Plume Passage	Groundshine following plume passage was calculated by interpolating and extrapolating doses based on 8-hour and 1-week DCFs (MACCS). MACCS2 performs exact numerical integration.	Potentially important for criticality (short half-life radionuclides), but groundshine dose component is usually small – Minor Impact

Table 6-2. Code Modifications to MACCS2 and Impact to DSA Calculation (Continued)

Error/Enhancement	Action	Impact to DSA MOI Dose Analysis
6. Nonprintable characters in site data file and FORTRAN Source Code	MACCS query of population counts and other information in site data file may lead to code crash due to suspected nonprintable ASCII characters or control codes in the file. MACCS2 has eliminated this factor.	Does not affect MACCS non debugging runs – No Impact to DSA calculations
7. Minor Changes to Input and Output	MACCS2 improved to allow: - 99.9^{th} quantile changed to show 99.5 quantile per NRC Reg. Guide 1.145 Variable DLBCST in CHRONC no longer allowed to have $0 cost for decontamination, to avoid potential division by zero errors.	Useful for some DSA calculations, but most DSA results will focus on 95^{th} percentile, direction independent results. The decontamination factor cost issue is not applicable to DSA calculations. - No Impact Overall.

6.1.2 Issues Associated with MACCS2

A Sandia National Laboratories SQA program was implemented in 1992. The SNL guidelines[13] (SNL, 1987; SNL, 1995; SNL, 1986; SNL, 1992; and SNL, 1989) followed the methodology established by IEEE software standards (IEEE, 1984). Of the five primary SNL software guideline volumes, two[14] were published after the completion of the original MACCS code. These documents demonstrate the development of the code was performed in a systematic way with each step thoroughly reviewed before the next step was taken. The other three volumes[15] were published during the development phase of the MACCS code and were in place before the beginning of the MACCS2 development. Although the guidelines were published after the completion of the MACCS code, the MACCS development followed a systematic method as did error reporting and correction processes associated with the code.

In the initial code development for MACCS2 the same systematic process was followed. A project plan was prepared as were draft versions of a development plan for the food model and for the inclusion of the new dose conversion factors. In addition, a draft test plan was developed. The draft test plan was followed through MACCS2 Version 1.02. However, the plans were never finalized and a formal SQA plan was not put into place.

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[13] - The SNL documentation is clearly described as guidance. The management directing the project may choose not to follow any part, or all, of the recommendations outlined in the guidelines.

[14] - The two volumes published after the beginning of the MACCS2 development were the Documentation volume and the Configuration Management volume. The Documentation volume (SNL, 1995) presents a description of documents needed for developing, maintaining, and defining software projects. The Configuration Management volume (SNL, 1992) presents a discussion of configuration management objectives and approaches throughout the software live cycle for software projects at SNL.

[15] - The three volumes published before the beginning of the MACCS2 development were Software Quality Planning volume, Standards, Practices, and Conventions volume, and Tools, Techniques, and Methodologies volume. The Software Quality Planning volume (SNL, 1987) presents an overview of procedures designed to ensure software quality. The Standards, Practices, and Conventions volume (SNL, 1986) presents standards and practices for developing and maintaining quality software at SNL and includes a description of the documents needed for a complete SQA package at SNL. The Tools, Techniques, and Methodologies volume (SNL, 1989) presents evaluations and a directory of software tools and methodologies available to SNL personnel.

In addition to early testing of the MACCS2 code by in-house staff, SNL contracted the University of New Mexico (UNM) to independently test the code during development. This testing was published in a draft document (Summa, 1996). The report focused on the following areas:

ATMOS Module: Calculation of the downwind relative air concentration (χ/Q) and of the diffusion parameters by using both the power law and the new look-up table methods

EARLY Module: Calculation of the acute thyroid dose, of the network evacuation centerline dose, of the radial evacuation peak dose, of the crosswind evacuation dose, and the dose when the evacuation speed changes

CHRONC Module: Testing of the ability to turn off the long-term phase and the decontamination model, comparison of intermediate phase and long-term phase doses, and calculation of the intermediate phase dose

The testing by UMN was done in an iterative manner. Errors discovered by UNM resulted in coding changes and a new version of the code. The new code version would then be retested by UNM for the function in question. This process would continue until the function worked correctly. The UNM testing did not include any of the preprocessors developed by SNL nor did it include the COMIDA food model developed at INEEL.

After the MACCS2 code was released, several new features of the MACCS2 code were verified against hand calculations at SRS (East 1997). These features were the calculation of the CCDF for the atmospheric concentration, and the vertical and horizontal diffusion parameters in the ATMOS module and the reporting of the peak dose both independent and dependent of sector in the EARLY module. The module functions tested worked properly.

As part of the MACCS2 SQA program evaluation, a review of the code's documentation and source code was performed. From that review, a number of undocumented changes from MACCS to MACCS2 were found. Many of the changes were simply a change in the upper and/or lower bound of the input parameter. Many of those input parameter changes can be attributed to the UNM testing effort. However, that effort was never published.

After the MACCS2 code had been released to the Radiation Safety Information Computation Center (RSICC) at Oak Ridge for distribution, an error was found during routine calculations by the DOE Area Office at Los Alamos National Laboratory.[16] This error involved the source term

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[16] This coding error (affecting only source term looping), and essentially the same error in looping on emergency response scenarios, was corrected in a local version of MACCS2 developed for Pantex Plant. Also incorporated was the Mills (1987) pool-fire model for aircraft crash fires, in addition to a new capability for sampling for as many as ten years of weather data. That Pantex version of MACCS2 underwent verification published by Hills et al. (1998).

looping function that produced erroneous results when four release plumes were specified. The coding error was introduced when the total number of radionuclides was increased from 825 to 900.[17] When this coding change was made, the dimensions of the variables associated with this change were properly increased, but the variables that were dependent on the changed variables were not modified. This led to a corruption of the data stored during each run and led to the subsequent erroneous results. See Appendix B for the Software Defect Notification.

In the interim before the completion of the MACCS2 backfit package, safety analysts using MACCS2 Version 1.12 should proceed with caution, using the guidance contained herein (Section 4). Alternatively, MACCS Version 1.5.11.1 can be applied with the appropriate dose conversion factor data, using the guidance provided in Appendix D of this report.[18]

In either case, independent confirmation and peer review of technical products is advised. "Spot checks" of key consequence calculations using an independent code calculation, or a set of spreadsheet or hand calculations, can frequently minimize or remove code result uncertainty while enhancing analyst confidence in code calculations

6.1.2.1 MACC2 Errors Not Important to DSA Calculations

Other errors exist in MACCS2, but these are determined to be negligible in DSA calculations where MOI doses are being estimated. In the first case, SNL developers reported an error in the emergency preparedness model (described in Appendix B), but this option is not used in obtaining MOI dose estimates, and thus is deemed of no impact to DSA calculations.

A second error is found in the deterministic health effects model. Although latent cancer deaths and injuries arising from exposure to radioactive materials is the primary health concern in nuclear safety, deterministic health effects are also of interest in some contexts. Latent cancer is a long-term health problem (incidence in some cases up to 70 year after exposure) and arises from relatively small internal doses (primarily from inhalation of alpha emitters). Deterministic health effects (called "acute" or "early" in MACCS2), on the other hand, arise from relatively larger intakes. These health effects, such as pneumonitis, manifest within a shorter time after intake, from days to perhaps a few years, depending on the size of the dose and the organ affected. MACCS2 includes a model for these health effects but, unfortunately, they are not calculated correctly.

The method used in MACCS2 to evaluate deterministic health effects is based on the model(s) given in a series of NUREG/CR-4214 reports (e.g., Abrahamson 1993). The equations in MACCS2 are correct, for most part, but their implementation is not. The issue is complex and

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[17] This is the number of available radionuclides in the Dose Conversion Factor database. MACCS2, is still limited to 150 radionuclides per execution.

[18] At the issuance of this report, Version 113.1 has been released, correcting the source-term "looping" errors. See Appendix F for additional detail.

will not be discussed fully here. Briefly, there is some confusion in the use of absorbed dose vs. adjusted dose (which has the RBE applied). For example, the LD_{50} and ED_{50} values used in MACCS2 are based on low-LET radiation, for which absorbed dose and adjusted dose are the same. However, for high-LET radiation (such as alpha emitters), the LD_{50} and ED_{50} should be based on adjusted dose, not absorbed dose. The calculations also need to account for the uncertainties in the parameters in the equations, and in differences in parameter values between low-LET and high-LET. In addition, the period for the effect to manifest is restricted to one year, whereas it should be at least five years. A technique has been published that correctly models these effects (Scott, 2003). Comparisons of calculations using the new technique with those from the MACCS2 code shows that MACCS2 overestimates the doses required to produce the deterministic health effects. A minor error is in the use of units: deterministic doses are measured in Gray, not Sievert. The latter should be used only for stochastic effects (cancer). Another minor error is including pneumonitis in the list of "acute injuries", whereas it is almost always fatal.

It should be noted, however, that although DSA accident analyses must include calculations of doses, calculations of health effects are not required. Therefore, the errors noted here are not relevant for DSA analyses.

In the interim before the completion of the MACCS2 upgrades and improvements, safety analysts using MACCS2 Version 1.12 should proceed with caution, using the guidance contained herein (Section 4). Alternatively, MACCS Version 1.5.11.1 can be applied with the appropriate dose conversion factor data, using the guidance provided in Appendix D of this report.

In either case, independent confirmation and peer review of technical products is advised. "Spot checks" of key consequence calculations using an independent code calculation, or a set of spreadsheet or hand calculations, can frequently minimize or remove code result uncertainty.

6.2 Outcome of Gap Analysis

The gap analysis for Version 1.12 of the MACCS2 software, based on requirements and criteria compliant with NQA-1 and 10 CFR 830, as contained in DOE (2003e), has been documented in the report, *Software Quality Assurance Improvement Plan: MACCS2 Gap Analysis,* (DOE, 2004). It was determined that MACCS2 code does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of MACCS2 for supporting safety analysis. Informed use of the software can be assisted by the current set of MACCS2 reports, as well as the present report. Furthermore, while SQA improvement actions are recommended for MACCS2, no evidence has been found of programming, logic, or other types of software errors in MACCS2 that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

Of the ten primary SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), two

requirements are met at an acceptable level, i.e., *Classification* (1) and *User Instructions* (7). A third requirement, *Error Notification and Corrective Action* (10), is partially met. Improvement actions are recommended for MACCS2 to fully meet requirement (10) criteria, and the remaining seven requirements, and these are listed in Table 6-3. This evaluation outcome is deemed acceptable because: (1) MACCS2 is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of MACCS2 is limited to those analytic applications for which the software is intended.

By order of priority, it is recommended that the following MACCS2 software improvement actions be taken:

1. correct known defects
2. upgrade user technical support activities
3. provide training on a regular basis, and
4. revise software documentation.

Performing these four primary actions should satisfactorily improve the SQA compliance status of MACCS2 relative to the primary evaluation criteria cited in this report.

A new software baseline set of documents is recommended for MACCS2 to demonstrate completion of item 4 (above), revise software documentation. The list of baseline documents for revision includes:

1. Software Quality Assurance Plan
2. Software Model Description, including, but not limited to,
    a. Software Requirements
    b. Software Design
3. User's Manual, including, but not limited to,
    a. User Instructions
    b. Test Case Description and Report
    c. Software Configuration and Control
4. Error Notification and Corrective Action Procedure.

Additionally, user documentation should be augmented to include error diagnostic advice and suggested input files for prototypic nuclear facility safety analysis problem types. Approximately two full-time equivalent years is conservatively estimated to upgrade MACCS2 software to be compliant with NQA-1-based requirements for existing software. While most of this effort is logically to be used by the code developer, independent review of the end products is necessary.

A new version of MACCS2, Version 1.13, has recently been released. It is recommended that this version be evaluated relative to the software improvement and baseline document recommendations, as well as the full set of SQA criteria discussed in the gap analysis report. If this version is found to be satisfactory, it should replace Version 1.12 as the designated version of the software for the toolbox.

It is recommended that MACCS2 user training for DOE safety analysis applications be conducted formally on, at minimum, an annual basis. Prerequisites for, and core knowledge needed by, the user prior to initiating MACCS2 applications should be documented by the code developer.

Approximately one FTE-month per year would be needed to maintain a web-based error notification and corrective action process for MACCS2. However, such a process has not been defined in depth for MACCS2 and the other designated toolbox codes.

Table 6-3. — Summary of Improvement Actions Identified in the Gap Analysis

No.	Criterion (*Sections refer to discussion in DOE (2004))	Reason Not Met	Remedial Action(s)
1.	SQA Procedures/Plans *(Section 4.2)	Earlier versions of MACCS (version 1.5.11.1 and older) followed SNL software engineering guidance. Although initially followed, SNL SQA Plan and Procedures for Version 1.12 of MACCS2 software were not explicitly followed.	As part of the new software baseline, the SQA Plan covering version 1.12 and successor versions of MACCS2 should be addressed as a stand-alone report or as part of another SQA document. Any new SQA procedures that provide prescriptive guidance to the MACCS2 software developers should be made available to a SQA evaluator for confirmatory review. • Document a written and approved SQA plan eliminating draft or non-compliant informal process of development. • Upgrade SQA program documentation, especially those procedures used for new features added in MACCS2.
2.	Requirements Phase *(Section 4.3)	Software Requirements documents for Version 1.12 of MACCS2 software, although filed for a 3 – 4 year period, were not maintained. Consequently a Software Requirements Document was never completed.	As part of the new software baseline for MACCS2, a concise listing of the software requirements should be documented. This can be reported as a stand-alone Software Requirements report, or as part of another MACCS2-specific document. Specific MACCS2 requirements need to be documented. Those from MACCS may be added to supplement the MACCS2 information, but are not as critical. In contrast, some MACCS-attributes are no longer present in the code, and it would facilitate understanding of the current code requirements to know which ones have been deleted.
3.	Design Phase *(Section 4.4)	A Software Design Document was not made available for the gap analysis. Thus, design information was not directly available. Instead, it was necessary to infer the intent of MACCS2 design from incomplete model description and user guidance documents, some of which address MACCS, not MACCS2.	As part of the new software baseline for MACCS2, software design information should be provided. This can be reported as a stand-alone report, or as part of another MACCS2-specific document, such as the model description report.

No.	Criterion {Sections refer to discussion in DOE (2004)}	Reason Not Met	Remedial Action(s)
4.	Implementation Phase *(Section 4.5)	Written documentation on implementation of Version 1.12 was not produced for MACCS2.	No action needed at this time. The gap analysis inferred from other documentation that source code and other software elements were finalized prior to transmittal of the code to RSICC.
5.	Testing Phase *(Section 4.6)	A Software Testing Report Document has not been produced for MACCS2, and therefore, test process and methodology could not be evaluated directly. Thus, testing process and methods had to be inferred from other information. A draft validation study has never been published.	A test document was prepared by the University of New Mexico (Summa, 1996), but never approved. As part of the new software baseline for MACCS2, this report should be finalized.
6.	Acceptance Test *(Section 4.8)	An Acceptance Test protocol was not provided to the gap analysis. No documentation exists that indicates how the code developers tested the code. There is no known formal procedure to assure that an installed version of MACCS2 is working properly.	As part of the new software baseline for MACCS2, an acceptance test process should be documented. This instruction can be made part of an upgraded User's Guide, and proceduralized in the installation files provided by RSICC or SNL.
7.	Configuration Control *(Section 4.9)	A MACCS2 Configuration and Control document was not provided for the gap analysis, despite indication that a configuration control system was in place for MACCS2. Files to support this area were not maintained.	It is recommended that a full-scope Software Configuration and Control document be issued as part of the new software baseline. If this document has been generated, then it should be made available for review.
8.	Error Notification *(Section 4.10)	An Error Notification and Corrective Action Report process is in place at SNL, but limited documentation was provided.	While a Software Problem Reporting system is apparently functional at SNL, written documentation should be provided to demonstrate its effectiveness.

7.0 SAMPLE CALCULATIONS

This section contains an overview of the MACCS2 input files and output for a sample calculation of a ground-level release of 1 curie of Pu-239. Four cases were run to model the following types of release:

- Non-buoyant (base case)
- Non-buoyant plume with building wake
- Buoyant plume
- Buoyant plume with building wake

Random stratified sampling was used with the number of samples set to 24 to sample each hour of the day (for 365 days) from the meteorological data file.

The next two sections summarize key features of the ATMOS and EARLY input files. Four separate ATMOS files were used to model the four release cases. Graphical results from the four cases are shown next. Finally, the output listing for the base case is given.

The main objective of this section is to provide sample input files that illustrate the guidance in this report and to show examples of the types of output that MACCS2 can provide.

7.1 ATMOS Input Overview

The ATMOS module uses two input files. These files contain the input data needed for the ATMOS module (A5_BASE.INP) and shown below in Figure 7-1, and a yearly meteorological data file which contains 365 days of meteorological conditions (METDATA.INP).

The following are the major assumptions associated with this analysis:

- The radial ring endpoints are at 0.1, 0.2, 0.3, 0.4, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0, 7.5, 8.0, and 10.0 km.
- The base case is assumed to be an open-area release (no buildings in the vicinity) so the initial vertical and horizontal dispersion coefficients are each set to the minimum value of 0.1. Also, the building height is set to its minimum value of 1.0.

  In the building wake cases, the building is assumed to have a height (H_b) of 42.5 ft (13 m) and width (W_b) of 296 ft (90 m). The initial horizontal dispersion coefficient is set to 21 m (W_b/4.3) and the initial vertical dispersion coefficient is set to 6 m (H_b/2.15).

- The base case is assumed to a non-buoyant plume so the sensible heat rate is specified to be zero.

  For the buoyant plume releases, the sensible heat rate is assumed to be 5 MW.

- One curie of Pu-239 is released over a ten-minute period.

- The inventory scaling factor (CORSCA) has been set equal to 3.7×10^{10} to convert the inventory units from curies to becquerels

- No wet deposition is assumed

- The dry deposition velocity is assumed to be 0.01 m/s, which corresponds to a particle with an aerodynamic equivalent diameter of 2 to 4 microns (Sehmel, 1978).

- The surface roughness length is specified as 10 cm to minimally credit the urban attributes of the operational area of the region of transport. MACCS (Jow, 1990) incorporates the change in the surface roughness using the model proposed in (AMS, 1977). In this model, the sigma z parameter is adjusted by applying the one-fifth power law to the quotient of the new surface roughness divided by the Prairie Grass surface roughness (3 cm) (Haugen, 1959)

The site meteorological data files are composed of hourly data for a specific calendar year of qualified data, at a measured wind speed height of 10 meters.

Figure 7-1. ATMOS Input File for Sample Case

```
*******************************************************************************
*
*         ATMOS FILE
*INPUT FILE IDENTIFIER
RIATNAM1001  'MACCS2 - Random Stratified Sampling (METCOND=5)'
*******************************************************************************
* GEOMETRY DATA BLOCK, LOADED BY INPGEO, STORED IN /GEOM/
*
* NUMBER OF RADIAL SPATIAL ELEMENTS
GENUMRAD001 21
*
* ENDPOINT DISTANCES TO RADIAL SPATIAL ELEMENTS (KILOMETERS)
GESPAEND001    0.10   0.20   0.30   0.40   0.50   1.00   1.50
GESPAEND002    2.00   2.50   3.00   3.50   4.00   4.50   5.00
GESPAEND003    5.50   6.00   6.50   7.00   7.50   8.00  10.00
*******************************************************************************
* ISOTOPE DATA BLOCK, LOADED BY INPISO, STORED IN /ISOGRP/, /ISONAM/
*
* NUMBER OF ISOTOPES
ISNUMISO001 1
*
* NUMBER OF ISOTOPE GROUPS
ISMAXGRP001 2
*
* WET AND DRY DEPOSITION FLAGS FOR EACH ISOTOPE GROUP
*              WETDEP     DRYDEP
ISDEPFLA001   .FALSE.    .FALSE.
ISDEPFLA002   .FALSE.    .TRUE.
*
* NUMBER OF PSEUDOSTABLE NUCLIDES (USED TO TRUNCATE THE DECAY CHAINS)
ISNUMSTB001  6
*
ISNAMSTB001     U-235     (DAUGHTER OF PU-239)
ISNAMSTB002     Th-231
ISNAMSTB003     Pa-231
ISNAMSTB004     Ac-227
ISNAMSTB005     Fr-223
ISNAMSTB006     Th-227
*
* ISOTOPE GROUP DATA FOR ISOTOPE GROUPS
*               NUCNAM     IGROUP
ISOTPGRP001     Pu-239       2
*ISOTPGRP002     Pu-238       2
*
******************************************************************************* WET
DEPOSITION DATA BLOCK, LOADED BY INPWET, STORED IN /WETCON/
*
* WASHOUT COEFFICIENT NUMBER ONE, LINEAR FACTOR
WDCWASH1001  9.5E-5  (JON HELTON AFTER JONES, 1986)
*
* WASHOUT COEFFICIENT NUMBER TWO, EXPONENTIAL FACTOR
WDCWASH2001  0.8  (JON HELTON AFTER JONES, 1986)
*******************************************************************************
* DRY DEPOSITION DATA BLOCK, LOADED BY INPDRY, STORED IN /DRYCON/
*
* NUMBER OF PARTICLE SIZE GROUPS
DDNPSGRP001  3
*
* DEPOSITION VELOCITY OF EACH PARTICLE SIZE GROUP (M/S)
```

```
DDVDEPOS001  0.001  0.005  0.01
*******************************************************************************
* DISPERSION PARAMETER DATA BLOCK, LOADED BY INPDIS, STORED IN /DISPY/, /DISPZ/
*
NUM_DIST001   0  (power-law fits used instead of dispersion tables)
*
*SIGMA = AX**B WHERE A AND B ARE VALUES FROM TADMOR GUR (1969)
*
* STABILITY CLASS: A        B        C        D        E        F
*
* LINEAR TERM OF THE EXPRESSION FOR SIGMA-Y, 6 STABILITY CLASSES
DPCYSIGA001   0.3658   0.2751   0.2089   0.1474   0.1046   0.0722
*
* EXPONENTIAL TERM OF THE EXPRESSION FOR SIGMA-Y, 6 STABILITY CLASSES
DPCYSIGB001    .9031    .9031    .9031    .9031    .9031    .9031
*
* LINEAR TERM OF THE EXPRESSION FOR SIGMA-Z, 6 STABILITY CLASSES
DPCZSIGA001   2.5E-4   1.9E-3       .2       .3       .4       .2
*
* EXPONENTIAL TERM OF THE EXPRESSION FOR SIGMA-Z, 6 STABILITY CLASSES
DPCZSIGB001    2.125   1.6021     .8543    .6532    .6021    .6020
*
*  LINEAR SCALING FACTOR FOR SIGMA-Y FUNCTION, NORMALLY 1
DPYSCALE001    1.
*
*  LINEAR SCALING FACTOR FOR SIGMA-Z FUNCTION,
*  NORMALLY USED FOR SURFACE ROUGHNESS LENGTH CORRECTION.
*  (Z1 / Z0) ** .2,   FOR Z1=10 CM, THEREFORE (10/3)**.2=1.27
DPZSCALE001    1.27
******************************************************************************* *
* EXPANSION FACTOR DATA BLOCK, LOADED BY INPEXP, STORED IN /EXPAND/
*
* TIME BASE FOR EXPANSION FACTOR (SECONDS)
PMTIMBAS001   180.
*
* BREAK POINT FOR FORMULA CHANGE (SECONDS)
PMBRKPNT001   3600.
*
* EXPONENTIAL EXPANSION FACTOR NUMBER 1
PMXPFAC1001   .2
*
* EXPONENTIAL EXPANSION FACTOR NUMBER 2
PMXPFAC2001   .25
*******************************************************************************
* PLUME RISE DATA BLOCK, LOADED BY INPLRS, STORED IN /PLUMRS/
*
* SCALING FACTOR FOR THE CRITICAL WIND SPEED FOR ENTRAINMENT OF A BOUYANT PLUME
* (USED BY FUNCTION CAUGHT)
PRSCLCRW001   1.
*
* SCALING FACTOR FOR THE A-D STABILITY PLUME RISE FORMULA
* (USED BY FUNCTION PLMRIS)
PRSCLADP001   1.
*
* SCALING FACTOR FOR THE E-F STABILITY PLUME RISE FORMULA
* (USED BY FUNCTION PLMRIS)
PRSCLEFP001   1.
*******************************************************************************
* WAKE EFFECTS DATA BLOCK, LOADED BY INPWAK, STORED IN /BILWAK/
* (minimum value specifcations for open area release)
* BUILDING WIDTH (METERS) {MACCS 1.5.11.1 Input}
* WEBUILDW001   1.0
```

```
*
* BUILDING HEIGHT (METERS) - FOR LIFT OFF CRITERION, BUOYANT PLUME (min. val.)
WEBUILDH001   1.0
*
* INITIAL VALUE OF SIGMA-Y [METERS] DUE TO WAKE EFFECTS (=Wb/4.3, minimum value)
SIGYINIT001    0.1
*
* INITIAL VALUE OF SIGMA-Z [METERS] DUE TO WAKE EFFECTS (=Hb/2.15, min. value)
SIGZINIT001    0.1
*
*******************************************************************************
* OUTPUT CONTROL DATA BLOCK, LOADED BY INPOPT, STORED IN /STOPME/, /ATMOPT/
*
* FLAG TO INDICATE THAT THIS IS THE LAST PROGRAM IN THE SERIES TO BE RUN
OCENDAT1001  .FALSE. (SET THIS VALUE TO .TRUE. TO SKIP EARLY AND CHRONC)
OCIDEBUG001  0
*
* NAME OF THE NUCLIDE TO BE LISTED ON THE DISPERSION LISTINGS
OCNUCOUT001  Pu-239
*******************************************************************************
* METEOROLOGICAL SAMPLING DATA BLOCK
*
* METEOROLOGICAL SAMPLING OPTION CODE:
* METCOD = 1, USER SPECIFIED DAY AND HOUR IN THE YEAR (FROM MET FILE),
*          2, WEATHER CATEGORY BIN SAMPLING,
*          3, 120 HOURS OF WEATHER SPECIFIED ON THE ATMOS USER INPUT FILE,
*          4, CONSTANT MET (BOUNDARY WEATHER USED FROM THE START),
*          5, STRATIFIED RANDOM SAMPLES FOR EACH DAY OF THE YEAR.
M1METCOD001  5
*
* LAST SPATIAL INTERVAL FOR MEASURED WEATHER
M2LIMSPA001  21
*
* BOUNDARY WEATHER MIXING LAYER HEIGHT
M2BNDMXH001   600.  (METERS)
*
* BOUNDARY WEATHER STABILITY CLASS INDEX
M2IBDSTB001  6      (F-STABILITY)
*
* BOUNDARY WEATHER RAIN RATE
M2BNDRAN001  5.     (MM/HR)
*
* BOUNDARY WEATHER WIND SPEED
M2BNDWND001  1.     (M/S)
*
*******************************************************************************
* START DAY
* M3ISTRDY001  237
* START HOUR
* M3ISTRHR001  1
*
* NUMBER OF RAIN DISTANCE INTERVALS FOR BINNING
* M4NRNINT001  6
*
* ENDPOINTS OF THE RAIN DISTANCE INTERVALS (KILOMETERS)
* NOTE: THESE MUST BE CHOSEN TO MATCH THE SPATIAL ENDPOINT DISTANCES
*       SPECIFIED FOR THE ARRAY SPAEND (10 % ERROR IS ALLOWED).
* M4RNDSTS001  0.2  0.5  1.0  1.5  2.0  3.5
*
* NUMBER OF RAIN INTENSITIY BREAKPOINTS
*M4NRINTN001   2
*
```

```
* RAIN INTENSITY BREAKPOINTS FOR WEATHER BINNING (MILLIMETERS PER HOUR)
* M4RNRATE001   1.  2.
*******************************************************************************
* NUMBER OF SAMPLES PER BIN
*
M4NSMPLS001  24
*
* INITIAL SEED FOR RANDOM NUMBER GENERATOR
M4IRSEED001  93
*******************************************************************************
* RELEASE DATA BLOCK, LOADED BY INPREL, STORED IN /ATNAM2/, /MULREL/
*
* SOURCE TERM RELEASE SPECIFIC INFORMATION
RDATNAM2001 'Unit Ci release Pu-239 w/ nonbuoyant (open area) - YR'
*
* TIME AFTER ACCIDENT INITIATION WHEN THE ACCIDENT REACHES GENERAL EMERGENCY
* CONDITIONS (AS DEFINED IN NUREG-0654), OR WHEN PLANT PERSONNEL CAN RELIABLY
* PREDICT THAT GENERAL EMERGENCY CONDITIONS WILL BE ATTAINED
*
RDOALARM001    0.00E+00
*
* NUMBER OF PLUME SEGMENTS THAT ARE RELEASED
RDNUMREL001     1
*
* SELECTION OF RISK DOMINANT PLUME
RDMAXRIS001     1
*
* REFERENCE TIME FOR DISPERSION AND RADIOACTIVE DECAY
RDREFTIM001       0.00
* CORRESPONDING TO LEADING EDGE WEATHER
*
* HEAT CONTENT OF THE RELEASE SEGMENTS (WATTS)
* A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
RDPLHEAT001   0.0
*
* HEIGHT OF THE PLUME SEGMENTS AT RELEASE (METERS)
* A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
RDPLHITE001  0.0
*
* DURATION OF THE PLUME SEGMENTS (SECONDS)
* A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
RDPLUDUR001   600.0
*
* TIME OF RELEASE FOR EACH PLUME (SECS FROM SCRAM)
* A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
RDPDELAY001   0.0
*
* PARTICLE SIZE DISTRIBUTION OF EACH ISOTOPE GROUP
* YOU MUST SPECIFY A COLUMN OF DATA FOR EACH OF THE PARTICLE SIZE GROUPS
*
*  V dep = 0.001 is for a filtered release
*  V dep = 0.005 is for HTO only
*  V dep = 0.010 is for an unfiltered release
*
*              0.001  0.005  0.010
RDPSDIST001    1.000  0.000  0.000
RDPSDIST002    0.000  0.000  1.000
*
*                NUCNAM      CORINV(Unit Ci Release)
RDCORINV001      Pu-239         1.00E+00
*RDCORINV002      Pu-238          0.00E+00
*
```

```
*  SCALING FACTOR TO ADJUST THE CORE INVENTORY
RDCORSCA001  3.7E+10 (Conversion of Curies to Becquerels)
*
* RELEASE FRACTIONS FOR ISOTOPE GROUPS IN RELEASE
* GROUP      XE/KR     I     CS     TE     SR     RU     LA     CE     BA    TRIT
RDRELFRC001   1.0   1.0    1.0    1.0    1.0    1.0    1.0    1.0    1.0    1.0
*
* RELEASE FREACTION APPLICATION TO INGROWTH DECAY PRODUCTS
* PRODUCED AFTER ACCIDENT INITIATION
RDAPLFRC001    PARENT
*
* REQUEST FOR ATMOSPHERIC OUTPUT INFORMATION
*
*            NUM0
TYPE0NUMBER    4
*
*            INDREL     INRAD
TYPE0OUT001      1          1
TYPE0OUT002      1          2
TYPE0OUT003      1         10
TYPE0OUT004      1         21    CCDF
*
*********************
.
```

7.2 EARLY Input Overview

The EARLY module uses two different input files, the file that contains the input data needed for the EARLY module (E1_TEDE.INP) shown below as Figure 7-2, and the dose conversion factor file (FGR_PU.INP) listed in the following as Figure 7-3.

The following are the major assumptions associated with this analysis:

- The assumed breathing rate is 3.33×10^{-4} cubic meters per second which is the DOE occupational breathing rate (DOE, 1998)
- A uniform population distribution of 0.0 people per square kilometer is assumed
- No shielding is assumed
- No evacuation and/or sheltering is assumed
- Results of interest are the centerline TEDE for all intervals

The last file needed by the EARLY module is the dose conversion factor file. The values within this file were generated with the FGRDCF code and are based on Federal Guidance Reports 11 and 12 (Eckerman, 1988 and Eckerman, 1993).

Figure 7-2. EARLY Input File for Sample Case.

```
*******************************************************************************
* GENERAL DESCRIPTIVE TITLE DESCRIBING THIS "EARLY" INPUT FILE
*
MIEANAM1001  'MACCS - TEDE'
*
* DCF FILE IDENTIFICATION
DCF_FILE001     'FGR_PU.INP'
*
* FLAG TO INDICATE THAT THIS IS THE LAST PROGRAM IN THE SERIES TO BE RUN
*
MIENDAT2001  .TRUE.    (SET THIS VALUE TO .TRUE. TO SKIP CHRONC)
*
* DISPERSION MODEL OPTION CODE:  1  *  STRAIGHT LINE
*                                2  *  WIND-SHIFT WITH ROTATION
*                                3  *  WIND-SHIFT WITHOUT ROTATION
*
MIIPLUME001  1
*
* NUMBER OF FINE GRID SUBDIVISIONS USED BY THE MODEL
*
MINUMFIN001  7    (3, 5 OR 7 ALLOWED)
*
* LEVEL OF DEBUG OUTPUT REQUIRED, NORMAL RUNS SHOULD SPECIFY ZERO
*
MIIPRINT001  0
*
* LOGICAL FLAG SIGNIFYING THAT THE BREAKDOWN OF RISK BY WEATHER CATEGORY
* BIN ARE TO BE PRESENTED TO SHOW THEIR RELATIVE CONTRIBUTION TO THE MEAN
*
*             RISBIN
*
MIRISCAT001   .FALSE.
*
* FLAG INDICATING IF WIND-ROSES FROM ATMOS ARE TO BE OVERRIDDEN
*
MIOVRRID001  .FALSE.  (USE THE WIND ROSE CALCULATED FOR EACH WEATHER BIN)
*******************************************************************************
* POPULATION DISTRIBUTION DATA BLOCK, LOADED BY INPOPU, STORED IN /POPDAT/
*
*PDPOPFLG001  FILE
*
PDPOPFLG001  UNIFORM
PDIBEGIN001  1   (SPATIAL INTERVAL AT WHICH POPULATION BEGINS)
PDPOPDEN001  0. (POPULATION DENSITY (PEOPLE PER SQUARE KILOMETER))
*******************************************************************************
* ORGAN DEFINITION DATA BLOCK, LOADED BY INORGA, STORED IN /EARDIM/ AND /ORGNAM/
*
*                ORGAN NAME             ORGFLG
*
*MIORGDEF001      'A-SKIN'               .FALSE.
*MIORGDEF002      'A-RED MARR'           .FALSE.
*MIORGDEF003      'A-LUNGS'              .FALSE.
*MIORGDEF004      'A-THYROIDH'           .FALSE.
*MIORGDEF005      'A-STOMACH'            .FALSE.
*MIORGDEF006      'A-LOWER LI'           .FALSE.
*MIORGDEF007      'L-EFFECTIVE'           .TRUE.
*MIORGDEF008      'L-RED MARR'           .FALSE.
*MIORGDEF009      'L-BONE SUR'           .FALSE.
*MIORGDEF010      'L-BREAST'             .FALSE.
```

```
*MIORGDEF011      'L-LUNGS'              .FALSE.
*MIORGDEF012      'L-THYROID'            .FALSE.
*MIORGDEF013      'L-LOWER LI'           .FALSE.
*MIORGDEF014      'L-BLAD WAL'           .FALSE.
*MIORGDEF015      'L-LIVER'              .FALSE.
*MIORGDEF016      'L-THYROIDH'           .FALSE.
*
*******************************************************************************
* SHIELDING AND EXPOSURE FACTORS, LOADED BY INDFAC, STORED IN /EADFAC/
*
* THREE VALUES OF EACH PROTECTION FACTOR ARE SUPPLIED,
* ONE FOR EACH TYPE OF ACTIVTY:
*
* ACTIVITY TYPE:
*     1 - EVACUEES WHILE MOVING
*     2 - NORMAL ACTIVITY IN SHELTERING AND EVACUATION ZONE
*     3 - SHELTERED ACTIVITY
*
* CLOUD SHIELDING FACTOR
*
*            EVACUEES  NORMAL  SHELTER
*
SECSFACT001      1.     1.     1.
*
* PROTECTION FACTOR FOR INHALATION
*
SEPROTIN001      1.     1.     1.
*
* BREATHING RATE (CUBIC METERS PER SECOND)
*
SEBRRATE001  3.33E-4  3.33E-4  3.33E-4
*
* SKIN PROTECTION FACTOR
*
SESKPFAC001      1.     1.     1.
*
* GROUND SHIELDING FACTOR
*
SEGSHFAC001      1.    1.     1.
*
* RESUSPENSION INHALATION MODEL CONCENTRATION COEFFICIENT (/METER)
*
*   RESCON = 1.E-4 IS APPROPRIATE FOR MECHANICAL RESUSPENSION BY VEHICLES.
*   RESHAF = 2.11 DAYS CAUSES 1.E-4 TO DECAY IN ONE WEEK TO 1.E-5, THE VALUE
*   OF RESCON USED IN THE FIRST TERM OF THE LONG-TERM RESUSPENSION EQUATION
*   USED IN CHRONC.
*
SERESCON001   1.0E-4     (RESUSPENSION IS TURNED ON)
*
* RESUSPENSION CONCENTRATION COEFFICIENT HALF-LIFE (SEC)
*
SERESHAF001   1.825E5  (2.11 DAYS)
*******************************************************************************
* EVACUATION ZONE DATA BLOCK, LOADED BY EVNETW, STORED IN /NETWOR/, /EOPTIO/
*
* SPECIFIC DESCRIPTION OF THE EMERGENCY RESPONSE SCENARIO BEING USED
*
EZEANAM2001  'NO EVACUATION OR SHELTERING'
*
* THE TYPE OF WEIGHTING TO BE APPLIED TO THE EMERGENCY RESPONSE SCENARIOS
* YOU MUST SUPPLY A VALUE OF 'TIME' OR 'PEOPLE'
*
```

```
EZWTNAME001  'PEOPLE'
*
*
* WEIGHTING FRACTION APPLICABLE TO THIS SCENARIO
*
EZWTFRAC001  1.000
*
* LAST RING IN THE MOVEMENT ZONE
*
EZLASMOV001      0    (NO EVACUATION)
*
* FIRST SPATIAL INTERVAL IN THE EVACUATION ZONE
*
****************************************************************************
* SHELTER AND RELOCATION ZONE DATA BLOCK, LOADED BY INPEMR,
*                                         STORED IN /INPSRZ/, /RELOCA/
*
* TIME TO TAKE SHELTER IN THE INNER SHELTER ZONE (SECONDS FROM OALARM)
*
*SRTTOSH1001       0.     (THERE IS NO INNER SHELTER ZONE)
*
* SHELTER DURATION IN THE INNER SHELTER ZONE (SECONDS FROM TAKING SHELTER)
*
*SRSHELT1001       0.     (THERE IS NO INNER SHELTER ZONE)
*
* LAST RING OF THE OUTER SHELTER ZONE
*
*SRLASHE2001       0      (THERE IS NO OUTER SHELTER ZONE)
*
* TIME TO TAKE SHELTER IN THE OUTER SHELTER ZONE (SECONDS FROM OALARM)
*
*SRTTOSH2001       0.     (THERE IS NO OUTER SHELTER ZONE)
*
* SHELTER DURATION IN THE OUTER SHELTER ZONE (SECONDS FROM TAKING SHELTER)
*
*SRSHELT2001       0.     (THERE IS NO OUTER SHELTER ZONE)
*
* DURATION OF THE EMERGENCY PHASE (SECONDS FROM PLUME ARRIVAL)
*
SRENDEMP001  86400.    (ONE DAY)
*
* CRITICAL ORGAN FOR RELOCATION DECISIONS
*
SRCRIORG001 'L-EFFECTIVE'
*
* HOT SPOT RELOCATION TIME (SECONDS FROM PLUME ARRIVAL)
*
SRTIMHOT001  86400.    (ONE DAY)
*
* NORMAL RELOCATION TIME (SECONDS FROM PLUME ARRIVAL)
*
SRTIMNRM001  86400.    (ONE DAY)
*
* HOT SPOT RELOCATION DOSE CRITERION THRESHOLD (SIEVERTS)
*
SRDOSHOT001  0.50   (50 REM DOSE TO RBM IN 1 WEEK TRIGGERS RELOCATION)
*
* NORMAL RELOCATION DOSE CRITERION THRESHOLD (SIEVERTS)
*
SRDOSNRM001  0.25    (25 REM DOSE TO RBM IN 1 WEEK TRIGGERS RELOCATION)
****************************************************************************
* EARLY FATALITY MODEL PARAMETERS, LOADED BY INEFAT, STORED IN /EFATAL/
```

```
*
* NUMBER OF EARLY FATALITY EFFECTS
*
EFNUMEFA001   0
*
*******************************************************************************
* EARLY INJURY MODEL PARAMETERS, LOADED BY INEINJ, STORED IN /EINJUR/
*
* NUMBER OF EARLY INJURY EFFECTS
*
EINUMEIN001  0
*
*******************************************************************************
* ACUTE EXPOSURE CANCER PARAMETERS, LOADED BY INACAN STORED IN /ACANCR/.
*
* NUMBER OF ACUTE EXPOSURE CANCER EFFECTS**
*
LCNUMACA001   0
*
* THRESHOLD DOSE FOR APPLYING THE DOSE DEPENDENT REDUCTION FACTOR
*
* LCDDTHRE001   0.0  (LOWEST DOSE FOR WHICH DDREFA WILL BE APPLIED)
*
* DOSE THRESHOLD FOR LINEAR DOSE RESPONSE (Sv)
*
* LCACTHRE001   1.5  (LINEAR-QUADRATIC MODEL IS NOT BEING USED)
*
*            ACNAME       ORGNAM  ACSUSC  DOSEFA DOSEFB  CFRISK  CIRISK  DDREFA
*
* LCANCERS001 'ICRP 60' 'L-EFFECTIVE' 1.0   1.0    0.0    5.0E-2  7.3E-2   1.0
*******************************************************************************
* RESULT 1 OPTIONS BLOCK, LOADED BY INOUT1, STORED IN /INOUT1/
* TOTAL NUMBER OF A GIVEN EFFECT (LATENT CANCER, EARLY DEATH, EARLY INJURY)
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPE1NUMBER    0
*******************************************************************************
* RESULT 2 OPTIONS BLOCK, LOADED BY INOUT2, STORED IN /INOUT2/
* FURTHEST DISTANCE AT WHICH A GIVEN RISK OF EARLY DEATH IS EXCEEDED.
* NUMBER OF DESIRED RESULTS OF THIS TYPE
*
TYPE2NUMBER  0
*******************************************************************************
* RESULT 3 OPTIONS BLOCK, LOADED BY INOUT3, STORED IN /INOUT3/
* NUMBER OF PEOPLE WHOSE DOSE TO A GIVEN ORGAN EXCEEDS A GIVEN THRESHOLD.
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPE3NUMBER  0
*******************************************************************************
* RESULT 4 OPTIONS BLOCK, LOADED BY INOUT4, STORED IN /INOUT4/
* 360 DEGREE AVERAGE RISK OF A GIVEN EFFECT AT A GIVEN DISTANCE.
* POSSIBLE TYPES OF EFFECTS ARE:
TYPE4NUMBER  0
*******************************************************************************
* RESULT 5 OPTIONS BLOCK, LOADED BY INOUT5, STORED IN /INOUT5/
* TOTAL POPULATION DOSE TO A GIVEN ORGAN BETWEEN TWO DISTANCES.
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPE5NUMBER    0
*******************************************************************************
* RESULT 6 OPTIONS BLOCK, LOADED BY INOUT6, STORED IN /INOUT6/
* CENTERLINE DOSE TO AN ORGAN VS DIST BY PATHWAY, PATHWAY NAMES ARE AS FOLLOWS:
*  PATHWAY NAME:
*    'CLD'     - CLOUDSHINE
*    'GRD'     - GROUNDSHINE
```

```
*     'INH ACU' - "ACUTE DOSE EQUIVALENT" FROM DIRECT INHALATION OF THE CLOUD
*     'INH LIF' - "LIFETIME DOSE COMMITMENT" FROM DIRECT INHALATION OF THE CLOUD
*     'RES ACU' - "ACUTE DOSE EQUIVALENT" FROM RESUSPENSION INHALATION
*     'RES LIF' - "LIFETIME DOSE COMMITMENT" FROM RESUSPENSION INHALATION
*     'TOT ACU' - "ACUTE DOSE EQUIVALENT" FROM ALL PATHWAYS
*     'TOT LIF' - "LIFETIME DOSE COMMITMENT" FROM ALL PATHWAYS
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPE6NUMBER     1
*
*             ORGNAM         PATHNM       I1DIS6    I2DIS6
*
TYPE6OUT001  'L-EFFECTIVE'    'TOT LIF'       1        21
*TYPE6OUT002  'L-EFFECTIVE'    'TOT LIF'       2         2
*TYPE6OUT003  'L-EFFECTIVE'    'TOT LIF'       3         3
*TYPE6OUT004  'L-EFFECTIVE'    'TOT LIF'       4         4
*******************************************************************************
* RESULT 7 OPTIONS BLOCK, LOADED BY INOUT7, STORED IN /INOUT7/
* CENTERLINE RISK OF A GIVEN EFFECT VS DISTANCE
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPE7NUMBER   0
*******************************************************************************
* RESULT 8 OPTIONS BLOCK, LOADED BY INOUT8, STORED IN /INOUT8/
* POPULATION WEIGHTED FATALITY RISK BETWEEN 2 DISTANCES
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPE8NUMBER   0
*******************************************************************************
* RESULT A OPTIONS BLOCK, LOADED BY INOUTA, STORED IN /INOUTA/
* PEAK TOTAL DOSE AT A DISTANCE
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPEANUMBER   1
*             ORGNAM            I1DISA    I2DISA
*
TYPEAOUT001  'L-EFFECTIVE'          1        21
*******************************************************************************
* RESULT B OPTIONS BLOCK, LOADED BY INOUTB, STORED IN /INOUTB/
* PEAK TOTAL DIRECT DOSE FOUND AT A SPATIAL GRID LOCATION
* NUMBER OF DESIRED RESULTS OF THIS TYPE
TYPEBNUMBER   16
*             ORGNAM            I1DISB    I2DISB
*
TYPEBOUT001  'L-EFFECTIVE'          3        1
TYPEBOUT002  'L-EFFECTIVE'          3        2
TYPEBOUT003  'L-EFFECTIVE'          3        3
TYPEBOUT004  'L-EFFECTIVE'          3        4
TYPEBOUT005  'L-EFFECTIVE'          3        5
TYPEBOUT006  'L-EFFECTIVE'          3        6
TYPEBOUT007  'L-EFFECTIVE'          3        7
TYPEBOUT008  'L-EFFECTIVE'          3        8
TYPEBOUT009  'L-EFFECTIVE'          3        9
TYPEBOUT010  'L-EFFECTIVE'          3       10
TYPEBOUT011  'L-EFFECTIVE'          3       11
TYPEBOUT012  'L-EFFECTIVE'          3       12
TYPEBOUT013  'L-EFFECTIVE'          3       13
TYPEBOUT014  'L-EFFECTIVE'          3       14
TYPEBOUT015  'L-EFFECTIVE'          3       15
TYPEBOUT016  'L-EFFECTIVE'          3       16
*******************************************************************************
.
```

Figure 7-3. Dose Conversion Factor File for Sample Case.

```
FGRDCF 06/18/02   12:22:20   BETA-TEST VERSION 1.10, MINOR FORTRAN FIXES 5/4/95
IMPLICIT DAUGHTER HALFLIVES (M) LESS THAN  90 AND LESS THAN 0.100 OF PARENT
        9 ORGANS DEFINED IN THE FILE:
GONADS
BREAST
LUNGS
RED MARR
BONE SUR
THYROID
REMAINDER
EFFECTIVE
SKIN(FGR)
        4 NUCLIDES DEFINED IN THE FILE:
Pu-238    W
Pu-239    W
Pu-240    W
Pu-241    W
          CLOUDSHINE  GROUND    GROUND    GROUND    INHALED   INHALED  INGESTION
                      SHINE 8HR SHINE 7DAY SHINE RATE ACUTE    CHRONIC
Pu-238
GONADS     6.560E-18 4.291E-14 9.011E-13 1.490E-18-1.000E+00 2.800E-05 2.330E-07
BREAST     1.270E-17 5.558E-14 1.167E-12 1.930E-18-1.000E+00 1.000E-09 8.410E-12
LUNGS      1.060E-18 2.267E-15 4.759E-14 7.870E-20-1.000E+00 1.840E-05 8.490E-12
RED MARR   1.680E-18 5.587E-15 1.173E-13 1.940E-19-1.000E+00 1.520E-04 1.270E-06
BONE SUR   9.300E-18 3.514E-14 7.378E-13 1.220E-18-1.000E+00 1.900E-03 1.580E-05
THYROID    4.010E-18 9.792E-15 2.056E-13 3.400E-19-1.000E+00 9.620E-10 7.990E-12
REMAINDER  1.990E-18 9.216E-15 1.935E-13 3.200E-19-1.000E+00 7.020E-05 6.000E-07
EFFECTIVE  4.880E-18 2.413E-14 5.068E-13 8.380E-19-1.000E+00 1.060E-04 8.650E-07
SKIN(FGR)  4.090E-17 2.776E-13 5.830E-12 9.640E-18-1.000E+00 0.000E+00 0.000E+00
Pu-239
GONADS     4.840E-18 1.768E-14 3.713E-13 6.140E-19-1.000E+00 3.180E-05 2.640E-07
BREAST     7.550E-18 2.238E-14 4.699E-13 7.770E-19-1.000E+00 9.220E-10 7.690E-12
LUNGS      2.650E-18 2.267E-15 4.760E-14 7.870E-20-1.000E+00 1.730E-05 7.740E-12
RED MARR   2.670E-18 3.456E-15 7.258E-14 1.200E-19-1.000E+00 1.690E-04 1.410E-06
BONE SUR   9.470E-18 1.673E-14 3.514E-13 5.810E-19-1.000E+00 2.110E-03 1.760E-05
THYROID    3.880E-18 5.126E-15 1.077E-13 1.780E-19-1.000E+00 9.030E-10 7.490E-12
REMAINDER  2.860E-18 4.838E-15 1.016E-13 1.680E-19-1.000E+00 7.560E-05 6.430E-07
EFFECTIVE  4.240E-18 1.057E-14 2.220E-13 3.670E-19-1.000E+00 1.160E-04 9.560E-07
SKIN(FGR)  1.860E-17 1.057E-13 2.220E-12 3.670E-18-1.000E+00 0.000E+00 0.000E+00
Pu-240
GONADS     6.360E-18 4.118E-14 8.649E-13 1.430E-18-1.000E+00 3.180E-05 2.640E-07
BREAST     1.230E-17 5.328E-14 1.119E-12 1.850E-18-1.000E+00 9.510E-10 7.970E-12
LUNGS      1.090E-18 2.249E-15 4.723E-14 7.810E-20-1.000E+00 1.730E-05 8.070E-12
RED MARR   1.650E-18 5.386E-15 1.131E-13 1.870E-19-1.000E+00 1.690E-04 1.410E-06
BONE SUR   9.260E-18 3.398E-14 7.137E-13 1.180E-18-1.000E+00 2.110E-03 1.760E-05
THYROID    3.920E-18 9.446E-15 1.984E-13 3.280E-19-1.000E+00 9.050E-10 7.510E-12
REMAINDER  1.960E-18 8.870E-15 1.863E-13 3.080E-19-1.000E+00 7.560E-05 6.430E-07
EFFECTIVE  4.750E-18 2.313E-14 4.857E-13 8.030E-19-1.000E+00 1.160E-04 9.560E-07
SKIN(FGR)  3.920E-17 2.644E-13 5.552E-12 9.180E-18-1.000E+00 0.000E+00 0.000E+00
Pu-241
GONADS     7.190E-20 6.653E-17 1.396E-15 2.310E-21-1.000E+00 6.820E-07 5.660E-09
BREAST     8.670E-20 7.229E-17 1.517E-15 2.510E-21-1.000E+00 3.060E-11 2.520E-13
LUNGS      6.480E-20 4.090E-17 8.584E-16 1.420E-21-1.000E+00 7.420E-09 4.450E-13
RED MARR   5.630E-20 4.003E-17 8.403E-16 1.390E-21-1.000E+00 3.360E-06 2.780E-08
BONE SUR   2.190E-19 1.385E-16 2.908E-15 4.810E-21-1.000E+00 4.200E-05 3.480E-07
THYROID    6.980E-20 4.522E-17 9.491E-16 1.570E-21-1.000E+00 1.240E-11 1.010E-13
REMAINDER  6.090E-20 4.291E-17 9.007E-16 1.490E-21-1.000E+00 1.310E-06 1.100E-08
EFFECTIVE  7.250E-20 5.558E-17 1.167E-15 1.930E-21-1.000E+00 2.230E-06 1.850E-08
SKIN(FGR)  1.170E-19 2.033E-16 4.268E-15 7.060E-21-1.000E+00 0.000E+00 0.000E+00
```

7.3 Results

Results for the four cases of the sample-problem involving a unit-curie release of Pu-239 are shown below in Figure 7-4. The results represent the centerline dose as output by MACCS2 with the Type Number 6 output option. The next section contains the output listing for the base case (non-buoyant plume) with the Type Number 6 output highlighted by a box border. The results of Figure 7-4 demonstrate the role that buoyancy and building wake effects can have on downwind exposures. Additional discussion on this topic is found in Appendix C.

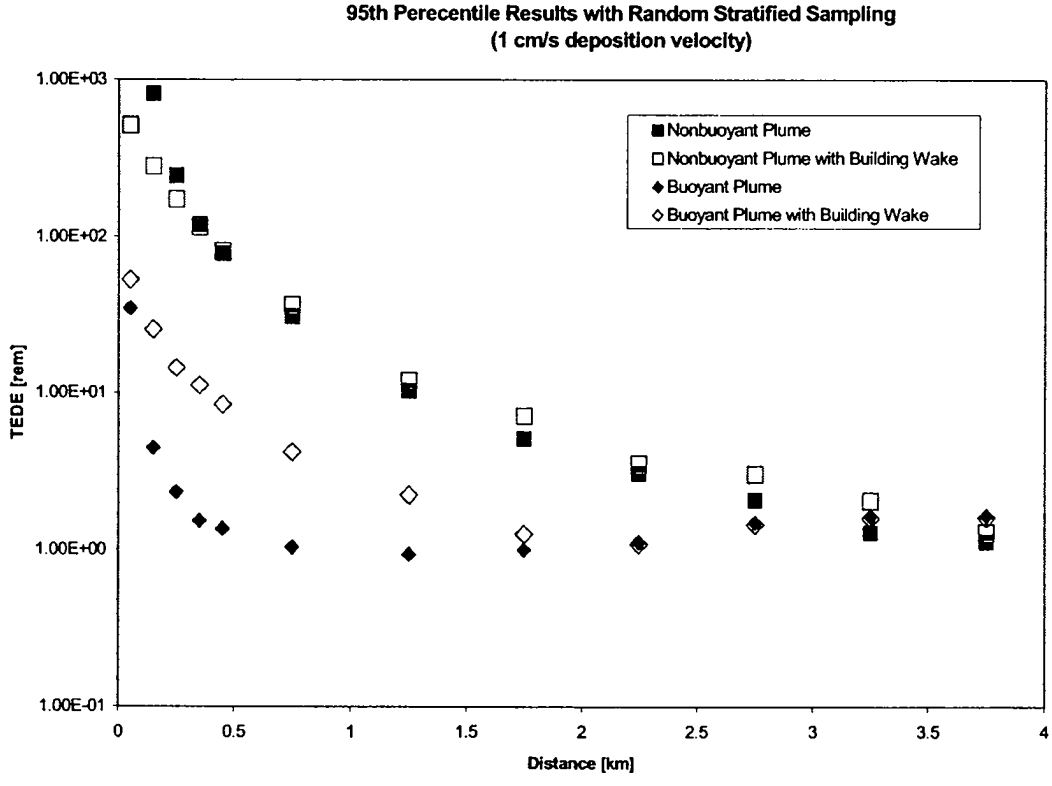

Figure 7-4. MACCS2 results for 4 cases of the sample problem Pu-239 unit curie release

Comparison to GENII 1.485 Results

The sample problem chosen for MACCS2 is the same as the one applied to GENII 1.485 and documented in the GENII guidance report (DOE 2003b). As noted in the previous section, four scenarios were addressed for MACCS2. However, two of them involved fires, which cannot be modeled with GENII 1.485 and therefore are not repeated in the present section. The two scenarios that could be analyzed with GENII are 1) no buoyancy and without building wake, and 2) no buoyancy and with building wake. The second case considers a building 13 m high and 90 m wide.

The objective of this section is to provide a comparison with GENII for the same scenarios executed with MACCS2, and to identify differences between the two codes that the user should consider when selecting a code for a specific purpose.

The following are the major assumptions associated with this analysis:

- The radial distances to the receptor in the GENII case are 150, 250, 350, 450, 750, 1250, 1750, 2250, 2750, 3250, 3750, 4250, 4750, 5250, 5750, 6250, 6750, 7250, 7750, and 9000 m. These correspond to the radial ring endpoints of 0.1, 0.2, 0.3, 0.4, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0, 7.5, 8.0, and 10.0 km used in the MACCS2 sample problem. (In MACCS2, the representative receptors are at the midpoints between the radial ring endpoints.) *In GENII 1.485, receptor distances less than 100 m are prohibited.*

- The base case is assumed an open-area release (no buildings in the vicinity) with a non-buoyant plume. The horizontal dispersion parameters (σ_ys) in GENII 1.485 are calculated in a manner identical to that of MACCS2. However, the vertical dispersion parameters (σ_zs) are calculated with distance-dependent coefficients, i.e., for distance x from the source, different sets of coefficients for $x < 100$m, $100\ \text{m} \le x \le 1000$ m, and $x > 1000$ m.

- In the building wake cases, the building is assumed to have a height of 42.5 ft (13 m) and width of 296 ft (90 m).

- One curie of ^{239}Pu is released over a ten-minute period. The default dose conversion factor (DCF) used in GENII 1.485 for ^{239}Pu is taken from ICRP-30 for lung clearance class Y, for which the inhalation DCF is 8.33×10^{-5} Sv/Bq. This default cannot be overridden by the user. In contrast, the MACCS2 analysis used class W for the ^{239}Pu, for which the DCF is 1.16×10^{-4} Sv/Bq. Thus, MACCS2 uses a DCF that is 1.4 times larger than used in GENII 1.485.

- No wet deposition is assumed.

- The default dry deposition velocity used in GENII 1.485 is 0.001 m/s. This is less than the value used in the MACCS2 sample problem (0.01 m/s). Although GENII 1.485 allows for dry deposition, it does not deplete the plume and therefore is overly conservative. Therefore, dry deposition was turned off in the GENII 1.485 runs.

- The surface roughness length is not specified in GENII 1.485.

- The assumed breathing rate is 3.3×10^{-4} m^3/s, which is the DOE occupational breathing rate (DOE, 1998). It is also the default GENII 1.485 value.
- The doses to the maximally exposed individuals at the specified distances are calculated. The population distribution is not needed.
- No shielding is assumed.
- Neither evacuation nor sheltering is assumed. GENII 1.485 cannot model these conditions.
- Results reported are the plume centerline TEDE value for 95th percentile meteorological conditions for all distances.

The site meteorological data file used was a joint-distribution file created based on the same hourly data used in the MACCS2 sample problem. It was for a specific calendar year of qualified data, measured at wind speed height of 10 meters.

GENII 1.485 was run repeatedly for all 16-wind sectors and receptor distances. Sectors are numbered clockwise from the south. Thus, S = 1, SSW = 2, etc. The base case problem considers no fire, no building wake, a distance of 150 m, and sector 4, that is, to the WSW, which typically had the largest doses for the weather data used. The 95th percentile χ/Q' (labeled E/Q in the output) for this sector at 150 m was 4.2×10^{-3} s/m^3 and the corresponding dose (TEDE) was 430 rem. (Only two significant figures are used in data transfers between subroutines in GENII 1.485, so some round-off error is expected. Thus, the expected result of 420 rem (i.e., 4.2×10^{-3} s/m^3)(1.02×10^5 rem-m^3/s) differed slightly from the output value of 430 rem.)

The results for the base case (no lofting, no wake) and case of building wake without lofting are given in Figure 7-5 as the solid curves. The results from MACCS2 for these same scenarios are included in the figure as dashed curves. For the base case, the MACCS2 results are somewhat larger at close-in distances but decrease much more rapidly with distance compared to GENII, the cross-over occurring at about 1,000 m. For the wake-effects case without lofting, the GENII results are lower at all distances compared to its base case. For MACCS2, the doses are very similar to its base case, being somewhat smaller than the base case for close-in distances but beyond about 400 m they are larger. The MACCS2 doses are larger than those from GENII at distances closer than about 3,500 m but are smaller at greater distances.

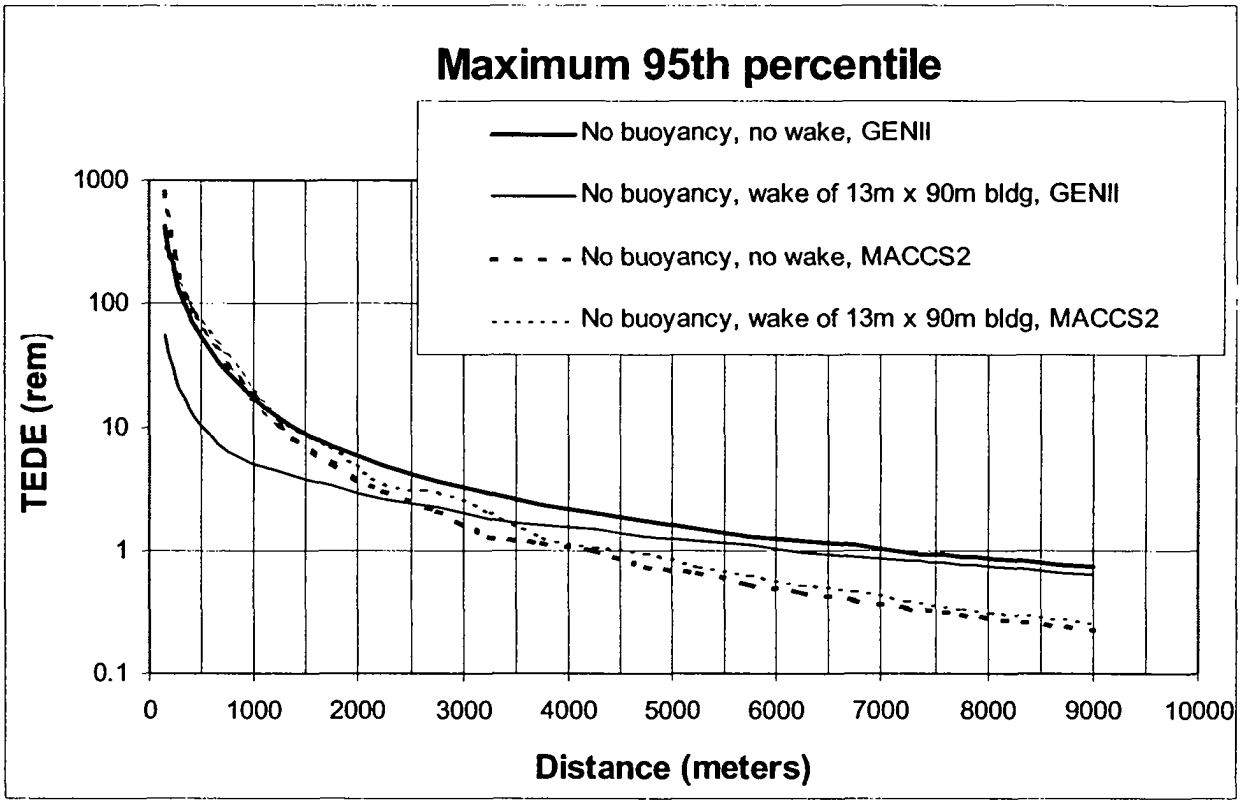

Figure 7-5. Comparison of MACCS2 with GENII for results at 95th percentile TEDE. Note: GENII produces maximum sector 95th percentile results whereas MACCS2 results are 95th direction-independent. GENII results are calculated for two cases only: (1) base case (no lofting, no wake) and (2) building wake without lofting. Sensible heat impact differences from a fire condition were not examined because GENII cannot treat this phenomenon.

The main sources for the differences between the two codes are attributed to the following factors:

- In the near-field (< several hundred meters), the MACCS2 results tend to be larger due to the dose conversion factor and vertical dispersion coefficient differences, and small differences in the wake model.
- In the transition to the far-field region and beyond about several hundred meters, the surface roughness factor impact to σ_z and the dry deposition depletion model in MACCS2 outweigh the dose conversion factor difference, and MACCS dose estimates fall below those of GENII at 1,000 m (base case) and 3,500 m (building wake case).
- In the two runs, GENII did not take into account dry deposition and thus the plume concentration will decrease only with increasing σ_y and σ_z. The two GENII curves decrease very slowly as a result. MACCS2 curves deplete via the dry deposition mechanism and tend to drop off more rapidly as a function of distance.
- For GENII, the plume σ_y and σ_z are initialized to some fraction of the building width and height, respectively and results in a smaller concentration for the wake results throughout the

region of transport. The MACCS2 model is slightly different in that there is a "cross-over" point produced because the no-wake result is depleted more readily as an effect of the simple deposition model depleting the concentration closest to the ground.

- The GENII code calculates the maximum sector 95th percentile results whereas MACCS2 results typically used are the 95th direction-independent. The two types of result can be close numerically, but will typically be different depending on the windrose of the region of transport.

7.4 Output File Listing (with Input Echo)

The output listing for the MACCS2 base case is given below. The output file contains echoes of the ATMOS and EARLY input files. Note that portions of the output listing of been deleted for space considerations. Author's notes in brackets signify where blocks of the output listing are missing. The output of interest in MACCS2 for DSA applications is the Type Number 6 output, which signifies centerline doses at a distance. A box border highlights the block of these results below. Following the output listing, changes to the base-case ATMOS files that were necessary to run the other three cases are also shown.

Nonbuoyant Plume (Base Case)

```
MACCS2  9/05/**   17:07:08   Version 1.12, Last Modified 7/01/96 by D. Chanin
 P1:  ATMOS USER INPUT (UNIT 24) = a5_base.INP
 P2:  EARLY USER INPUT (UNIT 25) = e1_tede.INP
 P3: CHRONC USER INPUT (UNIT 26) = ""
 P4:  METEOROLOGY DATA (UNIT 28) = metdata.INP
 P5:   SITE DATA INPUT (UNIT 29) = ""
 P6:       LIST OUTPUT (UNIT 06) = base5_1.OUT


 USER INPUT IS READ FROM UNIT 24
 RECORD IDENTIFIER FIELDS  11 CHARACTERS LONG ARE EXPECTED.
 THE FIRST 100 COLUMNS OF EACH INPUT RECORD ARE PROCESSED.
 THE MAXIMUM NUMBER OF IDENTIFIER RECORDS THAT MAY BE SAVED AS THE BASE CASE IS  1000.

 RECORD
 NUMBER                                    RECORD

       ********************************************************************************
       *
       *         ATMOS FILE
       *INPUT FILE IDENTIFIER
    1  RIATNAM1001  'MACCS2 - Random Stratified Sampling (METCOND=5)'
       ********************************************************************************
       * GEOMETRY DATA BLOCK, LOADED BY INPGEO, STORED IN /GEOM/
       *
       * NUMBER OF RADIAL SPATIAL ELEMENTS
    2  GENUMRAD001 21
       *
       * ENDPOINT DISTANCES TO RADIAL SPATIAL ELEMENTS (KILOMETERS)
    3  GESPAEND001    0.10   0.20   0.30   0.40   0.50   1.00   1.50
    4  GESPAEND002    2.00   2.50   3.00   3.50   4.00   4.50   5.00
    5  GESPAEND003    5.50   6.00   6.50   7.00   7.50   8.00  10.00
       ********************************************************************************
       * ISOTOPE DATA BLOCK, LOADED BY INPISO, STORED IN /ISOGRP/, /ISONAM/
       *
       * NUMBER OF ISOTOPES
    6  ISNUMISO001 1
       *
       * NUMBER OF ISOTOPE GROUPS
    7  ISMAXGRP001 2
       *
       * WET AND DRY DEPOSITION FLAGS FOR EACH ISOTOPE GROUP
       *              WETDEP     DRYDEP
    8  ISDEPFLA001   .FALSE.    .FALSE.
    9  ISDEPFLA002   .FALSE.    .TRUE.
       *
       * NUMBER OF PSEUDOSTABLE NUCLIDES (USED TO TRUNCATE THE DECAY CHAINS)
   10  ISNUMSTB001  6
       *
   11  ISNAMSTB001     U-235     (DAUGHTER OF PU-239)
   12  ISNAMSTB002     Th-231
   13  ISNAMSTB003     Pa-231
   14  ISNAMSTB004     Ac-227
   15  ISNAMSTB005     Fr-223
   16  ISNAMSTB006     Th-227
       *
       * ISOTOPE GROUP DATA FOR ISOTOPE GROUPS
       *               NUCNAM     IGROUP
   17  ISOTPGRP001     Pu-239       2
       *ISOTPGRP002     Pu-238       2
       *
       ********************************************************************************* WET
DEPOSITION DATA
       *
```

```
    * WASHOUT COEFFICIENT NUMBER ONE, LINEAR FACTOR
18  WDCWASH1001  9.5E-5  (JON HELTON AFTER JONES, 1986)
    *
    * WASHOUT COEFFICIENT NUMBER TWO, EXPONENTIAL FACTOR
19  WDCWASH2001  0.8  (JON HELTON AFTER JONES, 1986)
    ********************************************************************************
    * DRY DEPOSITION DATA BLOCK, LOADED BY INPDRY, STORED IN /DRYCON/
    *
    * NUMBER OF PARTICLE SIZE GROUPS
20  DDNPSGRP001  3
    *
    * DEPOSITION VELOCITY OF EACH PARTICLE SIZE GROUP (M/S)
21  DDVDEPOS001  0.001  0.005  0.01
    ********************************************************************************
    * DISPERSION PARAMETER DATA BLOCK, LOADED BY INPDIS, STORED IN /DISPY/, /DISPZ/
    *
22  NUM_DIST001   0  (power-law fits used instead of dispersion tables)
    *
    *SIGMA = AX**B WHERE A AND B ARE VALUES FROM TADMOR GUR (1969)
    *
    * STABILITY CLASS: A        B        C        D        E        F
    *
    * LINEAR TERM OF THE EXPRESSION FOR SIGMA-Y, 6 STABILITY CLASSES
23  DPCYSIGA001   0.3658   0.2751   0.2089   0.1474   0.1046   0.0722
    *
    * EXPONENTIAL TERM OF THE EXPRESSION FOR SIGMA-Y, 6 STABILITY CLASSES
24  DPCYSIGB001    .9031    .9031    .9031    .9031    .9031    .9031
    *
    * LINEAR TERM OF THE EXPRESSION FOR SIGMA-Z, 6 STABILITY CLASSES
25  DPCZSIGA001   2.5E-4   1.9E-3       .2       .3       .4       .2
    *
    * EXPONENTIAL TERM OF THE EXPRESSION FOR SIGMA-Z, 6 STABILITY CLASSES
26  DPCZSIGB001    2.125   1.6021     .8543    .6532    .6021    .6020
    *
    *  LINEAR SCALING FACTOR FOR SIGMA-Y FUNCTION, NORMALLY 1
27  DPYSCALE001    1.
    *
    *  LINEAR SCALING FACTOR FOR SIGMA-Z FUNCTION,
    *  NORMALLY USED FOR SURFACE ROUGHNESS LENGTH CORRECTION.
    *  (Z1 / Z0) ** .2,   FOR Z1=10 CM, THEREFORE (10/3)**.2=1.27
28  DPZSCALE001    1.27
    ********************************************************************************
    * EXPANSION FACTOR DATA BLOCK, LOADED BY INPEXP, STORED IN /EXPAND/
    *
    * TIME BASE FOR EXPANSION FACTOR (SECONDS)
29  PMTIMBAS001   180.
    *
    * BREAK POINT FOR FORMULA CHANGE (SECONDS)
30  PMBRKPNT001   3600.
    *
    * EXPONENTIAL EXPANSION FACTOR NUMBER 1
31  PMXPFAC1001   .2
    *
    * EXPONENTIAL EXPANSION FACTOR NUMBER 2
32  PMXPFAC2001   .25
    ********************************************************************************
    * PLUME RISE DATA BLOCK, LOADED BY INPLRS, STORED IN /PLUMRS/
    *
    * SCALING FACTOR FOR THE CRITICAL WIND SPEED FOR ENTRAINMENT OF A BOUYANT PLUME
    * (USED BY FUNCTION CAUGHT)
33  PRSCLCRW001   1.
    *
    * SCALING FACTOR FOR THE A-D STABILITY PLUME RISE FORMULA
    * (USED BY FUNCTION PLMRIS)
34  PRSCLADP001   1.
    *
    * SCALING FACTOR FOR THE E-F STABILITY PLUME RISE FORMULA
    * (USED BY FUNCTION PLMRIS)
35  PRSCLEFP001   1.
```

```
    ******************************************************************************
    * WAKE EFFECTS DATA BLOCK, LOADED BY INPWAK, STORED IN /BILWAK/
    * (minimum value specifcations for open area release)
    * BUILDING WIDTH (METERS) (MACCS 1.5.11.1 Input)
    * WEBUILDW001   1.0
    *
    * BUILDING HEIGHT (METERS) - FOR LIFT OFF CRITERION, BUOYANT PLUME (min. val.)
36  WEBUILDH001   1.0
    *
    * INITIAL VALUE OF SIGMA-Y [METERS] DUE TO WAKE EFFECTS (=Wb/4.3, minimum value)
37  SIGYINIT001    0.1
    *
    * INITIAL VALUE OF SIGMA-Z [METERS] DUE TO WAKE EFFECTS (=Hb/2.15, min. value)
38  SIGZINIT001    0.1
    *
    ******************************************************************************
    * OUTPUT CONTROL DATA BLOCK, LOADED BY INPOPT, STORED IN /STOPME/, /ATMOPT/
    *
    * FLAG TO INDICATE THAT THIS IS THE LAST PROGRAM IN THE SERIES TO BE RUN
39  OCENDAT1001  .FALSE. (SET THIS VALUE TO .TRUE. TO SKIP EARLY AND CHRONC)
40  OCIDEBUG001  0
    *
    * NAME OF THE NUCLIDE TO BE LISTED ON THE DISPERSION LISTINGS
41  OCNUCOUT001  Pu-239
    ******************************************************************************
    * METEOROLOGICAL SAMPLING DATA BLOCK
    *
    * METEOROLOGICAL SAMPLING OPTION CODE:
    * METCOD = 1, USER SPECIFIED DAY AND HOUR IN THE YEAR (FROM MET FILE),
    *          2, WEATHER CATEGORY BIN SAMPLING,
    *          3, 120 HOURS OF WEATHER SPECIFIED ON THE ATMOS USER INPUT FILE,
    *          4, CONSTANT MET (BOUNDARY WEATHER USED FROM THE START),
    *          5, STRATIFIED RANDOM SAMPLES FOR EACH DAY OF THE YEAR.
42  M1METCOD001  5
    *
    * LAST SPATIAL INTERVAL FOR MEASURED WEATHER
43  M2LIMSPA001  21
    *
    * BOUNDARY WEATHER MIXING LAYER HEIGHT
44  M2BNDMXH001   600.  (METERS)
    *
    * BOUNDARY WEATHER STABILITY CLASS INDEX
45  M2IBDSTB001  6      (F-STABILITY)
    *
    * BOUNDARY WEATHER RAIN RATE
46  M2BNDRAN001  5.     (MM/HR)
    *
    * BOUNDARY WEATHER WIND SPEED
47  M2BNDWND001  1.     (M/S)
    *
    ******************************************************************************
    * START DAY
    * M3ISTRDY001  237
    * START HOUR
    * M3ISTRHR001  1
    *
    * NUMBER OF RAIN DISTANCE INTERVALS FOR BINNING
    * M4NRNINT001  6
    *
    * ENDPOINTS OF THE RAIN DISTANCE INTERVALS (KILOMETERS)
    * NOTE: THESE MUST BE CHOSEN TO MATCH THE SPATIAL ENDPOINT DISTANCES
    *       SPECIFIED FOR THE ARRAY SPAEND (10 % ERROR IS ALLOWED).
    * M4RNDSTS001  0.2  0.5  1.0  1.5  2.0  3.5
    *
    * NUMBER OF RAIN INTENSITIY BREAKPOINTS
    *M4NRINTN001   2
    *
    * RAIN INTENSITY BREAKPOINTS FOR WEATHER BINNING (MILLIMETERS PER HOUR)
    * M4RNRATE001   1.  2.
```

```
    ******************************************************************************
    * NUMBER OF SAMPLES PER BIN
    *
48  M4NSMPLS001  24
    *
    * INITIAL SEED FOR RANDOM NUMBER GENERATOR
49  M4IRSEED001  93
    ******************************************************************************
    * RELEASE DATA BLOCK, LOADED BY INPREL, STORED IN /ATNAM2/, /MULREL/
    *
    * SOURCE TERM RELEASE SPECIFIC INFORMATION
50  RDATNAM2001 'Unit Ci release Pu-239 w/ nonbuoyant (open area) - YR'
    *
    * TIME AFTER ACCIDENT INITIATION WHEN THE ACCIDENT REACHES GENERAL EMERGENCY
    * CONDITIONS (AS DEFINED IN NUREG-0654), OR WHEN PLANT PERSONNEL CAN RELIABLY
    * PREDICT THAT GENERAL EMERGENCY CONDITIONS WILL BE ATTAINED
    *
51  RDOALARM001    0.00E+00
    *
    * NUMBER OF PLUME SEGMENTS THAT ARE RELEASED
52  RDNUMREL001     1
    *
    * SELECTION OF RISK DOMINANT PLUME
53  RDMAXRIS001     1
    *
    * REFERENCE TIME FOR DISPERSION AND RADIOACTIVE DECAY
54  RDREFTIM001       0.00
    * CORRESPONDING TO LEADING EDGE WEATHER
    *
    * HEAT CONTENT OF THE RELEASE SEGMENTS (WATTS)
    * A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
55  RDPLHEAT001   0.0
    *
    * HEIGHT OF THE PLUME SEGMENTS AT RELEASE (METERS)
    * A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
56  RDPLHITE001  0.0
    *
    * DURATION OF THE PLUME SEGMENTS (SECONDS)
    * A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
57  RDPLUDUR001   600.0
    *
    * TIME OF RELEASE FOR EACH PLUME (SECS FROM SCRAM)
    * A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
58  RDPDELAY001   0.0
    *
    * PARTICLE SIZE DISTRIBUTION OF EACH ISOTOPE GROUP
    * YOU MUST SPECIFY A COLUMN OF DATA FOR EACH OF THE PARTICLE SIZE GROUPS
    *
    *  V dep = 0.001 is for a filtered release
    *  V dep = 0.005 is for HTO only
    *  V dep = 0.010 is for an unfiltered release
    *
    *              0.001  0.005  0.010
59  RDPSDIST001    1.000  0.000  0.000
60  RDPSDIST002    0.000  0.000  1.000
    *
    *                NUCNAM      CORINV(Unit Ci Release)
61  RDCORINV001      Pu-239         1.00E+00
    *RDCORINV002      Pu-238          0.00E+00
    *
    *  SCALING FACTOR TO ADJUST THE CORE INVENTORY
62  RDCORSCA001  3.7E+10 (Conversion of Curies to Becquerels)
    *
    * RELEASE FRACTIONS FOR ISOTOPE GROUPS IN RELEASE
    * GROUP     XE/KR    I    CS    TE    SR    RU    LA    CE    BA   TRIT
63  RDRELFRC001   1.0  1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
    *
    * RELEASE FREACTION APPLICATION TO INGROWTH DECAY PRODUCTS
    * PRODUCED AFTER ACCIDENT INITIATION
```

```
    64  RDAPLFRC001     PARENT
        *
        * REQUEST FOR ATMOSPHERIC OUTPUT INFORMATION
        *
        *             NUM0
    65  TYPE0NUMBER     4
        *
        *             INDREL      INRAD
    66  TYPE0OUT001       1          1
    67  TYPE0OUT002       1          2
    68  TYPE0OUT003       1         10
    69  TYPE0OUT004       1         21     CCDF
        *
        *********************
        .
******** TERMINATOR RECORD ENCOUNTERED -- END OF BASE CASE USER INPUT ********


 USER INPUT PROCESSING SUMMARY - BASE CASE

 NUMBER OF RECORDS READ                          =  268
 NUMBER OF BLANK OR COMMENT RECORDS READ         =  198
 NUMBER OF TERMINATOR RECORDS                    =    1
 NUMBER OF RECORDS PROCESSED                     =   69
      NUMBER OF PROCESSED RECORDS DUPLICATED     =    0
      NUMBER OF PROCESSED RECORDS SORTED         =   69

*****************************************************************************************************
***



 Decay Chain #  Pu-239


 RELEASED INVENTORY OF ALL PLUMES
 Pu-239      3.70E+10

 READING FROM A WEATHER FILE WITH THE FOLLOWING HEADER:
 SAMPLE MET DATA FILE
 3/05/01  PROCESSED MET DATA FOR MACCS2 USE
      METEOROLOGICAL DATA FILE CONTAINS  255 HOURS OF OBSERVED RAIN DATA.
             ACCUMULATED RAIN MEASUREMENTS TOTALED   9.63 INCHES FOR THE YEAR.
             CONSTANT LID HEIGHTS (M) FOR 4 SEASONS =     600    600    600    600
             NON-ZERO WINDSPEEDS LESS THAN 0.5 M/S ARE SET TO 0.5 M/S


 USER INPUT IS READ FROM UNIT 25
 RECORD IDENTIFIER FIELDS  11 CHARACTERS LONG ARE EXPECTED.
 THE FIRST 100 COLUMNS OF EACH INPUT RECORD ARE PROCESSED.
 THE MAXIMUM NUMBER OF IDENTIFIER RECORDS THAT MAY BE SAVED AS THE BASE CASE IS  1000.

 RECORD
 NUMBER                                    RECORD

        ****************************************************************************
        * GENERAL DESCRIPTIVE TITLE DESCRIBING THIS "EARLY" INPUT FILE
        *
     1  MIEANAM1001  'MACCS - TEDE'
        *
        * DCF FILE IDENTIFICATION
     2  DCF_FILE001     'FGR_PU.INP'
        *
        * FLAG TO INDICATE THAT THIS IS THE LAST PROGRAM IN THE SERIES TO BE RUN
        *
     3  MIENDAT2001  .TRUE.    (SET THIS VALUE TO .TRUE. TO SKIP CHRONC)
        *
        * DISPERSION MODEL OPTION CODE:  1  *  STRAIGHT LINE
        *                                2  *  WIND-SHIFT WITH ROTATION
```

```
    *                                3  *  WIND-SHIFT WITHOUT ROTATION
    *
 4  MIIPLUME001  1
    *
    * NUMBER OF FINE GRID SUBDIVISIONS USED BY THE MODEL
    *
 5  MINUMFIN001  7     (3, 5 OR 7 ALLOWED)
    *
    * LEVEL OF DEBUG OUTPUT REQUIRED, NORMAL RUNS SHOULD SPECIFY ZERO
    *
 6  MIIPRINT001  0
    *
    * LOGICAL FLAG SIGNIFYING THAT THE BREAKDOWN OF RISK BY WEATHER CATEGORY
    * BIN ARE TO BE PRESENTED TO SHOW THEIR RELATIVE CONTRIBUTION TO THE MEAN
    *
    *             RISBIN
    *
 7  MIRISCAT001   .FALSE.
    *
    * FLAG INDICATING IF WIND-ROSES FROM ATMOS ARE TO BE OVERRIDDEN
    *
 8  MIOVRRID001  .FALSE.  (USE THE WIND ROSE CALCULATED FOR EACH WEATHER BIN)
    ****************************************************************************
    * POPULATION DISTRIBUTION DATA BLOCK, LOADED BY INPOPU, STORED IN /POPDAT/
    *
    *PDPOPFLG001  FILE
    *
 9  PDPOPFLG001  UNIFORM
10  PDIBEGIN001  1   (SPATIAL INTERVAL AT WHICH POPULATION BEGINS)
11  PDPOPDEN001  0. (POPULATION DENSITY (PEOPLE PER SQUARE KILOMETER))
    ****************************************************************************
    * ORGAN DEFINITION DATA BLOCK, LOADED BY INORGA, STORED IN /EARDIM/ AND /ORGNAM/
    *
    *                ORGAN NAME             ORGFLG
    *
    *MIORGDEF001      'A-SKIN'               .FALSE.
    *MIORGDEF002      'A-RED MARR'           .FALSE.
    *MIORGDEF003      'A-LUNGS'              .FALSE.
    *MIORGDEF004      'A-THYROIDH'           .FALSE.
    *MIORGDEF005      'A-STOMACH'            .FALSE.
    *MIORGDEF006      'A-LOWER LI'           .FALSE.
    *MIORGDEF007      'L-EFFECTIVE'           .TRUE.
    *MIORGDEF008      'L-RED MARR'           .FALSE.
    *MIORGDEF009      'L-BONE SUR'           .FALSE.
    *MIORGDEF010      'L-BREAST'             .FALSE.
    *MIORGDEF011      'L-LUNGS'              .FALSE.
    *MIORGDEF012      'L-THYROID'            .FALSE.
    *MIORGDEF013      'L-LOWER LI'           .FALSE.
    *MIORGDEF014      'L-BLAD WAL'           .FALSE.
    *MIORGDEF015      'L-LIVER'              .FALSE.
    *MIORGDEF016      'L-THYROIDH'           .FALSE.
    *
    ****************************************************************************
    * SHIELDING AND EXPOSURE FACTORS, LOADED BY INDFAC, STORED IN /EADFAC/
    *
    * THREE VALUES OF EACH PROTECTION FACTOR ARE SUPPLIED,
    * ONE FOR EACH TYPE OF ACTIVTY:
    *
    * ACTIVITY TYPE:
    *     1 - EVACUEES WHILE MOVING
    *     2 - NORMAL ACTIVITY IN SHELTERING AND EVACUATION ZONE
    *     3 - SHELTERED ACTIVITY
    *
    * CLOUD SHIELDING FACTOR
    *
    *            EVACUEES  NORMAL  SHELTER
    *
12  SECSFACT001      1.     1.     1.
    *
```

```
     * PROTECTION FACTOR FOR INHALATION
     *
13   SEPROTIN001       1.      1.      1.
     *
     * BREATHING RATE (CUBIC METERS PER SECOND)
     *
14   SEBRRATE001  3.33E-4  3.33E-4  3.33E-4
     *
     * SKIN PROTECTION FACTOR
     *
15   SESKPFAC001       1.      1.      1.
     *
     * GROUND SHIELDING FACTOR
     *
16   SEGSHFAC001       1.     1.      1.
     *
     * RESUSPENSION INHALATION MODEL CONCENTRATION COEFFICIENT (/METER)
     *
     *   RESCON = 1.E-4 IS APPROPRIATE FOR MECHANICAL RESUSPENSION BY VEHICLES.
     *   RESHAF = 2.11 DAYS CAUSES 1.E-4 TO DECAY IN ONE WEEK TO 1.E-5, THE VALUE
     *   OF RESCON USED IN THE FIRST TERM OF THE LONG-TERM RESUSPENSION EQUATION
     *   USED IN CHRONC.
     *
17   SERESCON001   1.0E-4      (RESUSPENSION IS TURNED ON)
     *
     * RESUSPENSION CONCENTRATION COEFFICIENT HALF-LIFE (SEC)
     *
18   SERESHAF001   1.825E5  (2.11 DAYS)
     ******************************************************************************
     * EVACUATION ZONE DATA BLOCK, LOADED BY EVNETW, STORED IN /NETWOR/, /EOPTIO/
     *
     * SPECIFIC DESCRIPTION OF THE EMERGENCY RESPONSE SCENARIO BEING USED
     *
19   EZEANAM2001  'NO EVACUATION OR SHELTERING'
     *
     * THE TYPE OF WEIGHTING TO BE APPLIED TO THE EMERGENCY RESPONSE SCENARIOS
     * YOU MUST SUPPLY A VALUE OF 'TIME' OR 'PEOPLE'
     *
               20  EZWTNAME001  'PEOPLE'
     *
     *
     * WEIGHTING FRACTION APPLICABLE TO THIS SCENARIO
     *
21   EZWTFRAC001  1.000
     *
     * LAST RING IN THE MOVEMENT ZONE
     *
22   EZLASMOV001     0    (NO EVACUATION)
     *
     * FIRST SPATIAL INTERVAL IN THE EVACUATION ZONE
     *
     ************************************************************************
     * SHELTER AND RELOCATION ZONE DATA BLOCK, LOADED BY INPEMR,
     *                                        STORED IN /INPSRZ/, /RELOCA/
     *
     * TIME TO TAKE SHELTER IN THE INNER SHELTER ZONE (SECONDS FROM OALARM)
     *
     *SRTTOSH1001       0.     (THERE IS NO INNER SHELTER ZONE)
     *
     * SHELTER DURATION IN THE INNER SHELTER ZONE (SECONDS FROM TAKING SHELTER)
     *
     *SRSHELT1001       0.     (THERE IS NO INNER SHELTER ZONE)
     *
     * LAST RING OF THE OUTER SHELTER ZONE
     *
     *SRLASHE2001       0      (THERE IS NO OUTER SHELTER ZONE)
     *
     * TIME TO TAKE SHELTER IN THE OUTER SHELTER ZONE (SECONDS FROM OALARM)
     *
```

```
    *SRTTOSH2001      0.    (THERE IS NO OUTER SHELTER ZONE)
    *
    * SHELTER DURATION IN THE OUTER SHELTER ZONE (SECONDS FROM TAKING SHELTER)
    *
    *SRSHELT2001      0.    (THERE IS NO OUTER SHELTER ZONE)
    *
    * DURATION OF THE EMERGENCY PHASE (SECONDS FROM PLUME ARRIVAL)
    *
 23 SRENDEMP001  86400.   (ONE DAY)
    *
    * CRITICAL ORGAN FOR RELOCATION DECISIONS
    *
 24 SRCRIORG001 'L-EFFECTIVE'
    *
    * HOT SPOT RELOCATION TIME (SECONDS FROM PLUME ARRIVAL)
    *
 25 SRTIMHOT001  86400.   (ONE DAY)
    *
    * NORMAL RELOCATION TIME (SECONDS FROM PLUME ARRIVAL)
    *
 26 SRTIMNRM001  86400.   (ONE DAY)
    *
    * HOT SPOT RELOCATION DOSE CRITERION THRESHOLD (SIEVERTS)
    *
 27 SRDOSHOT001  0.50  (50 REM DOSE TO RBM IN 1 WEEK TRIGGERS RELOCATION)
    *
    * NORMAL RELOCATION DOSE CRITERION THRESHOLD (SIEVERTS)
    *
 28 SRDOSNRM001  0.25   (25 REM DOSE TO RBM IN 1 WEEK TRIGGERS RELOCATION)
    ********************************************************************************
    * EARLY FATALITY MODEL PARAMETERS, LOADED BY INEFAT, STORED IN /EFATAL/
    *
    * NUMBER OF EARLY FATALITY EFFECTS
    *
 29 EFNUMEFA001   0
    *
    ********************************************************************************
    * EARLY INJURY MODEL PARAMETERS, LOADED BY INEINJ, STORED IN /EINJUR/
    *
    * NUMBER OF EARLY INJURY EFFECTS
    *
 30 EINUMEIN001  0
    *
    ********************************************************************************
    * ACUTE EXPOSURE CANCER PARAMETERS, LOADED BY INACAN STORED IN /ACANCR/.
    *
    * NUMBER OF ACUTE EXPOSURE CANCER EFFECTS**
    *
 31 LCNUMACA001   0
    *
    * THRESHOLD DOSE FOR APPLYING THE DOSE DEPENDENT REDUCTION FACTOR
    *
    * LCDDTHRE001   0.0  (LOWEST DOSE FOR WHICH DDREFA WILL BE APPLIED)
    *
    * DOSE THRESHOLD FOR LINEAR DOSE RESPONSE (Sv)
    *
    * LCACTHRE001   1.5  (LINEAR-QUADRATIC MODEL IS NOT BEING USED)
    *
    *            ACNAME       ORGNAM  ACSUSC  DOSEFA DOSEFB  CFRISK  CIRISK  DDREFA
    *
    * LCANCERS001 'ICRP 60' 'L-EFFECTIVE' 1.0   1.0    0.0    5.0E-2  7.3E-2   1.0
    ********************************************************************************
    * RESULT 1 OPTIONS BLOCK, LOADED BY INOUT1, STORED IN /INOUT1/
    * TOTAL NUMBER OF A GIVEN EFFECT (LATENT CANCER, EARLY DEATH, EARLY INJURY)
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
 32 TYPE1NUMBER    0
    ********************************************************************************
    * RESULT 2 OPTIONS BLOCK, LOADED BY INOUT2, STORED IN /INOUT2/
    * FURTHEST DISTANCE AT WHICH A GIVEN RISK OF EARLY DEATH IS EXCEEDED.
```

```
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
    *
33  TYPE2NUMBER  0
    ******************************************************************************
    * RESULT 3 OPTIONS BLOCK, LOADED BY INOUT3, STORED IN /INOUT3/
    * NUMBER OF PEOPLE WHOSE DOSE TO A GIVEN ORGAN EXCEEDS A GIVEN THRESHOLD.
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
34  TYPE3NUMBER  0
    ******************************************************************************
    * RESULT 4 OPTIONS BLOCK, LOADED BY INOUT4, STORED IN /INOUT4/
    * 360 DEGREE AVERAGE RISK OF A GIVEN EFFECT AT A GIVEN DISTANCE.
    * POSSIBLE TYPES OF EFFECTS ARE:
35  TYPE4NUMBER  0
    ******************************************************************************
    * RESULT 5 OPTIONS BLOCK, LOADED BY INOUT5, STORED IN /INOUT5/
    * TOTAL POPULATION DOSE TO A GIVEN ORGAN BETWEEN TWO DISTANCES.
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
36  TYPE5NUMBER     0
    ******************************************************************************
    * RESULT 6 OPTIONS BLOCK, LOADED BY INOUT6, STORED IN /INOUT6/
    * CENTERLINE DOSE TO AN ORGAN VS DIST BY PATHWAY, PATHWAY NAMES ARE AS FOLLOWS:
    *  PATHWAY NAME:
    *    'CLD'      - CLOUDSHINE
    *    'GRD'      - GROUNDSHINE
    *    'INH ACU' - "ACUTE DOSE EQUIVALENT" FROM DIRECT INHALATION OF THE CLOUD
    *    'INH LIF' - "LIFETIME DOSE COMMITMENT" FROM DIRECT INHALATION OF THE CLOUD
    *    'RES ACU' - "ACUTE DOSE EQUIVALENT" FROM RESUSPENSION INHALATION
    *    'RES LIF' - "LIFETIME DOSE COMMITMENT" FROM RESUSPENSION INHALATION
    *    'TOT ACU' - "ACUTE DOSE EQUIVALENT" FROM ALL PATHWAYS
    *    'TOT LIF' - "LIFETIME DOSE COMMITMENT" FROM ALL PATHWAYS
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
37  TYPE6NUMBER     1
    *
    *             ORGNAM        PATHNM      I1DIS6   I2DIS6
    *
38  TYPE6OUT001  'L-EFFECTIVE'    'TOT LIF'      1       21
    *TYPE6OUT002  'L-EFFECTIVE'    'TOT LIF'      2        2
    *TYPE6OUT003  'L-EFFECTIVE'    'TOT LIF'      3        3
    *TYPE6OUT004  'L-EFFECTIVE'    'TOT LIF'      4        4
    ******************************************************************************
    * RESULT 7 OPTIONS BLOCK, LOADED BY INOUT7, STORED IN /INOUT7/
    * CENTERLINE RISK OF A GIVEN EFFECT VS DISTANCE
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
39  TYPE7NUMBER   0
    ******************************************************************************
    * RESULT 8 OPTIONS BLOCK, LOADED BY INOUT8, STORED IN /INOUT8/
    * POPULATION WEIGHTED FATALITY RISK BETWEEN 2 DISTANCES
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
40  TYPE8NUMBER   0
    ******************************************************************************
    * RESULT A OPTIONS BLOCK, LOADED BY INOUTA, STORED IN /INOUTA/
    * PEAK TOTAL DOSE AT A DISTANCE
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
41  TYPEANUMBER   1
    *             ORGNAM            I1DISA   I2DISA
    *
42  TYPEAOUT001  'L-EFFECTIVE'          1       21
    ******************************************************************************
    * RESULT B OPTIONS BLOCK, LOADED BY INOUTB, STORED IN /INOUTB/
    * PEAK TOTAL DIRECT DOSE FOUND AT A SPATIAL GRID LOCATION
    * NUMBER OF DESIRED RESULTS OF THIS TYPE
43  TYPEBNUMBER   16
    *             ORGNAM            I1DISB   I2DISB
    *
44  TYPEBOUT001  'L-EFFECTIVE'          3       1
45  TYPEBOUT002  'L-EFFECTIVE'          3       2
46  TYPEBOUT003  'L-EFFECTIVE'          3       3
47  TYPEBOUT004  'L-EFFECTIVE'          3       4
48  TYPEBOUT005  'L-EFFECTIVE'          3       5
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   49  TYPEBOUT006  'L-EFFECTIVE'          3       6
   50  TYPEBOUT007  'L-EFFECTIVE'          3       7
   51  TYPEBOUT008  'L-EFFECTIVE'          3       8
   52  TYPEBOUT009  'L-EFFECTIVE'          3       9
   53  TYPEBOUT010  'L-EFFECTIVE'          3      10
   54  TYPEBOUT011  'L-EFFECTIVE'          3      11
   55  TYPEBOUT012  'L-EFFECTIVE'          3      12
   56  TYPEBOUT013  'L-EFFECTIVE'          3      13
   57  TYPEBOUT014  'L-EFFECTIVE'          3      14
   58  TYPEBOUT015  'L-EFFECTIVE'          3      15
   59  TYPEBOUT016  'L-EFFECTIVE'          3      16
       ********************************************************************************
       .
******** TERMINATOR RECORD ENCOUNTERED -- END OF BASE CASE USER INPUT ********


USER INPUT PROCESSING SUMMARY - BASE CASE

NUMBER OF RECORDS READ                          =  303
NUMBER OF BLANK OR COMMENT RECORDS READ         =  243
NUMBER OF TERMINATOR RECORDS                    =    1
NUMBER OF RECORDS PROCESSED                     =   59
     NUMBER OF PROCESSED RECORDS DUPLICATED     =    0
     NUMBER OF PROCESSED RECORDS SORTED         =   59

********************************************************************************************************
***



The list of defined organs from FGRDCF is as follows (A- is ACUTE and L- is LIFETIME):
   A-SKIN
   A-SKIN(FGR)
   L-GONADS
   L-BREAST
   L-LUNGS
   L-RED MARR
   L-BONE SUR
   L-THYROID
   L-REMAINDER
   L-EFFECTIVE

READING FROM A DOSE CONVERSION FILE WITH THE FOLLOWING HEADER:
FGRDCF 06/18/02   12:22:20   BETA-TEST VERSION 1.10, MINOR FORTRAN FIXES 5/4/95
IMPLICIT DAUGHTER HALFLIVES (M) LESS THAN  90 AND LESS THAN 0.100 OF PARENT

Processing DCFs for Pu-239
NO EVACUATION REQUESTED

CALCULATING A UNIFORM POPULATION DISTRIBUTION

1 THIS PROGRAM CURRENTLY ALLOWS THE GENERATION OF UP TO  394 RESULTS

YOU HAVE REQUESTED  58 RESULTS FROM "EARLY" COMPOSED OF:

   0 RESULTS OF TYPE 1
   0 RESULTS OF TYPE 2
   0 RESULTS OF TYPE 3
   0 RESULTS OF TYPE 4
   0 RESULTS OF TYPE 5
  21 RESULTS OF TYPE 6
   0 RESULTS OF TYPE 7
   0 RESULTS OF TYPE 8
  21 RESULTS OF TYPE A
  16 RESULTS OF TYPE B


     TRIAL        DAY       HOUR        BIN     PRBMET
         1          1          1          0   1.14E-04
```

```
 Each weather sequence has a probability of 1.142E-04

          2          1          2          0    1.14E-04
          3          1          3          0    1.14E-04
          4          1          4          0    1.14E-04
          5          1          5          0    1.14E-04
          6          1          6          0    1.14E-04
          7          1          7          0    1.14E-04
          8          1          8          0    1.14E-04
          9          1          9          0    1.14E-04

[Authors' Note:  Only small sample of 8760 trials are documented here]


     TRIAL        DAY       HOUR        BIN     PRBMET
       8751        365         15          0    1.14E-04
       8752        365         16          0    1.14E-04
       8753        365         17          0    1.14E-04
       8754        365         18          0    1.14E-04
       8755        365         19          0    1.14E-04
       8756        365         20          0    1.14E-04
       8757        365         21          0    1.14E-04
       8758        365         22          0    1.14E-04
       8759        365         23          0    1.14E-04
       8760        365         24          0    1.14E-04
1  DATE AND TIME OF RUN = MACCS2  9/05/**    17:07:08   Version 1.12, Last Modified 7/01/96 by D.
Chanin
   "ATMOS"  DESCRIPTION = MACCS2 - Random Stratified Sampling (METCOND=5)
                                                        PROB                           QUANTILES
PEAK       PEAK  PEAK
                                                     NON-ZERO   MEAN      50TH       90TH      95TH       99TH
99.5TH      CONS       PROB  TRIAL
 Source Term 1: Plume 1, at      0- .1 km
  Pu-239    Center Air Conc. (Bq-s/m3)       .9999  5.92E+08  1.97E+08  2.23E+09 NOT-FOUND NOT-FOUND
NOT-FOUND  2.74E+09  8.08E-02   23
  Pu-239    Ground Air Conc. (Bq-s/m3)       .9999  5.92E+08  1.97E+08  2.23E+09 NOT-FOUND NOT-FOUND
NOT-FOUND  2.74E+09  8.08E-02   23
  Pu-239    Center Ground Conc. (Bq/m2)      .9999  5.77E+06  1.97E+06  2.20E+07 NOT-FOUND NOT-FOUND
NOT-FOUND  2.62E+07  8.08E-02   23
  Total     Center Ground Conc. (Bq/m2)      .9999  5.77E+06  1.97E+06  2.20E+07 NOT-FOUND NOT-FOUND
NOT-FOUND  2.62E+07  8.08E-02   23
  Ground-Level Dilution, X/Q (s/m3)          .9999  1.97E-02  5.60E-03  7.93E-02 NOT-FOUND NOT-FOUND
NOT-FOUND  1.01E-01  8.08E-02   23
  Pu-239    Adjusted Source, Q (Bq)          .9999  3.41E+10  3.04E+10  3.15E+10  3.20E+10  3.32E+10
3.37E+10  3.67E+10  1.14E-04  941
  Plume Sigma-y (m)                          .9999  6.13E+00  5.39E+00  9.80E+00  1.26E+01 NOT-FOUND
NOT-FOUND  1.50E+01  3.11E-02  135
  Plume Sigma-z (m)                          .9999  3.85E+00  3.38E+00 NOT-FOUND NOT-FOUND NOT-FOUND
NOT-FOUND  6.56E+00  1.21E-01   11
  Plume Height  (m)                          .0000  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
0.00E+00  0.00E+00  0.00E+00    0
  Plume Arrival Time (s)                     .9999  3.60E+01  2.31E+01 NOT-FOUND NOT-FOUND NOT-FOUND
NOT-FOUND  1.00E+02  1.22E-01   23

 Source Term 1: Plume 1, at     .1- .2 km
  Pu-239    Center Air Conc. (Bq-s/m3)       .9999  5.87E+07  2.40E+07  2.06E+08 NOT-FOUND NOT-FOUND
NOT-FOUND  2.18E+08  8.08E-02   23
  Pu-239    Ground Air Conc. (Bq-s/m3)       .9999  5.87E+07  2.40E+07  2.06E+08 NOT-FOUND NOT-FOUND
NOT-FOUND  2.18E+08  8.08E-02   23
  Pu-239    Center Ground Conc. (Bq/m2)      .9999  5.85E+05  2.40E+05  2.06E+06 NOT-FOUND NOT-FOUND
NOT-FOUND  2.16E+06  8.08E-02   23
  Total     Center Ground Conc. (Bq/m2)      .9999  5.85E+05  2.40E+05  2.06E+06 NOT-FOUND NOT-FOUND
NOT-FOUND  2.16E+06  8.08E-02   23
  Ground-Level Dilution, X/Q (s/m3)          .9999  2.80E-03  7.26E-04  1.14E-02 NOT-FOUND NOT-FOUND
NOT-FOUND  1.46E-02  8.08E-02   23
  Pu-239    Adjusted Source, Q (Bq)          .9999  3.03E+10  3.02E+10  3.13E+10  3.18E+10  3.29E+10
3.34E+10  3.63E+10  1.14E-04  941
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  Plume Sigma-y (m)                          .9999  1.74E+01  1.30E+01  2.93E+01  3.68E+01 NOT-FOUND
NOT-FOUND  4.28E+01  3.11E-02  135
  Plume Sigma-z (m)                          .9999  1.04E+01  8.61E+00 NOT-FOUND NOT-FOUND NOT-FOUND
NOT-FOUND  1.83E+01  1.21E-01   11
  Plume Height  (m)                          .0000  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
0.00E+00  0.00E+00  0.00E+00    0
  Plume Arrival Time (s)                     .9999  1.08E+02  6.88E+01 NOT-FOUND NOT-FOUND NOT-FOUND
NOT-FOUND  3.00E+02  1.22E-01   23

 Source Term 1: Plume 1, at   2.5-3.0 km
  Pu-239   Center Air Conc. (Bq-s/m3)        .9999  2.21E+05  1.77E+05  4.54E+05  5.42E+05  7.01E+05
7.06E+05  7.16E+05  1.37E-03   55
  Pu-239   Ground Air Conc. (Bq-s/m3)        .9999  2.21E+05  1.77E+05  4.54E+05  5.42E+05  7.01E+05
7.06E+05  7.16E+05  1.37E-03   55
  Pu-239   Center Ground Conc. (Bq/m2)       .9999  2.21E+03  1.77E+03  4.52E+03  5.41E+03  7.01E+03
7.06E+03  7.16E+03  1.37E-03   55
  Total    Center Ground Conc. (Bq/m2)       .9999  2.21E+03  1.77E+03  4.52E+03  5.41E+03  7.01E+03
7.06E+03  7.16E+03  1.37E-03   55
  Ground-Level Dilution, X/Q (s/m3)          .9999  3.04E-05  7.45E-06  1.10E-04  1.69E-04 NOT-FOUND
NOT-FOUND  1.82E-04  4.42E-02   66
  Pu-239   Adjusted Source, Q (Bq)          .9999  2.22E+10  2.33E+10  3.06E+10  3.10E+10  3.19E+10
3.24E+10  3.47E+10  1.14E-04 6466
  Plume Sigma-y (m)                          .9999  2.42E+02  2.19E+02  3.70E+02  4.46E+02 NOT-FOUND
NOT-FOUND  5.94E+02  3.22E-02  135
  Plume Sigma-z (m)                          .9999  1.29E+02  5.70E+01  2.58E+02  7.09E+02  7.76E+02
8.07E+02  1.15E+03  1.14E-04 6970
  Plume Height  (m)                          .0000  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
0.00E+00  0.00E+00  0.00E+00    0
  Plume Arrival Time (s)                     .9999  1.95E+03  1.23E+03  4.91E+03 NOT-FOUND NOT-FOUND
NOT-FOUND  5.50E+03  8.50E-02   66

 Source Term 1: Plume 1, at  8.0-10.0 km
  Pu-239   Center Air Conc. (Bq-s/m3)        .9999  2.19E+04  1.67E+04  4.47E+04  5.89E+04  9.34E+04
1.06E+05  1.84E+05  1.14E-04 7681
  Pu-239   Ground Air Conc. (Bq-s/m3)        .9999  2.19E+04  1.67E+04  4.47E+04  5.89E+04  9.34E+04
1.06E+05  1.84E+05  1.14E-04 7681
  Pu-239   Center Ground Conc. (Bq/m2)       .9999  2.19E+02  1.66E+02  4.46E+02  5.87E+02  9.30E+02
1.06E+03  1.83E+03  1.14E-04 7681
  Total    Center Ground Conc. (Bq/m2)       .9999  2.19E+02  1.66E+02  4.46E+02  5.87E+02  9.30E+02
1.06E+03  1.83E+03  1.14E-04 7681
  Ground-Level Dilution, X/Q (s/m3)          .9999  4.01E-06  1.01E-06  1.27E-05  2.00E-05 NOT-FOUND
NOT-FOUND  3.06E-05  1.11E-02   66
  Pu-239   Adjusted Source, Q (Bq)          .9999  1.88E+10  2.07E+10  3.01E+10  3.05E+10  3.14E+10
3.17E+10  3.39E+10  1.14E-04 6466
  Plume Sigma-y (m)                          .9999  7.21E+02  5.64E+02  1.04E+03  1.17E+03  1.56E+03
NOT-FOUND  1.73E+03  5.59E-03  709
  Plume Sigma-z (m)                          .9999  2.00E+02  1.37E+02  5.04E+02  5.56E+02  6.96E+02
8.14E+02  1.15E+03  1.14E-04 1402
  Plume Height  (m)                          .0000  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
0.00E+00  0.00E+00  0.00E+00    0
  Plume Arrival Time (s)                     .9999  6.08E+03  4.06E+03  1.30E+04  1.68E+04 NOT-FOUND
NOT-FOUND  1.80E+04  4.18E-02   66
1 RESULT NAME = Source Term 1: Plume 1, at  8.0-10.0 km
                  Pu-239   Center Air Conc. (Bq-s/m3)
  1.00E-02  1.00E+00
  2.00E-02  1.00E+00
  3.00E-02  1.00E+00
  5.00E-02  1.00E+00
  7.00E-02  1.00E+00
  1.00E-01  1.00E+00
  2.00E-01  1.00E+00
  3.00E-01  1.00E+00
  5.00E-01  1.00E+00
  7.00E-01  1.00E+00
  1.00E+00  1.00E+00
  2.00E+00  1.00E+00
  3.00E+00  1.00E+00
  5.00E+00  1.00E+00
  7.00E+00  1.00E+00
```

```
  1.00E+01  1.00E+00
  2.00E+01  1.00E+00
  3.00E+01  1.00E+00
  5.00E+01  1.00E+00
  7.00E+01  1.00E+00
  1.00E+02  1.00E+00
  2.00E+02  1.00E+00
  3.00E+02  1.00E+00
  5.00E+02  9.98E-01
  7.00E+02  9.95E-01
  1.00E+03  9.90E-01
  2.00E+03  9.79E-01
  3.00E+03  9.57E-01
  5.00E+03  8.57E-01
  7.00E+03  7.24E-01
  1.00E+04  6.54E-01
  2.00E+04  4.54E-01
  3.00E+04  2.33E-01
  5.00E+04  7.88E-02
  7.00E+04  3.08E-02
  1.00E+05  7.65E-03
  1.84E+05  1.14E-04
```

[Authors' Note: Similar CCDF distributions as above are included in the output for the other plume results, but are not shown here.]

```
1  DATE AND TIME OF RUN = MACCS2  9/05/**   17:07:08   Version 1.12, Last Modified 7/01/96 by D.
Chanin
   "ATMOS"  DESCRIPTION = MACCS2 - Random Stratified Sampling (METCOND=5)
   "EARLY"  DESCRIPTION = MACCS - TEDE

 SOURCE TERM  1 OF  1:
    Unit Ci release Pu-239 w/ nonbuoyant (open area) - YR

 RESULTS FOR A SINGLE EMERGENCY RESPONSE COHORT WITHOUT ANY WEIGHTING FRACTIONS BEING APPLIED

    COHORT 1 = NO EVACUATION OR SHELTERING
```

9/05/** 17:07:08 PAGE 1		PROB	QUANTILES					
PEAK	PEAK PEAK							
		NON-ZERO	MEAN	50TH	90TH	95TH	99TH	99.5TH
CONS	PROB TRIAL							
CENTERLINE DOSE AT SOME DISTANCES (Sv)								
L-EFFECTIVE TOT LIF	0- .1 km	.9999	2.44E+01	8.26E+00	8.61E+01	NOT-FOUND	NOT-FOUND	NOT-FOUND
1.13E+02	8.08E-02 23							
L-EFFECTIVE TOT LIF	.1- .2 km	.9999	2.43E+00	9.98E-01	8.21E+00	NOT-FOUND	NOT-FOUND	NOT-FOUND
9.02E+00	8.08E-02 23							
L-EFFECTIVE TOT LIF	.2- .3 km	.9999	9.44E-01	4.32E-01	3.02E+00	3.09E+00	NOT-FOUND	NOT-FOUND
3.19E+00	1.95E-02 45							
L-EFFECTIVE TOT LIF	.3- .4 km	.9999	5.04E-01	2.48E-01	1.13E+00	1.27E+00	NOT-FOUND	NOT-FOUND
1.63E+00	1.19E-02 24							
L-EFFECTIVE TOT LIF	.4- .5 km	.9999	3.14E-01	1.64E-01	7.50E-01	8.22E-01	NOT-FOUND	NOT-FOUND
9.95E-01	1.18E-02 22							
L-EFFECTIVE TOT LIF	.5-1.0 km	.9999	1.24E-01	7.27E-02	2.87E-01	3.19E-01	3.77E-01	NOT-FOUND
3.82E-01	8.79E-03 46							
L-EFFECTIVE TOT LIF	1.0-1.5 km	.9999	4.47E-02	3.11E-02	9.70E-02	1.06E-01	1.26E-01	1.35E-01
1.38E-01	4.22E-03 7							
L-EFFECTIVE TOT LIF	1.5-2.0 km	.9999	2.27E-02	1.78E-02	4.45E-02	5.45E-02	7.04E-02	7.09E-02
7.13E-02	2.74E-03 1							
L-EFFECTIVE TOT LIF	2.0-2.5 km	.9999	1.36E-02	1.07E-02	2.80E-02	3.15E-02	3.65E-02	3.88E-02
4.37E-02	1.37E-03 501							
L-EFFECTIVE TOT LIF	2.5-3.0 km	.9999	9.14E-03	7.30E-03	1.97E-02	2.13E-02	2.47E-02	2.63E-02
2.96E-02	1.37E-03 55							
L-EFFECTIVE TOT LIF	3.0-3.5 km	.9999	6.59E-03	5.36E-03	1.25E-02	1.55E-02	2.11E-02	2.21E-02
2.44E-02	1.14E-03 91							
L-EFFECTIVE TOT LIF	3.5-4.0 km	.9999	4.94E-03	3.92E-03	1.04E-02	1.17E-02	1.54E-02	1.73E-02
2.10E-02	5.71E-04 744							

```
  L-EFFECTIVE TOT LIF        4.0-4.5 km   .9999  3.85E-03  3.05E-03  8.07E-03  1.00E-02  1.23E-02
1.35E-02  2.05E-02  2.28E-04 7757
  L-EFFECTIVE TOT LIF        4.5-5.0 km   .9999  3.10E-03  2.43E-03  6.26E-03  7.87E-03  1.10E-02
1.18E-02  1.81E-02  1.14E-04 6390
  L-EFFECTIVE TOT LIF        5.0-5.5 km   .9999  2.56E-03  2.08E-03  5.42E-03  6.84E-03  9.48E-03
1.07E-02  1.87E-02  1.14E-04 7607
  L-EFFECTIVE TOT LIF        5.5-6.0 km   .9999  2.14E-03  1.55E-03  4.16E-03  5.47E-03  8.36E-03
9.57E-03  1.60E-02  1.14E-04 8576
  L-EFFECTIVE TOT LIF        6.0-6.5 km   .9999  1.82E-03  1.33E-03  3.71E-03  4.82E-03  7.33E-03
8.75E-03  1.30E-02  3.42E-04  379
  L-EFFECTIVE TOT LIF        6.5-7.0 km   .9999  1.57E-03  1.19E-03  3.23E-03  4.18E-03  6.40E-03
7.34E-03  1.23E-02  1.14E-04 6331
  L-EFFECTIVE TOT LIF        7.0-7.5 km   .9999  1.37E-03  1.09E-03  2.73E-03  3.54E-03  5.92E-03
7.08E-03  1.11E-02  1.14E-04  213
  L-EFFECTIVE TOT LIF        7.5-8.0 km   .9999  1.20E-03  1.01E-03  2.45E-03  3.17E-03  5.17E-03
6.25E-03  1.17E-02  1.14E-04 2853
  L-EFFECTIVE TOT LIF       8.0-10.0 km   .9999  9.07E-04  7.43E-04  1.85E-03  2.42E-03  4.01E-03
4.90E-03  7.60E-03  1.14E-04 7681

 PEAK DOSE FOUND ON SPATIAL GRID (Sv)
  L-EFFECTIVE                 0- .1 km   .9999  2.38E+01  8.15E+00  8.37E+01 NOT-FOUND NOT-FOUND
NOT-FOUND  1.09E+02  8.08E-02   23
  L-EFFECTIVE                .1- .2 km   .9999  2.36E+00  9.89E-01  7.93E+00 NOT-FOUND NOT-FOUND
NOT-FOUND  8.67E+00  8.08E-02   23
  L-EFFECTIVE                .2- .3 km   .9999  9.15E-01  4.20E-01  3.00E+00  3.03E+00 NOT-FOUND
NOT-FOUND  3.06E+00  1.95E-02   45
  L-EFFECTIVE                .3- .4 km   .9999  4.88E-01  2.44E-01  1.12E+00  1.24E+00 NOT-FOUND
NOT-FOUND  1.56E+00  1.19E-02   24
  L-EFFECTIVE                .4- .5 km   .9999  3.04E-01  1.61E-01  7.43E-01  8.03E-01 NOT-FOUND
NOT-FOUND  9.47E-01  1.18E-02   22
  L-EFFECTIVE                .5-1.0 km   .9999  1.19E-01  7.20E-02  2.82E-01  3.14E-01  3.58E-01
NOT-FOUND  3.62E-01  8.79E-03   46
  L-EFFECTIVE               1.0-1.5 km   .9999  4.31E-02  3.09E-02  9.14E-02  1.03E-01  1.20E-01
1.28E-01  1.30E-01  4.22E-03    7
  L-EFFECTIVE               1.5-2.0 km   .9999  2.19E-02  1.73E-02  4.24E-02  5.08E-02  5.92E-02
6.31E-02  6.68E-02  2.74E-03    1
  L-EFFECTIVE               2.0-2.5 km   .9999  1.31E-02  1.05E-02  2.57E-02  3.06E-02  3.48E-02
3.68E-02  4.09E-02  1.37E-03  501
  L-EFFECTIVE               2.5-3.0 km   .9999  8.81E-03  7.15E-03  1.79E-02  2.08E-02  2.36E-02
2.50E-02  2.78E-02  1.37E-03  912
  L-EFFECTIVE               3.0-3.5 km   .9999  6.35E-03  4.84E-03  1.13E-02  1.28E-02  1.72E-02
1.96E-02  2.35E-02  1.14E-03   91
  L-EFFECTIVE               3.5-4.0 km   .9999  4.76E-03  3.84E-03  1.02E-02  1.13E-02  1.45E-02
1.62E-02  2.02E-02  1.26E-03 1247
  L-EFFECTIVE               4.0-4.5 km   .9999  3.71E-03  2.99E-03  7.85E-03  9.79E-03  1.21E-02
1.31E-02  1.90E-02  2.28E-04 7757
  L-EFFECTIVE               4.5-5.0 km   .9999  2.99E-03  2.37E-03  5.99E-03  7.35E-03  1.04E-02
1.12E-02  1.67E-02  1.14E-04 6390
  L-EFFECTIVE               5.0-5.5 km   .9999  2.46E-03  2.01E-03  5.20E-03  6.51E-03  9.14E-03
1.03E-02  1.73E-02  1.14E-04 7607
  L-EFFECTIVE               5.5-6.0 km   .9999  2.06E-03  1.51E-03  4.05E-03  5.25E-03  7.88E-03
9.11E-03  1.48E-02  1.14E-04 8576
  L-EFFECTIVE               6.0-6.5 km   .9999  1.75E-03  1.30E-03  3.58E-03  4.63E-03  6.91E-03
8.22E-03  1.24E-02  3.42E-04  379
  L-EFFECTIVE               6.5-7.0 km   .9999  1.51E-03  1.16E-03  3.08E-03  3.88E-03  6.09E-03
7.12E-03  1.18E-02  1.14E-04 6331
  L-EFFECTIVE               7.0-7.5 km   .9999  1.32E-03  1.07E-03  2.62E-03  3.38E-03  5.46E-03
6.38E-03  1.03E-02  1.14E-04 6331
1 9/05/**   17:07:08    PAGE   2          PROB                          QUANTILES
PEAK      PEAK  PEAK
                                        NON-ZERO   MEAN       50TH       90TH       95TH       99TH
99.5TH      CONS       PROB  TRIAL
 PEAK DOSE FOUND ON SPATIAL GRID (Sv)
  L-EFFECTIVE               7.5-8.0 km   .9999  1.16E-03  9.65E-04  2.36E-03  3.05E-03  4.80E-03
5.81E-03  1.07E-02  1.14E-04 2853
  L-EFFECTIVE              8.0-10.0 km   .9999  8.74E-04  7.28E-04  1.75E-03  2.29E-03  3.74E-03
4.54E-03  7.27E-03  1.14E-04 7681

 DOSE FOUND AT (R,THETA) LOCATION (Sv)
```

```
  Compass Sector  1 (N)       .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  2 (NNE)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  3 (NE)      .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  4 (ENE)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  5 (E)       .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  6 (ESE)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  7 (SE)      .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  8 (SSE)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector  9 (S)       .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 10 (SSW)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 11 (SW)      .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 12 (WSW)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 13 (W)       .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 14 (WNW)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 15 (NW)      .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45
  Compass Sector 16 (NNW)     .2- .3 km   .1418  6.25E-02  0.00E+00  5.57E-02  2.07E-01  2.06E+00
3.01E+00  3.06E+00  1.22E-03   45

 Successful completion of MACCS2 was achieved!
 This job required a total of     23.113 CPU seconds

    Input processing required       .160 CPU seconds
          Simulation required     21.152 CPU seconds
   Output processing required      1.801 CPU seconds
```

Non-buoyant Plume With Building Wake

The following changes were made to the ATMOS file for the base case to model the release of non-buoyant plume with building wake effects.

```
* BUILDING HEIGHT (METERS) - FOR LIFTOFF CRITERION W/ BUOYANT PLUME (42.5 ft)
WEBUILDH001    13.
*
* INITIAL VALUE OF SIGMA-Y [METERS] DUE TO WAKE EFFECTS (=Wb/4.3, Wb=296 ft)
SIGYINIT001     21.
*
* INITIAL VALUE OF SIGMA-Z [METERS] DUE TO WAKE EFFECTS (=Hb/2.15, Hb=42.5 ft)
SIGZINIT001     6.0
```

Buoyant Plume

The following changes were made to the ATMOS file for the base case to model the release of the buoyant plume released in an open area.

```
* HEAT CONTENT OF THE RELEASE SEGMENTS (WATTS)
* A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
RDPLHEAT001    5.0E+06 (for buoyant plume examples)
```

Buoyant Plume With Building Wake

The following changes were made to the ATMOS file for the base case to model the release of buoyant plume with building wake effects.

```
* BUILDING HEIGHT (METERS) - FOR LIFTOFF CRITERION W/ BUOYANT PLUME (42.5 ft)
WEBUILDH001    13.
*
* INITIAL VALUE OF SIGMA-Y [METERS] DUE TO WAKE EFFECTS (=Wb/4.3, Wb=296 ft)
SIGYINIT001     21.
*
* INITIAL VALUE OF SIGMA-Z [METERS] DUE TO WAKE EFFECTS (=Hb/2.15, Hb=42.5 ft)
SIGZINIT001     6.0
*
* HEAT CONTENT OF THE RELEASE SEGMENTS (WATTS)
* A VALUE SPECIFIED FOR EACH OF THE RELEASE SEGMENTS
RDPLHEAT001    5.0E+06 (for buoyant plume examples)
```

8.0 ACRONYMS & DEFINITIONS

ACRONYMS:

ALARA	As Low As Reasonably Achievable
ALI	Annual Limit on Intake
ALOHA	Areal Locations of Hazardous Atmospheres (designated toolbox software)
ANSI	American National Standards Institute
ARF	Airborne Release Fraction
ARR	Airborne Release Rate
BR	Breathing Rate
CDE	Committed Dose Equivalent (see definition below)
CEDE	Committed Effective Dose Equivalent (see definition below)
CFAST	Consolidated Fire and Smoke Transport Model (designated toolbox software)
CFR	Code of Federal Regulations
DAC	Derived Air Concentration
DBA	Design Basis Accident
DCF	Dose Conversion Factor
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DR	Damage Ratio
DSA	Documented Safety Analysis
EFCOG	Energy Facility Contractors Group
EH	DOE Office of Environment, Safety and Health
EIS	Environmental Impact Statement
EM	DOE Office of Environmental Management
EPIcode	Emergency Prediction Information code (designated toolbox software)
FRAMES	Framework for Risk Analysis in Multimedia Environmental Systems
GENII	Generalized Environmental Radiation Dosimetry Software System - Hanford Dosimetry System (Generation II) (designated toolbox software)
GEP	Good Engineering Practice
HT	Tritiated Hydrogen Gas
HTO	Tritium Oxide
ICRP	International Commission for Radiological Protection
IDCF	Inhalation Dose Conversion Factor
IEEE	Institute of Electrical and Electronics Engineers
IP	Implementation Plan
ISO	International Organization for Standardization
JFD	Joint Frequency Distribution
LANL	Los Alamos National Laboratory
LET	Linear Energy Transfer
LHS	Latin Hyper-cubed Square
LPF	Leak Path Factor
MACCS2	MELCOR Accident Consequence Code System 2 (designated toolbox software)
MAR	Material at Risk
MELCOR	Methods for Estimation of Leakages and Consequences of Releases (designated toolbox software)

MOI	Maximally Exposed Offsite Individual (see definition below)
NESHAPS	National Emissions Standards for Hazardous Air Pollutants
NNSA	National Nuclear Security Administration
NRC	Nuclear Regulatory Commission
OEP	Onsite Evaluation Point/Person (see definition below)
PNNL	Pacific Northwest National Laboratory
PSA	Probabilistic Safety Analysis (or Assessment)
RF	Respirable Fraction
RSICC	Radiation Safety Information Computational Center
SASG	Safety Analysis Software Group (see definition below)
SC	Safety Class
SC SSC	Safety Class Structures Systems or Components (see definition below)
SNL	Sandia National Laboratories
SQA	Software Quality Assurance
SS	Safety Significant
SSC	Systems Structures or Components
SSCs	Safety Structures Systems and Components (see definition below)
SS SSC	Safety Significant Structures Systems or Components (see definition below)
ST	Source Term
TEDE	Total Effective Dose Equivalent (see definition below)
TSR	Technical Safety Requirement
V&V	Verification and Validation
WSMS	Washington Safety Management Solutions
WSRC	Westinghouse Savannah River Company

Selected Terms and Definitions Used in Accident and Consequence Analysis & Software Quality Assurance

Absorbed Dose (D)- The energy absorbed by matter from ionizing radiation per unit mass of irradiated material at the place of interest in that material. The absorbed dose is expressed in units of rad (or gray) (1 rad = 0.01 gray).

Committed Dose Equivalent ($H_{T,50}$) - The dose equivalent calculated to be received by a tissue or organ over a 50-year period after the intake of a radionuclide into the body. It does not include contributions from radiation sources external to the body. Committed dose equivalent is expressed in units of rem (or sievert) (1 rem = 0.01 sievert).

Committed Effective Dose Equivalent (CEDE) - The sum of the committed dose equivalents ($H_{T,50}$) over a fifty-year period to various organs or tissues in the body, each multiplied by the appropriate weighting factor (w_T) -- that is $H_{E,50} = \Sigma\, w_T\, H_{T,50}$. CEDE is applicable to exposure from internally deposited radionuclides.

Documented Safety Analysis (DSA) – A documented analysis of the extent to which a nuclear facility can be operated safely with respect to workers, the public, and the environment, including a description of the conditions, safe boundaries, and hazard controls that provide the basis for ensuring safety. [10 CFR 830]

Gap Analysis — Evaluation of the Software Quality Assurance attributes of specific computer software against identified criteria.

Nuclear Facility — A reactor or a nonreactor nuclear facility where an activity is conducted for or on behalf of DOE and includes any related area, structure, facility, or activity to the extent necessary to ensure proper implementation of the requirements established by 10 CFR 830. [10 CFR 830]

Gray (Gy) - Systeme' International (SI) unit of absorbed dose. One gray is equal to an absorbed dose of 1 joule per kilogram. One Gy equals 100 rad.

Maximally Exposed Offsite Individual (MOI) - A theoretical offsite receptor defined to allow dose comparison with numerical offsite evaluation guides. The MOI is located at the maximum air concentration point (ground-level) at, or beyond the, DOE site boundary. The latter may occur with elevated or buoyant releases that do not land within the site boundary, but instead reach ground-level beyond the boundary (touchdown point).

Onsite Evaluation Point/Person (OEP) - A theoretical onsite receptor defined to allow dose comparison with numerical onsite evaluation guides. This point may be at a fixed distance (e.g. 100 m, 600 m, or 640 m), or located at the closest point on the facility or facility area exclusion zone. For elevated or buoyant releases that do not land within the exclusion zone, the OEP is the point beyond the exclusion zone where the maximum air concentration is located (touchdown point).

Rad - The unit of absorbed dose.

Rem - The unit of dose equivalent or effective dose equivalent. The rem is numerically equal to the absorbed dose in rad multiplied by a quality factor, distribution factor, and any other necessary modifying factor (1 rem = 0.01 sievert).

Safety Analysis and Design Software — Computer software that is not part of a structure, system, or component (SSC) but is used in the safety classification, design, and analysis of nuclear facilities to ensure

- proper accident analysis of nuclear facilities;
- proper analysis and design of safety SSCs; and
- proper identification, maintenance, and operation of safety SSCs.

Safety Analysis Software Group (SASG) — A group of technical experts formed by the Deputy Secretary in October 2000 in response to Technical Report 25 issued by the Defense Nuclear Facilities Safety Board (DNFSB). This group was responsible for determining the safety analysis and instrument and control (I&C) software needs to be fixed or replaced, establishing plans and cost estimates for remedial work, providing recommendations for permanent storage of the software and coordinating with the Nuclear Regulatory Commission on code assessment as appropriate.

Safety-Class Structures, Systems, and Components (SC SSCs) — SSCs, including portions of process systems, whose preventive and mitigative function is necessary to limit radioactive hazardous material exposure to the public, as determined from the safety analyses. [10 CFR 830]

Safety-Significant Structures, Systems, and Components (SS SSCs) — SSCs which are not designated as safety-class SSCs, but whose preventive or mitigative function is a major contributor to defense in depth and/or worker safety as determined from safety analyses. [10 CFR 830] As a general rule of thumb, SS SSC designations based on worker safety are limited to those systems, structures, or components whose failure is estimated to result in prompt worker fatalities, serious injuries, or significant radiological or chemical exposure to workers. The term serious injuries, as used in this definition, refers to medical treatment for immediately life-threatening or permanently disabling injuries (e.g., loss of eye, loss of limb). The general rule of thumb cited above is neither an evaluation guideline nor a quantitative criterion. It represents a lower threshold of concern for which an SS SSC designation may be warranted. Estimates of worker consequences for the purpose of SS SSC designation are not intended to require detailed analytical modeling. Consideration should be based on engineering judgment of possible effects and the potential added value of SS SSC designation. [DOE G 420.1-1]

Safety Software — Includes both safety system software and safety analysis and design software.

Safety Structures, Systems, and Components (SSCs) — The set of safety-class SSCs and safety-significant SSCs for a given facility. [10 CFR 830]

Safety System Software — Computer software and firmware that performs a safety system function as part of a structure, system, or component (SSC) that has been functionally classified as Safety Class (SC) or Safety Significant (SS). This also includes computer software such as human-machine interface software, network interface software, programmable logic controller (PLC) programming language software, and safety management databases that are not part of an SSC but whose operation or malfunction can directly affect SS and SC SSC function.

Sievert (Sv) - The Systeme' Internationale (SI) unit of any of the quantities expressed as dose equivalent. The dose equivalent in sievert is equal to the absorbed dose in gray multiplied by the quality factor (1 Sv = 100 rem).

Software — Computer programs, operating systems, procedures, and possibly associated documentation and data pertaining to the operation of a computer system. [IEEE Standard 610.12-1990, *IEEE Standard Glossary of Software Engineering Terminology*]

Toolbox Codes — A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and meeting minimum qualification standards. These codes shall be sufficiently verified and validated, and as such, applicable to support 10 CFR 830 DSAs. That is to say, the analysts using these codes do not need to present additional defense as to their qualification, provided that they are sufficiently qualified to use the codes and the input parameters are valid.

Total Effective Dose Equivalent (TEDE) - the sum of the deep dose equivalent (from external exposure) and the committed effective dose equivalent (from internal exposure). Note that the TEDE is equivalent to the EDE. For purposes of compliance, deep dose equivalent to the whole body may be used as effective dose equivalent for external exposures.

Whole Body - For the purposes of external exposure, head, trunk (including male gonads), arm above and including the elbow, or legs above and including the knee.

95th Percentile Consequence - A statistical level of consequence that is exceeded no more than five percent of the time based on site-characteristic meteorology. The offsite radiological exposure basis documented in Appendix A to DOE-STD-3009-94 and based on the method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to define the meteorological conditions assumed to be present for consequence analysis. Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based doses calculated for a postulated release to a downwind receptor location that would result in a dose that is exceeded 5% of the time (based on hourly averages). The specific meteorology or dilution factor leading to this dose

consequence is a function of release elevation, distance to the receptor, and (to some degree) the release duration. This consequence level is direction-independent, i.e. averaged over all 360° at the distance of interest. [See Position 3 in NRC Reg. Guide 1.145 and 5 Percent Overall Site χ/Q Value].

99.5 Percentile, Worst-Sector Consequence - A method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to define the meteorological conditions assumed to be present for consequence analysis. Given site-specific data, the sector 99.5th percentile meteorology is the set of meteorological conditions assumed during a postulated release to a downwind receptor location that would result in a dose that is exceeded 0.5% of the time (based on a yearly average) in one of sixteen 22.5° sectors. The highest of the sixteen 22.5° sectors is then defined as the 99.5 Percentile, Worst-Sector Meteorology/Consequence condition. This consequence level is then directionally based, and tends to exceed the 95th percentile consequence beyond approximately one mile for *most* sites.

The MOI dose consideration takes distance to the site boundary in each direction into account.

9.0 REFERENCES

Abrahamson, 1993, S. Abrahamson, M.A. Bender, B.B. Boecker, E.S. Gilbert, B.R. Scott, *Health Effects Models for Nuclear Power Plant Accident Consequence Analysis, Modification of Models Resulting From Addition of Effects of Exposure to Alpha-Emitting Radionuclides*, NUREG/CR-4214, Rev. 1, Part II (Scientific Bases for Health Effects Models), Addendum 2, LMF-136, Inhalation Toxicology Research Institute, Lovelace Biomedical and Environmental Research Institute, Albuquerque, NM, prepared for the U.S. Nuclear Regulatory Commission, Washington, DC, May 1993.

AIChE, 1996, Guidelines for Use of Vapor Cloud Dispersion Models, 2nd Edition. Publication 1439, American Institute of Chemical Engineers (AIChE) Center for Chemical Process Safety, New York, NY, 1996.

AMS, 1977, American Meteorological Society, *Workshop on Stability Classification Schemes and Sigma Curves – Summary and Recommendations*, Bulletin of the American Meteorological Society, 58, (1977).

AMS, 1978, American Meteorological Society, *Accuracy of Dispersion Models – A Position Paper of the AMS 1977 Committee on Atmospheric Turbulence and Diffusion*, Bulletin of the American Meteorological Society, 9 (8), (August 1978).

ANSI/ANS 1987, *American National Standard Institute/American Nuclear Society: Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry*, La Grange Park, IL, ANSI/ANS-10.4-1987.

Anspaugh, 1975, L.R. Anspaugh, J.H. Shinn, P.L. Phelps, and N.C. Kennedy, *Resuspension and Redistribution of Plutonium in Soils*, Health Physics, 29, 571-582, 1975.

Briggs, 1973, G. A. Briggs, *Lift Off of Buoyant Gas Initially on the Ground*," ADTL Contribution File No. 87, November 1973. Air Resources Atmospheric Turbulence and Diffusion Laboratory NOAA, Oak Ridge, TN.

Briggs, 1975, G. A. Briggs, Chapter 3, *Plume Rise Predictions*, in Lectures on Air Pollution and Environmental Impact Analysis, D. A. Haugen, ed., American Meteorological Society.

CFR, 1990, 10 CFR 100, *Reactor Site Criteria*, Title 10 Code of Federal Regulations Part 100, Office of the Federal Register, Washington, DC, January 1, 1990.

CFR, 1991, 10 CFR 20, *Standards for Protection Against Radiation*, Title 10 Code of Federal Regulations Part 20, Office of the Federal Register, Washington, DC, May 21, 1991.

CFR, 2001, 10 CFR 830, *Nuclear Safety Management Rule*, Title 10 Code of Federal Regulations Part 830, Office of the Federal Register, Washington, DC, January 10, 2001.

Chamberlain, 1953, A.C. Chamberlain, *Aspects of Travel and Deposition of Aerosol and Vapour Clouds*, Atomic Energy Research Establishment Report AERE-HP/R 1261, Harwell, United Kingdom, 1953.

Chanin, 1990, D.I. Chanin, J.L. Sprung, L.T. Ritchie, H-N Jow, and J.A. Rollstin, *MELCOR Accident Consequence Code System (MACCS). Volume 1: User's Guide*; H-N Jow, J.L.

Sprung, J.A. Rollstin, L.T. Ritchie, and D.I. Chanin, *Volume 2: Model Description*; J.A. Rollstin, D.I. Chanin, and H-N Jow, *Volume 3: Programmer's Reference Manual*; NUREG/CR-4691, Sandia National Laboratories, published by the U.S. Nuclear Regulatory Commission, Washington, DC, 1990.

Chanin, 1992a, D. Chanin, J. Rollstin, J. Foster, and L. Miller, *MACCS Version 1.5.11.1: A Maintenance Release of the Code*, Sandia National Laboratories, Albuquerque, NM, July 14, 1992.

Chanin, 1992b, D.I. Chanin, *A New Emergency Response Model for MACCS*, LA-SUB-94-67, prepared by Teledyne Engineering Consultants, Inc., Albuquerque, NM for Los Alamos National Laboratory, Los Alamos, NM, November 11, 1992.

Chanin, 1997, D. Chanin and M. Young, *Code Manual for MACCS2: Volume 1, User's Guide; Volume 1*, SAND97-0594, March 1997, Sandia National Laboratories, Albuquerque, NM.

Chanin, 1998, D. Chanin and M. Young, *Code Manual for MACCS2: Volume 1, User's Guide; Volume 2, Pre-Processor Codes COMIDA2, FGRDCF, IDCF2*; May 1998, M. Young, D. Chanin, and V. Banjac, *DOSFAC2 User's Guide*, NUREG/CR-6613, May 1998, Sandia National Laboratories, Albuquerque, NM.

DNFSB, 2000, Defense Nuclear Facilities Safety Board, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, Technical Report DNFSB/TECH-25, (January 2000).

DNFSB, 2002, Defense Nuclear Facilities Safety Board, *Recommendation 2002-1, Quality Assurance for Safety-Related Software* , (September 2002).

Dobbe 1990, C.A. Dobbe, E.R. Carlson, N.H. Marshall, E.S. Marwil, J.E. Tolli. *Quality Assurance and Verification of the MACCS Code, Version 1.5,* Idaho National Engineering Laboratory, Idaho Falls, ID, NUREG/CR-5376 (EGG-2566).

Dobbins, 1979, R.A. Dobbins, Atmospheric Motion and Air Pollution, John Wiley & Sons, New York.

DOE, 1992, B.S. Parks, *User's Guide for CAP88-PC*, Version 1.0, 402-B-92-001, U.S. Department of Energy, Las Vegas, NV, March 1992.

DOE, 1994, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports*, DOE-STD-3009-94, U.S. Department of Energy, Washington, DC, Change Notice 2 (April 2002).

DOE, 1994a, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities*, DOE-HDBK-3010-94, U.S. Department of Energy, Washington, DC, Change Notice 1 (January, 1999).

DOE, 1998, Implementation Guide for Use with DOE Order 440.1 Occupational Exposure Assessment, U.S. Department of Energy, Washington, D.C. DOE G 440.1-3.

DOE, 2000a, U.S. Department of Energy, *Appendix A, Evaluation Guideline,* DOE-STD-3009-94, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Reports* (January 2000).

DOE, 2000b, U.S. Department of Energy, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, DOE Response to TECH-25, Letter and Report, (October 2000).

DOE, 2002a, U.S. Department of Energy, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Reports*, DOE-STD-3009-94, Change Notice 2 (April 2002).

DOE, 2002b, Department of Energy, National Nuclear Security Agency, Selection of Computer Codes for DOE Safety Analysis Applications, DOE/NNSA-Germantown, MD, NNSA Report (2002).

DOE, 2003, U.S. Department of Energy, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1: Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, Report, (March 2003).

DOE/EH, 2003, U.S. Department of Energy (2003), *Designation of Initial Safety Analysis Toolbox Codes*, Letter, (March 28, 2003).

DOE, 2004a, *Software Quality Assurance Improvement Plan: GENII Gap Analysis*, U.S. Department of Energy, Washington DC (May 2004).

DOE, 2004b, *MACCS2 Computer Code Application Guidance for Documented Safety Analysis*, U.S. Department of Energy, Washington, DC (May 2004).

East, 1997, J.M. East, *Verification of MACCS2 Peak Dose Output (U)*, WSRC-TR-97-204, Westinghouse Savannah River Company, Aiken, SC (July 1998).

East, 1998, J.M. East and K.R. O'Kula, *MACCS Input Data Guidance for SRS Applications (U)*, WSRC-RP-98-00978, Westinghouse Savannah River Company, Aiken, SC (October 1998).

Eckerman 1988, K.F. Eckerman, A.B. Wolbarst, A.C.B. Richardson. *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion.* Federal Guidance Report No. 11, U.S. Environmental Protection Agency, Washington, DC, DE89-011065.

Eckerman 1993, K.F. Eckerman and J.C. Ryman. *External Exposure to Radionuclides in Air, Water, and Soil. Federal Guidance Report 12*, U.S. Environmental Protection Agency, Washington, DC, PB94-114451.

Eimutis, 1972, E.C. Eimutis and M.G. Konicek, *Derivations of Continuous Functions for the Lateral and Vertical Atmospheric Dispersion Coefficients*, Atm. Env.,6, pp. 859-863.

EPA, 1987, *On-Site Meteorological Program Guidance for Regulatory Modeling Applications*, EPA-450/4-87-013, Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC, June 1987.

EPA, 1988, K.F. Eckerman, A.B. Wolbarst, and A.C.B. Richardson, *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion*, Federal Guidance Report No. 11, U.S. Environmental Protection Agency, Washington, DC, 1988.

EPA, 1993, K.F. Eckerman and J.C. Ryman, *External Exposure to Radionuclides in Air, Water, and Soil*, Federal Guidance Report No. 12, U.S. Environmental Protection Agency, Washington, DC, 1993.

EPA, 1995a, *ALOHA, Areal Locations of Hazardous Atmospheres, User's Manual*, U.S. Environmental Protection Agency and National Oceanic and Atmospheric Administration, Washington, DC, June 1995.

EPA, 1995b, *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volume II – Description of Model Algorithms*, EPA-454/B-95-003b, U.S. Environmental Protection Agency, Research Triangle Park, NC, September 1995.

Fallon, 1982, R.D. Fallon, *Molecular Tritium Uptake in Southeastern U.S. Soils*, Soil Biol. Biochem., Vol. 14, pp. 553 to 556.

FEMA, 1990, *Handbook of Chemical Hazard Analysis Procedures*, Federal Emergency Management Agency, U.S. Department of Transportation, and U.S. Environmental Protection Agency, Washington, DC, 1990.

Gifford, 1975, F.A. Gifford, *Atmospheric Dispersion Models for Environmental Pollution Applications*, in Lectures on Air Pollution and Environmental Impact Analysis (D.A. Haugen, Ed.), American Meteorological Society, Boston, MA, page 45.

Gregory, 1998, J.J. Gregory, *MACCS2 Software Package, Software Defect Notification*, Sandia National Laboratories, Albuquerque, NM, Log Number: M2V1-12A, Dated: May 26, 1998.

Hanna, 1982, S.R. Hanna, G.A. Briggs, and R.P. Hosker, Handbook on Atmospheric Diffusion. DOE/TIC-11223, U.S. Department of Energy, Washington, DC, 1982.

Hanna, 2002, S.R. Hanna and R.E. Britter, Wind Flow and Vapor Cloud Dispersion at Industrial and Urban Sites, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

Haugen, 1959, D.A. Haugen, editor, *Project Prairie Grass: A Field Program in Diffusion*, Geophysical Research Papers, #59, Vol. III, Report AFCRC-TR-58-235, Air Force Cambridge Research Center, *Hanscom Field, MA, 1959.*

Healy, 1984, J.W. Healy, *Radioactive Cloud Dose Calculation*, in Atmospheric Sciences and Power Production, DOE/TIC-27601, D. Randerson, Editor, U.S. Department of Energy, Washington, DC, 1984.

Hills, 1998, C.R. Hills, D. I. Chanin, and C.L. Dickerman, *Validation Study of Available Models For Consideration of Explosive Releases at Pantex Plant*, RPT-30, Pantex Plant, Amarillo, TX (February 1998).

Hodgin, 1985, C.R. Hodgin, *The Terrain-Responsive Atmospheric Code (TRAC) for Plume Growth and Dispersion in Complex Terrain*, RFP-3683, Rockwell International, Golden, CO, April 3, 1985.

Holzworth, 1972, G.C. Holzworth, *Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution Throughout the Contiguous United States*, EPA Report AP-101, Environmental Protection Agency, Research Triangle Park, NC, p. 109, January 1972.

Homann 1994, S.G. Homann, *HOTSPOT Health Physics Codes for the PC. Hazards Control Department and the Emergency Preparedness and Response Program, Nonproliferation, Arms Control, and International Security Directorate*, UCRL-MA-106315 Lawrence Livermore National Laboratory, University of California, Livermore, California.

Hunter, 1993, C.H. Hunter, *Revised Onsite Meteorological Data for Emergency Planning Hazards Assessments*, Savannah River Technology Center, Westinghouse Savannah River Company, SRT-ETS-931167.

ICRP-26, 1977, *Recommendations of the ICRP*, Annals of the ICRP 1 (#3), ICRP Publication 26, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1977.

ICRP-30, 1979-82, *Limits for Intakes of Radionuclides by Workers*, Annals of the ICRP 2 (#3-4), 4 (#3-4), 6 (#2-3), 7, 8 (#1-4), and 19 (#4), ICRP Publication 30, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1979 - 1982.

ICRP-60, 1991, *1990 Recommendations of the International Commission of Radiological Protection*, Annals of the ICRP 21 (#1-3), ICRP Publication 60, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1991.

ICRP-66, 1994, *Human Respiratory Tract Model for Radiological Protection*, Annals of the ICRP 24 (#1-3), ICRP Publication 66, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1994.

ICRP-68/72, 2000, *The ICRP Database of Dose Coefficients: Workers and Members of the Public*, Version 1.0, CD-ROM of ICRP Publication 68 and 72, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 2000.

IEEE, 1984, *ANSI IEEE Standard for Software Quality Assurance Plans*, New York, 1984.

LANL, 1995, J.F. McInroy, *A True Measure of Exposure*, Los Alamos Science 23, p 235, Los Alamos National Laboratory, Los Alamos, NM, 1995.

Lombardi, 1998, D.A. Lombardi and W.R. Brock, *Use of HGSYSTEM/UF6 and MACCS for the Building 9204-2E Safety Analysis Report Consequence Analysis: General Overview and Comparison of Models*, ORNL/TM-13598, Oak Ridge National Laboratory (January 1998).

Mills, 1987. M. T. Mills, *Modeling the Release and Dispersion of Toxic Combustion Products from Chemical Fires*, Presented at International Conference on Vapor Cloud Modeling, November 2–4, 1987, Cambridge, MA.

Murphy, 1993. C.E. Murphy, Jr., *Tritium Transport and Cycling in the Environment*, Health Physics, 65, p. 683-697, (1993).

Napier, 1998, B.A. Napier, R.A. Peloquin, D.L Strenge, and J.V. Ramsdell, *GENII–The Hanford Environmental Radiation Dosimetry System*, Vol. 1, PNL-6584, Pacific Northwest National Laboratory, Richland, WA, 1998.

NEPA, 1993, *Recommendations for the Preparation of Environmental Assessments and Environmental Impact Statements*, NEPA report (no number), prepared for the Department of Energy, Office of NEPA Oversight, May 1993.

NCRP, 1996, National Council on Radiation Protection and Measurements, *Screening Models for Releases of Radionuclides to Atmosphere, Surface Water, and Ground*, NCRP No. 123.

NRC, 1972, *Onsite Meteorological Programs*, U.S. Nuclear Regulatory Commission Regulatory Guide 1.23 (February 1972).

NRC, 1977, *Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water-Cooled Reactors*, Regulatory Guide 1.111, U.S. Nuclear Regulatory Commission, Washington, DC, 1977.

NRC, 1979, *Assumptions Used for Evaluating the Potential Radiological Consequences of Accidental Nuclear Criticality in a Plutonium Processing and Fuel Fabrication Plant*, Regulatory Guide 3.35, U.S. Nuclear Regulatory Commission, Washington, DC, July 1979.

NRC, 1983, *Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants*, Regulatory Guide 1.145, U.S. Nuclear Regulatory Commission, Washington, DC, February 1983.

NRC, 1990a, *Severe Accident Risks: An Assessment for Five U. S. Nuclear Power Plants*, Sandia National Laboratory, Albuquerque, NM, NUREG-1150, Vol. 1.

NRC, 1990b, U.S. Nuclear Regulatory Commission, *Evaluation of Severe Accident Risks: Quantification of Major Input Parameters*, NUREG/CR-4551, Prepared by SNL for the USNRC (1990).

NRC, 1998, U.S. Nuclear Regulatory Commission, *Nuclear Fuel Cycle Facility Accident Analysis Handbook*, NUREG/CR-6410, Prepared by SAIC for the USNRC (1998).

NRC, 2003, *Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants*, U.S. Nuclear Regulatory Commission, Regulatory Guide 1.194, (June 2003).

O'Kula, 1998, K.R. O'Kula, J.M. East, A.H. Weber, A.V. Savion, and C.A. Mazzola, *Evaluation of Current Computer Models in the DOE Complex for SAR Analysis of Radiological Dispersion & Consequents*, WSRC-TR-96-0126, Savannah River Site, Aiken, SC.

O'Kula 2000, K.R. O'Kula and J.M. East, *Evaluating Compliance with DOE-STD-3009-94, Appendix A Requirements (U)*, 2000 American Nuclear Society/European Nuclear Society International Meeting, Washington, D.C. (November 2000).

O'Kula, 2001, K.R. O'Kula, *Crediting Tritium Deposition Velocity in Accident Analysis*, Eleventh EFCOG Safety Analysis Workshop, Milwaukee, WI (June 2001)

Peterson, 1993, V.L. Peterson, *Reference Computations of Public Dose and Cancer Risk from Airborne Releases of Plutonium*, RFP-4910 (formerly NSTR-015-93), Safety Analysis Engineering/Nuclear Safety, EG&G Rocky Flats, Inc., December 23, 1993.

Peterson, 1995, V.L. Peterson, *Reference Computations of Public Dose and Cancer Risk from Airborne Releases of Uranium and Class W Plutonium*, RFP-4965 (formerly NSTR-026-94), Nuclear Safety/Safety Analysis, EG&G Rocky Flats Inc., Golden, Colorado, June 6, 1995.

Randerson, 1984, D. Randerson, Ed., Atmospheric Science and Power Production, Department of Energy, DOE/TIC-27601 (1984).

RFRAG, 1994, *Rocky Flats Risk Assessment Guide*, prepared by Safety Analysis and Risk Assessment, Nuclear Safety Engineering, EG&G Rocky Flats, Inc., Golden, CO, Revision 3, September 30, 1994.

SAE, 1996, V.L. Peterson, *Calculations in Support of the SSAR Meteorological Statistics*, 96-SAE-029, Safety Analysis/Nuclear Engineering, Rocky Flats Environmental Technology Site, October 16, 1996.

Scott, 2003, B.R. Scott and V. L. Peterson, *Risk Estimates for Deterministic Health Effects of Inhaled Weapons Grade Plutonium*, Health Physics **85**, #3, 280-293, September 2003.

Sehmel, 1978, G.A. Sehmel and W.H. Hodgson, *A Model for Predicting Dry Deposition of Particles and Gases to Environmental Surfaces*, Battelle Pacific Northwest Laboratories, Richland, WA, PNL-SA-6721.

Slade, 1968, D.H. Slade (editor), *Meteorology and Atomic Energy*, U.S. Atomic Energy Commission, Office of Information Services, Washington, D.C., 1968.

Smith, 1995, B.J. Smith and K.K. Taylor, *Safety Analysis in Support of the Environmental Assessment for Consolidation and Interim Storage of Special Nuclear Material in Building 371*, NSTR-001-95, Safety Analysis/Nuclear Safety, EG&G Rocky Flats, Inc., Golden, CO, March 24, 1995.

SNL, 1987, *Sandia Software Guidelines: Volume 1: Software Quality Planning.* Sandia National Laboratories, Albuquerque, NM, SAND85-2344.

SNL, 1995, *Sandia Software Guidelines: Volume 2: Documentation.* Sandia National Laboratories, Albuquerque, NM, SAND85-2345.

SNL, 1986, *Sandia Software Guidelines: Volume 3: Standards, Pratices, and Conventions.* Sandia National Laboratories, Albuquerque, NM, SAND85-2346.

SNL, 1992, *Sandia Software Guidelines: Volume 4: Configuration Management.* Sandia National Laboratories, Albuquerque, NM, SAND85-2347.

SNL, 1989, *Sandia Software Guidelines: Volume 5: Tools, Techniques, and Methodologies.* Sandia National Laboratories, Albuquerque, NM, SAND85-2348.

Steele, 1998, C.M. Steel, T.L. Wald, and D.I. Chanin, *Plutonium Explosive Dispersal Modeling Using the MACCS2 Computer Code*, Los Alamos National Laboratory, LA-UR-98-1901 (June 1998).

Summa, 1996, K.J. Summa and F.E. Haskin. *Pre-Release Verification Testing of the MACCS2 Code.* University of New Mexico, Albuquerque, NM.

Sweet, 1984, C.W. Sweet, *The Relationship Between Tritiated Water Activities in Air, Vegetation and Soil Under Steady-state Conditions*, Health Physics, Vol. 47, No. 4, pp. 635-639.

Tadmor, 1969, J. Tadmor and Y. Gur, *Analytical Expressions for the Vertical and Lateral Dispersion Coefficients in Atmospheric Diffusion*, Atmospheric Environment **3**, Pergamon Press, Great Britain, pp 688, 1969.

Turner, 1970, D.B. Turner. Workbook of Atmospheric Dispersion Estimates. Education, and Welfare report PB-191482, U.S. Department of Health, Washington, DC (1970).

Turner, 1986, J.E. Turner, Atoms, Radiation, and Radiation Protection, Pergamon Press, New York, 1986.

Turner, 1994, D.B. Turner, Workbook of Atmospheric Dispersion Estimates, *An Introduction to Dispersion Modeling*, Lewis Publishers, Ann Arbor, MI, 1994.

WSRC, 1998, Westinghouse Savannah River Company, *MACCS Input Guidance for SRS Applications (U)*, WSRC-RP-98-00978, (October 1998).

A .H. Weber, 1996, and C.H. Hunter, *Estimating Dispersion from a Tornado Vortex and Mesocyclone (U)*, Savannah River Site, Aiken, SC, WSRC-TR-94-0386, Rev 2.

Yuan, 1993, Y.C. Yuan, S.Y. Chen, D. J. LePoire, and R. Rothman, *RISKIND – A Computer Program for Calculating Radiological Consequences and Health Risks from Transportation of Spent Nuclear Fuel*, ANL/EAIS-6, Rev. 0, Argonne National Laboratory, (February 1993).

Appendices

Appendix	Subject
A	Overview of Atmospheric Dispersion and Consequence Analysis
B	MACCS2 Software Defect Notices
C	Limited Parametric Study On MACCS/MACCS2 Treatment Of Plume Buoyancy And Wake Flow
D	Inputs and Recommendations for MACCS 1.5.11.1 Applications

APPENDIX A. OVERVIEW OF ATMOSPHERIC DISPERSION AND CONSEQUENCE ANALYSIS

Once the source term to the environment from a postulated accident condition has been calculated or estimated, the safety analyst must determine the concentration downwind to identified receptor locations. A robust safety analysis will apply a sound technical basis for predicting the transport and diffusion of the airborne plume. Often this is based on a dispersion model that applies environmental data specific to the facility and site under consideration.[19]

This section provides an overview of atmospheric dispersion methods, focusing on Gaussian methodology, and discusses radiological consequence analysis "back end". Recommendations are provided where appropriate for specific data or assumptions.

Dispersion Methodology & Summary Of DOE-STD-3009-94, Appendix A

Appendix A to DOE-STD-3009-94, Change Notice 2 (CN2), specifies an Evaluation Guideline for radiological exposure to the offsite receptor, and is to be applied in specifying SSCs (DOE, 2000). The numerical value of 25 rem is the Total Effective Dose Equivalent (TEDE). Dose estimates to be compared to the Evaluation Guideline (EG) are those received by a hypothetical maximally-exposed offsite individual (MOI) at the site boundary for an exposure period of two hours. The nominal exposure period of two hours may be extended to eight hours for release scenarios that occur over a prolonged period.

Appendix A to DOE-STD-3009-94 notes that the airborne pathway is of primary interest for nonreactor nuclear facilities. NUREG-1140 ("A Regulatory Analysis on Emergency Preparedness for Fuel Cycle and Other Radioactive Material Licenses") previously noted that, "for all materials of greatest interest for fuel cycle and other radioactive material licenses, the dose from the inhalation pathway will dominate the (overall) dose." For some types of facilities such as waste storage, the surface and groundwater pathways may be more important, but accident releases usually would be expected to develop more slowly than airborne releases.

The dose calculation references Regulatory Guide 1.145 of the Nuclear Regulatory Commission (NRC) for determination of the five percent overall site relative concentration (χ/Q, often referred to as the dilution factor) value at the exclusion area boundary (EAB). A straightline Gaussian model is to be applied with one-hour averaged χ/Q values for the entire course of plume duration for a period not to exceed eight hours. Text from Section A.3.3 of Appendix A on Dose Estimation (p. A-8 to A-9) states

> The relevant factors for dose estimation are receptor location, meteorological

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[19] The term dispersion is applied using the definition appearing as Footnote 2 in NRC Regulatory Guide 1.145 to encompass both transport (due to organized or mean airflow within the atmosphere) and diffusion (due to disorganized or random air motions) of the plume.

dispersion, and dose conversion values. . .

Dose Calculation Location. For the purposes of comparison to the EG, the comparison point is taken to be the location of a theoretical MOI standing at the site boundary. This location can also be beyond the DOE site boundary if a buoyant or elevate plume is not at ground level at the DOE site boundary. In such cases, the calculation location is taken at the point of maximum exposure, typically where the plume reaches ground level. It is DOE practice and expectation that onsite individuals, both workers and public are protected under the Emergency Response plans and capabilities of its sites. This protection, along with implementation of defense-in-depth and worker safety philosophy, Safety Significant (SS) (and indirectly, through SC) SSC designation, and DOE's safety management programs, address onsite safety. However, an annual assessment of any changes in the site boundary and potential effects on safety SSC classification should be performed in association with the required annual update of the DSA for a facility. Privatization and site turnover initiatives may affect these determinations.

Atmospheric Dispersion. The 95th percentile of the distribution of doses to the MOI, accounting for variations in distance to the site boundary as a function of direction, is the comparison point for assessment against the EG. The method used should be consistent with the statistical treatment of calculated χ/Q values described in regulatory position 3 of NRC Regulatory Guide 1.145 for the evaluation of consequences along the exclusion area boundary. The determination of distance to the site boundary should be made in accordance with the procedure outlined in position 1.2 of Regulatory Guide 1.145. NRC Regulatory Guide 1.23 describes acceptable means of generating the meteorological data upon which dispersion is based. Accident phenomenology may be modeled assuming straight-line Gaussian dispersion characteristics, applying meteorological data representing a 1-hour average for the duration of the accident. Accident duration is defined in terms of plume passage at the location of dose calculation, for a period not to exceed 8 hours. Prolonged effects, such as resuspension, need not be modeled. The accident progression should not be defined so that the MOI is not substantially exposed (i.e., using a release rate that is specifically intended to expose the MOI to only a small fraction of the total material released, or defining time and windspeed so that the plume has not reached the MOI). The exposure period begins from the time the plume reaches the MOI.

For ground releases, the calculated dose equates to the centerline dose at the site boundary. For elevated, thermally buoyant, or jet releases, plume touchdown may occur beyond the site boundary. As noted in the discussion of receptor location, these cases should locate the dose calculation at the point of maximum dose beyond the site boundary, which is typically at the point of plume touchdown.

Accidents with unique dispersion characteristics, such as explosions, may be modeled using phenomenon-specific codes more accurately representing the release conditions. Discussion should be provided justifying the appropriateness of the model to the specific

situation. For accident phenomena defined by weather extremes, actual meteorological conditions associated with the phenomena may be used for comparison to the EG.

The guidance provided herein uses the prescriptive requirements of Appendix A as a basis, and is applicable for performing DSAs compliant with Subpart B of 10 CFR 830.

Before discussing choice of a model, the key important environmental transport values are summarized.

Atmospheric Dispersion Parameters And Statistical Bases

Most radiological source terms may be treated as neutrally buoyant. By neutrally buoyant, it is assumed that the cloud[20] of released material has approximately the same density as air. This is normally a valid assumption for radioactive releases that are gaseous in nature that contain trace amounts of very fine particulates, aerosols, and gases. As the cloud is emitted and moves downwind, it is common practice based on convention and supporting experimental data, to assume a Gaussian distribution in both the crosswind (lateral) and vertical directions. For continuous releases, the mean wind speed dilutes the pollutant but the downwind dispersion is negligible. As the cloud moves downwind it grows progressively larger due to lateral and vertical diffusion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the downwind direction becomes more important. Accordingly, a puff is described by a three-dimensional Gaussian equation in contrast to the two-dimensional formulation for plumes.

Several meteorological parameters affect the shape and size of a neutrally buoyant cloud. These are discussed in the following sections.

Meteorological Parameters

Earlier it was noted that downwind dispersion of a radioactive plume may be thought of as a parallel process of transport and diffusion. In simplest terms, the transport term is mostly a function of wind and direction. The diffusion of the plume is due in large part to the atmospheric stability of the region of transport. The following sections discuss wind and direction and temperature profiles and their impact on conditions in the atmosphere.

Wind and Direction

Prevailing wind is a key determinant of the transport of the radioactive plume. In terms of importance to accident analysis calculations, wind is a vector quantity having both direction and

[20] In this report, "cloud" can mean either a continuous (plume) or short-term release (puff).

magnitude. The wind speed at the height of the release determines both the initial diffusion of the pollutant and the travel time to reach a given downwind receptor. The initial diffusion and the plume travel are both directly proportional to the wind speed. It is also a factor in determining the magnitude of atmospheric stability. Atmospheric turbulence (i.e., mechanical turbulence) is generated when adjacent parcels of air move at different speeds or move in different directions. Thus, a change in wind speed with height above the ground, or a variation in wind direction at a given height, causes mechanical turbulence – the effect may be described through the surface roughness length parameter. Mechanical turbulence is also generated when air interacts with some fixed object, such as the ground and obstacles such as vegetation and structures, or with a building, described by aerodynamic effects such as wake and cavity.

The horizontal wind direction at the height of the release determines the direction of transport. It is a vector and therefore does not affect the magnitude of the concentration of the pollutant within the plume. The horizontal wind direction, or more commonly, wind direction, is the first moment, or average, of a series of "instantaneous" wind direction measurements. By convention, the wind direction is 180 degrees out of phase with the downwind or transport direction.

Atmospheric turbulence is directly related to the variability of wind direction. The variability of wind direction is normally expressed in terms of the standard deviation, or second moment, of a series of "instantaneous" wind direction measurements over a selected observation period, normally fifteen minutes. The standard deviation, or second moment of the horizontal wind direction, σ_θ, is commonly used to characterize atmospheric turbulence by stability classes. Alternatively, the standard deviation of the vertical wind component, σ_φ, is sometimes used as a basis to describe the category of atmospheric turbulence.

Vertical Temperature Profiles

In addition to wind direction variation, another technique that is used to type atmospheric turbulence is to use vertical temperature gradient measurements ($\Delta T/\Delta Z$). When a parcel of air is displaced in the vertical plane, it will expand (if rising) or contract (if sinking) to adjust its pressure to that of its surroundings. The expansion or contraction is accompanied by an adiabatic temperature change. As a parcel rises, it cools. If the surrounding air is warmer, the parcel will be heavier than its surroundings and sink back toward its original position; and its motion ceases. On the other hand, if the surrounding air is cooler, the parcel will be lighter and continue to move upward. Similarly, if the air parcel sinks, it warms up as it contracts. If the surrounding air is cooler, the parcel will be lighter and rise back toward its original position; and its motion ceases. If the surrounding air is warmer, the parcel will be heavier and continue to sink.

Thus, turbulence is suppressed if the temperature profile of the air (the so-called lapse rate) is less than adiabatic (i.e., subadiabatic), and enhanced if greater than adiabatic (i.e., superadiabatic). The adiabatic lapse rate near ground is about –10.8 °C/km (-5.4 °F/1,000 feet). Superadiabatic lapse rates are associated with unstable atmospheric conditions and labeled A, B, or C stability classes, with Class A representing the most unstable set of conditions.

Subadiabatic lapse rates are associated with stable atmospheric conditions, inclusive of inversions (i.e., temperature increase with height) and labeled E, F, and G stability classes, with Class G representing the most stable conditions. Adiabatic lapse rates are associated with neutral atmospheric conditions and labeled as Class D. In practices, some sites limit the number of classes to six, with G stability class being combined with F stability. Alternatively, classes A and B can be combined (because they lead to lower doses) if stability class G is significant at the site.

The vertical temperature profile, in turn, affects atmospheric turbulence. The atmospheric layer near the ground is called the mixing, or the mixed layer. During daylight, the ground heats up, warming the air near the surface. The lapse rate near the surface thus becomes superadiabatic and buoyancy-driven vertical turbulence enhances in the existing mechanical turbulence due to ground roughness and wind shear. At night, the ground cools, causing the air near the surface to cool, and the lapse rate becomes subadiabatic and frequently inverted. Buoyancy-driven vertical turbulence thus suppresses the existing mechanical turbulence due to ground roughness and wind shear. At greater heights, a few hundred to a few thousand meters in altitude, the lapse rate may change. It is common for the turbulent lower atmosphere to be capped by lapse rate that is subadiabatic so that turbulent eddies rising from below are suppressed. This layer near ground is thus called the mixed layer, for this is where turbulence in the strongest due primarily to the frictional effects of the earth's surface and the convective heat transfer from the earth's surface.

Atmospheric Stability Classes

A comprehensive treatment of atmospheric dispersion is so complex that many approximations are needed to make it tractable. Since turbulence is random and chaotic, it cannot be parameterized and one must resort to empirical formulations. One early attempt to simplify the treatment of turbulence was to define atmospheric stability classes and associate a rate of lateral and vertical diffusion with each class as a function of downwind distance only. Although computations based on these stability classes provide only a rough approximation to reality, they have proved extremely useful and are still in use, although more accurate treatments are available. The more sophisticated modeling approaches typically require additional data that are often not available from a single Reg. Guide 1.23 (NRC, 1972) on-site weather tower. Wind direction variability and vertical temperature difference are the most common techniques that are employed. Wind direction variability provides the best approximation of mechanical turbulence, while vertical temperature difference approximates the buoyancy component.

The following sections provide key definitions associated with stability class and methods to discern the turbulence intensities that drive atmospheric dispersion.

Stability Class

The rate at which turbulence diffuses material depends upon the stability of the atmosphere. Seven stability classes (i.e., Pasquill-Gifford-Turner classes) have been defined. These classes, with the original descriptions and conditions of occurrence given by Pasquill (Turner, 1994), are:

A: Extremely Unstable (Strong superadiabatic). Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).

B: Moderately Unstable (Moderate superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 3 to 5 m/s range to dim sunshine with wind speeds < 2 m/s.

C: Slightly Unstable (Slight superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 5 to 6 m/s range to dim sunshine with wind speed in the 2 to 3 m/s range.

D: Neutral (Adiabatic). Normally occurs with moderate to dim sunshine, cloudy conditions, and at night, with wind speeds > 3 m/s. It also occurs with very strong wind speeds on either sunny or cloudy days.

E: Slightly Stable (Slight subadiabatic with or without inversion). Normally occurs at night or early morning with some cloud cover and with wind speeds in 2 to 5 m/s range.

F: Moderately Stable (Moderate subadiabatic with inversion). Normally occurs at night or early morning with little cloud cover and with relatively low wind speeds (< 3 m/s).

G: Extremely Stable (Strong subadiabatic with inversion). Normally occurs at night or early morning with very light to nearly zero wind speed.

Unstable conditions result in rapid lateral and vertical diffusion of pollutants (i.e., wide plumes), whereas stable conditions result in slow lateral and vertical diffusion (i.e., narrow plumes). The latter will lead to higher air concentrations from ground-level releases.

Although Class A is not rare, it is not as common as Classes B through F. Class D is the most common stability class for many DOE sites. This is due to the large number of combinations that can result in Class D stability. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally Class D. Classes E and F are the most common stability classes at night.

Note that the meteorological conditions used as a basis for DOE-STD-1027-92 Hazard Characterization, Attachment 1 are D stability and 4.5 m/s wind speed. This set of conditions is also used as a basis by chemical process industry for determining limits on chemical inventories, and is representative of most U.S. regions (29 CFR 1910.119).

Dispersion Conditions For Accident Analysis

In calculating plume concentrations, and subsequently consequences to the receptor, both "unfavorable" and "typical" dispersion conditions are of special interest in accident analyses. For accident analysis consideration of the offsite MOI receptor, unfavorable meteorology should be based on site data. In practice, this is the dilution factor (χ/Q) that coupled with the source

term would lead to doses that are exceeded no more than five percent of the time. The method should be conservative or consistent to the discussion in the NRC Regulatory Guide 1.145 (Position 3) as summarized in Appendix A to DOE-STD-3009-94, CN2. The 95th percentile of the distribution of doses to the MOI, accounting for variation in distance to the site boundary as a function of direction, is the comparison basis for assessment against the EG.

The size of the data set used in the meteorological assessments should be sufficiently large that it is representative of long-term meteorological trends at most sites. Meteorological data, qualified and meeting requirements of Regulatory Guide 1.23 (NRC, 1972), available at most DOE sites should be applied that is representative of long-term trends. A five-year dataset is desirable, but a one-year data set can be applied under the right circumstances.[21] In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations, such as Class F stability and 1.0 m/s to 1.5 m/s wind speed, as an interim measure.

It should be noted that in the long run, site meteorological data is always preferred over default conditions for accident analysis.

For example, Hunter (1993) evaluated Savannah River Site data and found the 95th percentile conditions varied with release height, and receptor distance. For most facility MOI distances, it was determined that 95th percentile conditions were E stability and

- 1.7 m/s wind speed (release height of 0 m – 10 m)

- 2.1 m/s wind speed (20-m release height), and

- 3.0 m/s wind speed (60-m release height).

- For mitigated hazard analysis, DOE has not established guidance for evaluating the mitigated benefit of SSCs. Both median statistical basis (i.e., 50th percentile) and 95th percentile bases have been applied to determine onsite receptor doses. While other measures of "typical" could be applied, each is problematic. The mean (i.e., average) and the mode (i.e., peak) of a distribution, unlike the median, not heavily influenced by outliers (abnormally small or large values). For a bimodal distribution, which can often occur , the mean may fall between the peaks (i.e., modes) of the distribution and thus be comparatively infrequent, which could not be considered "typical". (The median could also be atypical in this sense but it has a relevant meaning.) In addition, if mode were chosen as "typical", a bimodal distribution could give two valid choices if the peaks are nearly as large.

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[21] In Regulatory Guide 1.194, this subject is discussed as follows: "The NRC staff considers 5 years of hourly observations to be representative of long-term trends at most sites. With sufficient justification of its representativeness, the minimum meteorological data set is one complete year (including all four seasons) of hourly observations" (NRC, 2003).

- Evaluation of site data for determining 95th and 50th percentile conditions has historically been of two types. A Joint Frequency Distribution (JFD) sampling of site hourly data sorts *all* data from high relative concentration to low relative concentration and identifies various percentile conditions by ranking the full data set. Another basis is use of a random sampling technique in which a sample of the full data is randomly selected and then typically sorted into pre-assigned consequence bins (normally chosen to find high-consequence conditions). An example of this approach is Latin Hypercube Sampling (LHS).

- JFD sampling is usually done for a standard set of release conditions (e.g., hour duration, ground-level release). The random sampling basis is normally determined on an accident case-by-case basis. The JFD profile tends to be composed of more data points and is generally "smoother".

Gaussian Model For Neutrally Buoyant Plumes

The choice of a dispersion model depends on factors such as the phase of safety analysis, complexity of facility, complexity of the accident sequence, and site topography and its affect on environmental transport conditions. Simply put, the most comprehensive, realistic computer model is not the best choice for all safety analysis situations. In most situations, peer-reviewed engineering calculations and spreadsheet analyses employing a Gaussian atmospheric dispersion model are sufficient. Data requirements are typically less demanding and more readily verified than for more complex models. Ultimately, the accident analysis is more scrutable and technically defensible during independent review if based on the Gaussian model.

The simple, straight-line Gaussian dispersion equation is used as the basis for a majority of the models used in DOE safety analysis of accidental releases. It is the basis for radionuclide inventories defining Hazard Category 2 and 3 facilities in DOE-STD-1027-92, CN 2. And, as noted earlier, for compliance with Appendix A of DOE-STD-3009, and comparison with the EG, the Gaussian model can readily estimate time-integrated air concentrations (typical units of Ci-s/m^3 for radiological releases) at downwind locations and is recommended for most accident conditions (Figure A-1). While more sophisticated models are becoming more commonplace, especially in situations where complexities in physical or chemical properties, terrain, or nearby buildings influence the dispersion of radiological material, the data demands for these approaches may be prohibitive. However, for these situations, the basic Gaussian dispersion model can be modified to accommodate release and dispersion effects that are influenced by surface features or source term characteristics.

The user should exercise care over the distance for which the Gaussian model is applied. The American Meteorological Society (AMS) published a position paper indicating that the Gaussian model is estimated to be accurate within a factor of two for distances of 0.1 to 10 – 20 km when onsite meteorological tower data are available, and conditions are reasonably steady and horizontally homogeneous (AMS, 1978). Beyond 20 km and closer than 100 m should be considered to be order-of-magnitude estimates at best. Aerodynamic wakes, rough or urban terrain, and dispersion under very stable conditions and slow wind speeds introduce more uncertainty into the Gaussian model predictions.

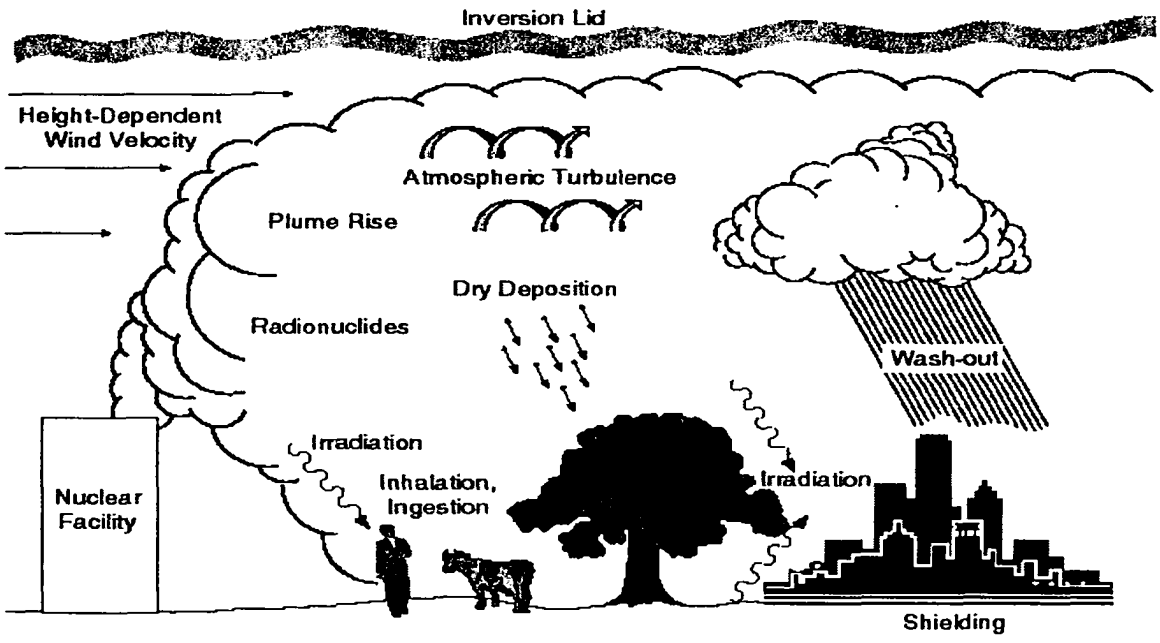

Figure A-1. Basic Processes Occurring During Accidental Release and Dose Pathways

For energetic releases, other models may be employed, as allowed under Appendix A of DOE-STD-3009-94, CN2. However, data requirements for alternative model types may preclude use to support most DSA applications. Alternative techniques have been applied to modify a standard Gaussian model and thereby apply it to cases normally outside the regime of Gaussian applicability (Steele, 1998).

It is the responsibility of the analyst to make the final determination of a dispersion basis. The value of a complex, more realistic computer model with associated data demands, the requirements of the specific application, and the phase of the safety analysis must be weighed.

Recommendation: Apply the Gaussian model as a first choice. Accident phenomenology may be modeled assuming straight-line Gaussian dispersion characteristics, applying meteorological data representing a 1-hour average for the duration of the accident.

Use other special-purpose approaches as warranted for unique release situations, e.g. detonation or blast accident scenarios. Consider appropriate modifications for addressing weather extremes, such as tornado or high-wind conditions.

Basic Gaussian Equations

Intrinsic to the assumptions underlying the Gaussian approximation of atmospheric dispersion, as a plume is transported downwind, its horizontal expansion is essentially unlimited[22]. Vertical expansion is limited by the earth's surface and aloft under inversion conditions. The downward expansion of the plume must obviously stop at the ground, while upward expansion may be stopped if there is a stable layer (i.e., a "cap") at the top of the mixing layer. This cap acts as a lid to rising "thermals" of air, thus restricting the range and magnitude of vertical turbulence. The plume is often considered to "reflect" off of both the ground and the top of the mixing layer, causing the *vertical* profile to become increasingly uniform as the plume proceeds downwind.

The amount of atmospheric dilution and dispersion is usually expressed in terms of χ/Q, where χ is the concentration of the pollutant in air at some downwind location. For these formulations, χ represents either the instantaneous concentration (e.g.,Ci/m^3 or Bq/m^3) or the time-integrated concentration (e.g., $Ci\text{-}s/m^3$ or $Bq\text{-}s/m^3$), and Q is the rate of release (e.g., Ci/s or Bq/s) of the pollutant, or total source strength (e.g., Ci or Bq) of the pollutant. The units of χ/Q are s/m^3 whether the instantaneous or time-integrated releases are considered. Thus, χ/Q is the concentration of the pollutant in air at the receptor per unit source rate, or time-integrated concentration per unit source. The instantaneous concentration of the pollutant in air at the receptor is thus the product of χ/Q and the rate of release of the pollutant.

The Gaussian plume model (Slade, 1968), when not constrained in the vertical by the ground or the top of the mixed layer, is expressed as:

$$\frac{\chi(x,y,z,h)}{Q} = \frac{1}{2\pi u \sigma_y \sigma_z} e^{-y^2/2\sigma_y^2} \left[e^{-(z-h)^2/2\sigma_z^2} \right] \qquad (1)$$

where x is the distance of the receptor downwind from the release point, y is the horizontal cross-wind distance of the receptor from the centerline of the plume, z is the distance of the receptor above the ground, h is the height of the plume centerline above the ground, σ_y is the standard deviation of the horizontal Gaussian distribution (i.e., the "half width"), σ_z is the standard deviation of the vertical Gaussian distribution (i.e., the "half thickness"), and u is the wind speed at 10 m height, the standard measurement height. The constant, 2π, is implicit in a Gaussian distribution, and is the product of lateral and vertical components each contributing $(2\pi)^{0.5}$.
Note that the downwind distance x does not appear explicitly in this equation since downwind distance is an independent variable. The x dependence is implicit, as the σ_y and σ_z are functions of x only, for a given stability class. The wind speed (u) represents the direct dilution of the pollutant as soon as it is released into the atmosphere. The lateral and vertical Gaussian

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[22] Horizontal, or lateral, plume expansion may be somewhat limited by physical barriers, such as buildings and topographic obstacles, but these are normally treated as special cases.

coefficients (σ_y, σ_z) approximate the diffusion or dispersion in the atmosphere as the plume is transported downwind.

The bracketed term in equation (1) defines the vertical distribution. If hazardous material released in the plume is reflected from the ground and from the top of the mixed layer, this term must be modified. This is done mathematically by adding multiple mirror source terms. The bracketed term in equation (1) thus is replaced with:

$$\left[e^{-(z-h)^2/2\sigma_z^2} + e^{-(z+h)^2/2\sigma_z^2} + \sum_{n=1}^{N} \left(e^{-(z-h-2nL)^2/2\sigma_z^2} + e^{-(z+h-2nL)^2/2\sigma_z^2} + e^{-(z-h+2nL)^2/2\sigma_z^2} + e^{-(z+h+2nL)^2/2\sigma_z^2} \right) \right] \tag{1a}$$

The term before the summation in the preceding equation is the ground reflection component since perfect reflection is assumed. The series of terms after the summation represent the perfect reflection of first the top of the plume and later the bottom of the plume on the top of the mixed layer. L represents the height of the top of the mixed layer and the summation is over the number (N) of reflections to be considered. The contribution of the summation term is minor, especially for distances close to the source and for larger values of L; also, the higher order terms contribute progressively less and the series is normally terminated after only a few terms. For example, in the MACCS code (Chanin, 1990), the series is terminated at $N = 5$. For a ground-level release (i.e., $h = 0$), the first two exponential terms become equivalent. Each of these terms subsequently becomes a value of one when the receptor is at ground level (i.e., $z = 0$). In these cases, the "2" in the denominator of equation (1) cancels out with the "2" in the numerator, if the summation term is ignored, as is often done. The maximum concentration occurs at plume centerline (i.e., $y = 0$). Thus, if the summation term is ignored, the Gaussian equation simplifies to a centerline condition:

$$\frac{\chi(x, y = 0, z = 0, h = 0)}{Q} = \frac{1}{\pi u \sigma_y \sigma_z} \tag{2}$$

Strictly speaking, the numerator in the above expression is slightly greater than one because of the contribution of the summation term. Equation (2), which is now only a function of downwind distance of the receptor, is often used for the MOI, as the plume centerline concentration represents a conservative value.

Similarly, a puff model using a Gaussian formulation may be used for instantaneous or near-instantaneous releases of hazardous material

$$\chi(x, y, z; H) = \frac{Q_T}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp\left[-\frac{1}{2} \left(\frac{y}{\sigma_y} \right)^2 \right] \left\{ \exp\left[-\frac{1}{2} \left(\frac{z-H}{\sigma_z} \right)^2 \right] + \exp\left[-\frac{1}{2} \left(\frac{z+H}{\sigma_z} \right)^2 \right] \right\} \tag{3}$$

where:

Q_T = total source term [Ci]

σ_x = longitudinal dispersion coefficient, representing the standard deviation of the concentration distribution in the downwind axis direction [m] (AIChE, 1996).

The horizontal and vertical dispersion coefficients, σ_y and σ_z, required in the Gaussian dispersion equation are obtained either from site-specific meteorological measurements (standard deviations of wind angles) or indirectly through estimating an atmospheric stability class for which standard dispersion coefficients have been established. If the necessary meteorological measurements are not available, several methods for determining stability class may be used. The differences between puff and plume dispersion handled with the Gaussian dispersion equation should be taken into account when applying the model. Methods for calculating puff dispersion coefficients have been addressed by Turner (1970), Gifford (1977), and Hanna (1982).

Extreme Weather Conditions

Section A.3 of Appendix A to DOE-STD-3009-94, CN2, indicates, "For accident phenomena defined by weather extremes, actual meteorological conditions associated with the phenomena may be used for comparison to the EG". A common weather extreme that is frequently addressed in many DSAs is that due to tornadoes.

The accident analysis should at minimum consider two periods for subsequent exposure evaluation: (1) that due to meteorological conditions from the tornado impact or strike itself; and (2) a second, prolonged period. The latter period would account for aerodynamic re-entrainment and resuspension acting to transport radiological material from the facility into the environment. The first period would be modeled with a design basis accident dilution factor (Ψ/Q) designated for a specific class tornado and applied for the distance from the facility to the receptor. The second period is modeled using a standard consequence model for an exposure period of no longer than eight hours, to be consistent with the time period specification discussed in Appendix A to DOE-STD-3009-94, CN2.

For the initial strike period, the appropriate Fujita scale should be applied. For most safety analysis this is either Fujita - 2 (F2) or F3. Figure A-2 shows the maximum time-integrated ground-level centerline air concentration (s/m^3) vs. downwind distance (km) for different mean translational speeds of the F2 tornado (Weber and Hunter, 1996). The consequence analysis should pick a maximum Ψ/Q for the assumed translational speed. For example, the translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers. This exposure should be added to that obtained for the MOI distance using the standard 95^{th} percentile condition to estimate the full exposure due to the event.

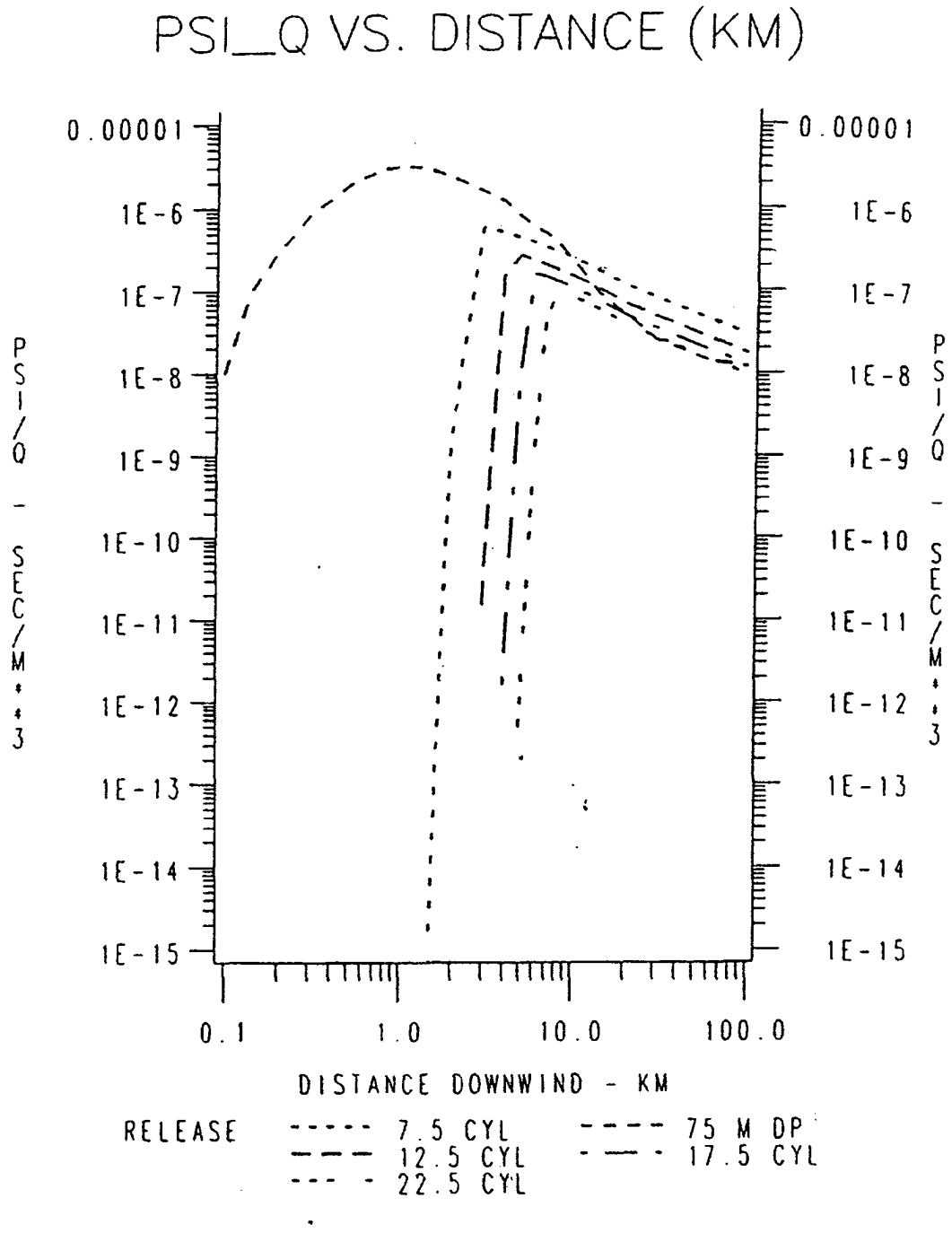

Figure A-2. The maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km) for different mean translational speeds from 7.5m/s to 22.5 m/s. The downdraft speed is 10 m/s and the height of the cylindrical mesocyclone is 3500 m (from Weber and Hunter, 1996).

Mixing Layer Height

For an evaluation of χ/Q that includes reflections from the ground and the top of the mixing layer, an estimate of the depth of the mixing layer is required. This height varies throughout the day and throughout the seasons. During clear nights, when inversions are present, the mixed layer is relatively low, while during sunny days the mixing layer is much higher. The magnitude of these heights can be obtained from balloon soundings or from remote sensing techniques, such as acoustic or radar soundings. In the absence of such data, regional tables can be consulted, such as those of Holzworth (1972).

Recommendation: Base mixing layer height on seasonal averages and day/night time of day. Apply archived site or laboratory meteorological data. If this is not applicable, use regional data as default input values.

Dispersion Parameters

Many schemes have been proposed for establishing the magnitudes of σ_y and σ_z. Most of these are based on empirical curve fitting of data that were taken during experiments over flat grassland (Haugen, 1959). One commonly used curve-fitting method is that of Tadmor and Gur (1969), in which each σ is expressed as a power law:

$$\sigma = a\,x^{b} + c \tag{4}$$

where a, b, and c are empirical constants, given in Table A-1 as used in the MACCS/MACCS2 code; the units of x and σ are given in meters. In MACCS, the c term of σ_z has been set to zero for mathematical convenience, which has required adjustments to the a and b values.

Table A-1. Fitting Constants for σy and σz - Tadmor and Gur (as used in MACCS2 code; See Dobbins (1979))

Curve Fitting Constant	ATMOSPHERIC STABILITY CLASS					
	A	B	C	D	E	F
a_y	0.3658	0.2751	0.2089	0.1474	0.1046	0.0722
a_z	0.00025	0.0019	0.2	0.3	0.4	0.2
b_y	0.9031	0.9031	0.9031	0.9031	0.9031	0.9031
b_z	2.125	1.6021	0.8543	0.6532	0.6021	0.6020
c_y	0.0	0.0	0.0	0.0	0.0	0.0
c_z	0.0	0.0	0.0	0.0	0.0	0.0

Another commonly used curve-fitting method is that of Briggs (1973), for which each σ is expressed as

$$\sigma = a\,x(1 + bx)^{-½} \tag{5}$$

where a and b are constants, given in Table A-2.

Table A-2. Fitting Constants for σ_y and σ_z from Briggs

Curve Fitting Constant	ATMOSPHERIC STABILITY CLASS					
	A	B	C	D	E	F
	Open-Country Conditions					
a_y	0.22	0.16	0.11	0.08	0.06	0.04
a_z	0.20	0.12	0.08	0.06	0.03	0.016
b_y	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001
b_z	0	0	0.0002	0.0015	0.0003	0.0003
	Urban Conditions					
a_y	0.32	0.32	0.22	0.16	0.11	0.11
a_z	0.24	0.24	0.20	0.14	0.08	0.08
b_y	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004
b_z	0.001	0.001	0	0.0003	0.00015	0.00015

The most commonly used curves are the Pasquill-Gifford curves based on measurements at Project Prairie Grass in the mid-1950s. They are found in Slade (1968), and are based on three-minute averaging times. An empirical formula derived the Pasquill-Gifford parameters has the following form for σ_y and σ_z, and is based on work published by Yuan (1993), where

$$\sigma_y(x) = (0.000246\,\sigma_\theta^2 + 0.00576\,\sigma_\theta + 0.066)\,x^{0.9031}$$

and (6)

$$\sigma_z(x) = a\,x^b + c.$$

Coefficients and constants for various downwind distances and stability classes are given in Table A-3. The Tadmor-Gur and Briggs formulations, as well as others, give results that are nearly the same for some ranges and stability classes. However, they may differ by a factor of two or more for other ranges/classes. The coefficients given in the above tables, and in other Gaussian models, are based on fitting curves to observational data of plumes released over flat grassland. In the case of the Briggs model, an adjustment for urban conditions has also been made. The Pasquill-Gifford formulations also specify different coefficients for different ranges of distance. It should be noted that the database underlying the empirical curve fits is valid for distances between 100 m and 1,000 m.

For distances less than about 100 m, these coefficients generally do not provide a good fit to the observations and the models are generally considered approximate. This is due to the fact that Gaussian models, with the underlying assumption of steady-state, do not perform well in the near-field.

In practice, the concentration at close-in receptor distances is frequently influenced by the physical presence of the facility from which the plume is released, as well as neighboring structures. Often, building wake effects are important for these smaller distances but the above coefficients ignore the enhancement of vertical turbulence from wake effects, down washing into the cavity behind the building, as well as recirculation. These effects can influence concentrations, and building geometry correction factors are often applied.

Recommendation: Consult with the laboratory or site meteorology organization responsible for recording and maintaining site data, and request a best-fit set of dispersion parameters for the region of transport applicable to the analysis. As a default, apply Tadmor-Gur, Briggs, or Pasquill-Gifford dispersion parameter sets, based on site-specific and surface roughness characteristics.

Table A-3. Pasquill-Gifford Dispersion Coefficients (Eimutis, 1972)

Applicable Distance, m	Coefficients				
	Stability Class	σ_θ	a	b	c
x > 1,000	A	25	0.00024	2.094	-9.6
	B	20	0.055	1.098	2.0
	C	15	0.113	0.911	0.0
	D	10	1.26	0.516	-13.0
	E	5	6.73	0.305	-34.0
	F	1.5	18.05	0.18	-48.6
100< x <1,000	A	25	0.00066	1.941	9.27
	B	20	0.0382	1.149	3.3
	C	15	0.113	0.911	0.0
	D	10	0.222	0.725	-1.7
	E	5	0.211	0.678	-1.3
	F	1.5	0.086	0.74	-0.35
x<100	A	25	0.192	0.936	0.0
	B	20	0.156	0.922	0.0
	C	15	0.116	0.905	0.0
	D	10	0.079	0.881	0.0
	E	5	0.063	0.871	0.0
	F	1.5	0.053	0.814	0.0

Special Gaussian Modeling Considerations

Plume Meander

The above expressions are for short-duration clouds released over relatively smooth terrain. However, as time passes after the initial release, larger sized eddies, mostly in the horizontal direction, may affect the cloud. Shifts in wind direction become likely with time, and the cloud will tend to change direction, or meander. The meander factor is especially important for longer duration releases. For a receptor that remains immersed in the plume for some time, meandering effectively widens the plume (i.e., increases horizontal dispersion) and thus decreases χ/Q. One formulation of the plume meander factor[23], the one used in MACCS (Chanin, 1990), but initially attributed to Gifford (1975) is

$$meander\ factor = (plume\ duration\ /\ time\ base)^{n} \quad (7)$$

where the time base is typically 10 minutes and the exponent n is 0.2 for plume duration of one hour or less and 0.25 for greater duration. The σ_y is increased by this meander factor and accordingly, the plume-centerline χ/Q would accordingly be reduced by this factor. The plume meander factor is never allowed to be less than one, and the experimental basis is limited to periods no longer than 100 hours.

Example: For a two hour release and a time base of ten minutes, the plume meander factor is $[(2\ hr)\ (60\ min/hr)\ /10\ min]^{0.25} = 1.86$.

An alternative formulation (NRC 1980) is

$$meander\ factor = (2 \times plume\ duration)^{1/3} \quad (8)$$

where the plume duration is in hours (minimum of 0.5 hours). This gives results similar, but not identical, to those shown in equation (7).

A different type, and larger meander factor occurs under conditions that are very close to adverse meteorology for ground-level releases (i.e., very stable conditions with light wind speeds). Under such conditions, large eddies are present in the stably stratified atmosphere which augment the magnitude of the lateral turbulence. This theoretical effect was first empirically determined from tracer studies performed in the mid-1970s. After careful review of the results of the tracer study, the Nuclear Regulatory Commission (NRC) incorporated this meander factor in Regulatory Guide 1.145 (NRC, 1983), and acknowledged it in several of their atmospheric dispersion models. The Regulatory Guide does not advise using this factor for relatively higher stability classes (A, B, and C).

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[23] The meander factor is also called the plume expansion factor.

The embedded equations in these models can simply be described by an augmentation of the lateral turbulence:

$$\Sigma_y = M\sigma_y \quad (9)$$

where Σ_y is the augmented lateral turbulence, and M is the meander factor.

The value of M increases for more stable conditions (i.e., from E to G stability class) and as wind speeds approach calm. This is exactly opposite to the aerodynamic building wake factor that is very small under these meteorological conditions, but increases significantly as the wind speeds increase and the stability class becomes neutral or slightly unstable.

Recommendation: Apply the Gifford model for recalibrating the time basis of the set of dispersion parameters to the release duration of interest.

Surface Roughness

Surface roughness affects the magnitude of mostly vertical turbulence, and hence, vertical atmospheric dispersion. The rougher the surface of the region of transport, the larger the turbulent eddies that are formed when the plume encounters the earth's surface. If the terrain is not smooth, which is frequently the case, a linear scaling factor needs to be introduced to increase the effective value of σ_z. A common approach to quantifying the "roughness" factor, is based on AMS (1977) and is usually expressed as:

$$roughness\ factor = (z_1/z_0)^{0.2} \quad (z_1 \geq z_0) \quad (10)$$

where z_1 is the roughness length of the terrain over which the plume is passing and z_0 is the comparison standard length, normally taken as 3 cm, which represents the roughness factor associated with flat terrain. A rule of thumb suggests that z_1 is approximately one-tenth of the physical height of local obstacles. The roughness factor cannot be less than unity. Because σ_z is increased by the roughness factor, the plume-centerline χ/Q is proportionally reduced by this amount. For grasslands, the roughness length is estimated to be 10 cm. In this case, the roughness factor is $(10/3)^{0.2} = 1.27$. For terrain that includes grasslands, trees, mountains, and cities, the average roughness length commonly applied ranges from 30 cm to 100 cm. Other surface roughness lengths and their subsequent correction factors are shown in Table A-4. (Note that in the Briggs formulation of σ_y and σ_z, this roughness factor is already taken into account in that different coefficients are used for open-country and urban terrain.). McElroy and Pooler first developed "urban" dispersion coefficients in the 1960's (1968). As a rough rule of thumb, the vertical dispersion increases by one stability class for urban areas (i.e., an atmospheric condition resulting in F stability in rural environments becomes E stability in urban environments).

Recommendation: Apply a roughness correction to adjust the vertical dispersion parameterization for the region of transport-based recommendations from the American Meteorological Society (1977).

Table A-4. Surface Roughness Lengths for Characteristic Surface Types

(See Jow (1990) – Volume 2. MELCOR Accident Consequence Code System (MACCS), Model Description, NUREG/CR-4691, SAND86-1562, Sandia National Laboratories, Albuquerque, NM (1990).

Surface Type	Surface Roughness Length z_0 (cm)	Roughness Factor (Eqn. 10)	Scaling Factor for Dilution Factor
Tall Grass, Cropland	10 – 15	1.27 – 1.38	0.79 – 0.72
Countryside	30	1.58	0.63
Suburban	100	2.02	0.50
Forests	20 – 200	1.46 – 2.32	0.68 - 0.43
Urban	100 – 300	2.02 – 2.51	0.50 – 0.40

Depletion Processes

While atmospheric dispersion processes are the major types affecting cloud concentration, others exist that can both remove both gases and particulates from the cloud and reinsert other radioactive species back into the atmosphere. The removal processes are dry deposition, which results from impaction, gravitation settling and fallout of material from the plume, and wet deposition, or precipitation scavenging. Reinsertion of material back into the atmosphere is termed resuspension and will be discussed in more detail in the next section. These mass transfer processes are very important in determining the ultimate fate of small respirable particulates.

Dry Deposition

The physical characteristics of particulate and aerosol radionuclide species will tend to remove this component from a released cloud. Two common models for removal are the source depletion model and the surface depletion model. The source depletion model is computationally simple, in which the rate at which material in the cloud are deposited to the ground as the product of the ground level concentration of the materials, and the dry deposition velocity of the material (Chamberlain, 1953). The approach uniformly depletes the cloud. However, this treatment does not perturb the normal distribution of the concentration in the vertical direction, an assumption that is valid during neutral or unstable atmospheric conditions.

Another approach is the surface depletion method. It is computationally more complex, and depletes the source primarily at the cloud/earth interface. Use of the surface model changes the source material distribution in the cloud.

The parameterization of dry deposition processes is usually accomplished by the use of a deposition velocity. Deposition velocity (v_d) is a mass-transfer boundary condition at the atmosphere-ground surface interface in atmospheric dispersion and transport models. The deposition velocity is defined as a deposition flux (F_d) divided by the airborne concentration of radioactive material (χ):

$$v_d = F_d/\chi \qquad (11)$$

In reality, the deposition velocity is a function of the particle size. The larger the particle, the larger its deposition velocity up to the Stokes velocity limit. From various field experiments conducted over the years, dry deposition velocities range from 0.001 – 180 cm/s for particulates, while for gases it ranges from 0.002 – 26 cm/s.

Dispersion models such as MACCS2 permit the treatment of particle sizes and assign different deposition velocities to each of user-prescribed particle size bins. The challenge facing the analyst is to assign radioactive material into these bins that has been generated under accident conditions. More than fifty variables exist that can influence the magnitude of the rate of dry deposition removal. These are categorized into micrometeorological, depositing material, and surface variable categories.

Typically, simplifying assumptions are made, based on radionuclide species, chemical form, and whether the emitted radioactive material is filtered or non-filtered. For noble gases and tritiated hydrogen gas (HT), no deposition should be modeled. For filtered particulate releases, the deposition velocity is assumed to 0.001 m/s. This dry deposition velocity corresponds to a particle with an approximate aerodynamic equivalent diameter (AED) of 0.2 μm to 0.4 μm (Sehmel, 1978).[24] For unfiltered particulate releases, such as through cracks and open breaches assumed in the accident conditions, the deposition velocity is assumed to 0.01 m/s. This dry deposition velocity corresponds to a particle with an approximate AED of 2 μm to 4 μm. Tritium oxide is normally taken to have a deposition velocity of 0.005 m/s (Murphy, 1993, Fallon, 1982 and Sweet, 1984).

Wet Deposition

Wet deposition through precipitation, depletes the plume to some degree. This phenomenon is difficult to parameterize due to its dependency on cloud physics variables which themselves vary over time and space. All types of precipitation (i.e., rain, snow, hail), passing through the plume will collect particulates and also scavenge soluble gases. Wet deposition can be approximated by the following correction factor to a dispersion model:

$$D_w = \exp(-vx/u) \qquad (12)$$

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[24] From DOE-HDBK-3010-94, the Aerodynamic Equivalent Diameter (AED): the diameter of a sphere of density 1 g/cm^3 that exhibits the same terminal velocity as the particle in question. The AED is proportional to the product of the [spherical equivalent diameter] and [material density of an aerosol particle].$^{0.5}$ Thus for plutonium oxide (density of 11.46 g/cm3, the spherical equivalent diameter is approximately 3 μm for an AED of 10 μm. Another term frequently used in accident analysis with distributions of various sizes particles is the Activity Mass Median Diameter (AMAD). The AMAD is the diameter of the particle for which half the activity is associated with particles larger than and half the activity associated with particles smaller than this size particle.

where D_w represents the wet deposition and ν represents a washout coefficient (s^{-1}), which itself is a complex function of precipitation particle size spectrum, precipitation rate, radioactive or hazardous chemical particle size distribution, and the solubility of the effluent. As previously, x is the downwind distance of the plume centerline from its release point, and u is the wind speed. Families of empirical curves have been developed for various rainfall rates (mm/h) to estimate the washout coefficient. This procedure is made more complex by the spatial variability of the rainfall. Frequently, rainfall rates vary significantly within a rainfall event, and different washout coefficients may need to be applied to various segments of the plume as it travels to the receptor.

Wet deposition is not modeled in consequence calculations for either the MOI receptor, or the onsite receptors supporting Mitigated Hazard Analysis. While not applicable to deterministic safety analysis, it is usually credited as part of a site's historical data patterns in probabilistic safety assessments (PSAs).

In addition to these mass-transfer processes, in-growth and decay of radioactive releases constantly occur during the transport and dispersion process. The process of in-growth and decay of radioactive isotopes in the plume is a function of the travel time and the half-life of each specific radionuclide that is present in the plume. In practice, this effect is appreciable with radioisotopes of half-life on the same order or shorter than the time to reach the receptor under consideration. For non-reactor facilities, inadvertent criticality would be the primary accident type for which this factor is important.

Decay changes to the population of parent nuclide can be represented by the following factor:

$$A_i = A_i(t)/A_0 = \exp -(\lambda_i t) = \exp -(\lambda_i x/u) \qquad (13)$$

Where A_i represents the relative decrease, i.e., Activity at time t, relative to activity at time 0, or $A_i(t)/A_0$, through decay of the i^{th} radionuclide species, λ_i is the half-life of the i^{th} radionuclide species, and the time is represented by the components x, the downwind distance, and u, the mean wind speed. In this case t = 0 at the time of release into the environment.

Recommendation: Either the source or surface model for depletion may be used in accident analysis. Do not model dry deposition for noble gases or tritium gas (HT or T_2). For filtered particulate releases, the deposition velocity can be taken as 0.001 m/s. For unfiltered releases, the deposition velocity is 0.01 m/s. Tritium oxide (HTO or T_2O) has been characterized with a deposition characteristic of 0.005 m/s. Do not credit wet deposition for DSA accident conditions. Account for decay and in-growth if the initial radionuclides involved at the start of the accident condition have half-lives shorter than the travel time to the receptor.

Resuspension

Deposition addresses mass-transfer from the plume to the ground surface. Resuspension processes are essentially the opposite of deposition processes, in which material that has already been deposited from the plume, or which has been on the ground for a period of time, is re-

entrained by the wind. This re-entrainment and release from the ground of particulates is termed resuspension. The particulates are reintroduced into the atmosphere where it can be transported to a new location. While this effect can be non-negligible for DOE facilities in high-wind, environments without significant intervening vegetation, Appendix A to DOE-STD-3009-94, CN2 indicates that resuspension "need not be modeled".

Recommendation: The analyst need not explicitly account for resuspension in the dose calculation of an accident condition for a DSA.

Deposition and Reemission of Tritium

While dry deposition behavior is observed for most non-noble gas radioactive species and results in diminished plume concentrations as a function of downwind transport, tritium in particular, deposits and re-emits through mechanisms that are distinct from other radionuclides. The major biophysical processes are

- Initial settling to ground
- HT conversion to HTO by soil
- HTO uptake by plants (and partial conversion to organically-bound tritium)
- HTO re-emission from soil and plant
- Uptake by vegetation root systems
- Transport into deeper soil regions.

In evaluating tritium-containing plumes in accident analysis, it is important to recognize that tritium will tend to move in the hydrogen pool throughout the environment. For tritiated water vapor, this will mean rapid uptake depending on difference in concentration. Furthermore, re-emission of tritium from soil and vegetation will take place after plume passage. The latter phenomenon usually takes place on a time scale much longer than the initial removal from the plume (Murphy, 1993).

Plume Rise Mechanisms

Two physical processes can vertically propel a neutrally buoyant plume to a higher level above the ground from its initial point of release. Both of these mechanisms are collectively called plume rise. The first mechanism is termed momentum plume rise, in which the velocity of the release (i.e., efflux velocity) vertically propels the plume due to the excess momentum of the release itself. Accordingly, this is termed momentum plume rise.

The other plume rise mechanism is through buoyancy. Buoyancy plume rise occurs if the temperature of the release is warmer than the ambient air. It is also important to account for stack tip downwash of the plume under high wind speed conditions and plume downwash into the wake and cavity behind the building if the release is from a vent or small stack. A brief discussion follows on both of these plume rise components, and how they interact with forces that tend to downwash. Lastly a series of equations are identified that can be integrated into an atmospheric transport and dispersion model to account for the magnitude of these effects.

Momentum Rise

The estimation of the momentum rise component requires knowledge of the efflux velocity at the point of release, the wind speed at the point of release, and the diameter of the stack through which the effluent is released. In short, the efflux velocity varies inversely with the stack diameter. The efflux velocity is directed vertically, while the wind speed is directed horizontally. Therefore, the ratio of efflux velocity to wind speed determines the initial plume rise. As the plume is transported downwind, the momentum from the efflux velocity vanishes and the wind speed bends the plume over into the horizontal plane. Any additional plume rise beyond the point of release only occurs due to plume buoyancy.

Plume Rise and Entrainment Methods

NRC Regulatory Guides 1.111 and 1.145 define a "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977, 1983). Open-field, "parking lot" dispersion calculations assume non-stack releases, but with no influence of neighboring structures. Releases can be considered to be ground-level if the point of release is below the height of the facility in question and collocated buildings. The intermediate case of releases that occur in the range between 2.5 times the height of adjacent buildings and the building height, escape the building wake under certain conditions, become completely entrained into the building wake under certain conditions, or behave as a "mixture" of these types for still other conditions (NRC, 1998). Several rules of thumb are presented in this section to guide analysis under these conditions.

The NRC guidance differs moderately from the EPA Good Engineering Practice (GEP) stack height criteria. Applying the EPA criterion, the entire effluent escapes the influence of the facility structures if the stack height is 1.5 times the height of the nearest facility structure plus either the height or width of that structure, whichever is larger. For releases from structures that meet GEP stack height criteria, and under neutral or unstable stability conditions, the following equation applies:

$$h_{pr} = 1.44d\,[v_e/u]^{0.667}\,[x/d]^{0.333} - C \qquad (14)$$

where h_{pr} is the plume rise (m), v_e is the efflux velocity (m/s), u is the wind speed (m/s), x, the downwind distance (m), and d, the diameter of the stack (m). This equation shows the

relationship between the two opposing parameters, v_e, and u. C is the downwash correction factor, which is represented by:

$$C = 3[1.5 - v_e/u]d \tag{15}$$

Under stable (e.g., E-G stability classes) atmospheric conditions, the following two empirical equations are evaluated

$$hpr = 4\,[F_m/S]^{0.25} \tag{16a}$$

and

$$hpr = 1.5[S]^{-0.1666}[F_m/u]^{0.333}\,, \tag{16b}$$

and the smaller value is chosen. In Equations 16a and 16b, the momentum flux, $F_m = v_e^2(0.5d)^2$, and the stability parameter $S = g/T[-d\theta/dz]$. For these equations, g represents gravitational acceleration (m/s^2), T is the ambient temperature (K), and $d\theta/dz$ is the potential temperature lapse rate (K/m), which is related to the actual lapse rate.

For plume rise from non-GEP stacks or building vents, empirical relationships from field studies have been developed, where the v_e/u ratio is the driving parameter. When the v_e/u ratio is >5, the vertically-directed momentum flux (i.e., escape building effects) dominates the horizontally-directed (i.e., capture building effects) wind speed, and the release is treated as elevated. This means that although the release emanated from a vent, it still will fully escape the aerodynamic effects of nearby buildings due to the high momentum flux coupled with low wind speed, and the GEP stack height equations apply. On the other end of the spectrum, when the v_e/u ratio is <1, the release is ground level and no plume rise occurs. Two intermediate cases were also developed from field studies. These are the partially entrained and the partially elevated cases and are expressed in terms of an entrainment coefficient, E_t. The entrainment coefficient is defined as the fraction of the plume entrained in the wake and cavity of the building.

Partially Entrained: For cases where the v_e/u ratio is less than 5, but greater than 1.5, a portion of the plume is entrained and the remainder of the plume remains elevated. An entrainment coefficient can be calculated for this case as follows:

$$E_t = 0.30 - 0.06v_e/u \tag{17}$$

Partially Elevated: For cases where the v_e/u ratio is greater than or equal to 1, but less than or equal to 1.5, an entrainment coefficient can be calculated for this case as follows:

$$E_t = 2.58 - 1.58v_e/u \tag{18}$$

In both of these cases, the elevated portion of the plume is subject to plume rise, while the entrained portion of the plume is downwashed to ground level. Building wake effects are discussed in more detail in a later section.

Buoyancy Rise

Buoyancy effects usually arise if significant sensible heat is contained in the cloud being released. For nonreactor DOE facilities, the primary sources of these cloud types are through postulated explosion or fire events. The estimation of the buoyancy component requires knowledge of the effluent and ambient temperatures at the point of release. If the effluent temperature is higher, positive (i.e., upward) buoyancy occurs, while for a cold or dense cloud, negative buoyancy will occur. The latter condition is normally associated with certain types of chemical releases, more so than for radiological releases. The stability class of the atmosphere is also a very important parameter to account for, as it affects the magnitude of the buoyancy plume rise.

Buoyancy rise is usually calculated in two steps. The first is the initial rise and is dependent on the stability class. The second one is the gradual rise and is independent of stability class. The larger of the two is then selected as representative.

Initial Plume Rise: For stability classes A – D, and buoyancy fluxes less than 55 m^4/s^3, the plume rise is given by (Briggs, 1971)

$$\Delta h = 21.425\ F_b^{3/4}\ u^{-1} \tag{19}$$

where F_b is the buoyancy flux, and is evaluated from

$$F_B = g\ Q_h/\pi\ C_p\ \rho_a\ T_a \tag{19a}$$

with units of $[m^4/s^3]$. In this equation, g is the gravitational acceleration, C_p is the specific heat of effluent gases, ρ_a is the density of air, and T_a is the ambient air temperature.

For fluxes greater than 55 m^4/s^3, the plume rise is given by

$$\Delta h = 38.71\ F_b^{3/5}\ u^{-1}. \tag{20}$$

For stability classes E - G, the plume rise is given by (Randerson 1984)

$$\Delta h = 2.6\ [F_b/(u\ S)]^{1/3}. \tag{21}$$

In calm conditions, a better approximation is provided by

$$\Delta h = 4\ F_b^{1/4}\ S^{3/8}. \tag{22}$$

In Equations 21 and 22, S is a stability parameter with units of inverse time squared (t^{-2}), and is defined in Volume 2 of Chanin et al. (1990).

Gradual Plume Rise: The second portion of plume rise, gradual plume rise, is applicable to unstable to neutral conditions and can be calculated from

$$\Delta h = 1.6\, F_b^{1/3}\, x^{2/3}\, u^{-1}. \qquad (23)$$

The buoyancy flux from a fire is $F_b = 8.79 \times 10^{-6}\, \Omega$, where Ω is the rate of release of sensible energy in watts (W).

MACCS2 applies Equation 23 for stability classes A – D, and Equation 21 for E and F stability classes. Several methods are used in MACCS2 to cap the height of the plume rise, such as: (1) reaches 300 F_b/u^3 (Briggs, 1975); (2) when the plume centerline has reached the height of the top of the mixing layer; or (3) when one hour has elapsed. The Briggs model is based on data obtained from industrial stacks, and assumes negligible stack radius leading to the environment.

Another model is that from Mills (1987). It is based on an area (pool) fire and is more correct for facility accident analysis where the assumed fire has compromised or breached an area in the facility. The Mills method adjusts the Briggs effective release height to a lower value using

$$H_{Mills} = \{ (H_{Briggs})^3 + (R/\gamma)^3 \}^{1/3} - R/\gamma \quad \text{where} \qquad (24)$$

where H_{Brigg} = effective release height estimated with the Briggs approach

R = radius of burning pool

γ = entrainment coefficient for buoyant plume rise.

An area or full facility fire event would fall in this category.

Several significant issues exist in modeling a fire event in accident analysis and the ensuing release into the environment. These include

- Sensible heat released
- Fire plume history
- Radiological material involvement in the fire.

Sensible heat – The fraction of the heat of combustion that is not radiated is available to cause a temperature increase in the air and other gases emitted in the plume. This energy is sensible heat and will act to effectively increase the height of release. The radiated fraction can vary with the nature of the fire, but a typical value is ~0.3, implying a sensible heat release of 0.7. However, for indoor fires in complex facilities, the fraction can vary with heat being radiated to structures (walls and ceilings) rather than being available for heating of air and other gases escaping into the environment.

Fire plume history – Another uncertainty that exists is the temporal nature of the fire. For the same amount of radiological material released, short duration fires will lead to larger dose than longer fires due to less crosswind meander.

Radiological material involvement – Depending on facility type and location of radiological hazards with respect to the combustible loading, the fire may have a radiological component that is evenly distributed in time, localized to certain intervals, or some combination. The radioactive release history may not correspond numerically to the sensible heat release.

Thus fires represent complex phenomenology that can demand an inordinate level of precision relative to the purpose of accident analysis. While MACCS and other codes allow use of an effective height model based on sensible heat released, the uncertainties in fire duration, sensible heat, and radiological material involvement introduce a significant burden to the analyst to defend. The outcome of an even a successful defense to this level of detail may be difficult to interpret against the requirements of the accident analysis process.

Recommendation(s):

External (outdoor) fires: Determine the sensible heat fraction for well-defined fires. Credit only sensible heat fraction for the thermal buoyancy effect. Assume shortest duration consistent with fire sequence definition.

Internal (indoor fires: Assume no sensible heat release for release to environment. Assume shortest duration consistent with fire sequence definition.

If the source term analysis can defend the amount of sensible energy, the temporal history, and the spatial distribution, then this phenomenon may be modeled in the consequence analysis. If this cannot be defended adequately, then the source term from fire should be estimated using recommended five-factor methodology, and the consequent environmental model should assume a short duration fire, occurring as a ground-level release.

Building Wake Effects

As shown in an earlier section, releases from vents and small stacks can be entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs. Figure A-3 depicts the wake and cavity zones downwind of a nuclear facility. The downwind direction is x, the facility height is H_B, and A_B is the projected cross-sectional area of the building most influencing the flow of the plume. For most bounding, screening purposes, A_B may be assumed to be the surface area of the largest wall of the building nearest the receptor. To a first approximation, the extent of the cavity zone may be taken to be approximately a downwind distance of $2.5\ A_B^{0.5}$. Similarly, the wake zone may extend to roughly ten times $A_B^{0.5}$.

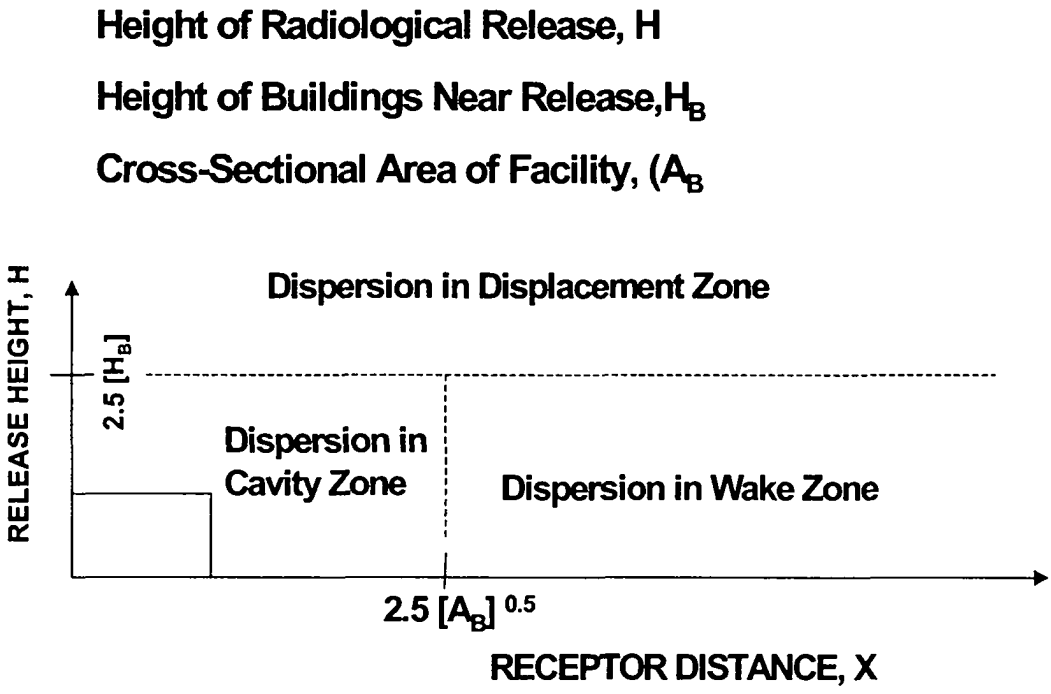

Figure A-3. Cavity and Wake Zones downwind of a Building Structure (Constant Wind Direction from Left to Right).

In order to account for aerodynamic effects of the building, the ground level dilution factor equation is modified

$$\chi/Q = (u\,[\pi\sigma_y\sigma_z + cA])^{-1} \tag{25}$$

where c is the building shape factor, usually taken to be 0.5, A is the smallest cross-sectional area of the building, u is the 10-meter height wind speed and the σ_z is corrected for the wake effect.

This formulation is to be applied in the context of NRC Regulatory Guide 1.145 for non-stack releases, e.g., vent and other building penetrations (NRC, 1983). Building wake effects tend to be appreciable occur under windy conditions, while the plume meander effects (discussed earlier) are more likely under light wind conditions.

An approximate form for the wake zone concentration of airborne release from a "squat" (length and width are > height) facility, up to a receptor distance of 10 building heights ($10H_B$) is given by Turner (1970),

$$\chi/Q \approx 1/\{u\,\pi\,\sigma'_y\,\sigma'_z\} \tag{26}$$

where $\sigma'_y = 0.35\ h_w + 0.067(x - 3\ H_B)$
$\sigma'_z = 0.7\ h_w + 0.067(x - 3\ H_B)$,
$h_w = 0.866\ [(\text{Facility Length})^2 + (\text{Facility Width})^2]$.

The dispersion parameters for this condition are those found in EPA (1995b), and the distance, x, is measured from the facility center.

For screening purposes, several empirical formulas are available for the cavity and wake zone concentrations. A suggested set is found in NCRP (1996).

MACCS/MACCS2 Building Wake and Plume Liftoff

In assessing the capabilities of MACCS and MACCS2 for releases into building wakes, both codes assume initial crosswind and vertical dimensions of the plume are increased through mixing with ambient air caused by the turbulent wake. The dimensions are based on user input for the initial plume dispersion parameters in the lateral (σ_{y0}) and vertical (σ_{z0}) directions, and adjust the initial plume to (width)/4.3 and (height)/2.15, respectively.

Both MACCS and MACCS2 apply a simple approach for determining escape of a buoyant plume from its point of release. It is based on a liftoff criterion that states the plume rise will occur for wind speeds at the release height below a critical wind speed value, u_c, determined by (Briggs, 1973)

$$u_c = \{9.09\ (8.79 \times 10^{-6}\ (\text{Sensible Heat Release Rate (W)}))/\text{Facility Height}\}^{0.33} \quad (27)$$

and will be entrained for wind speeds above u_c. The limitation with this approach is that although the plume is not allowed to rise, the code does not simulate mixing in the cavity behavior nor plume downwash. The only change is to increase plume dimensions to the extent discussed earlier (Lombardi, 1998).

The MACCS2 User's Guide recommends that the code not be applied for estimating doses at distances less than 0.5 km from laboratory or industrial-scale facilities (Chanin and Young, 1998). This is acknowledging the large degree of uncertainty in the modeling of building effects on plume release, as well as the range of applicability for the dispersion parameterization.

Recommendation: Use of open field, ground-level release conditions in the dispersion model, minimizing or eliminating the influence of nearby buildings will be bounding *in most cases.* In the case of receptor(s) within a downwind distance influenced by facility or neighboring structures, the MACCS/MACCS2 model should be used with caution. Apply appropriate scaling factor for the dilution factor and resulting doses based on receptor position in the cavity or building wake regions.

A parametric study is reported in Appendix C of this document to show the combined effects of buoyancy and building wakes on ground-level, plume-centerline χ/Q predictions by MACCS for two different wind speed conditions.

Radiological Consequences

This section provides guidance to the safety analyst regarding evaluation of radiological doses and health risks. It discusses the different types of radiation and the effect radiation can have on the human body, its organs, and its tissues. The factors that must be considered in estimating the dose a receptor may receive following the atmospheric release of radioactive material are covered in detail. Finally, the health risks associated with radiological doses and the standards for radiation protection, in terms of allowed dose or air concentration, are discussed.

Radiological doses can arise from exposure to clouds of radioactive material and fallout from the cloud, and from exposure to prompt (direct) radiation from a criticality. The modes of exposure include:

- inhalation of radioactive material (particulates and gases) in a cloud,
- inhalation of particulates from fallout that have been resuspended by traffic or by wind,
- ingestion of food products and water contaminated by fallout from the cloud,
- gamma radiation from the plume (cloudshine)[25],
- gamma radiation from particulates deposited on the ground from fallout (groundshine),
- skin contamination from fallout, and
- prompt (direct) neutron and gamma radiation from a criticality.[26]

Of especial concern to many DOE non-reactor facilities are inadvertent criticality events and exposure to actinide particulates. In the case of a criticality, doses arise from both the plume of fission products that may be released and from the prompt radiation. The primary contributor to dose from a criticality plume is cloudshine, although actinide particulates can also be important for an unfiltered release. Prompt radiation from a criticality is of concern only for workers located near the accident site. The distance of concern for prompt radiation depends upon the size of the criticality (number of fissions) and the amount of shielding (as from concrete walls) between the worker and the site of the criticality. On the other hand, for actinide exposure, inhalation of plutonium particulates is the primary radiological concern; cloudshine, groundshine, skin contamination, and ingestion doses are insignificant in comparison (Peterson, 1993). Inhalation of enriched uranium particulates is of lesser concern and inhalation of depleted

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[25] Cloudshine also may contain a contribution from beta radiation and its attendant *bremsstrahlung* (discussed below), but this is normally minor compared to the gamma radiation.

[26] Note: MACCS2 does not model the extremely near-field neutron transport and resultant dose such as is important for assessing criticality doses to nearby workers. It can however be used for assessing public exposures due to released fission products.

uranium particulates is trivial by comparison (Peterson, 1995). For uranium, chemical toxicity is normally of greater concern than is the radioactivity.

Types of Radiation

Four types of radiation are important in accident analysis for DOE nuclear facilities: alpha (α), beta (β), gamma (γ), and neutron. The α, β, and γ radiations are emitted from atomic nuclei during radioactive disintegration (or decay) of the nucleus. The neutron radiation is emitted when a nucleus fissions (breaks into fragments), such as during an inadvertent criticality[27]. Alpha particles are energetic (fast-moving) helium nuclei - consisting of two protons and two neutrons, with a charge of +2[28]. Beta particles are energetic electrons, of charge -1, or positrons, of charge +1 - they have a mass about 0.01% that of the alpha particle. Gamma radiation consists electromagnetic waves, or photons - gamma rays have energy similar to that of X-rays, and, being photons, have neither charge nor mass. Gamma radiation typically accompanies alpha and beta radiation. Neutron radiation consists of energetic neutrons. Neutrons are particles with zero charge and mass similar to that of protons, that is, about 25% of the mass of alpha particles. When radiation strikes an organ or tissue of the body, they can deposit some or all of their energy, causing damage. The manner of energy deposition varies with the type of radiation. Some types of radiation, principally alpha and beta, deposit energy primarily by ionization. Upon striking an atom, an electron is stripped off, and the atom is said to be ionized. The two charged particles thus formed – the electron and the ion – are referred to as an ion-pair. The electron that is stripped off the atom may be sufficiently energetic that it can cause further ionization. The amount of ionization created depends upon the mass, charge, and energy of the particle. Particulate radiation (α, β, and neutron) can also deposit their energy through the dissociation of molecules and through elastic scattering, which causes heating

Alpha-decay energy is typically on the order of several MeV (mega-electron volts)[29]. For example, plutonium, uranium, and americium all emit alpha particles with energies on the order of 5 MeV. Because an alpha particle is doubly charged and massive, it can ionize many atoms that it may encounter. For example, an alpha particle traveling through air will create on the order of 50,000 ion pairs for each centimeter it travels. Because it creates so much ionization, it deposits its energy quickly, and penetrates only a short distance into a tissue.

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[27] Neutrons can also be produced through (α,n) reactions, in which an alpha particle strikes the nucleus of an atom, causing the emission of a neutron. This is generally not important for dose calculations as the additional dose from the neutron radiation is balanced by the decreased dose from the lost alpha particle.

[28] The basic unit of charge is that of the electron, but with a reversal of sign. The charge of an electron is -1.60×10^{-19} coulomb.

[29] An electron volt is the kinetic energy of an electron after being accelerated through an electric potential difference of one volt. It is equal to 1.60×10^{-19} joule.

Beta-decay energy is typically on the order of tens of keV to a few MeV. For example, the beta-decay energy of ^{241}Pu is 21 keV. During beta decay, the emitted electron (or positron) is accompanied by a neutrino (or anti-neutrino), with which is shares the energy. The beta-decay energy is the sum of the energies of the electron and neutrino. Thus, for ^{241}Pu, the maximum energy the electron can have is 21 keV; normally, it will have only ~ 1/3 of this. Because the beta particle is singly charged and not very massive, it cannot create nearly the amount of ionization as can an alpha particle. For example, a beta particle traveling through air will create on the order of 100 ion pairs for each centimeter it travels. In addition to causing ionization, beta particles also can be scattered elastically by atomic electrons. Because a beta particle doesn't lose its energy as rapidly as does an alpha particle, and because of elastic scattering, it can penetrate more deeply into tissue. However, it travels an irregular path in tissue because of elastic scattering. This gives rise to the emission of electromagnetic radiation called *bremsstrahlung* (German for "braking radiation"), which in turn can deposit its energy in the surrounding tissue.

The energy of a gamma ray is typically on the order of tens of keV to a few MeV. For example, the energy of one of the (several possible) gamma rays that accompanies the alpha decay of ^{239}Pu is 52 keV. A gamma photon will typically create only about one ion-pair per centimeter in air. A gamma photon can also lose its energy through Compton scattering from electrons and even from interactions with the nucleus of an atom, although the latter are minor in comparison with photoionization and Compton scattering. Gamma radiation is capable of penetrating deeply into the human body.

The energy of a fission neutron is typically on the order of a few keV to about 10 MeV. Because the neutron has no charge, it will not create many ion-pairs. It loses it energy primarily through elastic scattering. However, it can also cause nuclear transformations, especially when it has slowed (through elastic scattering) and become a "thermal" neutron. These nuclear transformations can lead to the emission of other radiation, such as α and γ. Neutron absorption through nuclear transformation is primarily by hydrogen and nitrogen in the body. Elastic scattering of neutrons is primarily by the hydrogen in the body. Like gamma radiation, neutron radiation is very penetrating.

Radioactivity

The *Système International d'Unités* (SI) unit of radioactivity, or simply *activity*, is the *becquerel* (*Bq*). It is equal to one *disintegration per second* (*dps*). The more commonly used, or traditional, unit of activity is the *curie* (*Ci*), and is equal to

$$1 \text{ Ci} = 3.7 \times 10^{10} \text{ Bq}. \qquad (28.a)$$

This unit was derived from the activity of radium. The activity of one gram of ^{226}Ra was originally defined as one *Ci*. (Modern measurements, however, show that the activity of one gram of ^{226}Ra is slightly less than one *Ci*.) Conversely,

$$1 \text{ Bq} = 2.7 \times 10^{-11} \text{ Ci}. \qquad (28.b)$$

The activity per unit mass is called *specific activity* and is measured in units such as *Bq/kg* or *Ci/g*. Thus, the specific activity of ^{226}Ra was originally defined as one *Ci/g*. The specific activity of a mixture of radionuclides is the sum, over all the radionuclides in the mixture, of the products of specific activities and mass fractions.

The activity of a sample of any given radionuclide decreases exponentially with time, providing it is not being created by the decay of another radionuclide. If N is the number of atoms of a specific type of radionuclide in a sample of material, the change in this number, dN, in a small interval of time, dt, is proportional to N and to dt. This is written

$$dN = -\lambda N\, dt \tag{29}$$

where the negative sign is needed to show that N decreases with increasing time. The constant of proportionality, λ, is called the decay (or transformation) constant and is measured in inverse time units, such as s^{-1}. The disintegration rate, or activity (A), is given by

$$A = -dN / dt = \lambda N \tag{30}$$

The solution to equation (29) is

$$N = N_0\, e^{-\lambda t} \tag{31}$$

where N_0 is the number of atoms at time $t = 0$. Thus, equation (30) can be written

$$A = A_0\, e^{-\lambda t} \tag{31}$$

where $A_0 = \lambda N_0$ is the activity at time $t=0$.

Because the decay is exponential, the time interval to decrease the number of atoms in a sample by a given factor is a constant. For example, the time to decrease by a factor of two, called the half-life ($t_{½}$), is obtained by inverting equation (31):

$$t_{½} = -(1/\lambda) \ln (½ N_0 / N_0) = (1/\lambda) \ln (2) = 0.693 / \lambda. \tag{32}$$

The half-life of ^{239}Pu, for example, is 2.44×10^4 years and that of ^{235}U is 7.1×10^8 years. The specific activity of ^{235}U is therefore about 3×10^4 times smaller than that of ^{239}Pu, which is the reason it doesn't present as great a radiological hazard as ^{239}Pu for a given mass.

Effects of Radiation on the Body

Radiation damages the body as it deposits its energy (primarily through ionization) in organs and tissues. Because alpha radiation can be stopped by the body's epithelium (outer layer of dead skin cells), it poses no external hazard to the body; rather, its hazard is through inhalation and ingestion. Beta radiation can penetrate the skin (barely) to cause some damage; beta radiation can also damage the eye. Like alpha radiation, its damage comes principally from inhalation and ingestion, although less so than from alpha radiation. Gamma radiation and neutrons, on the other hand, cause damage as they penetrate the body directly from external sources; material that emits gamma radiation and neutrons can, of course, be inhaled or ingested, but this is not the

normal mode of exposure considered in DSAs. Skin contamination from fallout causes tissue damage principally from β radiation.

Both short-term and long-term exposures are important. External radiation (from cloudshine, groundshine, skin contamination, or prompt radiation) typically gives a short-term, or even instantaneous dose, whereas internal radiation (from inhalation and ingestion) gives a long-term (committed) dose. A long-term dose can also arise from continual exposure to external radiation, as in a work place. If a radioactive particle is inhaled or ingested, it will cause damage as long as it remains in the body, because it contains many radioactive atoms that continue to disintegrate. If an organ or tissue is irradiated for an extended time, it can develop cancer or suffer other deleterious effects.

Dose Evaluation

The effects of exposure to ionizing radiation were originally defined in terms of the amount of ionization in air produced by gamma radiation and X-rays. The unit used was the *Roentgen* (*R*), now defined as the ratio $\Delta Q/\Delta m$, where ΔQ is the sum of all charges of one sign produced in air when all the electrons liberated by photons in a mass Δm of air are completely stopped in air. It is equal to 2.58×10^{-4} coulombs produced in one kg of air. This is equivalent to 1.61×10^{15} ion-pairs produced per kg of air or an energy deposited of 87.3 erg per gram of air (Turner, 1986). Absorption of 1 *R* of radiation in tissue corresponds to about 95 ergs per gram of tissue.

Today, dose is expressed as an absorbed dose, i.e., the amount of energy deposited in matter, or as an equivalent dose, a measure of damage done in tissue. The traditional unit of absorbed dose is the *rad* and is defined as 100 ergs absorbed in one gram of material, slightly greater than the *rep*. The newer (*SI*) unit is the *gray* (*Gy*) and is defined as one joule absorbed in one kilogram of material. Thus,

1 Gy = 100 rad

This definition applies to any type of radiation absorbed in any type of material.

The dose of most interest in accident analysis is the equivalent dose, as this is a measure of the biological damage. The amount of damage depends upon the type of radiation as well as the amount of energy absorbed. The equivalent dose, H_T, to a particular tissue *(T)* is equal to the absorbed dose, D_T, in that tissue times a radiation-weighting factor, w_R

$$H_T = w_R D_T \quad (33)$$

where w_R is a measure of the amount of damage done by the radiation.[30] If more than one type of radiation impacts the tissue, H_T is calculated by summing over all radiation types. Table A-4 gives the radiation weight factors (ICRP-60, 1991) for the four radiation types considered here.

[30] The definitions given here are taken from the *1990 Recommendations of the International Commission on Radiological Protection* (ICRP-60, 1991). In earlier recommendations of the ICRP, the terminology was a little different. The following table gives the old and new terminology.

Old Terminology	New Terminology
Quality Factor	Radiation Weighting Factor
Dose Equivalent	Equivalent Dose
Committed Dose Equivalent	Committed Equivalent Dose
Effective Dose Equivalent	Effective Dose
Committed Effective Dose Equivalent	Committed Effective Dose

The effective dose is not identical to the effective dose equivalent in that the organ weighting factors are slightly different (Table 8) and the organs included in "remainder" are different. A similar statement can be made for the differences between committed effective dose and committed effective dose equivalent.

Table A-4. Radiation Weighting Factors

Type, Energy Range		Radiation Weighting Factor, w_R
Alpha	any energy	20
Beta	any energy	1
Gamma	any energy	1
Neutrons	< 10 keV	5
	10 keV to 100 keV	10
	>100 keV to 2 MeV	20
	>2 MeV to 20 MeV	10
	> 20 MeV	5

The traditional unit for equivalent dose is the *rem* (roentgen-equivalent, man). The newer (*SI*) unit is the sievert (*Sv*). The relation between them is the same as between *gray* and *rad:*

1 Sv = 100 rem.

The radiation-weighting factor is related to the stopping power of the material, expressed as *Linear Energy Transfer* (*LET*)

$$LET = dE / dx \qquad (34)$$

where *dE* is the average energy locally imparted to the medium by a charged particle traversing the distance *dx*. Alpha and beta particles have high and low LET, respectively. Gamma radiation, although not a charged particle, is considered equivalent to low LET radiation. Neutrons have a moderate to high LET, depending upon their kinetic energy.

The definition of equivalent dose does not differentiate between short-term and long-term dose, or between external and internal exposure. A related term is committed equivalent dose, which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults (such as workers) or 70 years for children (as in the general population); it does not include external exposures. The committed equivalent dose is thus a subset of the equivalent dose. This has led to some confusion as it has led some workers to use (incorrectly) equivalent dose exclusively for external radiation, apparently as a counterpoint to committed equivalent dose, which is used exclusively for internal radiation. A new term, total organ dose equivalent (TODE), is now used to indicate the sum of the external (short-term) and internal (committed, long-term) doses to *an organ or tissue* (CFR, 1991).

Doses are also calculated for the body as a whole. This is done by summing over all organs the product of an organ weighting factor and the equivalent dose for that organ. This sum is called the effective dose (formerly, the effective dose equivalent (EDE) – a term still used). The organ

weighting factors represent the fraction of the total health risk resulting from uniform whole-body irradiation that could be attributed to that particular tissue or organ. These factors are between zero and one; their sum over all organs and tissues is one. The weighting factors for the various organs are shown in Table A-5, as taken from ICRP-60 (1991). For comparison, the ICRP-26 (1977) values are also shown, as they are still in use at many sites and laboratories.

Table A-5. Organ Weighting Factors

Organ	Organ Weighting Factor	
	ICRP-26	ICRP-60
Bladder	-	0.05
Bone Marrow (red)	0.12	0.12
Bone Surface (skeleton)	0.03	0.01
Breast	0.15	0.05
Colon	-	0.12
Esophagus	-	0.05
Gonads	0.25	0.20
Liver	-	0.05
Lung	0.12	0.12
Skin	-	0.01
Stomach	-	0.12
Thyroid	0.03	0.05
Remainder	0.30	0.05

A term similar to effective dose is committed effective dose (formerly, the committed effective dose equivalent – CEDE, a term still used), which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults, or 70 years for children. However, it does not include external exposures. Committed effective dose is thus a subset of effective dose. However, as with equivalent dose *cf.* committed equivalent dose, confusion has arisen in that some workers use (incorrectly) effective dose to refer to only external radiation, because committed effective dose refers only to internal radiation. A new term, total effective dose equivalent (TEDE), is now used to indicate the sum of the external (short-term) and the internal (committed, long-term) effective doses (CFR, 1991).

Types of Dose

Doses arise from both internal and external exposures, as noted above. The internal exposures consist of inhalation (from the plume and from resuspension) and ingestion. The external exposures are from cloudshine, groundshine, skin deposition, and direct (prompt) radiation from a criticality. These are discussed individually below. See the discussion earlier in this chapter

for the calculation of the amount of material that falls out from a plume; this is important for the discussions of resuspension, ingestion, groundshine, and skin deposition.

Uptake Through Inhalation

Inhalation dose from a cloud to a given organ or tissue from a given isotope (*i*) is the product of the amount of respirable radioactive material released (M_i), atmospheric dispersion factor (χ/Q), breathing rate (*BR*), and dose conversion factor (DCF_i)

$$\text{Dose}_i = M_i \times \chi/Q \times BR \times DCF_i \quad (35)$$

assuming the receptor remains exposed for the duration of the plume. The total dose to the organ or tissue is the sum over all isotopes inhaled. The amount of respirable material released (M_i) is the product of the material at risk (*MAR*), damage ratio (*DR*), leakpath factor (*LPF*), airborne release fraction (*ARF*), respirable fraction (*RF*), and the atmospheric dispersion factor (χ/Q). The dose conversion factors are discussed below.

Breathing Rate

The breathing rates for the for various activities, as have been used in accident analyses for the past several years at many DOE sites, are given in Table A-6 (ICRP-2, 1977 and ICRP-30, 1979-82). The value used in the development of DOE-STD-1027-92 (Change Notice 1) tables is 3.5 x 10^{-4} m^3/s. ICRP-66 (1994) gives revised breathing for the "reference human"[31]. These are also listed in Table A-6. Still other breathing rates are appropriate for other individuals, such as infants, the elderly, and the infirm, and for other levels of activity (ICRP-66, 1994). The analyst needs to choose which breathing rate is appropriate for the scenario being evaluated, taking into account the possible need to be consistent with earlier analyses.

Recommendation: Based on the DOE (1998) directive, it is advised to apply the breathing rate of 3.33 x 10^{-4} m^3/s in dose calculations.

[31] The reference human is male, 30 years old, height 176 cm (5 feet, 9 inches), and weight 73 kg (161 lb).

Table A-6. "Reference Human" Breathing Rates for Various Levels of Activity

Activity Level	Breathing Rate (m^3/s)
ICRP-2, ICPR-30, DOE 1998	
Chronic	2.66×10^{-4}
Light	3.33×10^{-4}
Heavy	3.47×10^{-4}
ICRP-66	
Sleep	1.25×10^{-4}
Rest, sitting	1.50×10^{-4}
Light exercise	4.17×10^{-4}
Heavy exercise	8.33×10^{-4}

Biokinetic Model and Dose Conversion Factors

Once radioactive material enters the lungs, it begins to migrate to other parts of the body. A portion is transferred directly to the blood and another portion to the stomach. Transfer of the material directly from the lungs into the blood depends upon where in the lungs it is deposited and how soluble it is. Material is also cleared from the lungs by means of the body's mucociliary mechanism and then swallowed, thus entering the gastro-intestinal (GI) tract. The fraction (f_l) of the material that passes from the GI tract into the blood (primarily from the small intestine) depends the solubility of the material. For some radionuclides, such as iodine, the transfer to the blood is nearly complete ($f_l = 1.0$). For others, such as plutonium, the portion transferred to the blood is much less than 1%; the remainder is excreted. Once the material enters the blood, it can be carried to any part of the body. From there, it may preferentially target a given organ or tissue, as determined by the chemical properties of the radioactive material and the nature of the organ or tissue. For example, plutonium and americium become preferentially attached to bone surface (LANL, 1995), and tritium ultimately mixes uniformly with all tissues and organs.

The residence time of a radioactive particle in the lungs depends in part upon the solubility of the material. Three broad categories have been defined, and specify a characteristic half-time for inhaled material to clear from the pulmonary region of the lung to the blood and the gastrointestinal tract (Eckerman, 1988):

- Y: Radionuclides in insoluble compounds typically remain in the lungs for a long time; these are of Solubility Class Y (for years), also called Lung Clearance Class Y.
- W: Radionuclides in moderately soluble compounds remain in the lungs for weeks; these are of Solubility Class W (for weeks), also called Lung Clearance Class W.
- D: Radionuclides in soluble compounds remain in the lungs for only a short time; these are of Solubility Class D (for days), also called Lung Clearance Class D.

According to Federal Guidance Report #11 (EPA, 1988), plutonium compounds can be Class Y (the oxides[32]) or Class W (all other Pu compounds). There are no Class D Pu compounds. Americium compounds are only Class W. Uranium compounds can be Class Y (UO_2 and U_3O_8), Class W (UO_3, UF_4, and UCl_4), or Class D (UF_6, UO_2F_2, and $UO_2(NO_3)_2$). Fission products are of all three classes. Should these compounds be involved in a fire, their chemical nature may change. For example, a plutonium salt (as in certain residues), which is class W, may change to an oxide (class Y) in a fire. However, such conversion will probably not be complete. To be conservative, it is best to assume that the resultant chemical form is the one that gives the largest dose; in the case of plutonium salts, for example, it is conservative to assume they remain class W.

In ICRP Publication 60, the lung clearance class term was dropped in favor of the term lung absorption type. Absorption types fast (F), medium (M), and slow (S) broadly correspond to older lung clearance classes of D, W, and Y (ICRP, 1990).

Dose Conversion Factors

The amount of biological damage that radioactive material may inflict on an organ or tissue is given by the Dose Conversion Factor (DCF) mentioned above. The DCFs take into account the migration of the radioisotope within the body, the decay of the radioisotope, and the formation of daughter isotopes that may be radioactive. For inhalation, this is typically expressed in units of Sv/Bq (or rem/Ci), that can be converted to Sv/g (or rem/g) by multiplying by the specific activity.

The older system of DCFs for a large number of radionuclides is given in Federal Guidance Report #11 (EPA, 1988). FGR 11 contains DCFs based on weighting factors from ICRP 26 (ICRP, 19770 and organ/tissue models documented in ICRP 30 and 48 (ICRP, 1979a to 1982c, and ICRP, 1986). The DCF values in FGR 11 are based on exposure to an adult worker and a particle size of 1.0 μm Activity Median Aerodynamic Diameter (AMAD).[33] The values are applied uniformly for all ages in the general public population and all release conditions.

ICRP Publication 68 provides updated dosimetry for radiation workers, while ICRP 72 covers the general public. Both include age specific models and parameters (ICRP, 1995). The DCFs contained in these reports are based on ICRP 1990 Recommendation on radiation protection standards in Publication 60 (ICRP, 1991a) and as well as the revised kinetic and dosimetric model of the respiratory tract in Publication 66 (ICRP, 1994). The inhalation DCFs in ICRP Publication 68 are for the CEDE and assume either 1.0 μm or 5.0 μm AMAD particle sizes. The inhalation DCFs in ICRP 72 are only for the CEDE and a 1.0 μm AMAD particle.

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[32] Plutonium hydroxides have subsequently been added to Class Y.

[33] The AMAD signifies that fifty percent of the activity in the aerosol is associated with particles of aerodynamic diameter greater than the AMAD.

A combined data set is now available from the ICRP (1999) that not only provides dosimetric information for both worker and general public populations, but extends the parameter space of the ICRP Publications 68 and 72. The combined data gives inhalation dose coefficients for ten aerosol sizes (0.001 μm to 10 μm AMAD) as well as ingestion coefficients. Effective doses and equivalent doses for all important tissues for a range of integration times (1, 7 and 30 days, 1, 5, 10, 20, 30, and 45 years) are given, together with the dose coefficients to age 70 years.

The Nuclear Regulatory Commission and at least one NRC Agreement State have granted license amendments to allow use of the newer ICRP 68/72 dosimetry. The newer data have been approved for use at several DOE sites.

Inhalation (Resuspension)

Dose from resuspension inhalation is primarily of concern after plume passage. The ground concentration (GC_i) of a given isotope (i) under a plume can be calculated by the method discussed earlier, which also discusses resuspension factor (F_r) of this material. The resuspension inhalation dose to a given organ or tissue from this isotope is the product of the ground concentration, resuspension factor, breathing rate, and DCF_i for that organ and radionuclide.

$$Dose_i = GC_i \times F_r \times BR \times DCF_i \quad (36)$$

The total dose to the organ or tissue is the sum of the doses from all isotopes resuspended. Correction factors can also be applied, as appropriate, to account for the receptor being off-centerline (if the GC_i was calculated for plume centerline) and for shielding, such as for the receptor being indoors. Off-centerline considerations and shielding are normally of greater importance for resuspension inhalation than for plume inhalation because resuspension takes place over an extended period and the routine activities of the receptors should be taken into account. This is especially important for inhalation doses to the public. The comparative magnitude of the resuspension dose depends on the amount material deposited on the ground from the plume. If the amount is large, the resuspension inhalation dose over a period of days, weeks, or months can be as large as, or even larger than, the direct inhalation dose from the plume. For dry deposition, the size distribution of the particulates released in an accident is important; very small particles have small deposition velocities, leading to small ground concentrations. For wet deposition, particles of all sizes can be washed out by precipitation. If an accidental release of radioactive particulates occurs during a period of rain or snow, the subsequent resuspension inhalation dose will be much larger than it would be otherwise.

It is noted that the guidance in DOE-STD-3009-94, CN2, Appendix A allows resuspension to be ignored.

Ingestion

Fallout of particulates from a plume may contaminate water and food supplies. The uptake of radionuclides by plants and animals, and their transfer into the food chain for humans, is a very

complex process and beyond the scope of this guidebook. Several models have been developed and incorporated into computer models for atmospheric dispersion and consequence assessment. Consumption of contaminated food products is not restricted to persons living near the site of an accidental release, as the food products may transported to another location for processing, and consuming in still another location. The ingestion dose must therefore be calculated separately from the other doses (from inhalation, etc.). It is not to be added to the doses from the other modes of intake unless it is clear that the receptor for the ingestion dose is the same as the receptor for the other modes of intake.

Once the amount of radioactive material ingested has been determined, the dose can be calculated by multiplying this amount by the DCF for ingestion. Tables of ingestion DCFs for a large number of radionuclides are available from both the older FGR 11/12 series as well as the ICRP 72 series. Like the inhalation DCFs, the units of the DCFs are Sv/Bq (or rem/Ci).

For calculations supporting DSA preparation, ingestion is ignored.

Cloudshine

The amount of gamma radiation (and beta, if appropriate) received by a receptor from a plume of radioactive material depends upon the location of the receptor relative to the plume. The greatest dose would be received by a receptor in the plume centerline, of course, and dose conversion factors have been developed for such a receptor. The assumptions made in deriving these DCFs are that (1) the plume is uniform and semi-infinite ("semi" because the plume extends upward from the ground, but not downward) and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide and the DCF, integrated over the duration of the plume. The doses from all the radionuclides must then be summed. Cloudshine DCFs are expressed in units of $(Sv\text{-}m^3)/(Bq\text{-}s)$.

The cloudshine doses calculated using the DCFs from Federal Guidance Report #12 are conservative because of the assumptions that the receptor is standing upright in a uniform, semi-infinite cloud. The plume, of course, is neither uniform nor semi-infinite, the receptor may not be at plume centerline (and the plume may even be elevated), the receptor may be sheltered, and the receptor may not be standing up. Each of these factors would tend to reduce the dose. Corrections for finite cloud size and distribution (Gaussian) and for receptor locations off-centerline are included in several computer models of atmospheric dispersion and consequence assessment. However, for typical MOI dose-to-an-individual calculations supporting DSA preparation, the effect of structural shielding is conservatively not taken into account.[34]

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[34] In FGR 12 (EPA 1993), the EPA allows the use of a groundshine shielding factor of 0.7 (unitless) to take account of these factors for an individual assumed to be located outdoors

Groundshine

The treatment of groundshine is similar to that of cloudshine. The amount of gamma radiation received by a receptor from radioactive material deposited on the ground (fallout) depends upon the location of receptor relative to the fallout. The greatest dose would be received by a receptor at the center of the fallout, of course, and dose conversion factors have been developed for such a receptor. The assumptions made in deriving groundshine DCFs are that (1) the material is uniformly distributed on the surface or in the soil for an infinite distance in every horizontal direction, and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide on (or in) the ground and the DCF, integrated over the duration of the exposure (i.e., how long the receptor is present to receive groundshine). The groundshine doses from all the radionuclides must then be summed. The concentration to be used in the calculation is either an areal concentration (Bq/m^2), if the material is only on the surface, or a volume concentration (Bq/m^3), if mixed with the soil. Groundshine DCFs are expressed in units of either $(Sv\text{-}m^2)/(Bq\text{-}s)$ for surface contamination, or $(Sv\text{-}m^3)/(Bq\text{-}s)$ for soil contaminated down to a specified depth.

Typically, the groundshine doses calculated using the DCFs the two data series are conservative because of the assumptions that the receptor is standing upright on a uniformly contaminated, infinite plane. The fallout, of course, is neither uniform nor infinite and the receptor may not be the middle of it. Furthermore, surface irregularities (surface roughness and uneven terrain) tend to shield the receptor, the receptor may be sheltered, and the receptor may be elevated. Each of these factors would tend to reduce the dose. Corrections for finite size and distribution of the fallout pattern, and for receptor locations off-centerline, are included in several computer models of atmospheric dispersion and consequence assessment. The safety analyst may also wish to consider additional dose reduction factors associated with sheltering or surface roughness / unevenness.

In calculating groundshine doses, the time variation of the ground concentration at the receptor's location must be considered. In the early stages of plume passage, the ground concentration is increasing, the concentration reaching a peak at the end of plume passage. Resuspension of the particulates then erodes the amount of contamination. The dose received from groundshine therefore must consider not only the exposure duration of the receptor, but also the period during which the exposure is attained. Such considerations are included in several computer models of atmospheric dispersion and consequence assessment.

Skin Deposition

Doses from skin deposition are normally of short duration (a few hours) because of decontamination of the skin. The only radionuclides of importance for skin contamination are the beta emitters. Beta particles can penetrate the surface layer of dead skin cells and damage the cells directly beneath. Experiments show that for beta radiation in the 200 keV to 2 MeV range, the absorbed dose to these cells is about 0.2 rad/s for a surface contamination of 1 Ci/m^2 (Healy, 1984). Because the radiation-weighting factor for beta radiation is one (Table A-4), this equates

to a dose rate of 5.4×10^{-14} (Sv-m^2)/(Bq-s). This dose rate must then be integrated over the duration, T, that the material is on the skin prior to decontamination to give the skin DCF

$$DCF_{skin} = 5.4\times10^{-14} (1 - e^{-\lambda T}) / \lambda \quad (37)$$

The dose to the exposed skin from a given beta-emitting isotope (i) for a receptor at (or under) plume centerline is

$$Dose_{i,skin} = AC_i \times V_d \times DCF_{skin} \times F \quad (38)$$

where AC_i is the ground-level air concentration of this isotope, V_d is the deposition velocity to the skin (on the order of 1 cm/s or less, depending upon the particle size distribution), and F is the fraction of the plume duration that the receptor is exposed to the plume. Correction factors need to be applied for receptors off-centerline or that are sheltered. The total skin dose will be the sum of the contributions from all the beta-emitters that are deposited on the skin.

Direct (Prompt) Dose

Doses from criticalities arise from both the plume of fission products that may be released and from prompt radiation, i.e., the gamma rays and neutrons that are emitted during the brief (millisecond) energy burst(s) during the criticality spike(s). The doses from the plume of fission products are included in the discussions above and won't be repeated here.

The prompt dose depends only upon the number of fissions in the criticality, the distance to the receptor, and the amount of intervening shielding material, such as concrete. The gamma and neutron doses should be quantified using nuclear engineering principles.

Shielding is expressed in terms of the amount of intervening concrete, or the equivalent if other shielding materials are involved. In the case of gamma radiation, the dose is reduced by a factor of 2.5 for the first eight inches of concrete, a factor of 5.0 for the first foot, and a factor of 5.5 for each additional foot. For neutron radiation, the dose is reduced by a factor of 2.3 for the first eight inches of concrete, a factor of 4.6 for the first foot, and a factor of 20 for each additional foot.

Prompt dose is important for the immediate worker, i.e., one within some tens of meters from the accident, but is rarely important for persons more distant. The dose to a collocated worker at a distance of 100 m is normally small and the dose to the public is negligible.

Health Risks

The discussion in the following sections is added for completeness, because the DOE-STD-3009-94, CN2 Appendix A calculation is concluded upon calculation of individual doses.

Once doses have been calculated, the corresponding health risks can be determined. This is done by multiplying doses by stochastic risk factors. Latent Cancer Fatalities (LCFs) are the health risks of most interest. The term "latent" indicates that the estimated cancer fatalities would occur

sometime in the future, within the next 50 years for adults, or the next 70 years for the general population, which includes children. One can also calculate latent cancer occurrences (fatal plus non-fatal), genetic effects, etc., but these are not normally evaluated in safety analyses. The stochastic risk factor depends upon the type of radiation and the organ considered.

High-LET Radiation

In the case of alpha emitters, such as Pu and U, the only organs of importance for cancer risk are the lungs, liver, and bone surface (Abrahamson, 1993). The stochastic risk factors for cancer fatalities for these organs are shown in Table A-7. For these three organs, the stochastic risk factors are linear and continuous. Earlier models, based on ICRP-26 (1977), used a linear-quadratic model. The new model, based on ICRP-60 (1991), is linear but may be discontinuous for some radionuclides. The Abrahamson (1993) values (Table A-7) differ from the earlier ones (ICRP-26): the lung factor is about four times larger, the bone skeleton factor is about ten times smaller, and liver is about three times smaller than the earlier values. The values in Table A-7 are for high-LET radiation (alpha particles). Table A-7 does not give the stochastic risk factor for committed effective dose, as the total cancer risk should be calculated as the sum of the individual organ cancer risks [Σ (dose $\times$ stochastic factor)]. The other organs of the body do not contribute significantly to cancer risk from exposure to alpha radiation and have been ignored.

Table A-7. Stochastic Risk Factors for Alpha-Emitters (Abrahamson, 1993)

ORGAN	RISK FACTOR *(LCF/rem)*
Bone Surface	6.0×10^{-7}
Lungs	8.0×10^{-5}
Liver	1.5×10^{-5}

Example: A calculation of committed inhalation doses to a certain receptor from a release of plutonium gives a bone-surface dose of 0.353 rem, a lung dose of 0.112 rem, and a liver dose of 0.0787 rem; the effective dose (whole body) was 0.0351 rem. (The effective dose includes contributions from all organs, not just the three mentioned here.) For this individual, the LCF risk would therefore be $(0.353)(6.0 \times 10^{-7}) + (0.112)(8.0 \times 10^{-5}) + (0.0787)(1.5 \times 10^{-5}) = 1 \times 10^{-5}$ LCF. This means that only one person in 10^5 would die of cancer from this exposure. Note that although the bone dose is larger than the doses to the other organs, the lung dose is more important in terms of cancer risk, as seen in this example.

Low-LET Radiation

For low-LET radiation (beta and gamma radiation), the latent cancer risk is normally calculated from the committed effective dose, although the individual organ cancer risks could also be summed. ICRP-60 (1991) recommends using a stochastic risk factor of 5×10^{-4} LCF/rem

(5×10^{-2} LCF/Sv) for the whole population, or 4×10^{-4} LCF/rem (4×10^{-2} LCF/Sv) for adult workers, based on the committed effective dose. (The factor for the public is higher than for adult workers because the public consists of a mixture of individuals with varying degrees of resistance to hazardous materials, including children, the elderly, and the infirm. This includes the cancer risk to all organs, unlike the treatment of alpha radiation, which considers only the three organs of Table A-7 to be important for cancer risk.) This ICRP-60 recommendation has been adopted by the Environmental Protection Agency for the evaluations of Environmental Assessments (EAs) (NEPA, 1993). Had this factor been used in the above example, the LCF risk to that individual would have been $(0.0351)(5 \times 10^{-4}) = 1.75 \times 10^{-5}$ LCF, or about 75% higher than obtained from using Table A-7 data. This low-LET risk factor is not recommended for alpha-emitters (high LET).

Acute Health Risks

Doses received in a short period (acute doses) may cause acute health risks, if large enough. A dose from gamma or neutron radiation, such as from a criticality, is the primary concern here. Table A-8 (adapted from Turner (1986)) summarizes the health effects associated with varying levels of gamma radiation.

Table A-8. Acute Radiation Effects for Gamma Radiation

DOSE (rad)	HEALTH EFFECT
0 -25	No detectable effect
25 - 100	Some biological damage; recovery probable
100 - 300	More damage; recovery probable but not assured
300 – 600	Fatalities occur in about half the population
> 600	Death expected

An acute, whole-body, gamma-ray dose of about 450 – 500 rad would probably be fatal to about half the population within about 30 days. This dose is known as LD_{50}, sometimes called $LD_{50/30}$, where "LD" means Lethal Dose. Because gamma radiation has a radiation-weighting factor of one (Table A-4) the doses in Table A-8 could also have been labeled in rem. Presumably, neutron doses (in rem) would give similar effects.

An acute dose from inhalation of plutonium or uranium, i.e., the dose received in a few hours or days, is normally very small. All of the isotopes of plutonium and uranium have half-lives of many years; therefore, the inhalation dose received by a person during the first few days following an acute exposure via the inhalation pathway will only be a small fraction of the lifetime dose. Accordingly, an acute health effect requires a very large amount of plutonium to

be released. For example, in order for a person at a distance of about 2 km from the release site to get a dose large enough to cause pneumonitis (the first prompt health effect to occur), an airborne release of about 100 kg of respirable plutonium would be required (Peterson, 1993). Such a large release is extremely unlikely. Therefore, *acute* health effects need not be considered for releases of plutonium or uranium.

Radiation Protection

Radiation protection of the worker is governed by the As Low As Reasonable Achievable (ALARA) principle. Control of internal exposure to radionuclides is based on the limitation of the sum of current and future doses from annual intake (i.e., the committed effective dose equivalent) rather than of annual dose. If it is found that limits on committed dose have been exceeded for a worker, corrective actions are needed to limit further exposure.

The primary guides for worker annual exposure are 5 rem for effective dose equivalent, 50 rem to individual organs or tissues (except the lens of the eye), and 15 rem to the lens of the eye. Two types of derived guides are used to implement this. These are the Annual Limit on Intake (ALI) and the Derived Air Concentration (DAC). The ALI is the annual intake of a radionuclide that would result in a radiation dose to the reference man equal to the relevant primary guide. The DAC is the air concentration of a radionuclide that would result in an intake corresponding to its ALI, if breathed for a work-year (2,000 hours).

The above guidance of comparing the annual exposure limit (primary guide) with the full 50-year (or 70-year) committed effective dose received is found in several DOE and EPA documents. For dose calculations supporting DSAs, the dose should be calculated using the full fifty-year commitment, following conservative health protection and radiological practices. The newer dose conversion factor methodology and biokinetics models as described in ICRP 60, 66, and ICRP 68/72 are recommended. The older FGR guidance can be used as an alternative should local agreements still support use of the earlier dose conversion data.

APPENDIX B. SOFTWARE DEFECT NOTIFICATIONS

MACCS2 Software Package Sandia National Laboratories	**Software Defect Notification**

1. Date: 5/26/98
2. Log Number: M2V1-12A
3. Computer Code: ☒ MACCS2 ☐ COMIDA2 ☐ FGRDCF ☐ IDCF2 ☐ DOSFAC2
4. Computer Code Version Number: Version 1.12
5. Defect Classification: ☒ Major ☐ Minor
6. Does the defect still exist? ☒ Yes ☐ No · Defect to be corrected in MACCS2 V1.13

7. Brief Description of Defect:
When multiple source terms are specified in a single calculation, that is, when the source term change case is invoked in the ATMOS input file by specifying a change record set (ref. Section 5.11 of MACCS2 User's Guide, Vol. 1, SAND97-0594, NUREG/CR-6613), certain parameters specified to be changed will be incorrectly implemented. The source term change case parameters that are involved in the defect are: PSDIST (particle size distribution by group), SIGYINIT and SIGZINIT (initial values for σ_y and σ_z), BUILDH (building height), and some of the released inventory in the fourth plume segment. The source term change case parameters that are not affected by the defect are: PLHEAT (plume heat), PLHITE (plume height), PLUDUR (plume duration), PDELAY (plume release time), REFTIM (plume reference time point), and the inventories of the first 3 plume segments.

8. Brief Description of Evaluation/Impact:
Parameters PSDIST, SIGYINIT, SIGZINIT, BUILDH, and the inventory of the 4th plume segment will be incorrectly implemented if they are specified to be changed in the source terms that follow the initial source term specification. The specified changes for these parameters are actually implemented in the previously defined source term. For example, suppose a user specifies an initial source term with 4 plume segments and then uses 5 source term change cases for a total of 6 source terms in the calculation. In each new source term the following parameters are specified to be changed: plume duration, initial σ_y and σ_z specifications, and release fractions for all 4 plume segments. The 4th plume segment inventory and the σ_y and σ_z values which will be corrupted in the first 5 source terms, all other source term parameters will be implemented correctly (the only entirely correct source term is the 6th and final one).

9. Recommendations:
Avoid using the source term change case feature in MACCS2, or only specify changes for the unaffected parameters listed in Item 7 above.

10. Expected Corrective Actions:
The defect will be corrected in the next release of MACCS2 (Version 1.13)

Julie Gregory	Julie Gregory	5/26/98
Recorded by	Signature	Date

MACCS2 Software Package Sandia National Laboratories	**Software Defect Notification**

1. Date: 5/26/98
2. Log Number: M2V1-12B
3. Computer Code: ☒ MACCS2 ☐ COMIDA2 ☐ FGRDCF ☐ IDCF2 ☐ DOSFAC2
4. Computer Code Version Number: Version 1.12
5. Defect Classification: ☒ Major ☐ Minor
6. Does the defect still exist? ☒ Yes ☐ No Defect to be corrected in MACCS2 V1.13

7. Brief Description of Defect:
   When multiple (up to 3) emergency response scenarios are specified in the EARLY input file (ref. Section 6.6.1 of MACCS2 User's Guide, Vol. 1, SAND97-0594, NUREG/CR-6613), certain parameters specified in a new emergency response definition will cause errors to result in the EARLY module calculation. The parameters that are involved in the defect are: RESCON (resuspension concentration coefficient) and RESHAF (resuspension concentration halflife); although these two parameters are not typically used in an alternate emergency response strategy, they potentially may be used. All other parameters that may be specified in an alternate emergency response do not involve the defect.

8. Brief Description of Evaluation/Impact:
   Specification of new values for the parameters RESCON and RESHAF in an alternate emergency response scenario in the EARLY input will result in erroneous results (not only for the alternate scenario, but for the initially specified response scenario).

9. Recommendations:
   Do not define alternate emergency response scenarios that involve the parameters RESCON or RESHAF.

10. Expected Corrective Actions:
    The defect will be corrected in the next release of MACCS2 (Version 1.13)

Julie Gregory		5/26/98
Recorded by	Signature	Date

APPENDIX C. LIMITED PARAMETRIC STUDY ON MACCS/MACCS2 TREATMENT OF PLUME BUOYANCY AND WAKE FLOW

A limited parametric study was performed of the models used in MACCS/MACCS2 to incorporate the effects of buoyancy and a building wake on atmospheric dispersion of plumes from an accidental release.[35] The following cases were run in the limited parametric study.

Table C-1. Cases for Limited Parametric Study on Plume Buoyancy and Wake Flow

Case Description	Atmospheric Stability Class D		SRS 50% Meteorological Conditions
	Wind Speed of 4.5 m/s	Wind Speed of 2.3 m/s	
Simple Gaussian Plume[1]	•	•	
Plume with Building Wake Effects[2]	•	•	
Buoyant Plume[3]	•	•	
Buoyant Plume with Building Wake Effects[2,3]	•	•	•

[1] Nonbuoyant plume released under open-field conditions

[2] Building has dimensions of 20-m high x 50-m wide x 50-depth

[3] Rate of sensible heat release, 10 MW

In the parametric study centerline χ/Q dilution factors for ground-level releases based on a 30-minute averaging time are calculated for each case with the assumption of no plume depletion from deposition mechanisms. Dilution factors are calculated at downwind distances of 100 m, 200 m, 500m, 1 km, 5 km, and 10 km. The critical wind speed calculated for a 20-m high facility and with concurrent 10 MW sensible heat release, using the Briggs threshold equation is 3.4 m/s (Equation (27) in Appendix A of this report).

Results for the 4.5-m/s cases are shown in Figure C-1, and results for the 2.3-m/s cases are shown in Figure C-2. The case for SRS median (50^{th} percentile) meteorological conditions is shown in both figures and serves as a baseline case to facilitate comparisons between the two sets of results.

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[35] The calculations were performed using MACCS 1.5.11.1 but similar results as presented in this appendix would be expected with MACCS2.

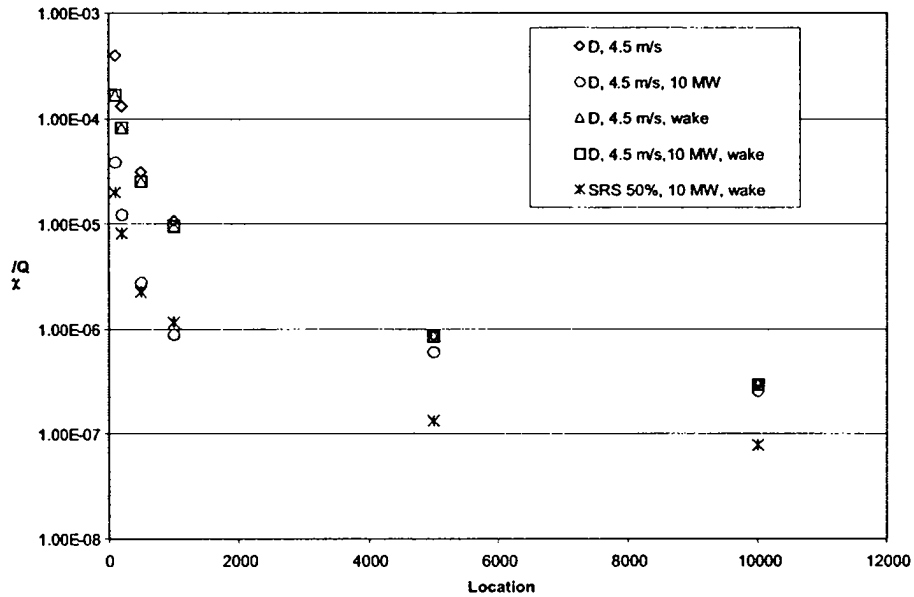

Figure C-1. MACCS results for buoyant plume with building wake effects (4.5 m/s wind speed)

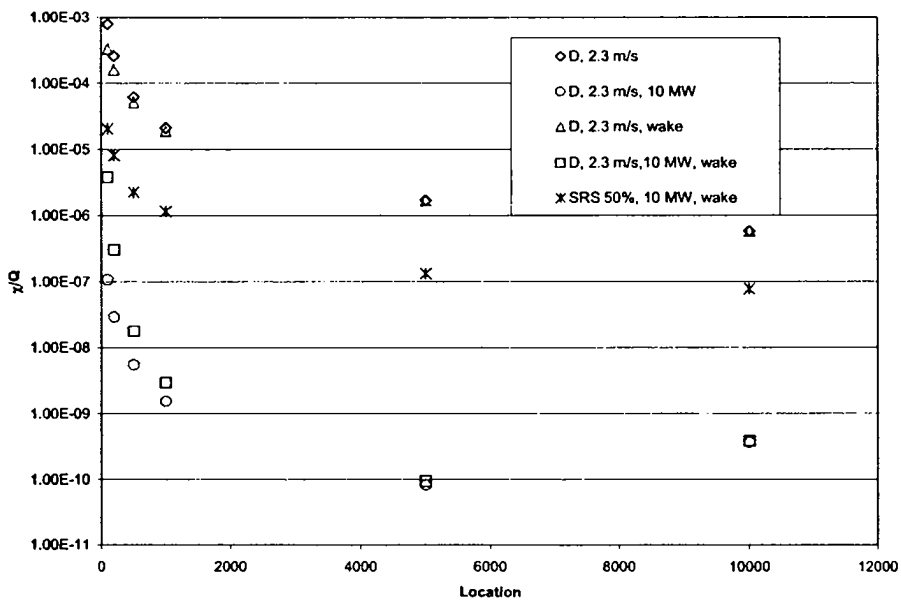

Figure C-2. MACCS results for buoyant plume with building wake effects (2.3 m/s wind speed)

General trends that are observed in both figures are as follows:

- The highest centerline χ/Q values (representing highest downwind concentrations) are calculated with the simple Gaussian plume cases. Adding buoyancy and/or wake effects reduces ground-level concentrations with respect to the simple Gaussian plume case. Buoyancy induces plume rise that results in lower ground-level concentrations. The building wake increases the initial dispersion of the plume in the horizontal and vertical directions, resulting in lower ground-level centerline concentrations. For the building dimensions used in the calculations, building-wake effects essentially become insignificant for non-buoyant plumes at distances beyond 1 km. For the 2.3-m/s and 4.5-m/s sets of results, the calculated downwind concentrations at distances of ≥1 km for the building-wake cases with the non-buoyant plumes are within 10% (slightly lower) of those for the corresponding simple Gaussian plume.

- The lowest centerline χ/Q values (representing lowest downwind concentrations) are calculated with the buoyant plume case. For the building dimensions and sensible heat rate input considered in the limited parametric analysis, the plume rise has a larger effect in reducing ground level consideration than does the building-wake effect. The explanations for why the combined effects of buoyant-plume and wake effects produce higher downwind concentrations compared to those from buoyant-plume effects alone are discussed below. Different phenomena are responsible for this trend for the two wind speeds used in the analysis.

With a wind speed of 4.5 m/s that is above the 3.4 m/s liftoff criterion, the results for the combined effects of plume buoyancy and the building wake are identical to those calculated for building-wake effects alone. MACCS uses a liftoff criterion that is based on a critical wind speed that is a function of the buoyancy flux and the building height. The buoyancy flux is directly proportional to the sensible heat rate of release as discussed in the body of this document. If wind speed is high enough, then the plume does not escape the building wake and the buoyancy has no effect. The critical wind speed (liftoff criterion) defines the maximum wind speed that will allow the buoyant plume to escape from the wake and rise as it travels downwind. Both a high sensible heat rate and small building height support a high critical wind speed. For the first two non-wake cases (D stability and 4.5 m/s wind speed), the results indicate that the 10 MW sensible heat provides about an order of magnitude lower dilution factor than without sensible heat. The effect is important close-in but grows negligibly small after 3 to 4 km. For the sensible heat rate input and building dimensions considered, because the 4.5 m/s wind speed implies that the plume is not escaping, MACCS is initializing the plume dimensions in the same manner for the wake cases regardless of whether 10 MW sensible heat is added. For the 50-m square and 20-m high facility assumed, the initial plume lateral and vertical dimensions are σ_{y0} = 50 m/4.3 = 11.6 m, and σ_{z0} = 20 m/2.15 = 9.3 m.

The wind speed of 2.3 m/s is below the 3.4 m/s critical wind speed, and the results of Figure C-2 show that plume buoyancy is now factored into the results. Here the downwind concentrations for the combined effects of plume buoyancy and the building wake are substantially lower than those calculated for building-wake effects alone. They are also slightly higher than those

calculated for plume-buoyancy effects alone for distances in the first 1000 m to 2000 m. For the case combining the effects of plume buoyancy and the building wake, the plume rises but the increased dispersion from the building wake increases the vertical spread of the plume and increases concentrations in the portion of the plume that contacts the ground. Thus, the ground-level concentrations are higher compared to those from a buoyant plume released in an open field for the first 2000 meters of plume travel. After this distance the dilution factors are about the same.

With D stability, and plume rise "allowed", the model applied in MACCS is Equation (23) of Appendix A of this report. Applying this formulation indicates that plume rise would continue until a distance of approximately 5820 m at which point the plume has grown to the mixing layer height (~1000 m). From that distance to points farther downwind the dilution factors for the thermally buoyant cases (with and without wake effects) start increasing and in time will be similar to the non-buoyant cases.

For additional insights, comparisons can be made between the 2.3-m/s and 4.5-m/s wind speed results for similar cases. First to be examined are the cases involving nonbuoyant plumes, namely, the simple Gaussian plume and plume with building wake effects. For both of these the 2.3-m/s wind speed concentrations are approximately twice as large as the corresponding 4.5-m/s wind speed concentrations. This trend reflects the inverse proportionality of downwind concentration with respect to wind speed in the Gaussian model as shown in Equations (1) and (2) from Appendix A of this report. In the other two cases that involve buoyant plumes, the trend is drastically different. For buoyant plumes, the 4.5-m/s wind speed yields higher concentrations that are more than a magnitude higher than the corresponding 2.3-m/s wind speed concentrations. The plume rise from buoyancy is more pronounced under lower wind speed conditions.

Similar comparisons have been reported previously. One study compared the relative capabilities for MACCS2 and an updated WAKE model from HGSYSTEM/UF_6 for a large facility release, with and without wake effects and plume buoyancy (Lombardi, 1998). It was concluded that MACCS was limited in its treatment of close-in, wake-impacted releases, and also in predicting all or nothing entrainment based on ambient wind speed alone.

The authors of this report recommend MACCS results be carefully reviewed and checked with independent calculations for cases where sensible heat and building wake influence effects are included. It is important to be aware that the combined effects of buoyant-plume and wake effects generally produce higher downwind concentrations compared to those from buoyant-plume effects alone. Only well-defined fires (time sequence, spatial definition, and sensible heat release) should be modeled with any atmospheric code, especially in terms of the initial plume behavior. Furthermore, the MACCS-predicted consequences for the first several hundred meters of plume travel should be applied cautiously.

APPENDIX D. INPUTS AND RECOMMENDATIONS FOR MACCS 1.5.11.1 APPLICATIONS

Section 4.0 of the main body of the report provides guidance for specifying inputs when using the MACCS2 computer code. This appendix provides parallel guidance for specifying inputs when using the earlier version of the code, namely, MACCS 1.5.11.1 (referred to as simply MACCS in the discussion below).

General Notes

For MACCS, all values not in quotes must be in UPPER case.

Quote marks should be single straight quote marks (i.e. 'input value') not smart quotes marks (i.e. ‘input value’)

The MACCS naming convention for input parameters is as follows:

Characters one and two indicate the date block

Characters three to eight indicate the variable name

Characters nine to eleven indicate the line of data being entered (there must always be eleven characters in the input parameter name)

The MACCS naming convention for user requested output is as follows:

Characters one to five indicate the output type

Characters six to eleven indicate either the number of requested input or the specific output requested

The discussion in this section is based on the MACCS User's Guide (Chanin, 1990) and the MACCS Model Description (Volumes 1 and 2, Chanin, 1990). For each section of input, page-specific references to the MACCS User's Guide (NUREG/CR-4691, Vol. 1 – page X-Y) is provided. This will allow the DOE safety analyst to review the original report from the SNL code developer to check directly a specific variable.

ATMOS Input File

The particular ATMOS input file commented upon here is used because it is one of the sample files (e.g., IN1A.INP) supplied with the software from RSICC.

This section of the document addresses variables that may be changed during a normal execution of MACCS for input into a safety basis document or must be selected by the user for a specific location. If a variable is not explicitly mentioned, it need not be changed.

Identification Data Block (RI) *NUREG/CR-4691, Vol. 1 – p. 12*

Variable ATNAM1 (ATMOS input file identifier line)
Line within MACCS IN1A.INP sample file:

```
RIATNAM1001  'IN1A.INP, SURRY, SAMPLE PROBLEM A, ATMOS INPUT'
```

For a specific application:
Change to a descriptive title for this execution of MACCS.

Geometry Data Block (GE) *NUREG/CR-4691, Vol. 1 – p. 13*

Variable NUMRAD and SPAEND (Number of radial grid endpoints and locations of radial grid endpoints)
Lines within MACCS IN1A.INP sample file:

```
GENUMRAD001  26
*
GESPAEND001      .16       .52      1.21      1.61      2.13
GESPAEND002     3.22      4.02      4.83      5.63      8.05
GESPAEND003    11.27     16.09     20.92     25.75     32.19
GESPAEND004    40.23     48.28     64.37     80.47    112.65
GESPAEND005   160.93    241.14    321.87    563.27    804.67
GESPAEND006  1609.34
```

For a specific application:

If population data is being used, the MACCS grid supplied in the software package transmittal should be sufficient. However, distances past 80.5 km (50 miles) should be eliminated. If a consequence at a single receptor point is required, the following lines, or similar lines, may be used:

```
GENUMRAD001  35
*
GESPAEND001    0.20   0.30   0.40   0.50   0.60   0.70   0.80
GESPAEND002    0.90   1.00   1.50   2.00   2.50   3.00   3.50
GESPAEND003    4.00   4.50   5.00   5.50   6.00   6.50   7.00
GESPAEND004    7.50   8.00   8.50   9.00   9.50  10.00  10.50
GESPAEND005   11.00  11.50  12.00  12.50  15.00  20.00  30.00
```

If the location of interest is not a midpoint of two of these endpoints, the two closest to the location may be changed.

Note:

If meteorological data is sampled based on binning of like conditions, values must be included here that are within 10% of the rain interval endpoints that are specified though the RNDSTS variable of the M4 data block.

Nuclide Data Block (IS) *NUREG/CR-4691, Vol. 1 – p. 14*

Variable NUMISO (Number of radionuclides)
Line within MACCS IN1A.INP sample file:

```
ISNUMISO001 60
```

For a specific application:
Change to the number of radionuclides being released. This number must be 150 or less. If the number of radionuclides is greater than 150, either the inventory must be divided into groups with a maximum of 150 radionuclides, or only those radionuclides that contribute to the overall TEDE should be retained. A useful rule of thumb is approximately 0.1% - below which radionuclides are not considered because they contribute insignificantly to the dose.

Variable WETDEP and DRYDEP (Wet and dry deposition flags as inputted by DEPFLA)
Line within MACCS IN1A.INP sample file:

```
ISDEPFLA001     .FALSE.    .FALSE.
ISDEPFLA002     .TRUE.     .TRUE.
ISDEPFLA003     .TRUE.     .TRUE.
ISDEPFLA004     .TRUE.     .TRUE.
ISDEPFLA005     .TRUE.     .TRUE.
ISDEPFLA006     .TRUE.     .TRUE.
ISDEPFLA007     .TRUE.     .TRUE.
ISDEPFLA008     .TRUE.     .TRUE.
ISDEPFLA009     .TRUE.     .TRUE.
```

For a specific application:
For the noble gases group, both values should be set to ".FALSE." For the other groups, the first value should always be ".FALSE." indicating no wet deposition. When dry deposition is used, the second value should be set to ".TRUE."

Variable MAXGRP (Number of chemical groups)
Line within MACCS IN1A.INP sample file:

```
ISMAXGRP001 9
```

For a specific application:
This is simply the total number of groups determined above with a minimum value of 1 (all radionuclides are modeled in the same manner) and a maximum

value of 10. Typically this value will be 3 or less (group 1 – noble gases, group 2 – tritiated water vapor, and group 3 – all other radionuclides).

Variable NUCNAM, PARENT, IGROUP, and HAFLIF (Radionuclide name, parent radionuclide, chemical group, and half-life as inputted by OTPGRP)
Line within MACCS IN1A.INP sample file:

```
ISOTPGRP001     CO-58       NONE       6       6.160E+06
ISOTPGRP002     CO-60       NONE       6       1.660E+08
ISOTPGRP003     KR-85       NONE       1       3.386E+08
  .
  .
  .
ISOTPGRP060     CM-244      NONE       7       5.712E+08
```

For a specific application:
The selection of the chemical groups is based on similar release fractions and plume removal mechanisms (i.e. wet and dry deposition). For example, both noble gases and tritiated water vapor have a release fraction of 1.0, but the noble gases are not subjected to either removal mechanism while tritiated water vapor can be removed by both wet and dry deposition mechanisms. Thus, noble gases would be in one chemical group, and tritiated water vapor would be in another.

Wet Deposition Data Block (WD) *NUREG/CR-4691, Vol. 1 – p. 17*

These values should not be changed.

Dry Deposition Data Block (DD) *NUREG/CR-4691, Vol. 1 – p. 18*

Variable NPSGRP (Number of dry deposition velocity groups)
Line within MACCS IN1A.INP sample file:

```
DDNPSGRP001    1
```

For general application:
Set this value to the maximum number of dry deposition velocities groups to be used in a majority of site analyses. Typically this value will be 3 (one group will be for releases passing through a filtration system; one group will be for releases straight to environment; and one group will be for tritiated water vapor).

Variable VDEPOS (Dry deposition velocities)
Line within MACCS IN1A.INP sample file:

```
DDVDEPOS001    0.01    (VALUE SELECTED BY S. ACHARYA, NRC)
```

For general application:

Typically, the line will be:

```
DDVDEPOS001   0.001  0.005 0.010
```

The dry deposition velocity of 0.001 m/s is appropriate for releases passing through a filter before being released into the atmosphere as well as those not passing through a filter depending on release and environmental conditions. The 0.001-m/s deposition velocity is consistent with a particle with an aerodynamic equivalent diameter (AED) of 0.2 to 0.4 microns (Sehmel, 1978). The dry deposition velocity of 0.005 m/s is an approximate value for tritiated water vapor (Fallon, 1983; Sweet, 1984). The dry deposition velocity of 0.01 m/s is appropriate for unfiltered releases straight into environment and corresponds to particles with an AED between 2 to 5 microns (Sehmel, 1978).

Additional discussion on the topic was presented earlier in Appendix A, and in the NRC reference for recommended MACCS inputs (NRC, 1990b).

Dispersion Data Block (DP) *NUREG/CR-4691, Vol. 1 – p. 19*

Variable YSCALE (Scaling factor for sigma y)
Line within MACCS IN1A.INP sample file:

```
DPYSCALE001    1.
```

For a specific application:
Normally this value should not be changed. However, if a duration longer than 10 hours is absolutely needed. This value may be changed to calculate a dose from a release of up to 100 hours (the upper valid range of the model). The longer release duration correction factor is calculated by dividing the new duration in seconds by 180 seconds and raising the quotient to the 0.25 power. The release duration (variable PLUDUR in the RD data block) must be set equal to 180 seconds. If the user changes the 180-second basis, e.g. use of a new dispersion set with a ten-minute basis, then this must be reflected in the calculation.

Variable ZSCALE (Scaling factor for sigma z)
Line within MACCS IN1A.INP sample file:

```
DPZSCALE001    1.27
```

For general application:
The calculation of this variable is discussed in Appendix A under surface

roughness, and is calculated as $(z_{new}/z_{ref})^{0.2}$, where the quotient of the new and reference surface roughness length is raised to the power of 0.2 Thus, the scaling factor as a function of surface roughness length , which approximately equals one-tenth of the height of roughness obstacles (Hanna, 2002), is

Obstacle Height	30 cm	100 cm	10 m
Surface Roughness Length	3 cm	10 cm	100 cm
σz correction	1.	1.27	2.02

The surface roughness parameter is region-of-transport specific and should be changed to be consistent for the environment surrounding facility in question.

Variable CYSIGA, CYSIGB, CZSIGA, and CZSIGB (Linear and Exponential Terms for sigma y and sigma z)
Line within MACCS IN1A.INP sample file:

```
DPCYSIGA001   0.3658   0.2751   0.2089   0.1474   0.1046   0.0722
DPCYSIGB001    .9031    .9031    .9031    .9031    .9031    .9031
DPCZSIGA001   2.5E-4   1.9E-3      .2       .3       .4       .2
DPCZSIGB001    2.125   1.6021    .8543    .6532    .6021    .6020
```

For a specific application:
These values should be set once for the dispersion parameter set being applied. However, if an individual location has a specific set of linear and exponential terms for sigma y (σ_y) and sigma z (σ_z), then those values should be used.

Plume Meander Data Block (PM) *NUREG/CR-4691, Vol. 1 – p. 21*

Variable TIMBAS (Time base for the parameterization of the plume meander adjustment factor (seconds).)
Line within MACCS IN1A.INP sample file:

```
PMTIMBAS001    600.   (10 MINUTES)
```

For general application:

This value should be set once and not changed.

If the values based on the Project Prairie Grass are being used as given in the sample MACCS input, set the value to three minutes (180. s) (NRC, 1990b).

If another set of dispersion coefficients are being used, the value should be consistent with the time-basis of those experiments.

Plume Rise Data Block (PR) *NUREG/CR-4691, Vol. 1 – p. 23*

These values should not be changed.

Wake Effects Data Block (WE) *NUREG/CR-4691, Vol. 1 – p. 24*

Note: The building size may not be credited if a stack release is being modeled.

Variable BUILDW (Width of the building)
Line within MACCS IN1A.INP sample file:

```
WEBUILDW001   40.  *  SURRY
```

For a specific application:
Normally this value should be set equal to its minimum value of 1.0, and implies no credit is taken for the size of the building. If the building is credited, the width should be set equal to the average of the sides of the building. Use of this parameter will initialize the plume lateral standard deviation, σ_{y0}, to W/4.3 (Chanin, 1990).

Variable BUILDH (Height of the building)
Line within MACCS IN1A.INP sample file:

```
WEBUILDH001   50.  *  SURRY
```

For a specific application:
Normally this value should be set equal to its minimum value of 1.0, and implies no credit is taken for the size of the building. If the building is credited, the value used here is the actual height of the building, H, and the initial vertical standard deviation, σ_{z0}, will be set to H/2.15 (Chanin, 1990).

Release Description Data Block (RD) *NUREG/CR-4691, Vol. 1 – p. 25*

NOTE: All values in this data block may be changed using a change case.

Variable ATNAM2 (Source term identifier)
Line within MACCS IN1A.INP sample file:

```
RDATNAM2001 'SECOND DRAFT 1150, WORST CASE SOURCE TERM FOR EARLY FATALITIES'
```

For a specific application:
Change the entire character string to identify the source term.

Note:

A unique identifier must be used for each case

Variable NUMREL (Number of plume segments being released)
Line within MACCS IN1A.INP sample file:

```
RDNUMREL001          2
```

For a specific application:
Change to the number (≤ 4) of plume segments defined in the source term. If more than four plume segments are defined, the activity of consecutive source terms may be added together if they have the same release duration, release height, and sensible heat rate. The release duration of the combined plume segments is the same as the individual plume segments.

Variable REFTIM (Representative time point for each plume)
Line within MACCS IN1A.INP sample file:

```
RDREFTIM001        0.00       0.50
```

For a specific application:
The representative time point for each plume should be zero (0.00).

Variable PLHEAT (Sensible heat rate of each plume segment)
Line within MACCS IN1A.INP sample file:

```
RDPLHEAT001      3.7E+6      1.7E5
```

For a specific application:

If the sensible heat rate is credited and the release mechanism is an explosion, the energy of the event can be divided by sixty seconds, as a conservative reduction. This will underpredict the sensible heat rate of the event by at least an order of magnitude as explosions are normally much less than one minute in duration.

The sensible heat option in MACCS should be applied only for well-defined fires. Credit only sensible heat fraction for the thermal buoyancy effect, and apply conservative spatial factors to account for area-type fires. Assume shortest duration consistent with fire sequence definition.

Variable PLHITE (Release height of each plume segment)
Line within MACCS IN1A.INP sample file:

```
RDPLHITE001         0.         0.
```

For a specific application:
If the release height is not defined in the given source term, this value should be set equal to zero meters for each plume segment. If the release is elevated and the release height is not at least 2.5 times the tallest collocated building height, the release height is set equal to zero.

Variable PLUDUR (Plume duration of each plume segment)
Line within MACCS IN1A.INP sample file:

```
RDPLUDUR001       1800.     22000.
```

For a specific application:
If the release duration is not defined in the given source term, this value should be set equal to 180 seconds (or the value of TIMBAS defined in the expansion factor data block) for each plume segment. The value range on this parameter is from the TIMBAS value (180 seconds) to 36000 seconds (10 hours). Release duration of longer than 10 hours are calculated by setting the duration of the plume segment to TIMBAS and applying the appropriate YSCALE factor

Variable PDELAY (Start time of each plume segment)
Line within MACCS IN1A.INP sample file:

```
RDPDELAY001       3700.     10000.
```

For a specific application:
Sequential plumes may not overlap. Therefore, the start time of each plume must be at or after the end of the preceding plume. In other words, the start time for a plume segment "i" must be ≥ the sum of the start time and release time of the previous plume segment (plume segment "i-1").

Variable PSDIST (Dry deposition velocity bin distribution)
Line within MACCS IN1A.INP sample file:

```
RDPSDIST001       1.
RDPSDIST002       1.
RDPSDIST003       1.
RDPSDIST004       1.
RDPSDIST005       1.
RDPSDIST006       1.
RDPSDIST007       1.
RDPSDIST008       1.
RDPSDIST009       1.
```

For a specific application:

A dry deposition velocity distribution must be specified for each chemical group even if dry deposition is turned off for that group. The dry deposition bins were defined in variable VDEPOS. As discussed previously, a dry deposition velocity of 0.001 m/s is appropriate for filtered releases. Similarly, a dry deposition velocity of 0.005 m/s is an approximate value for tritiated water vapor. A dry deposition velocity of 0.01 m/s is appropriate for unfiltered releases into the environment.

Variable CORINV (Inventory available for release into the environment)

Line within MACCS IN1A.INP sample file:

```
RDCORINV001     CO-58         3.223E+16
RDCORINV002     CO-60         2.465E+16
RDCORINV003     KR-85         2.475E+16
  .
  .
  .
RDCORINV060     CM-244        2.596E+15
```

For a specific application:

Enter the radionuclides and their associated inventories for the specific application. The radionuclides here do not need to be entered in the same order as provided in the default listing.

Variable CORSCA (Inventory scaling factor)

Line within MACCS IN1A.INP sample file:

```
RDCORSCA001   0.715  *  SURRY
```

For a specific application:

This value is most often used to scale the inventory units of curies to the MACCS required value of becquerels (Bq). However, the value may be used to scale the inventory to meet any need.

Variable RELFRA (Fraction of inventory released in each plume segment)

Line within MACCS IN1A.INP sample file:

```
RDRELFRC001 1.0E+0 6.8E-1 6.4E-1 1.7E-1 4.2E-3 2.3E-3 1.6E-4 4.0E-4 6.3E-3
RDRELFRC002 4.3E-3 9.5E-3 2.4E-3 1.4E-1 6.8E-2 4.7E-4 6.8E-3 7.1E-3 5.4E-2
```

For a specific application:

A value must be specified for each chemical group and plume segments. The fraction of release is applied uniformly in to all radionuclides within a chemical group.

Output Control Data Block (OC) *NUREG/CR-4691, Vol. 1 – p. 32*

Variable ENDAT1 (Flag for Ending Code Execution)
Line within MACCS IN1A.INP sample file:

```
OCENDAT1001  .FALSE. (SET THIS VALUE TO .TRUE. TO SKIP EARLY AND CHRONC)
```

For a specific application:
Normally this value should not be changed.

Variable IDEBUG (Debug Flag)
Line within MACCS IN1A.INP sample file:

```
OCIDEBUG001  0
```

For a specific application:
Normally this value should not be changed. However, the novice use will find it helpful to set the debug to a higher value and compare the MACCS results with hand calculations using the equations in the code documentation.

Variable NUCOUT (Radionuclide to be listed on the dispersion listings)
Line within MACCS IN1A.INP sample file:

```
*OCNUCOUT001  CS-137
```

For a specific application:
Normally this value should not be changed. However, when intermediate results are desired, this value should be set equal to the dominant radionuclide.

Meteorological Sampling Data Block (M1) *NUREG/CR-4691, Vol. 1 – p. 34*

Variable METCOD (Meteorological sampling specification)
Line within MACCS2 IN1A.INP sample file:

```
* METEOROLOGICAL SAMPLING DATA BLOCK
*
* METEOROLOGICAL SAMPLING OPTION CODE:
*
* METCOD = 1, USER SPECIFIED DAY AND HOUR IN THE YEAR (FROM MET FILE),
*          2, WEATHER CATEGORY BIN SAMPLING,
*          3, 120 HOURS OF WEATHER SPECIFIED ON THE ATMOS USER INPUT FILE,
*          4, CONSTANT MET (BOUNDARY WEATHER USED FROM THE START),
*          5, STRATIFIED RANDOM SAMPLES FOR EACH DAY OF THE YEAR.
*
M1METCOD001  2
```

For a specific application:
For DSA applications, weather category bin sampling (METCOD=2) or stratified random sampling (METCOD=5) is specified.

Boundary Weather Data Block (M2) *NUREG/CR-4691, Vol. 1 – p. 36*

Note: The values in this data block must always be defined. When constant meteorological conditions are chosen (METCOD = 4), the input values represent the constant meteorological conditions. In all other cases, they represent the meteorological data if the plume has not traversed the entire grid in 120 hours.

Variable LIMSPA (Index of last radial endpoint for measured meteorological data)
Line within MACCS IN1A.INP sample file:

```
M2LIMSPA001  25
```

For a specific application:
This value should be set equal to the index of the last spatial interval

Variable BNDMXH (Boundary weather mixing layer height)
Line within MACCS IN1A.INP sample file:

```
M2BNDMXH001  1000.  (METERS)
```

For a specific application:
This value should be set equal to the appropriate mixing height for the selected stability class.

Variable IBDSTB (Boundary weather stability class)
Line within MACCS IN1A.INP sample file:

```
M2IBDSTB001  4      (D-STABILITY)
```

For a specific application:
This value should be set equal to the numeric index of the desired stability class.

Variable BNDWND (Boundary weather windspeed)
Line within MACCS IN1A.INP sample file:

```
M2BNDWND001  5.     (M/S)
```

For a specific application:
This value should be set equal to the desired windspeed.

Fixed Start Time Data Block (M3) *NUREG/CR-4691, Vol. 1 – p. 37*

Note: The values in this data block must be defined if METCOD does not equal 2 or 5.

Variable ISTRDY (Index of start day from meteorological data file)
Line within MACCS IN1A.INP sample file:

```
M3ISTRDY001  157    (START TIME FOR PEAK ECONOMIC COST OF SAMPLE PROBLEM A)
```

For a specific application:
This line should not be changed.

Variable ISTRHR (Index of start hour from meteorological data file)
Line within MACCS IN1A.INP sample file:

```
M3ISTRHR001  10     (START TIME FOR PEAK ECONOMIC COST OF SAMPLE PROBLEM A)
```

For a specific application:
This line should not be changed.

Meteorological Bin Sampling Data Block (M4) *NUREG/CR-4691, Vol. 1 – p. 38*

Variable NSMPLS (Number of samples per bin)
Line within MACCS IN1A.INP sample file:

```
M4NSMPLS001  4  (THIS NUMBER SHOULD BE SET TO 4 FOR RISK ASSESSMENT)
```

For a specific application:
This value should be set equal once to 10 and then not changed

Variable IRSEED (Random Number Generator Seed)
Line within MACCS IN1A.INP sample file:

```
M4IRSEED001  79
```

For a specific application:
This value should be selected based on the meteorological data associated with a specific location, then not changed. This is done by selecting a set of

representative base source terms, and then executing the code for each possible seed. From the resultant MOI TEDE values, the seed parameter value can be selected by the user.

EARLY Input File

Similar to the ATMOS discussion, this section of the document addresses variables that may be changed during a normal execution of MACCS 1.5.11.1 for input into a safety basis document, or must be selected by the user for a specific location. If a variable is not explicitly mentioned, it need not be changed. The particular EARLY input file commented upon here is used because it is one of the sample files (e.g., IN2A.INP) supplied with the software from RSICC.

Miscellaneous Data Block (MI) *NUREG/CR-4691, Vol. 1 – p. 46*

Variable EANAM1 (EARLY input file identifier line)
Line within MACCS IN2A.INP sample file:

```
MIEANAM1001  ' IN2A.INP, MODIFIED 6/92, SURRY, SAMPLE PROBLEM A, EARLY INPUT'
```

For a specific application:
Change to a descriptive title for this execution of MACCS

Variable IPLUME (Dispersion model option code)
Line within MACCS IN2A.INP sample file:

```
MIIPLUME001  2
```

For a specific application:

This value should be set once to 1 and then not changed.

Variable IPRINT (Debug Flag)
Line within MACCS IN2A.INP sample file:

```
MIIPRINT001  0
```

For a specific application:
Normally this value should not be changed. However, the novice use will find it helpful to set the debug to a higher value and compare the MACCS results with hand calculations using the equations in the code documentation.

Variable RISCAT (Logical flag for consequences by contribution to mean)
Line within MACCS IN2A.INP sample file:

```
MIRISCAT001    .FALSE.
```

For a specific application:
Normally this value should not be changed. However, the novice use will find it helpful to set the value to ".TRUE." and compare the MACCS results with hand calculations using the equations in the code documentation.

Variable OVRRID (Logical flag for overriding the code calculated windrose)
Line within MACCS IN2A.INP sample file:

```
MIOVRRID001   .FALSE.   (USE THE WIND ROSE CALCULATED FOR EACH WEATHER BIN)
```

For a specific application:
Normally this value should not be changed. However, if this value should be set equal to ".TRUE.", then the user-calculated windrose is inputted using the WINROS parameter that is described next.

Variable WINROS (probabilities of the wind blowing from the site into each of the 16 compass sectors (rotating clockwise from N to NNW when OVRRID parameter is set equal to ".TRUE.")

For a specific application:
Normally this parameter is not used.

Population Distribution Data Block (PD) *NUREG/CR-4691, Vol. 1 – p. 49*

Variable POPFLG (Flag indicating whether a population file of uniform population is being used)
Line within MACCS IN2A.INP sample file:

```
PDPOPFLG001   FILE
```

For a specific application:
This value should be changed once to "UNIFORM" and then not changed

Variable IBEGIN (Index of radial endpoint where the population begins)
Line within MACCS IN2A.INP sample file:

```
*PDIBEGIN001  1    (SPATIAL INTERVAL AT WHICH POPULATION BEGINS)
```

For a specific application:
This line should be changed once by removing the comment indicator (the asterisk) from the beginning of the line.

Variable POPDEN (Uniform population density of the region)
Line within MACCS IN2A.INP sample file:

```
*PDPOPDEN001  50. (POPULATION DENSITY (PEOPLE PER SQUARE KILOMETER))
```

For a specific application:
This line should be changed once by removing the comment indicator (the asterisk) from the beginning of the line, and the value changed to zero (0.). After the line has been changed once, it will not need to be changed again.

Organ Definition Data Block (OD) *NUREG/CR-4691, Vol. 1 – p. 51*

Variable NUMORG (Number of organs to be considered)
Line within MACCS IN2A.INP sample file:

```
ODNUMORG001   10
```

For a specific application:
This value should be changed once to 2 and then not changed

Variable ORGNAM (Number of organs to be considered)
Line within MACCS IN2A.INP sample file:

```
ODORGNAM001 'SKIN', 'EDEWBODY', 'LUNGS', 'RED MARR', 'LOWER LI', 'STOMACH',
ODORGNAM002 'THYROIDH', 'BONE SUR', 'BREAST', 'BLAD WAL'
```

For a specific application:
This value should be changed to the following

```
ODORGNAM001 'NULL', 'EFFECTIVE'
```

After, the line has been changed once, it will not need to be changed again.

Shielding and Exposure Data Block (SE) *NUREG/CR-4691, Vol. 1 – p. 53*

Variable CSFACT (Cloudshine shielding factor)
Line within MACCS IN2A.INP sample file:

```
SECSFACT001      1.     0.75     0.6   *  SURRY SHELTERING VALUE
```

For a specific application:

The cloudshine shielding factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable PROTIN (Inhalation protection factor)
Line within MACCS IN2A.INP sample file:

```
SEPROTIN001      1.      0.41      0.33  * VALUES FOR NORMAL ACTIVITY AND
```

For a specific application:

The inhalation protection factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable SKPFAC (Skin absorption protection factor)
Line within MACCS IN2A.INP sample file:

```
SESKPFAC001  1.0      0.41      0.33    * VALUES FOR NORMAL ACTIVITY AND
```

For a specific application:

The skin absorption protection factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable GSHFAC (Groundshine shielding factor)
Line within MACCS IN2A.INP sample file:

```
SEGSHFAC001      0.5    0.33    0.2   * VALUE FOR NORMAL ACTIVITY SELECTED BY
```

For a specific application:

The groundshine shielding factor for all three activity levels should be set equal to one (1.) and then not changed.

Variable BRRATE (Breathing rate)
Line within MACCS IN2A.INP sample file:

```
SEBRRATE001  2.66E-4  2.66E-4  2.66E-4
```

For a specific application:

The breathing rate for all three activity levels should be set equal to 3.33E-04 m^3/s (DOE, 1998), as discussed earlier. Note that the basis for DOE-STD-1027-92 hazard categorization is slighter higher at 3.47E-04 m^3/s.

Variable RESCON (Resuspension inhalation model concentration coefficient)
Line within MACCS IN2A.INP sample file:

```
SERESCON001   1.E-4      (RESUSPENSION IS TURNED ON)
```

For a specific application:

This value should be set once and not changed. Per DOE-STD-3009-94 Appendix A, resuspension does not need to be included in the DSA calculations of TEDE. If resuspension is to be turned off, set the value equal to zero (0.). If resuspension is to be applied, this value does not need to be changed.

Evacuation Zone Data Block (EZ) *NUREG/CR-4691, Vol. 1 – p. 55*

Variable LASMOV (Index of last radial ring involved in the evacuation)
Line within MACCS IN2A.INP sample file:

```
EZLASMOV001     15    (EVACUEES DISAPPEAR AFTER TRAVELING TO 20 MILES)
```

For a specific application:

This value should be set once to zero (0) and then not changed.

Shelter and Relocation Data Block (SR) *NUREG/CR-4691, Vol. 1 – p. 58*

Variable ENDEMP (Duration of the emergency phase)
Line within MACCS IN2A.INP sample file:

```
SRENDEMP001  604800.   (ONE WEEK)
```

For a specific application:

This value of the emergency phase in units of seconds, should be set once to 86400. (24 hours) and then not changed. This is the minimum value allowed by MACCS and represent conservative implementation of the prescribed exposure duration of 2 hours (or 8 hours for slow-developing release scenarios) (DOE, 1994).

Variable TIMHOT (Time for hot-spot relocation)
Line within MACCS IN2A.INP sample file:

```
SRTIMHOT001  43200.    (ONE-HALF DAY)
```

For a specific application:

This value should be set once to 86400 (24 hours) and then not changed.

Variable CRIORG (Critical organ for relocation)
Line within MACCS IN2A.INP sample file:

```
SRCRIORG001 'EDEWBODY'
```

For a specific application:

This value should be set once to "EFFECTIVE" and then not changed.

Early Fatality Data Block (EF) *NUREG/CR-4691, Vol. 1 – p. 63*

Variable NUMEFA (Number of early fatality effects)
Line within MACCS IN2A.INP sample file:

```
EFNUMEFA001   3
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Early Injury Data Block (EI) *NUREG/CR-4691, Vol. 1 – p. 67*

Variable NUMEIN (Number of early injury effects)
Line within MACCS IN2A.INP sample file:

```
EINUMEIN001   7
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Latent Cancer Data Block (LC) *NUREG/CR-4691, Vol. 1 – p. 69*

Variable NUMACA (Number of acute exposure cancer effects)
Line within MACCS IN2A.INP sample file:

```
LCNUMACA001    7
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type One Output - Health Effects Data Block (T1) *NUREG/CR-4691, Vol. 1 – p. 75*

Variable NUM1 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE1NUMBER    27
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Two Output – Early Fatality Radius Data Block (T2) *NUREG/CR-4691, Vol. 1 – p. 77*

Variable NUM2 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE2NUMBER  1
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Three Output – Population Exceed Dose Threshold Data Block (T3) *NUREG/CR-4691, Vol. 1 – p. 78*

Variable NUM3 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE3NUMBER  3
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Four Output – Average Individual Risk Data Block (T4) *NUREG/CR-4691, Vol. 1 – p. 79*

Variable NUM4 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE4NUMBER  5
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Five Output – Population Dose Data Block (T5) *NUREG/CR-4691, Vol. 1 – p. 81*

Variable NUM5 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE5NUMBER      3
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

Type Six Output – Centerline Dose at Distance Data Block (T6) *NUREG/CR-4691, Vol. 1 – p. 82*

Variable NUM6 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE6NUMBER      0
```

For a specific application:
This value should be set equal to the number of desired results.

Variable ORGNAM, PATHNM, I1DIS6, and I2DIS6 (Organ name, pathway name, inner spatial interval, and outer spatial interval as input by OUT)
Line within MACCS IN2A.INP sample file:

```
*TYPE6OUT001  'RED MARR'    'TOT ACU'      1        19      (0-50 MILES)
*TYPE6OUT002  'LUNGS'       'TOT ACU'      1        19      (0-50 MILES)
*TYPE6OUT003  'EDEWBODY'    'TOT LIF'      1        26      (0-1000 MILES)
```

For a specific application:

The comment indicator (the asterisk) should be removed from the output definition. The organ name should be change to "EFFECTIVE". The pathway name should be changed to "TOT LIF". The inner and outer spatial intervals (radii) should be set equal to the ring encompassing the receptor location. If the release is elevated or heated and the MOI is located within several kilometers of the release location, the MOI may not be located at the closest site boundary but at the point of plume touch down. In this case, the inner and outer spatial intervals should be reset to encompass the location of the plume touch down.

Type Seven Output – Centerline Risk vs. Distance Data Block (T7) *NUREG/CR-4691, Vol. 1 – p. 84*

Variable NUM7 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE7NUMBER     0
```

For a specific application:

This value should not be changed.

Type Eight Output – Population Weighted Risk Data Block (T8) *NUREG/CR-4691, Vol. 1 – p. 86*

Variable NUM8 (Number of requested outputs)
Line within MACCS IN2A.INP sample file:

```
TYPE8NUMBER    2
```

For a specific application:

This value should be set once to zero (0) and the rest of the lines within the block should be commented out and then not changed.

APPENDIX E: RADIONUCLIDE CHEMICAL GROUPING, HALF-LIFE, AND PARENT RADIONUCLIDE

For input into the MACCS ATMOS input file, the chemical group, half-life, and parent of each radionuclide is needed. Table E1 gives this information. The parent and half-life information is taken from [Young, 1998]. The chemical group information is taken from [Powers, 1988] with the tetravalent and trivalent groups combined into one group as well as main group I and II.

Table E1. Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
AC-223	PA-227	8	1.32E+02
AC-224	PA-228	8	1.04E+04
AC-225	NONE	8	8.64E+05
AC-226	NONE	8	1.04E+05
AC-227	RA-227	8	6.87E+08
AC-228	NONE	8	2.21E+04
AG-102	NONE	9	7.74E+02
AG-103	NONE	9	3.94E+03
AG-104	AG-104M & CD-104	9	4.15E+03
AG-104M	NONE	9	2.01E+03
AG-105	NONE	9	3.54E+06
AG-106	NONE	9	1.44E+03
AG-106M	NONE	9	7.27E+05
AG-108	NONE	9	1.42E+02
AG-108M	NONE	9	4.01E+09
AG-109M	NONE	9	3.96E+01
AG-110	NONE	9	2.46E+01
AG-110M	NONE	9	2.16E+07
AG-111	NONE	9	6.44E+05
AG-112	NONE	9	1.12E+04
AG-115	NONE	9	1.20E+03
AL-26	NONE	8	2.26E+13
AL-28	MG-28	8	1.34E+02
AM-237	NONE	8	4.38E+03
AM-238	CM-238	8	5.88E+03
AM-239	NONE	8	4.28E+04
AM-240	NONE	8	1.83E+05
AM-241	BK-245, WPU-241, & YPU-241	8	1.36E+10
AM-242	NONE	8	5.77E+04
AM-242M	NONE	8	4.79E+09
AM-243	WPU-243 & YPU-243	8	2.33E+11
AM-244	NONE	8	3.64E+04
AM-244M	NONE	8	1.56E+03
AM-245	WPU-245 & YPU-245	8	7.38E+03
AM-246	NONE	8	2.34E+03
AM-246M	NONE	8	1.50E+03

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
AR-37	NONE	1	3.03E+06
AR-39	CL-39	1	8.48E+09
AR-41	NONE	1	6.58E+03
AS-69	NONE	9	9.12E+02
AS-70	SE-70	9	3.16E+03
AS-71	NONE	9	2.33E+05
AS-72	NONE	9	9.36E+04
AS-73	SE-73 & SE-73M	9	6.94E+06
AS-74	NONE	9	1.53E+06
AS-76	NONE	9	9.48E+04
AS-77	GE-77	9	1.40E+05
AS-78	GE-78	9	5.44E+03
AT-207	NONE	4	6.48E+03
AT-211	NONE	4	2.60E+04
AT-215	FR-219	4	6.00E+00
AT-216	FR-220	4	1.80E+01
AT-217	FR-221	4	3.23E-02
AT-218	PO-218	4	2.00E+00
AU-193	HG-193 & HG-193M	6	6.35E+04
AU-194	NONE	6	1.42E+05
AU-195	AU-195M, HG-195, & HG-195M	6	1.58E+07
AU-195M	NONE	6	3.05E+01
AU-198	AU-198M	6	2.33E+05
AU-198M	NONE	6	1.99E+05
AU-199	PT-199	6	2.71E+05
AU-200	AU-200M & PT-200	6	2.90E+03
AU-200M	NONE	6	6.73E+04
AU-201	NONE	6	1.58E+03
BA-126	NONE	3	5.79E+03
BA-128	NONE	3	2.10E+05
BA-131	BA-131M & LA-131	3	1.02E+06
BA-131M	NONE	3	8.76E+02
BA-133	BA-133M	3	3.39E+08
BA-133M	NONE	3	1.40E+05
BA-135M	NONE	3	1.03E+05
BA-137M	NONE	3	1.53E+02
BA-139	NONE	3	4.96E+03
BA-140	NONE	3	1.10E+06
BA-141	NONE	3	1.10E+03
BA-142	NONE	3	6.36E+02
BE-10	NONE	3	5.05E+13
BE-7	NONE	3	4.61E+06

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
BI-200	NONE	9	2.18E+03
BI-201	NONE	9	6.48E+03
BI-202	NONE	9	6.01E+03
BI-203	AT-207 & PO-203	9	4.23E+04
BI-205	PO-205	9	1.32E+06
BI-206	NONE	9	5.39E+05
BI-207	AT-211 & PO-207	9	1.20E+09
BI-210	NONE	9	4.33E+05
BI-210M	NONE	9	9.46E+13
BI-211	AT-215 & PB-211	9	1.28E+02
BI-212	AT-216 & PB-212	9	3.63E+03
BI-213	AT-217	9	2.74E+03
BI-214	AT-218 & PB-214	9	1.19E+03
BK-245	NONE	8	4.27E+05
BK-246	NONE	8	1.58E+05
BK-247	ES-251	8	4.35E+10
BK-249	CM-249	8	2.76E+07
BK-250	ES-254M	8	1.16E+04
BR-74	KR-74	4	1.52E+03
BR-74M	NONE	4	2.49E+03
BR-75	NONE	4	5.88E+03
BR-76	KR-76	4	5.83E+04
BR-77	KR-77	4	2.02E+05
BR-80	BR-80M	4	1.04E+03
BR-80M	NONE	4	1.59E+04
BR-82	NONE	4	1.27E+05
BR-83	SE-83	4	8.60E+03
BR-84	NONE	4	1.91E+03
C-11	NONE	8	1.22E+03
C-14	NONE	8	1.81E+11
CA-41	NONE	3	4.42E+12
CA-45	K-45	3	1.41E+07
CA-47	NONE	3	3.91E+05
CA-49	NONE	3	5.23E+02
CD-104	NONE	9	3.46E+03
CD-107	NONE	9	2.34E+04
CD-109	IN-109	9	4.01E+07
CD-113	NONE	9	2.93E+23
CD-113M	NONE	9	4.29E+08
CD-115	AG-115	9	1.92E+05
CD-115M	AG-115	9	3.85E+06
CD-117	NONE	9	8.96E+03
CD-117M	NONE	9	1.21E+04

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
CE-134	NONE	8	2.59E+05
CE-135	NONE	8	6.34E+04
CE-137	CE-137M & PR-137	8	3.24E+04
CE-137M	NONE	8	1.24E+05
CE-139	PR-139	8	1.19E+07
CE-141	LA-141	8	2.81E+06
CE-143	LA-143	8	1.19E+05
CE-144	NONE	8	2.46E+07
CF-244	NONE	8	1.16E+03
CF-246	NONE	8	1.29E+05
CF-248	FM-252	8	2.88E+07
CF-249	FM-253	8	1.11E+10
CF-250	BK-250, ES-250, & FM-254	8	4.12E+08
CF-251	ES-251 & FM-255	8	2.83E+10
CF-252	NONE	8	8.32E+07
CF-253	NONE	8	1.54E+06
CF-254	NONE	8	5.23E+06
CL-36	NONE	4	9.49E+12
CL-38	NONE	4	2.23E+03
CL-39	NONE	4	3.34E+03
CM-238	NONE	8	8.64E+03
CM-240	CF-244	8	2.33E+06
CM-241	NONE	8	2.83E+06
CM-242	AM-242 & CF-246	8	1.41E+07
CM-243	NONE	8	8.99E+08
CM-244	AM-244 & AM-244M	8	5.71E+08
CM-245	AM-245 & BK-245	8	2.68E+11
CM-246	AM-246, AM-246M, & BK-246	8	1.49E+11
CM-247	NONE	8	4.92E+14
CM-248	NONE	8	1.07E+13
CM-249	NONE	8	3.85E+03
CM-250	NONE	8	2.18E+11
CO-55	NONE	7	6.31E+04
CO-56	NI-56	7	6.80E+06
CO-57	NI-57	7	2.34E+07
CO-58	CO-58M	7	6.12E+06
CO-58M	NONE	7	3.29E+04
CO-60	CO-60M	7	1.66E+08
CO-60M	NONE	7	6.28E+02
CO-61	NONE	7	5.94E+03
CO-62M	NONE	7	8.35E+02

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
CR-48	NONE	7	8.27E+04
CR-49	NONE	7	2.53E+03
CR-51	MN-51	7	2.39E+06
CS-125	NONE	2	2.70E+03
CS-126	BA-126	2	9.84E+01
CS-127	NONE	2	2.25E+04
CS-128	BA-128	2	2.34E+02
CS-129	NONE	2	1.15E+05
CS-130	NONE	2	1.79E+03
CS-131	NONE	2	8.37E+05
CS-132	NONE	2	5.59E+05
CS-134	CS-134M	2	6.50E+07
CS-134M	NONE	2	1.04E+04
CS-135	CS-135M, XE-135, & XE-135M	2	7.25E+13
CS-135M	NONE	2	3.18E+03
CS-136	NONE	2	1.13E+06
CS-137	NONE	2	9.46E+08
CS-138	XE-138	2	1.93E+03
CU-60	NONE	2	1.39E+03
CU-61	NONE	2	1.23E+04
CU-62	ZN-62	2	5.84E+02
CU-64	NONE	2	4.57E+04
CU-66	NI-66	2	3.06E+02
CU-67	NONE	2	2.23E+05
DY-155	HO-155	8	3.60E+04
DY-157	HO-157	8	2.92E+04
DY-159	HO-159	8	1.25E+07
DY-165	NONE	8	8.40E+03
DY-166	NONE	8	2.94E+05
ER-161	NONE	8	1.17E+04
ER-165	NONE	8	3.73E+04
ER-169	NONE	8	8.04E+05
ER-171	NONE	8	2.71E+04
ER-172	NONE	8	1.77E+05
ES-250	NONE	8	7.56E+03
ES-251	NONE	8	1.19E+05
ES-253	FM-253 & MD-257	8	1.77E+06
ES-254	NONE	8	2.38E+07
ES-254M	NONE	8	1.41E+05
EU-145	GD-145 & TB-149	8	5.13E+05
EU-146	NONE	8	3.98E+05
EU-147	GD-147 & TB-151	8	2.07E+06
EU-148	NONE	8	4.71E+06

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
EU-149	NONE	8	8.04E+06
EU-150A	NONE	8	4.54E+04
EU-150B	NONE	8	1.08E+09
EU-152	NONE	8	4.20E+08
EU-152M	NONE	8	3.36E+04
EU-154	NONE	8	2.78E+08
EU-155	SM-155	8	1.56E+08
EU-156	SM-156	8	1.31E+06
EU-157	NONE	8	5.45E+04
EU-158	NONE	8	2.75E+03
F-18	NONE	4	6.59E+03
FE-52	NONE	7	2.98E+04
FE-55	CO-55	7	8.51E+07
FE-59	NONE	7	3.85E+06
FE-60	NONE	7	3.15E+12
FM-252	NONE	8	8.17E+04
FM-253	NONE	8	2.59E+05
FM-254	NONE	8	1.17E+04
FM-255	ES-254M	8	7.23E+04
FM-257	MD-257	8	8.68E+06
FR-219	AC-223	2	1.26E+03
FR-220	AC-224	2	2.74E+01
FR-221	NONE	2	2.88E+02
FR-222	AC-226	2	8.64E+02
FR-223	NONE	2	1.31E+03
GA-65	NONE	9	9.12E+02
GA-66	GE-66	9	3.38E+04
GA-67	GE-67	9	2.82E+05
GA-68	NONE	9	4.08E+03
GA-70	NONE	9	1.27E+03
GA-72	ZN-72	9	5.08E+04
GA-73	NONE	9	1.77E+04
GD-145	NONE	8	1.37E+03
GD-146	NONE	8	4.17E+06
GD-147	TB-147	8	1.37E+05
GD-148	NONE	8	2.93E+09
GD-149	TB-149	8	8.12E+05
GD-151	TB-151	8	1.04E+07
GD-152	EU-152M	8	3.41E+21
GD-153	TB-153	8	2.09E+07
GD-159	NONE	8	6.68E+04

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
GE-66	NONE	9	8.17E+03
GE-67	NONE	9	1.12E+03
GE-68	NONE	9	2.49E+07
GE-69	AS-69	9	1.41E+05
GE-71	AS-71	9	1.02E+06
GE-75	NONE	9	4.97E+03
GE-77	NONE	9	4.07E+04
GE-78	NONE	9	5.22E+03
H-3	NONE	10	3.89E+08
HF-170	NONE	8	5.76E+04
HF-172	TA-172	8	5.90E+07
HF-173	TA-173	8	8.64E+04
HF-175	TA-175	8	6.05E+06
HF-177M	NONE	8	3.08E+03
HF-178M	NONE	8	9.78E+08
HF-179M	NONE	8	2.17E+06
HF-180M	NONE	8	1.98E+04
HF-181	NONE	8	3.66E+06
HF-182	HF-182M	8	2.84E+14
HF-182M	NONE	8	3.69E+03
HF-183	NONE	8	3.84E+03
HF-184	NONE	8	1.48E+04
HG-193	HG-193M	9	1.26E+04
HG-193M	NONE	9	4.00E+04
HG-194	TL-194 & TL-194M	9	8.20E+09
HG-195	HG-195M & TL-195	9	3.56E+04
HG-195M	NONE	9	1.50E+05
HG-197	HG-197M & TL-197	9	2.31E+05
HG-197M	NONE	9	8.57E+04
HG-199M	NONE	9	2.56E+03
HG-203	NONE	9	4.03E+06
HO-155	NONE	8	2.88E+03
HO-157	NONE	8	7.56E+02
HO-159	NONE	8	1.98E+03
HO-161	ER-161	8	9.00E+03
HO-162	HO-162M	8	9.00E+02
HO-162M	NONE	8	4.08E+03
HO-164	HO-164M	8	1.74E+03
HO-164M	NONE	8	2.25E+03
HO-166	DY-166	8	9.65E+04
HO-166M	NONE	8	3.78E+10
HO-167	NONE	8	1.12E+04

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
I-120	XE-120	4	4.86E+03
I-120M	NONE	4	3.18E+03
I-121	XE-121	4	7.63E+03
I-122	XE-122	4	2.17E+02
I-123	XE-123	4	4.75E+04
I-124	NONE	4	3.61E+05
I-125	XE-125	4	5.20E+06
I-126	NONE	4	1.12E+06
I-128	NONE	4	1.50E+03
I-129	TE-129	4	4.95E+14
I-130	NONE	4	4.45E+04
I-131	TE-131 & TE-131M	4	6.95E+05
I-132	I-132M & TE-132	4	8.28E+03
I-132M	NONE	4	5.02E+03
I-133	TE-133 & TE-133M	4	7.49E+04
I-134	TE-134	4	3.16E+03
I-135	NONE	4	2.38E+04
IN-109	NONE	9	1.51E+04
IN-110A	SN-110	9	4.15E+03
IN-110B	NONE	9	1.76E+04
IN-111	SN-111	9	2.45E+05
IN-112	NONE	9	8.64E+02
IN-113M	NONE	9	5.97E+03
IN-114	NONE	9	7.19E+01
IN-114M	NONE	9	4.28E+06
IN-115	IN-115M	9	1.61E+23
IN-115M	CD-115	9	1.61E+04
IN-116M	NONE	9	3.25E+03
IN-117	CD-117, CD-117M, & IN-117M	9	2.63E+03
IN-117M	CD-117 & CD-117M	9	6.99E+03
IN-119	IN-119M	9	1.44E+02
IN-119M	NONE	9	1.08E+03
IR-182	NONE	6	9.00E+02
IR-184	NONE	6	1.09E+04
IR-185	NONE	6	5.04E+04
IR-186A	NONE	6	5.69E+04
IR-186B	PT-186	6	6.30E+03
IR-187	NONE	6	3.78E+04
IR-188	NONE	6	1.49E+05
IR-189	PT-189	6	1.15E+06
IR-190	IR-190M	6	1.05E+06
IR-190M	IR-190N	6	4.32E+03

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
IR-190N	NONE	6	1.12E+04
IR-191M	NONE	6	4.94E+00
IR-192	NONE	6	6.40E+06
IR-192M	NONE	6	7.60E+09
IR-194	NONE	6	6.89E+04
IR-194M	NONE	6	1.48E+07
IR-195	IR-195M	6	9.00E+03
IR-195M	NONE	6	1.37E+04
K-38	NONE	2	4.58E+02
K-40	NONE	2	4.04E+16
K-42	NONE	2	4.45E+04
K-43	NONE	2	8.14E+04
K-44	NONE	2	1.33E+03
K-45	NONE	2	1.20E+03
KR-74	NONE	1	6.90E+02
KR-76	NONE	1	5.33E+04
KR-77	NONE	1	4.48E+03
KR-79	RB-79	1	1.26E+05
KR-81	KR-81M & RB-81	1	6.62E+12
KR-81M	NONE	1	1.30E+01
KR-83M	BR-83	1	6.59E+03
KR-85	KR-85M	1	3.38E+08
KR-85M	NONE	1	1.61E+04
KR-87	NONE	1	4.58E+03
KR-88	NONE	1	1.02E+04
LA-131	NONE	8	3.54E+03
LA-132	NONE	8	1.73E+04
LA-134	CE-134	8	4.00E+02
LA-135	CE-135	8	7.02E+04
LA-137	CE-137 & CE-137M	8	1.89E+12
LA-138	NONE	8	4.26E+18
LA-140	NONE	8	1.45E+05
LA-141	BA-141	8	1.41E+04
LA-142	BA-142	8	5.55E+03
LA-143	NONE	8	8.54E+02
LU-169	NONE	8	1.23E+05
LU-170	HF-170	8	1.73E+05
LU-171	NONE	8	7.10E+05
LU-172	NONE	8	5.79E+05
LU-173	HF-173	8	4.32E+07
LU-174	NONE	8	1.04E+08
LU-174M	NONE	8	1.23E+07

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
LU-176	NONE	8	1.14E+18
LU-176M	NONE	8	1.32E+04
LU-177	YB-177	8	5.80E+05
LU-177M	NONE	8	1.39E+07
LU-178	YB-178	8	1.70E+03
LU-178M	NONE	8	1.36E+03
LU-179	NONE	8	1.65E+04
MD-257	NONE	8	1.87E+04
MD-258	NONE	8	4.75E+06
MG-28	NONE	3	7.53E+04
MN-51	NONE	7	2.77E+03
MN-52	MN-52M	7	4.83E+05
MN-52M	FE-52	7	1.27E+03
MN-53	NONE	7	1.17E+14
MN-54	NONE	7	2.70E+07
MN-56	NONE	7	9.28E+03
MO-101	NONE	7	8.77E+02
MO-90	NONE	7	2.04E+04
MO-93	MO-93M, TC-93, & TC-93M	7	1.10E+11
MO-93M	NONE	7	2.47E+04
MO-99	NONE	7	2.38E+05
N-13	NONE	8	5.98E+02
NA-22	NONE	2	8.21E+07
NA-24	NONE	2	5.40E+04
NB-88	NONE	7	8.58E+02
NB-89A	NONE	7	3.96E+03
NB-89B	NONE	7	7.32E+03
NB-90	MO-90	7	5.26E+04
NB-93M	NONE	7	4.29E+08
NB-94	NONE	7	6.40E+11
NB-95	NB-95M	7	3.04E+06
NB-95M	NONE	7	3.12E+05
NB-96	NONE	7	8.41E+04
NB-97	NB-97M & ZR-97	7	4.33E+03
NB-97M	ZR-97	7	6.00E+01
NB-98	NONE	7	3.09E+03
ND-136	NONE	8	3.04E+03
ND-138	NONE	8	1.81E+04
ND-139	ND-139M	8	1.78E+03
ND-139M	NONE	8	1.98E+04
ND-141	ND-141M & PM-141	8	8.96E+03
ND-141M	PM-141	8	6.24E+01

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
ND-147	PR-147	8	9.49E+05
ND-149	NONE	8	6.23E+03
ND-151	NONE	8	7.46E+02
NE-19	NONE	1	1.72E+01
NI-56	NONE	6	5.27E+05
NI-57	NONE	6	1.30E+05
NI-59	NONE	6	2.37E+12
NI-63	NONE	6	3.03E+09
NI-65	NONE	6	9.07E+03
NI-66	NONE	6	1.97E+05
NP-232	NONE	8	8.82E+02
NP-233	AM-237	8	2.17E+03
NP-234	AM-238, WPU-234, & YPU-234	8	3.80E+05
NP-235	AM-239, WPU-235, & YPU-235	8	3.42E+07
NP-236A	NONE	8	3.63E+12
NP-236B	AM-240	8	8.10E+04
NP-237	U-237	8	6.75E+13
NP-238	NONE	8	1.83E+05
NP-239	U-239	8	2.03E+05
NP-240	NONE	8	3.90E+03
NP-240M	U-240	8	4.44E+02
O-15	NONE	5	1.22E+02
OS-180	NONE	6	1.32E+03
OS-181	NONE	6	6.30E+03
OS-182	IR-182 & PT-186	6	7.92E+04
OS-185	IR-185	6	8.12E+06
OS-189M	RE-189	6	2.16E+04
OS-190M	NONE	6	5.94E+02
OS-191	OS-191M	6	1.33E+06
OS-191M	NONE	6	4.69E+04
OS-193	NONE	6	1.08E+05
OS-194	NONE	6	1.89E+08
P-30	NONE	8	1.50E+02
P-32	NONE	8	1.23E+06
P-33	NONE	8	2.19E+06
PA-227	NONE	8	2.30E+03
PA-228	NONE	8	7.92E+04
PA-230	NONE	8	1.50E+06
PA-231	TH-231 & U-231	8	1.03E+12
PA-232	NONE	8	1.13E+05
PA-233	NONE	8	2.33E+06
PA-234	PA-234M	8	2.41E+04
PA-234M	NONE	8	7.02E+01

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
PB-195M	NONE	9	9.48E+02
PB-198	NONE	9	8.64E+03
PB-199	NONE	9	5.40E+03
PB-200	BI-200	9	7.74E+04
PB-201	BI-201 & PO-205	9	3.38E+04
PB-202	BI-202 & PB-202M	9	9.46E+12
PB-202M	BI-202	9	1.30E+04
PB-203	BI-203	9	1.87E+05
PB-205	NONE	9	4.51E+14
PB-209	PO-213 & TL-209	9	1.17E+04
PB-210	PO-214	9	7.03E+08
PB-211	PO-215	9	2.17E+03
PB-212	PO-216	9	3.83E+04
PB-214	PO-218	9	1.61E+03
PD-100	NONE	6	3.14E+05
PD-101	NONE	6	2.98E+04
PD-103	AG-103	6	1.47E+06
PD-107	RH-107	6	2.05E+14
PD-109	NONE	6	4.83E+04
PM-141	SM-141 & SM-141M	8	1.25E+03
PM-142	SM-142	8	4.05E+01
PM-143	NONE	8	2.29E+07
PM-144	NONE	8	3.14E+07
PM-145	NONE	8	5.58E+08
PM-146	NONE	8	1.75E+08
PM-147	NONE	8	8.27E+07
PM-148	NONE	8	4.64E+05
PM-148M	NONE	8	3.57E+06
PM-149	ND-149	8	1.91E+05
PM-150	NONE	8	9.65E+03
PM-151	ND-151	8	1.02E+05
PO-203	NONE	5	2.20E+03
PO-205	NONE	5	6.48E+03
PO-207	AT-207	5	2.10E+04
PO-210	BI-210	5	1.20E+07
PO-211	AT-211 & BI-211	5	5.16E-01
PO-212	BI-212	5	3.05E-07
PO-213	BI-213	5	4.20E-06
PO-214	BI-214 & RN-218	5	1.64E-04
PO-215	RN-219	5	1.78E-03
PO-216	RN-220	5	1.50E-01
PO-218	RN-222	5	1.83E+02

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
PR-136	ND-136	8	7.86E+02
PR-137	NONE	8	4.60E+03
PR-138	ND-138	8	8.70E+01
PR-138M	NONE	8	7.56E+03
PR-139	ND-139 & ND-139M	8	1.62E+04
PR-142	PR-142M	8	6.89E+04
PR-142M	NONE	8	8.76E+02
PR-143	CE-143	8	1.17E+06
PR-144	PR-144M	8	1.04E+03
PR-144M	NONE	8	4.32E+02
PR-145	NONE	8	2.15E+04
PR-147	NONE	8	8.16E+02
PT-186	NONE	6	7.20E+03
PT-188	NONE	6	8.81E+05
PT-189	NONE	6	3.91E+04
PT-191	NONE	6	2.42E+05
PT-193	AU-193 & PT-193M	6	1.58E+09
PT-193M	NONE	6	3.74E+05
PT-195M	NONE	6	3.47E+05
PT-197	PT-197M	6	6.59E+04
PT-197M	NONE	6	5.66E+03
PT-199	NONE	6	1.85E+03
PT-200	NONE	6	4.50E+04
PU-234	CM-238	8	3.17E+04
PU-235	NONE	8	1.52E+03
PU-236	NP-236B	8	8.99E+07
PU-237	AM-237	8	3.91E+06
PU-238	AM-238 & NP-238	8	2.77E+09
PU-239	AM-239 & NP-239	8	7.59E+11
PU-240	AM-240, NP-240, & NP-240M	8	2.06E+11
PU-241	NONE	8	4.54E+08
PU-242	AM-242	8	1.19E+13
PU-243	NONE	8	1.78E+04
PU-244	NONE	8	2.60E+15
PU-245	NONE	8	3.78E+04
PU-246	NONE	8	9.37E+05
RA-222	FR-222 & TH-226	3	3.80E+01
RA-223	FR-223	3	9.88E+05
RA-224	AC-224	3	3.16E+05
RA-225	NONE	3	1.28E+06
RA-226	AC-226	3	5.05E+10
RA-227	NONE	3	2.53E+03
RA-228	NONE	3	1.81E+08

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
RB-79	NONE	2	1.37E+03
RB-80	SR-80	2	3.40E+01
RB-81	RB-81M & SR-81	2	1.65E+04
RB-81M	NONE	2	1.92E+03
RB-82	NONE	2	7.80E+01
RB-82M	NONE	2	2.23E+04
RB-83	SR-83	2	7.45E+06
RB-84	NONE	2	2.83E+06
RB-86	NONE	2	1.61E+06
RB-87	KR-87 & SR-87M	2	1.48E+18
RB-88	KR-88	2	1.07E+03
RB-89	NONE	2	9.12E+02
RE-177	NONE	6	8.40E+02
RE-178	NONE	6	7.92E+02
RE-180	OS-180	6	1.46E+02
RE-181	OS-181	6	7.20E+04
RE-182A	OS-182	6	4.57E+04
RE-182B	NONE	6	2.30E+05
RE-184	NONE	6	3.28E+06
RE-184M	NONE	6	1.43E+07
RE-186	NONE	6	3.26E+05
RE-186M	NONE	6	6.31E+12
RE-187	W-187	6	1.58E+18
RE-188	RE-188M	6	6.11E+04
RE-188M	NONE	6	1.12E+03
RE-189	NONE	6	8.75E+04
RH-100	PD-100	6	7.49E+04
RH-101	PD-101 & RH-101M	6	1.01E+08
RH-101M	PD-101	6	3.75E+05
RH-102	NONE	6	9.15E+07
RH-102M	NONE	6	1.79E+07
RH-103M	NONE	6	3.37E+03
RH-105	RU-105	6	1.27E+05
RH-106	NONE	6	2.99E+01
RH-106M	NONE	6	7.92E+03
RH-107	NONE	6	1.30E+03
RH-99	NONE	6	1.38E+06
RH-99M	NONE	6	1.69E+04
RN-218	RA-222	1	2.10E+03
RN-219	NONE	1	3.96E+00
RN-220	RA-224	1	5.56E+01
RN-222	NONE	1	3.30E+05
RU-103	NONE	6	3.39E+06
RU-105	NONE	6	1.60E+04
RU-106	NONE	6	3.18E+07
RU-94	NONE	6	3.11E+03
RU-97	NONE	6	2.51E+05
S-35	NONE	5	7.55E+06
SB-115	NONE	9	1.91E+03

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
SB-116	TE-116	9	9.48E+02
SB-116M	NONE	9	3.62E+03
SB-117	NONE	9	1.01E+04
SB-118M	NONE	9	1.80E+04
SB-119	NONE	9	1.37E+05
SB-120A	NONE	9	9.53E+02
SB-120B	NONE	9	4.98E+05
SB-122	NONE	9	2.33E+05
SB-124	SB-124M	9	5.20E+06
SB-124M	SB-124N	9	9.30E+01
SB-124N	NONE	9	1.21E+03
SB-125	NONE	9	8.74E+07
SB-126	SB-126M	9	1.07E+06
SB-126M	NONE	9	1.14E+03
SB-127	SN-127	9	3.33E+05
SB-128A	SN-128	9	6.24E+02
SB-128B	NONE	9	3.24E+04
SB-129	NONE	9	1.56E+04
SB-130	NONE	9	2.40E+03
SB-131	NONE	9	1.38E+03
SC-43	NONE	8	1.40E+04
SC-44	SC-44M	8	1.41E+04
SC-44M	NONE	8	2.11E+05
SC-46	NONE	8	7.24E+06
SC-47	CA-47	8	2.90E+05
SC-48	NONE	8	1.57E+05
SC-49	CA-49	8	3.44E+03
SE-70	NONE	5	2.46E+03
SE-73	SE-73M	5	2.57E+04
SE-73M	NONE	5	2.34E+03
SE-75	BR-75	5	1.04E+07
SE-77M	NONE	5	1.75E+01
SE-79	NONE	5	2.05E+12
SE-81	SE-81M	5	1.11E+03
SE-81M	NONE	5	3.44E+03
SE-83	NONE	5	1.35E+03
SI-31	NONE	8	9.44E+03
SI-32	NONE	8	1.42E+10
SM-141	SM-141M	8	6.12E+02
SM-141M	NONE	8	1.36E+03
SM-142	NONE	8	4.35E+03
SM-145	EU-145	8	2.94E+07
SM-146	EU-146	8	3.25E+15
SM-147	NONE	8	3.34E+18
SM-151	PM-151	8	2.84E+09
SM-153	NONE	8	1.68E+05
SM-155	NONE	8	1.33E+03
SM-156	NONE	8	3.38E+04

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
SN-110	NONE	9	1.44E+04
SN-111	NONE	9	2.12E+03
SN-113	NONE	9	9.94E+06
SN-117M	IN-117	9	1.18E+06
SN-119M	IN-119	9	2.53E+07
SN-121	NONE	9	9.74E+04
SN-121M	NONE	9	1.73E+09
SN-123	NONE	9	1.12E+07
SN-123M	NONE	9	2.40E+03
SN-125	NONE	9	8.33E+05
SN-126	NONE	9	3.15E+12
SN-127	NONE	9	7.56E+03
SN-128	NONE	9	3.55E+03
SR-80	NONE	3	6.00E+03
SR-81	NONE	3	1.53E+03
SR-82	NONE	3	2.16E+06
SR-83	NONE	3	1.17E+05
SR-85	SR-85M	3	5.60E+06
SR-85M	NONE	3	4.17E+03
SR-87M	Y-87	3	1.01E+04
SR-89	RB-89	3	4.36E+06
SR-90	NONE	3	9.18E+08
SR-91	NONE	3	3.42E+04
SR-92	NONE	3	9.76E+03
TA-172	NONE	7	2.21E+03
TA-173	NONE	7	1.31E+04
TA-174	NONE	7	4.32E+03
TA-175	NONE	7	3.78E+04
TA-176	W-176	7	2.91E+04
TA-177	W-177	7	2.04E+05
TA-178A	NONE	7	5.59E+02
TA-178B	NONE	7	7.92E+03
TA-179	W-179	7	5.74E+07
TA-180	NONE	7	3.15E+20
TA-180M	NONE	7	2.92E+04
TA-182	HF-182M & TA-182M	7	9.94E+06
TA-182M	NONE	7	9.50E+02
TA-183	HF-183	7	4.41E+05
TA-184	HF-184	7	3.13E+04
TA-185	NONE	7	2.94E+03
TA-186	NONE	7	6.30E+02

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
TB-147	NONE	8	5.94E+03
TB-149	NONE	8	1.49E+04
TB-150	NONE	8	1.18E+04
TB-151	NONE	8	6.34E+04
TB-153	NONE	8	2.02E+05
TB-154	NONE	8	7.70E+04
TB-155	DY-155	8	4.60E+05
TB-156	TB-156M & TB-156N	8	4.61E+05
TB-156M	NONE	8	8.78E+04
TB-156N	NONE	8	1.80E+04
TB-157	DY-157	8	4.73E+09
TB-158	NONE	8	4.73E+09
TB-160	NONE	8	6.25E+06
TB-161	NONE	8	5.97E+05
TC-101	MO-101	7	8.52E+02
TC-104	NONE	7	1.09E+03
TC-93	TC-93M	7	9.90E+03
TC-93M	NONE	7	2.61E+03
TC-94	NONE	7	1.76E+04
TC-94M	RU-94	7	3.12E+03
TC-95	NONE	7	7.20E+04
TC-95M	NONE	7	5.27E+06
TC-96	TC-96M	7	3.70E+05
TC-96M	NONE	7	3.09E+03
TC-97	RU-97	7	8.20E+13
TC-97M	RU-97	7	7.52E+06
TC-98	NONE	7	1.32E+14
TC-99	MO-99 & TC-99M	7	6.72E+12
TC-99M	MO-99	7	2.17E+04
TE-116	NONE	5	8.96E+03
TE-121	I-121	5	1.47E+06
TE-121M	NONE	5	1.33E+07
TE-123	I-123	5	3.15E+20
TE-123M	I-123	5	1.03E+07
TE-125M	NONE	5	5.01E+06
TE-127	SB-127	5	3.37E+04
TE-127M	SB-127	5	9.42E+06
TE-129	SB-129	5	4.18E+03
TE-129M	SB-129	5	2.90E+06
TE-131	SB-131 & TE-131M	5	1.50E+03
TE-131M	SB-131	5	1.08E+05
TE-132	NONE	5	2.82E+05
TE-133	TE-133M	5	7.47E+02

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
TE-133M	NONE	5	3.32E+03
TE-134	NONE	5	2.51E+03
TH-226	AC-226	8	1.85E+03
TH-227	PA-227 & U-231	8	1.62E+06
TH-228	AC-228 & PA-228	8	6.03E+07
TH-229	NONE	8	2.31E+11
TH-230	NONE	8	2.43E+12
TH-231	NONE	8	9.19E+04
TH-232	NONE	8	4.43E+17
TH-234	NONE	8	2.08E+06
TI-44	NONE	8	1.49E+09
TI-45	NONE	8	1.11E+04
TL-194	NONE	9	1.98E+03
TL-194M	NONE	9	1.97E+03
TL-195	PB-195M	9	4.18E+03
TL-197	NONE	9	1.02E+04
TL-198	PB-198 & TL-198M	9	1.91E+04
TL-198M	NONE	9	6.73E+03
TL-199	PB-199	9	2.67E+04
TL-200	PB-200	9	9.40E+04
TL-201	PB-201	9	2.63E+05
TL-202	PB-202M	9	1.06E+06
TL-204	NONE	9	1.19E+08
TL-206	NONE	9	2.52E+02
TL-207	BI-211	9	2.86E+02
TL-208	BI-212	9	1.84E+02
TL-209	BI-213	9	1.32E+02
TM-162	YB-162	8	1.30E+03
TM-166	YB-166	8	2.77E+04
TM-167	YB-167	8	7.98E+05
TM-170	NONE	8	1.11E+07
TM-171	ER-171	8	6.05E+07
TM-172	ER-172	8	2.29E+05
TM-173	NONE	8	2.97E+04
TM-175	NONE	8	9.12E+02
U-230	PU-234 & PU-234	8	1.80E+06
U-231	PU-235 & PU-235	8	3.63E+05
U-232	NP-232 & PA-232	8	2.27E+09
U-233	NP-233	8	5.00E+12
U-234	NP-234, PA-234, & PA-234M	8	7.71E+12
U-235	NONE	8	2.22E+16
U-236	NP-236B	8	7.38E+14
U-237	NONE	8	5.83E+05

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
U-238	NONE	8	1.41E+17
U-239	NONE	8	1.41E+03
U-240	NONE	8	5.08E+04
V-47	NONE	7	1.96E+03
V-48	CR-48	7	1.40E+06
V-49	CR-49	7	2.85E+07
W-176	NONE	7	8.28E+03
W-177	RE-177	7	8.10E+03
W-178	RE-178	7	1.87E+06
W-179	NONE	7	2.25E+03
W-181	RE-181	7	1.05E+07
W-185	TA-185	7	6.49E+06
W-187	NONE	7	8.60E+04
W-188	NONE	7	6.00E+06
XE-120	NONE	1	2.40E+03
XE-121	NONE	1	2.41E+03
XE-122	NONE	1	7.24E+04
XE-123	NONE	1	7.49E+03
XE-125	CS-125	1	6.12E+04
XE-127	CS-127	1	3.15E+06
XE-129M	NONE	1	6.91E+05
XE-131M	NONE	1	1.03E+06
XE-133	I-133 & XE-133M	1	4.53E+05
XE-133M	I-133	1	1.89E+05
XE-135	I-135 & XE-135M	1	3.27E+04
XE-135M	I-135	1	9.17E+02
XE-138	NONE	1	8.50E+02
Y-86	Y-86M & ZR-86	8	5.31E+04
Y-86M	NONE	8	2.88E+03

Table E1. (cont.) Radionuclides Chemical Grouping, Half-Life, and Parent Information

Radionuclide	Parent	Group	T 1/2 (s)
Y-87	NONE	8	2.89E+05
Y-88	NONE	8	9.21E+06
Y-90	Y-90M	8	2.30E+05
Y-90M	NONE	8	1.15E+04
Y-91	SR-91 & Y-91M	8	5.06E+06
Y-91M	SR-91	8	2.98E+03
Y-92	SR-92	8	1.27E+04
Y-93	NONE	8	3.64E+04
Y-94	NONE	8	1.15E+03
Y-95	NONE	8	6.42E+02
YB-162	NONE	8	1.13E+03
YB-166	NONE	8	2.04E+05
YB-167	NONE	8	1.05E+03
YB-169	LU-169	8	2.77E+06
YB-175	TM-175	8	3.62E+05
YB-177	NONE	8	6.84E+03
YB-178	NONE	8	4.44E+03
ZN-62	NONE	9	3.33E+04
ZN-63	NONE	9	2.29E+03
ZN-65	GA-65	9	2.11E+07
ZN-69	ZN-69M	9	3.42E+03
ZN-69M	NONE	9	4.95E+04
ZN-71M	NONE	9	1.41E+04
ZN-72	NONE	9	1.67E+05
ZR-86	NONE	8	5.94E+04
ZR-88	NB-88	8	7.21E+06
ZR-89	NB-89A & NB-89B	8	2.82E+05
ZR-93	Y-93	8	4.83E+13
ZR-95	Y-95	8	5.53E+06
ZR-97	NONE	8	6.08E+04

APPENDIX F. USER NOTES FOR MACCS2 VERSION 1.13.1 (RSICC, MARCH 2004)

```
--------------------------  MACCS2 VERSION 1.13  --------------------

------------------------------------------------------------------------
HISTORY of MACCS2
------------------------------------------------------------------------

The release history of MACCS2 is as follows:

MACCS2 1.12 was released in April 1997.

MACCS2 1.13, released to the NRC in September 2001, was created to correct
deficiencies found in MACCS2 1.12 and introduce an interface for
WinMACCS, a Windows front end developed to support MACCS2 uncertainty
analysis.  The FORTRAN compiler was changed from LAHEY to DIGITAL Visual
FORTRAN Professional 6.6A.

MACCS2 1.13.1, released to the user community in January 2004, is essentially
the same as version 1.13.  The only change in MACCS2 was to modify the
default
temp file name.  The default temp file in MACCS2 1.13 is MACCS3.tmp.  The
default temp file for MACCS2 1.13.1 and MACCS2 1.12 is MACCS2.tmp. The
FORTRAN compiler used was changed to COMPAQ Visual FORTRAN Professional
6.6B.

For details regarding the history leading up to MACCS2, see NUREG/CR-6613,
Vol. 1.

Since versions 1.13 and 1.13.1 are essentially the same, the following
discussion uses 1.13 generically to refer to either version.

------------------------------------------------------------------------
MODIFICATIONS MADE TO CREATE MACCS2 1.13 FROM MACCS2 1.12
------------------------------------------------------------------------
1) Add a validate-only option to allow input to be validated without
running the calculation. For "Validate" execution, the content of the
MACCS2.TMP file is the same as it is for MACCS2 1.12 with the sole difference
being that the 13-character text string VALIDATE_ONLY appears on line number
seven as shown in the following example:

IN1A.INP
IN2A.INP
IN3A_N.INP
METSUR.INP
SURSIT.INP
LISTA_N.OUT
VALIDATE_ONLY

2) Added support for status files to allow access to MACCS2- and
FORTRAN-generated error messages created during the execution of MACCS2.
The outcome of MACCS2 is communicated through files MaxStat.log and
FortErr.log. MaxStat.log contains the string "OK" if MACCS2 terminates
```

with no error. MaxStat.log contains the string "NO" followed by an informative message if MACCS2 detects an error. If MACCS2 crashes due to an undetected error, trace information is appended to FortErr.log.

3) MACCS2 was modified to optionally read the path and name of the file Maccs2.tmp as a program argument. The file name argument is preceded by an argument set to '-i'. For example, MACCS2 can be initiated from a command prompt window with the following command:

```
>MACCS2.exe -i "d:\My Maccs Files\maccs.tmp"
```

3) Improve error handling in Function IMNTGR, Subroutine XERROR, and Subroutine RANDOM.

4) Resolve an error related to inconsistent results when using the source-term loop feature to analyze multiple releases. The bug was resolved by Modifying Subroutine PUTSTM as follows:

Changed A0/A1 dimensions from 3432 to 3732 to match length of
COMMON /MULREL/
Changed ILNTHA from 3432 to 3732 to reflect length of
COMMON /MULREL/
ILNTHA of 15 changed to 17; ILNTHD of 2911 changed to 2914

This fix resolves defect notifications M2V1-12A and M2V1-12B, both issued on 5/26/98.

5) Because of difficulties compiling program under the new compiler, the scratch file on unit 22 was renamed temp99.

6) Commented out the following unused line in Subroutine WGTMET:

```
      IMXHT(I,J)=MOD(MRAIN(I,J)/1000,100)
```

7) A new subroutine was added, namely CHECK_SIGMA_Y.
This subroutine checks sigma-y values (for all stability classes) at the maximum downwind distance (SPAEND(NUMRAD)) to see if the plume is so large as to "wrap around" to the release point and thus cover an area greater than a semicircle (going to 2.15 sigma-y, or the 10% level)

9) Debug information written to output file was removed from Subroutine LTPROJ.

10) Improve calculation of TDECON, the time when the projected dose satisfies long term criterion, by avoiding taking the log of 0. Modification was in Subroutine LTMACT.

11) MACCS2 incorrectly reported the foodchain doses from leafy vegetables and did not report the doses from grains. This was resolved by modifying Subroutine DOSGET to correct the crop index as follows:

```
MACCS2 1.12:
      DOSE(9) = DOSE(9) + TERM *
 1   ACU_DOSE(INDORG,2,INIOTH(IANG,IRAD),IFALLOUT,INUC)
```

```
MACCS2 1.13:
      DOSE(9) = DOSE(9) + TERM *
     1   ACU_DOSE(INDORG,1,INIOTH(IANG,IRAD),IFALLOUT,INUC)

-------------------------------------------------------------------------
Contents of Distribution CD
-------------------------------------------------------------------------
The complete MACCS2 software package is distributed in folder
Software & Related Files\ in the following subfolders on the
distribution CD:
COMIDA2
DOSFAC2
FGRDCF
MACCS2

Folder MACCS2\ contains the MACCS2 code and the files required to run
the 14 MACCS2 sample problems.

The preprocessors COMIDA2, DOSFAC2 and FGRDCF are not required to
use MACCS2.  The preprocessors may be used to create input files
containing dose conversion factor (DCF) or food pathway data not included
with the sample problem files.

CHAIN is a program used to view the decay chain data file FGR1112.IDX.  This
file is used by FGRDCF.

READEM is a program used to view FGR dose coefficients based on Federal
Guidance Reports 11 and 12.

All executables were compiled using Compaq Visual FORTRAN Professional 6.6B
on Windows XP Professional.

The binary files created by Comida2 that are used as input to MACCS2
(namely SAMP_A.BIN and SAMP_D.BIN) must be created by versions of COMIDA2
compiled with the same compiler as that of MACCS2.

-------------------------------------------------------------------------
HARDWARE AND SOFTWARE REQUIREMENTS
-------------------------------------------------------------------------
IBM-compatible 486/DX or Pentium PC running Windows NT, 2000 or XP.

-------------------------------------------------------------------------
INSTALLATION INSTRUCTIONS
-------------------------------------------------------------------------
Create a Maccs Suite folder.

Copy each of the CD folders (MACCS2, COMIDA2, etc.) into this folder.

Remove the read-only permission from the files and the folders. To do this,
right click on the files/folder and select Properties. Uncheck the Read
Only radio button. Click OK.

The MACCS2/ directory contains 14 sample problems.  The MACCS2 outputs from
the 14 sample problem runs are provided in the *.OUT files on the
distribution CD.  The contents of the ATMOS, EARLY, and CHRONC input
```

files are echoed in the *.OUT files generated for each MACCS2 run. A description of the sample problems are provided in Section 4.4 of the Code Manual for MACCS2: Volume 1, User's Guide.

Dose Conversion Factor (DCF) Files

Four DCF files are included

DOSDATA.INP - Created by an old version of DOSFAC and which contains the 60 radionuclides and 19 Organs considered most important for consequence analysis
of commercial reactor accidents.

DOSDATA.NEW - Created by DOSFAC2. Contains 60 radionuclides and 20 Organs. The DCFs are slightly different than in DOSDATA.INP.

DOSD825.INP - Created by FGRDCF and which contains all of the 825 radionuclides
accessed by FGRDCF.

DOSD60.INP - Created by FGRDCF and contains the 60 radionuclides contained in DOSDATA.INP. However, DCFs are different.

IDCF2 is no longer supported, hence these files are not included.

The MACCS2 DCF input file name is specified by the user in the EARLY input file by the DCF_FILE input parameter. The user must specify the drive and directory containing the DCF input file if the files are not contained in the subdirectory containing the MACCS2 executable.

The input files required for the FGRDCF and DOSFAC2 preprocessor sample problems can be identified by the .SEL extension. The FGRDCF and DOSFAC2 preprocessors may be exercised using the following commands:

FGRDCF: RUNFGR filename
DOSFAC2: DOSFACPC filename

where filename does not include the .SEL extension.
RUNEM.bat will run all of the DOSFAC2 sample problems provided.
The MACCS2 DCF input files created by these two preprocessors are filename.inp.

COMIDA2 food pathway preprocessor

The COMIDA2-generated MACCS2 input file name is user specified in the CHRONC input file by the BIN_FILE input parameter. The user must specify the drive and directory containing the COMIDA2 MACCS2 input files if the files are not contained in the subdirectory containing the MACCS2 executable.

If a COMIDA2-generated input file is used in a MACCS2 analyses, the DCF file specified in the EARLY input file must be the same DCF file used to generate the COMIDA2 MACCS2 input file.

The COMIDA2 input files associated with problem PROB can be identified by PROB.INP, PROB.VAR, and PROB.PAR. DOSDATA.INP AND DOSD825.INP files are DCF files required as input to the COMIDA2 sample problems and are specified in the PROB.INP file. The COMIDA2 sample problems may be run by typing:

```
RUNEM
```

or they may be run individually as follows:

```
RUNCOM2 PROB
```

where PROB is one of the COMIDA2 *.INP filenames without the .INP extension.

EXECUTION OF MACCS2 FROM A COMMAND PROMPT WINDOW

To execute the MACCS2 sample problems, open a command prompt window. Change to the MACCS2/ directory. Type the following command:

```
  RUNEM
```

This will regenerate the .OUT files in the MACCS2/ directory, overwriting the provided set of output files.

A single MACCS2 run is initiated by calling the RunMACCS2.bat file and specifying six MACCS2 input and output file names. On the command line, the user must specify the ATMOS, EARLY, CHRONC, meteorological, site, and output file names. Sample problem A_O, for example, may be initiated with the following command line:

```
RunMACCS2 IN1A IN2A IN3A_O METSUR SURSIT LISTA_O
```

IN1A.INP is the ATMOS input filename
IN2A.INP is the EARLY input filename
IN3A_O.INP is the CHRONC input filename
METSUR.INP is the meteorological data input filename
SURSIT.INP contains site specific data
LISTA_O.OUT is the name of the output file to which the MACCS2 output is to be
written.

Double quotes, "", can be inserted in place of filenames not required when a run does not use a complete set of six input filenames.

Any FORTRAN error generated causing an abnormal termination to MACCS2 is written to a file called FortErr.log.

Any MACCS2 error generated that is caught by MACCS2 will be written to a file called MaxStat.log.

All executables on this CD were compiled with Compaq Visual FORTRAN Professional 6.6B on a Windows XP Professional platform. These can be executed on Windows XP Pro, 2000 and Windows NT platforms. Other platforms

have not been tested.

COMPILING FOR PC SYSTEMS

Files containing a LAHEY-FORTRAN source compatible with MACCS2 1.12 has not been included in this distribution, but is available upon request. MACCS2 1.13.1 was compiled using Compaq Visual FORTRAN Professional 6.6B on a Windows XP Pro platform. It was not tested against any other compiler.

The makefile fconsole.mak in the MACCS2/ directory contains the compiler and linker settings used to create MACCS2. This file was created by Visual Studio. Additional compiler and linker settings for the preprocessor and utility programs are in Comida2.mak in the COMIDA2/ directory, Dosfac2.mak in the DOSFAC2/ directory, and Fgrdcf.mak, Chain.mak and Readem.mak in the FGRDCF/ directory.

COMPILING FOR NON-PC SYSTEMS

The MACCS2 package includes a file of machine dependent subroutines which must be modified for non-PC environments. These subroutines are provided in MXXMICRO.FOR. Testing on Non-PC systems has not been done for MACCS2 version 1.13.

KNOWN ISSUES

---

1. There is a slight difference (less than .5%) in the results between MACCS2 1.12 and MACCS2 1.13 due to the change in the FORTRAN compiler.

2. There are three entries on the CD corresponding to the filename Dosdata.inp. These are not all identical. Within subdirectories MACCS2 and COMIDA2, Dosdata.inp corresponds to an older dose conversion factor file with the following header:

```
MACCS File DOSDATA.INP: Changed by D. CHANIN25-JUN-92, 09:53:47
Seven new organs added with MACCS Version 1.5.11.1
      19 ORGANS DEFINED IN THIS FILE:
```

The user will not be able to recreate this file given the data on this CD. This file is used for the MACCS2 sample problems and the creation of the COMIDA2 binary file SAMP_A.BIN. Within subdirectory DOSFAC2, Dosdata.inp corresponds to a newer file that is created by running DOSFAC2 using internal defaults set within the Dosfac2 executable. The header of this file is as follows:

```
DOSFAC2 VERSION 1.12.0.0, DOSFAC2 LAST MODIFIED 01/09/2004.
RUN DATE: 01/09/2004, 15:53:22
      20 ORGANS DEFINED IN THIS FILE:
```

Within the subdirectories MACCS2/ and COMIDA2/, this file is named DOSDATA.NEW. It is not used in any of the MACCS2 sample problems.

```
-------------------------------------------------------------------------
This software was written by Sandia National Laboratories with support from
Sigma Software LLC and AQ Safety Inc. For problems with the installation or
with
using MACCS2, you may contact Nate Bixler by email at nbixler@sandia.gov or
by phone at (505)845-3144.
```

SEPARATION

PAGE

ALOHA Computer Code Application Guidance for Documented Safety Analysis

Final Report

U.S. Department of Energy
Office of Environment, Safety and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

June 2004

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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the ALOHA computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the ALOHA documentation provided by the code developer. ALOHA is one of six computer codes designated by DOE's Office of Environmental, Safety and Health as a toolbox code for safety analysis.

Suggestions for corrections or improvements to this document should be addressed to –

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REVISION STATUS

Page/Section	Revision	Change
1. Entire Document	1. Final Draft for Review	1. Original Issue
2. Entire Document	2. Final Report	2. Updated all sections per review comments.

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EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications (DOE, 2002b). The Areal Locations of Hazardous Atmospheres (ALOHA) code is one of the designated toolbox codes.

ALOHA may require some degree of quality assurance improvement before meeting current SQA standards. In the interim period before these changes are completed, ALOHA is still considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available user's manual information.

The ALOHA guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

Use of the information contained here, although not ensuring correct use of ALOHA in each analytical context, will minimize potential user errors and the likelihood of ALOHA use outside its regime of applicability.

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1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and the variability in guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its recommendation to the DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the Board's concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include:

(i) identification of a suite of accident analysis software that is widely used in the DOE Complex, and

(ii) issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regime in accident analysis, default inputs, and special conditions for use.

Safety analysis software for the DOE "toolbox" status was designated by the DOE Office of Environment, Safety and Health (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications*, (http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf), and includes version 5.2.3 of the Areal Locations of Hazardous Atmospheres (ALOHA) code.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in the body of this report. This code-specific document will be maintained and updated until a minimum qualification software package is completed.

The contents of this report are applicable in the interim period until measures are completed to

bring ALOHA into compliance with defined SQA standards. The primary objective of the guidance report is to provide information on the use of ALOHA for supporting DOE safety basis accident analysis. Specifically, the report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Overcoming known vulnerabilities and avoiding code errors
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications
- Default input value recommendations for site-independent parameters, and
- Citations of currently available SQA documentation.

Thus, this report is intended to complement existing ALOHA user's documentation. The latter tends to be much broader in coverage of the full range of capabilities of ALOHA and the spectrum of inputs that might be needed depending upon the application, but lack cohesive and targeted guidance for particular applications such as DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The ALOHA guidance document is written using the following set of sections. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830 (CFR, 2001). More information follows on the scope and purpose of this document. The next major section is a summary description of ALOHA. A third section discusses applicable regimes for using ALOHA in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, succeeds this section. Following this discussion are sections on special conditions for use of the software and software limitations. A sample case is then provided, followed by acronyms and definitions, references, and appendices.

1.1 Background: Overview of Toolbox Software in Context of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software will be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as "toolbox" codes (DOE, 2002b). Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

The ALOHA guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

1.3 Purpose

The ALOHA code, while part of the toolbox collection of software, still may require SQA upgrades prior to meeting current established standards for software. However, until these SQA upgrades are completed so that ALOHA meets current established standards for software, ALOHA can be applied safely by following the guidance contained in this report. Once SQA upgrades are finalized with ALOHA, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of ALOHA in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

Even though ALOHA was developed as a tool for emergency response and emergency preparedness/planning, it is also widely used throughout the DOE complex to support 10 CFR 830 safety analysis. Note that this guidance document does not specifically address application issues related to emergency response or emergency preparedness/planning.

It is recognized that other computer codes besides ALOHA exist that perform similar source term and downwind concentration calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for many accident analysis

applications that involve chemical spills. The relative merits of using a different computer program or using a hand calculation for a given application is a judgment that must be made by the analyst on a case-by-case basis.

The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program. As part of this program, the Chemical Dispersion and Consequence Assessment (CDCA) Working Group (WG) was established to address issues and evaluate methodologies in the CDCA domain. Other WGs were also established for other domains of safety analysis (i.e., fire analysis, explosion analysis, spill source term analysis, in-facility transport analysis, and radiological dispersion and consequence assessment). The CDCA WG (also referred to as WG 6) issued a report that identifies and evaluates methodologies and computer codes to support CDCA applications (Lazaro, 1997). Also of interest is the WG 3 report, which performed a similar function for source term analysis of spills (Brereton, 1997).

The CDCA WG 6 report identified the ALOHA computer code as a recommended code that is "applicable to generally broad safety basis documentation applications." The ALOHA code was similarly recommended by the Spills WG 3 report. In addition to code recommendations, both the Spills WG 3 report and the CDCA WG 6 report also provide a broad set of recommended "best practices" for modeling chemical releases to the atmosphere for safety analysis applications.

This report builds upon the WG 3 and WG 6 work to provide guidance and recommendations that are targeted to the use of the ALOHA code to calculate source terms and downwind concentrations for safety analysis applications.

2.0 SUMMARY DESCRIPTION OF THE ALOHA CODE

This section provides a summary form description of the ALOHA. A brief overview is given with additional information to follow in other sections and appendices of the report to provide more in-depth coverage of topics such as the principles of source term development for analysis of accidents that involve chemical inventories, the interface with dispersion conditions in the atmosphere, and the overall assessment of toxicological exposure to receptors.

2.1 ALOHA Code Development

The current version (as of January 2004) of the ALOHA code is version 5.2.3, was released in 1999.[1] ALOHA is a public domain code that is part of a system of software that is known as the Computer-Aided Management of Emergency Operations (CAMEO) that was developed to plan for and respond to chemical emergencies. It is also widely used throughout the DOE complex for safety analysis applications, which is the focus of this document. The United States Environmental Protection Agency (EPA), through its Chemical Emergency Preparedness and Prevention Office (CEPPO), and the National Oceanic and Atmospheric Administration (NOAA) Office of Response and Restoration jointly sponsor ALOHA. ALOHA can be downloaded free of charge from the EPA website (http://www.epa.gov/ceppo/cameo/aloha.htm). An accompanying user's manual can also be obtained at the website (NOAA, 1999a). An online help is also built into the code and a technical staff is available to address user questions (NOAA, 1999b).

The ALOHA code has evolved over the years to add capabilities, improve algorithms, and correct errors. Appendix C contains a reproduction of website information on the developmental history of the ALOHA code from the early 1980s to the present. (http://response.restoration.noaa.gov/cameo/alohafaq/history.html).

ALOHA runs either on Macintosh or in Microsoft Windows™ (version 95 or later) on IBM-compatible personal computers. ALOHA requires a least 1 megabyte (MB) of RAM and about 2.5 MB of hard disk space.

Information sources for the technical details of the ALOHA algorithms are from the ALOHA User's manual (NOAA, 1999a), the online help with ALOHA 5.2.3 (NOAA, 1999b), the APAC WG reports (Brereton, 1997; Lazaro, 1997), a NOAA report (Evans, 1993) and a draft NOAA theoretical description memorandum (for ALOHA 5.0) (Reynolds, 1992). Information from ALOHA websites is also used:

- http://www.epa.gov/ceppo/cameo/instruct.htm
- http://www.nwn.noaa.gov/sites/hazmat/cameo/aloha.html

- [1] A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report.

- http://response.restoration.noaa.gov/cameo/aloha.html

Whenever possible, an attempt was made to verify any information that was in the draft NOAA theoretical description memorandum through use of the others sources of information.

2.2 Overview of ALOHA Models

ALOHA performs calculations for chemical source terms and resulting downwind concentrations. Source term calculations determine the rate at which the chemical material is released to the atmosphere, release duration, and the physical form of the chemical upon release.[2] The term cloud is used in this document to refer to the volume that encompasses the chemical emission. In general, the released chemical may be a gas, a vapor, or an aerosol. The aerosol release may consist of either solid (e.g., fume, dust) or liquid (e.g., fog, mist, spray) particles that are suspended in a gas or vapor medium.[3] Liquid particles are also referred to as droplets.

The analyst specifies the chemical and then characterizes the initial boundary conditions of the chemical with respect to the environment through the source configuration input. The ALOHA code allows for the source to be defined in one of four ways (i.e., direct source, puddle source, tank source, or pipe source) in order to model various accident scenarios. The source configuration input is used to either specify the chemical source term or to provide ALOHA with the necessary information and data to calculate transient chemical release rates and physical state of the chemical upon release. ALOHA calculates time-dependent release rates for up to 150 time steps (NOAA, 1999a). ALOHA then averages the release rates from the individual time steps over one to five averaging periods, each lasting at least one minute (NOAA, 1999a). The five averaging periods are selected to most accurately portray the peak emissions. The five average release rates are inputs to the ALOHA algorithms for atmospheric transport and dispersion (NOAA, 1999a). ALOHA tracks the evolution of the mean concentration field of the five

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[2] More sophisticated source term algorithms found in some other computer codes will also model the energetic effects of the release (e.g., as would occur with a fire or explosion) to include the impact of the initial momentum and buoyancy. ALOHA ignores these effects that can lead to initial puff or plume rise, which is sometimes modeled through an effective, elevated release height. The ALOHA approach of ignoring initial puff or plume rise is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release when plume depletion from deposition effects are ignored, as is done in ALOHA.

[3] The ALOHA code user's manual cautions that the ALOHA code does not model particulate transport phenomena (e.g., gravitational settling). Generally, particulate transport phenomena can be ignored with little error, but it is up to the analyst to make a determination of whether a passive atmospheric transport or dense-gas transport model is most appropriate. ALOHA has both models, and information in this document will provide guidance on their use. In the case of low concentrations of very fine airborne particles, it is reasonable to neglect transport phenomena peculiar to particulate and to assume that the particles remain suspended and act as a passive scalar contaminant that follows the flow field (Hanna, 2002). Under high concentrations of particles, the density of the cloud may be high enough that dense gas transport phenomena may be important.

separate chemical clouds and calculates the concentration at a given time and location through superimposition. ALOHA limits releases to one hour.

Evolution of the mean concentration field of the chemical cloud is calculated through algorithms that model turbulent flow phenomena of the atmosphere. The prevailing wind flows and associated atmospheric turbulence serve to transport, disperse[4], and dilute the chemical cloud that initially forms at the source. For an instantaneous release or release of short duration, the chemical cloud will travel downwind as a puff. In contrast, a plume will form for a sustained or continuous release.

The wind velocity is a vector term defined by a direction and magnitude (i.e., wind speed). The wind direction and wind speed determine where the puff or plume will go and how long it will take to reach a given downwind location. For sustained or continuous releases, the wind speed has the additional effect of stretching out the plume and establishing the initial dilution of the plume (i.e., determines the relative proportion of ambient air that initially mixes with the chemical source emission). Atmospheric turbulence causes the puff or plume to increasingly mix with ambient air and grow (disperse) in the lateral and vertical direction as it travels downwind. Longitudinal expansion also occurs for a puff. These dispersion effects further enhance the dilution of the puff or plume. The two sources of atmospheric turbulence are mechanical turbulence and buoyant turbulence. Mechanical turbulence is generated from shear forces that result when adjacent parcels of air move at different velocities (i.e., either at different speeds or directions)[5]. Fixed objects on the ground such as trees or buildings increase the ground roughness and enhance mechanical turbulence in proportion to their size. Buoyant turbulence arises from vertical convection and is greatly enhanced by the formation of thermal updrafts that are generated from solar heating of the ground.

The ALOHA code considers two classes of atmospheric transport and dispersion based upon the assumed interaction of the released cloud with the atmospheric wind flow.

- For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, ALOHA treats the released chemical as neutrally buoyant.[6] A neutrally

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[4] The term dispersion is sometimes used in the literature to describe the combined effects of advection (transport by the bulk motion of the wind flow) and turbulent diffusion (spreading) and other times, particularly in meteorological publications, to describe only the turbulent diffusion component. The latter, narrower sense is used in this document.

[5] Atmospheric flows experience a change in speed with height due to the friction of the earth's surface in slowing down the wind adjacent to it.

[6] In the strictest sense, neutrally buoyant conditions exist when the density difference between the released chemical cloud and ambient air is small. A positively buoyant cloud is produced when the cloud density is significantly less than that of the ambient air. The positive buoyancy induces puff or plume rise that results in an effective elevated release. The ALOHA code does not account for these positive buoyancy effects, but instead models the release as neutrally buoyant. This approach is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release.

buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

- Conversely, if the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either neutrally buoyant or dense-gas type of atmospheric transport and dispersion.[7] In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind, and the cloud alters the atmospheric wind field in its vicinity. Dense-gas releases can potentially occur with gases that have a density greater than air due to either a high molecular weight or being sufficiently cooled. A chemical cloud with sufficient aerosol content can also result in the bulk cloud density being greater than that of the ambient air. Dense-gas releases undergo what has been described in the literature as "gravitational slumping". Gravitational slumping is characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release.

Appendix A contains a more in-depth discussion of the neutrally buoyant model and the dense gas model that are used in ALOHA for atmospheric transport and dispersion calculations.

In addition to the source term and downwind concentration calculations, ALOHA allows for the specification of concentration limits for the purpose of consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). ALOHA refers to these concentration limits as level-of-concern (LOC) concentrations. Safety analysis work uses the Emergency Response Planning Guidelines (ERPGs) and Temporary Emergency Exposure Limits (TEELs) for assessing human health effects for both facility workers and the general public (Craig, 2001). While ERPGs and TEELs are not explicitly a part of the ALOHA chemical database[8], ALOHA allows the user to input any value, including an ERPG or TEEL value, as the LOC concentration. The LOC value is superimposed on the ALOHA generated plot of downwind concentration as a function of time to facilitate comparison. In addition, ALOHA will generate a footprint that shows the area (in terms of longitudinal and lateral boundaries) where the ground-level concentration reached or exceeded the LOC during puff or plume passage (the footprint is most useful for emergency response applications) (Figure 2-1).

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[7] ALOHA uses the terminology heavy gas in place of dense gas.

[8] The ALOHA chemical database incorporates two sets of concentration limits that are used in the chemical industry to address worker safety issues: (1) immediately dangerous to life or health (IDLH) and (2) threshold limit value – time weighted average (TLV-TWA). Note that ALOHA 5.3 that was released in March 2004 just prior to the issuance of this report does have ERPGs and TEELs as part of the chemical database.

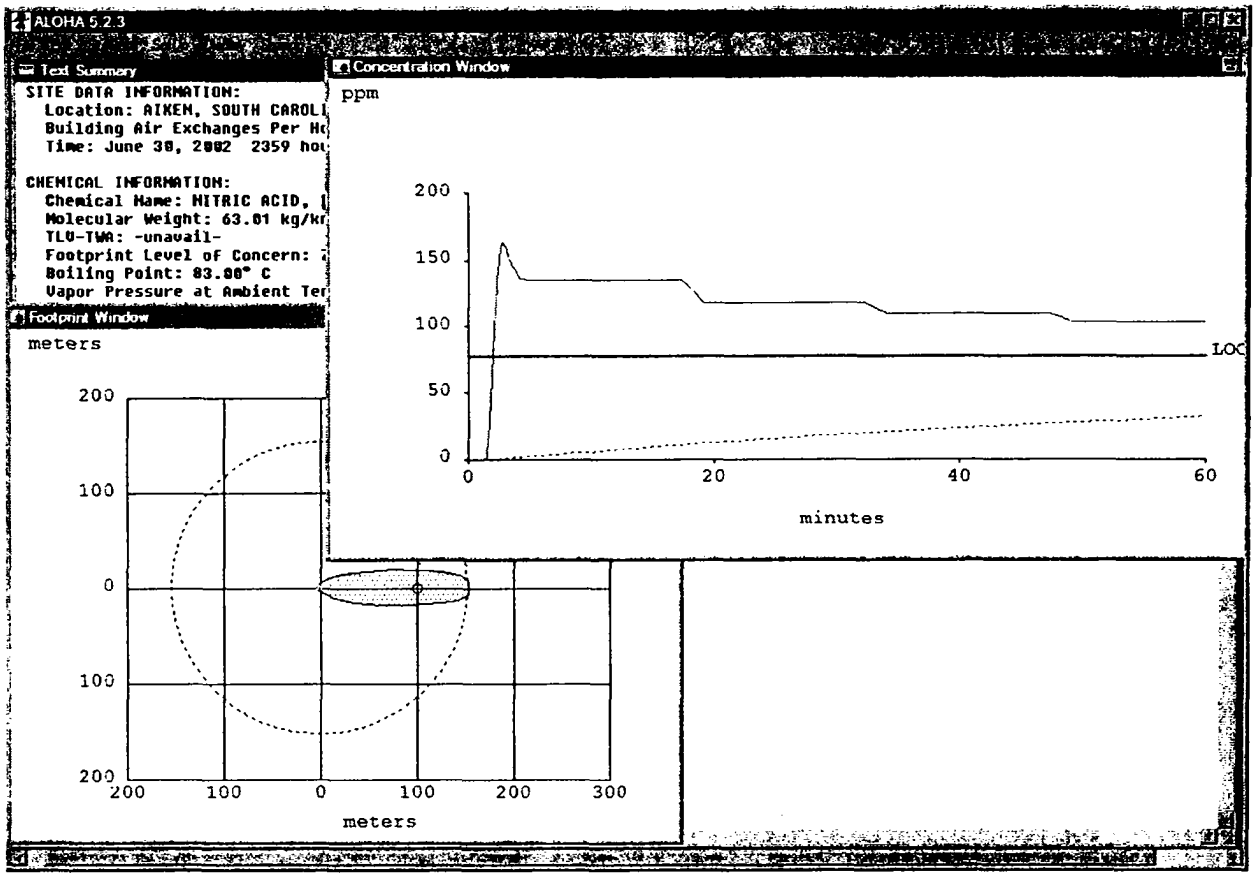

Figure 2-1. ALOHA Graphical Output.

2.3 ALOHA Software Quality Assurance

The validation and verification (V&V) efforts for ALOHA are not formally documented and do not appear to be part of a systematic quality assurance (SQA) plan (DNFSB, 2000). Some SQA information can be found in a document that is posted on the NOAA website (NOAA, 1998) and in a draft quality assurance report (Evans, 1994) as summarized below. Benchmark comparisons have been made with the results from the ARCHIE (FEMA, 1989) and CHEMS-PLUS (Little, 1988) computer models. Comparisons with field data were also made with the following results reported (NOAA, 1998; Evans, 1994).

- Source term prediction for non-boiling pool evaporation – All ALOHA predictions were within 42% of measured evaporation rates.

- Source term prediction for liquefied propane – About 83% of ALOHA predictions were within a factor of two of measured vaporization rates.

- Atmospheric transport and dispersion predictions with Gaussian model – ALOHA predictions of mean downwind concentrations tended to underestimate measured field

concentrations at distances of 200 meters or more and overestimate concentrations closer in.

- Atmospheric transport and dispersion predictions with dense-gas model for releases of ammonia, liquefied petroleum gas, liquefied natural gas, and dinitrogen tetroxide – ALOHA predictions were not compared directly with field measurements, but compared with results from the DEGADIS model that was calibrated to 12 trials from field experiments (Spicer, 1989). About 70% of DEGADIS predictions were within a factor of two of measured field concentrations. ALOHA predictions of mean downwind concentrations were on average conservative with respect to DEGADIS predictions.

- Atmospheric transport and dispersion predictions with dense-gas model for hydrogen fluoride (HF) releases –ALOHA predictions of mean downwind concentrations were on average 48% of the measured field data.

3.0 APPLICABLE REGIMES

The objective of this section is to present a discussion of ALOHA applicability from two perspectives: (1) in terms of its overall function as a key step in accident analysis; and (2) noting the phenomenological regimes in which it provides an approximate model of dispersion in the environment and the resulting toxicological exposure to downwind individuals (receptors).

3.1 Overall Application in Safety Analysis

The ALOHA code is designated for the toolbox under the area of applicability of chemical release and dispersion and consequence assessment. A code of this type of is used primarily to calculate the release rate to the atmosphere of a chemical involved in an accident scenario and the resulting instantaneous or time-averaged concentration of a chemical downwind from the accident. Because the DOE does not have an evaluation guideline for chemicals, the chemical concentration calculated is not used to distinguish safety-class designation for systems, structures, and components. A typical use of chemical consequence results is to confirm the selection of safety significant systems, structures, and components for worker protection.

Occasionally, chemical concentrations are used to help set limits on chemical inventory, and this may present more of a safety implication. When these code calculations are used to help set inventory limits, they have a direct effect on values used in technical safety requirements, and the quality of the calculation may be very important. Again, it is important to note that a hand calculation can often be used to verify this value.

In this context of setting limits on chemical inventory, analysts have generally applied the American Industrial Hygiene Association (AIHA) ERPGs[9] and TEELs [10] for the purpose of

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[9] The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The ERPGs are estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

> ***ERPG-1**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*
>
> ***ERPG-2**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*
>
> ***ERPG-3**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

assessing human health effects for both facility workers and the general public (Craig, 2001). Recently, another alternative has become available to analysts. The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) has been developing acute exposure guideline levels (AEGLs) to assist federal and state agencies and private sector organizations with their need for short-term hazardous chemical exposure information in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h).[11]

Since the DOE has not provided definitive evaluation guidelines for chemical exposures for use in DSAs, the specific use of ERPGs, TEELs, and AEGLs in accident analysis remains largely an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001). In some cases, surrogate values for inventory limits (such as EPA or OSHA limits) can also be used.

3.2 Phenomenological Regimes of Applicability

The atmospheric transport and dispersion algorithms of ALOHA are based on Gaussian and dense-gas models. These models are best suited for specific types of conditions. The chief phenomenological regimes for applying ALOHA include:

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[10] The temporary emergency exposure limits (TEELs) are another set of chemical-specific concentrations that correspond to varying levels of health effects (Craig, 2001). TEELs have been developed since ERPGs are available only for a limited number of chemicals. The TEELs consist of (a) ERPG values for all chemicals for which ERPGs have been published and surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values), and (b) Permissible Exposure Limit - TWA (PEL-TWA) values for all chemicals for which PEL-TWA values have been published and surrogate PEL-TWA values for additional chemicals (i.e., the TEEL-0 values) (Craig, 2001). PEL-TWA values are developed by the Occupational Safety & Health Administration (OSHA) for use in limiting worker exposures to airborne chemicals (CFR, 1999). Most people are not expected to experience any adverse health effects to accident exposures at the TEEL-0 level (Craig, 2001).

[11] The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) is developing AEGLs in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h) and three severity levels as defined below:

AEGL-1: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

- Temporal regime – These models are best suited for "short" duration plumes, ranging from approximately several minutes to several hours (ALOHA limits the duration to one hour).
- Spatial regime - These models have high uncertainty close to the source, especially where the influence of structures or other obstacles is still significant. Dispersion influenced by several, collocated facilities, within several hundred meters of each other should be modeled with care. Similarly, ALOHA imposes a downwind distance limit of ten kilometers (six miles). The rationale behind the distance limit of ten kilometers and the one-hour time limit that is noted above is that meteorological conditions are likely to vary with location and change after significant passage of time. Long-range projections of toxicological exposures are better calculated with mesoscale, regional models that are able to account for multiple weather observations.
- Terrain variability – These models are inherently flat-earth models, and perform best over regions of transport where there is minimal variation in terrain.
- Extreme weather – These models do not apply to extreme weather conditions such as tornadoes.

4.0 INPUTS AND RECOMMENDATIONS

4.1 Overview of ALOHA Input Menus

Users of ALOHA enter input data mainly through two menus that are labeled "Site Data" and "Set up" on the menu bar (Figure 4-1). Preliminary information about the location of the accidental release and date and time are entered through a series of dialog boxes that are accessed through the Site Data menu. The chemical that is released and the initial and boundary conditions associated the postulated accident scenario are input through a series of dialog boxes that are accessed through the Set up menu. In addition, an ERPG or TEEL value can be entered as the LOC value under the menu labeled "Display" ("Options" submenu) or alternatively saved as the default LOC in the chemical library.

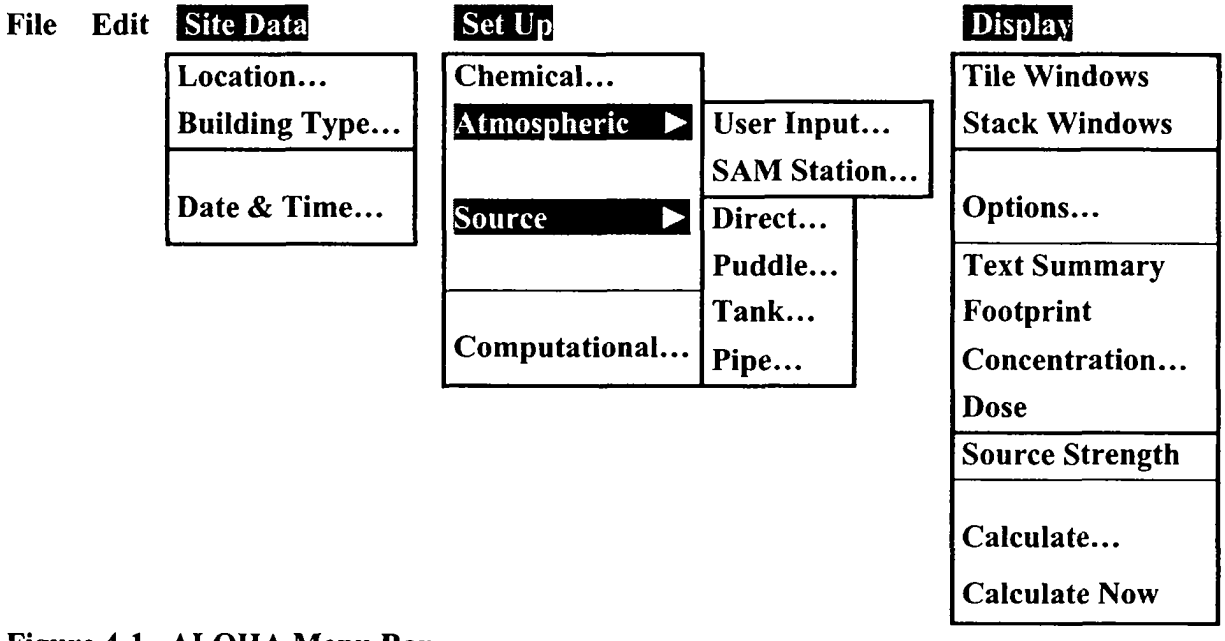

Figure 4-1. ALOHA Menu Bar.

For each numerical input, ALOHA typically allows for a variety of units (both metric and British) to be used. The user must therefore identify the particular units to be used among those offered by ALOHA and input the numerical value on the basis of the units that have chosen for the given input parameter. Frequently, an ALOHA dialog box presents one or more pre-defined options that the user may select through the use of selection bubbles, but generally the user is not limited to these options as a space for numerical values to be input as an alternative is usually available (Figure 4-2).

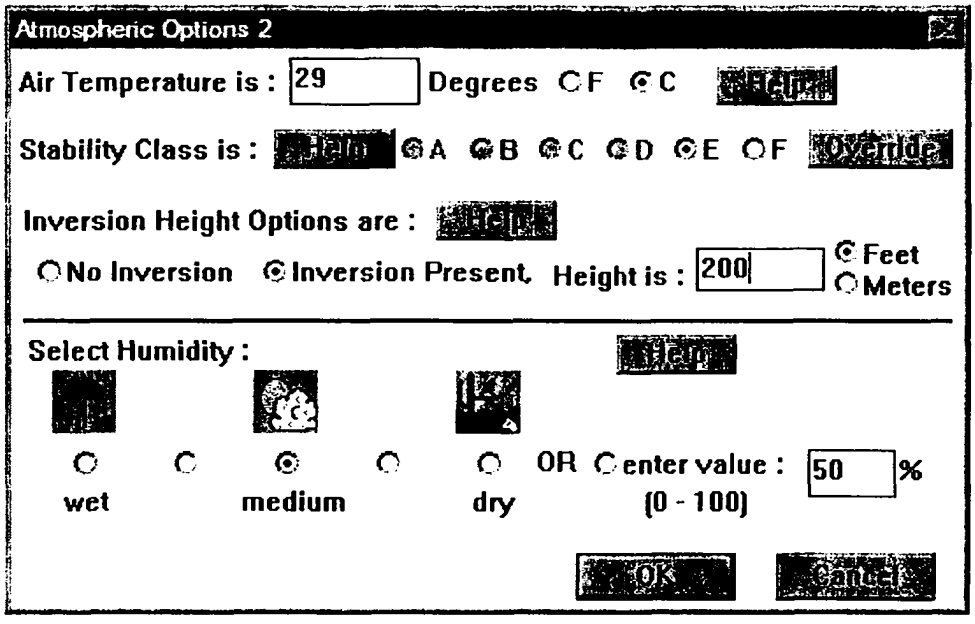

Figure 4-2. Sample ALOHA Dialog Box for Data Entry.

4.2 Input Recommendations for Site Data Parameters

The following submenus are included under the Site Data menu:

- Location
- Building Type
- Date and Time

4.2.1 LOCATION

More than 500 U.S. cities as well as some Canadian cites are part of the ALOHA library. The library includes the elevation, longitude, and latitude of each city. The longitude and latitude, along with the time and date inputs that are discussed later, are used to estimate the incoming solar radiation (Reynolds, 1992). The amount of incoming solar radiation on a puddle influences the evaporation rate. ALOHA uses the elevation input to determine ambient air pressure (Reynolds, 1992).

Recommendation: Choose the city in closest proximity to the location of interest or add a new city to the library by entering its name along with the elevation, longitude, and latitude of the city.

4.2.2 BUILDING TYPE

Building parameters related to infiltration are entered through the dialog box under the Building Type submenu. Choices for the building type are (i) enclosed office building, (ii) single storied

building, or (iii) double storied building. The user selects one the above three choices or alternatively enters the number of air changes per hour (allowable range is 0.01 to 60 exchanges per hour) (NOAA, 1999b). The user also identifies the building surroundings as either sheltered (with trees, bushes, etc.) or unsheltered.

Recommendation: ALOHA uses the information entered here to determine indoor infiltration and to estimate indoor concentration and chemical dose at a location. ALOHA assumes that all doors and windows are closed. DSA analysis conservatively takes no credit for sheltering or evacuation. As a result, safety analysts do generally not use the indoor concentration and chemical dose calculated by ALOHA.

4.2.3 DATE AND TIME

The user is provided with the option to use either the internal clock or set a constant time and date. Time is based on a 24-hour clock. ALOHA uses this input, along with the location data, to determine the incoming solar radiation based upon the position of the sun.

Recommendation: Set a constant time that is consistent with the input specification for the atmospheric stability class (discussed in a later section). For example, stable atmospheric conditions occur at night or early morning. Unstable atmospheric conditions occur during the day. Neutral atmospheric conditions can occur either at day or night. For analysis of a daytime release, the evaporation rate increases with increasing solar influx. A conservative approach for unstable and neutral atmospheric conditions is to set the date to a mid-summer day (e.g., June 30th) and the time to around noon (e.g., 12:00). Any year may be specified since the results can be expected to be insensitive to the year input (ALOHA, however, will prompt the user to check his entry if the year is more than 10 years away from the current year).

4.3 Input Recommendations for Set Up Parameters (Scenario Definition)

The following submenus are included under the Set Up menu:

- Chemical Information
- Atmospheric Options
- Source
- Computational Preferences

4.3.1 CHEMICAL INFORMATION

Over 1000 chemicals are part of the chemical library.

Recommendation: Choose chemical of concern from chemical library list or enter new chemical into library. An ALOHA dialog box will prompt the user to enter the following information for the new chemical.

- Chemical name

- Molecular weight
- Boiling point
- Critical pressure
- Critical temperature
- Default level of concern
- Density (gas)
- Density (liquid)
- Diffusivity (molecular)
- Freezing point (normal)
- Heat capacity (gas, constant pressure)
- Heat capacity (liquid, constant pressure)
- IDLH
- TLV-TWA
- Vapor pressure

Information on what properties are required to support each source configuration option and atmospheric transport and dispersion type is given in Table 4-1 (NOAA, 1999a).

Table 4-1 Use of Chemical Property Data

Property	Direct Source		Puddle Source		Tank Source		Pipe Source	
	Gaussian	Heavy Gas	Gaussian	Heavy Gas	Gaussian	Heavy Gas	Gaussian	Heavy Gas
Chemical Name	●	●	●	●	●	●	●	●
Molecular Weight	●	●	●	●	●	●	●	●
Boiling Point	●[1]	●	●	●	●	●	●	●
Critical Pressure	●[1]	●[2]	●	●	●	●	●	●
Critical Temperature	●[1]	●[2]	●	●	●	●	●	●
Gas Density		●		●		●		●
Freezing Point			●	●	●	●		
Gas Heat Capacity		●	●	●	●	●	●	●
Liquid Heat Capacity			●	●	●	●		
Vapor Pressure		●[2]						

1 Required only if direct source term is expressed in volume or volume rate units. That is, these properties are not required if source term is expressed in mass or mass rate units.

2 Either the vapor pressure is required or both the critical pressure and critical temperature is required.

4.3.2 ATMOSPHERIC OPTIONS

ALOHA allows meteorological conditions to be entered from a portable monitoring station. For accident analysis purposes, however, the user enters the meteorological data manually. Note that ALOHA does not handle extreme weather conditions such as tornadoes Appendix B summarizes an approach that has been used at Savannah River Site for tornadoes.

ALOHA requires input for the following meteorological parameters.

- Wind speed
- Wind direction

- Measurement height of wind speed
- Ground roughness
- Cloud cover
- Air temperature
- Stability class
- Inversion height
- Humidity

In calculating puff or plume concentrations, both "unfavorable" and "typical" dispersion conditions are of special interest in accident analyses. For accident analysis consideration of the offsite receptor, unfavorable meteorology is ideally based on site data. In defining unfavorable meteorological conditions for chemical releases, it seems reasonable to follow the practices that are used for radiological consequence analysis. Unfavorable meteorology refers to the meteorology that coupled with the source term would lead to doses (or concentration exposures for chemicals) that are exceeded less than five percent of the time. The method should be conservative or consistent to the discussion in the NRC Regulatory Guide 1.145 (Position 3) (NRC, 1983) as summarized in Appendix A to DOE-STD-3009-94, CN2 (DOE, 2002a). The 95^{th} percentile result of the distribution of doses (or concentration exposures for chemicals) to the offsite receptor, accounting for variation in distance to the site boundary as a function of direction, is generally the consequence result of interest. The median or the 50^{th} percentile result of the consequence distribution is usually the basis for typical meteorological conditions. The determination of the meteorological conditions that correspond to 50^{th} and 95^{th} percentile consequence results will require the simultaneous consideration of both atmospheric stability class and wind speed (the effect of ambient temperature on chemical vapor pressure may also be considered for scenarios that involve pool evaporation).

Meteorological variables such as wind speed and solar radiation affect both the evaporation rate and the amount of dilution of the puff or plume during atmospheric transport. Generally, these variables affect the evaporation rate and atmospheric dilution in opposite ways with regard to the effect produced on downwind concentrations. For example, higher wind speeds increase the evaporation rates, but also support greater dilution of the plume. Similarly, higher solar radiative influx and warmer temperatures also increase the evaporation rates, but typically support atmospheric conditions that are less stable and more dispersive. Meteorologists at Savannah River Site (SRS) studied these effects and concluded that the dominant influence of the meteorological variables generally occurs with atmospheric dispersion and dilution (Hunter, 1993). Higher downwind concentrations are associated with stable atmospheric conditions and low wind speeds (Hunter, 1993).

The size of the data set used in the meteorological assessments should be sufficiently large that it is representative of long-term meteorological trends at most sites. Meteorological data, qualified and meeting requirements of Regulatory Guide 1.23 (NRC 1972), available at most DOE sites

should be applied that is representative of long-term trends. A five-year data set is desirable, but a one-year data set can be applied under the right circumstances.[12]

In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes (EPA, 1999). See Appendix A for a fuller discussion on the role of wind speed and atmospheric stability class on downwind puff or plume concentrations, especially as these parameters relate to the Gaussian transport and dispersion models for neutrally buoyant releases. For elevated releases, the lofted plume must travel further downwind with stable atmospheric conditions before reaching the ground and exposing receptors to the hazardous contaminant. Therefore, neutral or even unstable stability conditions may produce the most unfavorable meteorological conditions for receptors close to the elevated release.

It should be noted that in the long run, site data is normally preferable over the default conditions for accident analysis. Meteorologists evaluated SRS data and found the conditions associated with 95th percentile results varied with release height, and receptor distance (Hunter, 1993). For most facility distances to the offsite boundary, it was determined for neutrally buoyant plumes that 95th percentile results correspond to conditions of E stability and the following wind speeds.[13]

- 1.7 m/s wind speed (release height 0 m – 10 m)
- 2.1 m/s wind speed (20-m release height), and
- 3.0 m/s wind speed (60-m release height).

Finally, note that the specification of the atmospheric stability class in ALOHA should be consistent with inputs for location, date and time, wind speed, surface roughness length, and cloud cover. Algorithms are used within ALOHA to inform the user of which atmospheric stability classes are consistent with other data that the user has entered for these parameters.

Guidance for each meteorological parameter required by ALOHA follows.

Wind Speed

ALOHA accepts 10-m reference elevation wind speeds in the range of 1 m/s to 60 m/s (NOAA, 1999b). ALOHA can accommodate wind speed values that are representative of other heights since inputs are required for both the wind speed and the corresponding height for this wind

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[12] In Regulatory Guide 1.194, this subject is discussed as follows: "The NRC staff considers five years of hourly observations to be representative of long-term trends at most sites. With sufficient justification of its representativeness, the minimum meteorological data set is one complete year (including all four seasons) of hourly observations." (NRC, 2003)

[13] The cited wind speeds reflect the value at the release height (at 10 m for the 0 m – 10 m release height range).

speed. The height input parameter for the wind speed is discussed separately in a later section of this document.

Recommendation: As discussed above, statistical analysis of site-specific, wind speed measurements is the preferred approach for specifying wind speed. The determination of the meteorological conditions that correspond to the 50th and 95th percentile consequence results will require the simultaneous consideration of both atmospheric stability class and wind speed (ambient temperature may also be considered for scenarios that involve pool evaporation).

In general, higher downwind concentrations (i.e., unfavorable meteorological conditions) are associated with lower wind speeds. In lieu of site-specific meteorological data, the following default wind speeds may be considered for each atmospheric stability class (Lazaro, 1997). More discussion of the interplay between wind speed and atmospheric stability in establishing typical and unfavorable meteorological conditions is presented later in the context of the input for atmospheric stability class. Also, performing a parametric study among the various combinations of wind speed and atmospheric stability classes can provide useful insights about the role of wind speed and atmospheric stability class in determining unfavorable meteorological conditions.

	Atmospheric Stability Class					
	A	B	C	D	E	F
Default Wind Speed [m/s]	2.0	*	*	4.5	1.5	1.5

* Lazaro (1997) does not specify default wind speeds for B and C stability classes. The 2.0 m/s default wind speed value that is specified for A stability class would seem to be a reasonably conservative choice based on information presented later in this section, as well as in Appendix A, for atmospheric stability class and wind speed.

Wind Direction

The wind direction is specified as the direction from which the wind is blowing. This information is entered in either units of degrees true, or in one- to three-letter directional terms. For example, the wind blowing from the north-northeast is indicated by entering either NNE or 22.5 degrees.

Wind directions expressed in degrees and letter terms correspond as follows:

- N = 0 degrees or 360 degrees
- NNE = 22.5 degrees
- NE = 45 degrees
- ENE = 67.5 degrees
- E = 90 degrees
- ESE = 112.5
- SE = 135 degrees

- SSE = 157.5 degrees
- S = 180 degrees
- SSW = 202.5 degrees
- SW = 225 degrees
- WSW = 247.5 degrees
- W = 270 degrees
- WNW = 292.5 degrees
- NW = 315 degrees
- NNW = 337.5 degrees

Recommendation: For accident analysis calculations, any direction may be input. The calculated concentrations for a given downwind distance that are calculated by ALOHA are insensitive to direction input.

Measurement Height for Wind Speed

ALOHA accounts for the variation of wind speed with distance from the earth's surface as caused by friction. Therefore, ALOHA needs the height that is associated with the wind speed that is entered. From discussions with ALOHA technical staff, the atmospheric transport and dispersion calculations of ALOHA are based on either the wind speed at the release height or at 3 meters for release heights of 3 meters or less.

Recommendation: The input for this parameter must be consistent with the value that is input for the wind speed (that was discussed in a previous section above). If the value for wind speed input into ALOHA is based on site measurements at a known height, then that height should be input. Generally, portable weather monitoring stations are mounted approximately 3 meters high. Typically, the NWS measures and reports wind speeds at 10 meters. When using the generally accepted, default combination of F stability class and 1.5 m/s wind speed or the equivalent for analysis of ground-level releases of neutrally buoyant plumes, specifying a 10-meter measurement height is expected to yield a more conservative result than that obtained from specifying a 2-meter measurement height. With a 10-meter measurement height specification, ALOHA will calculate a wind speed at 2 meters that is less than 1.5 m/s for use in the Gaussian plume model, and the Gaussian plume model predicts downwind concentrations that are inversely proportional to wind speed as shown in Appendix A.

Ground Roughness

ALOHA accepts input of "open country" or "urban or forest" to characterize the surface roughness. Alternatively, ALOHA accepts input of a roughness length (z_o) between 0.001 centimeters and 200 centimeters (NOAA, 1999b). How ALOHA uses this input depends upon whether ALOHA is performing a heavy-gas or Gaussian dispersion calculation as discussed below (NOAA, 1999b).

For a heavy-gas dispersion calculation, ALOHA limits z_o to a maximum 10 centimeters. ALOHA will set z_o to the value entered by the user when the value is 10 centimeters or less. ALOHA uses a maximum z_o value of 10 centimeters whenever the user enters a value that is greater than 10 centimeters.

For a Gaussian dispersion calculation, ALOHA will either use a z_o value of 3 centimeters or 100 centimeters. The 3-cm value corresponds to terrain that is characterized as "open country". In open country, the roughness elements are small and widely spaced (e.g., open fields, parking lots). The 100-cm value corresponds to terrain that is characterized as "urban or forest" and that would be characteristic of residential housing developments, industrial areas or forests. ALOHA will set z_o to the 3-cm value whenever the user enters a value that is 20 centimeters or less. ALOHA uses a z_o value of 100 centimeters whenever the user enters a value that is greater than 20 centimeters. ALOHA uses the ground roughness input to determine which set of vertical dispersion coefficients (σ_z) will be used in the calculation. Two different sets of σ_z curves are used by ALOHA for rural and urban environments, respectively.[14]

The different approaches for heavy-gas dispersion and Gaussian dispersion are consistent with the observation that surface roughness has less influence on dense-gas releases in comparison with neutrally buoyant releases (Lazaro, 1997).

Various tables of z_o as a function of terrain attributes are found in the literature (Lazaro, 1997; Hanna, 2002). In addition, the ALOHA online help (NOAA, 1999b) provides the following guidance from Brutsaert (1982).

Surface description	z_o (cm)
Mud flats, ice	0.001
Smooth tarmac (airport runway)	0.002
Large water surfaces (average)	0.01-0.06
Grass (lawn to 1 cm high)	0.1
Grass (airport)	0.45
Grass (prairie)	0.64
Grass (artificial, 7.5 cm high)	1.0
Grass (thick to 10 cm high)	2.3
Grass (thin to 50 cm)	5.0
Wheat stubble plain (18 cm)	2.44

[14] The Gaussian plume equation makes use of both a vertical dispersion coefficient (σ_z) and a horizontal dispersion coefficient (σ_y). Typically, dispersion modeling uses different sets of σ_y and σ_z dispersion coefficients for open country (often referred to as rural) and urban applications. ALOHA, however, uses the same set of σ_y dispersion coefficients for both open country and urban applications (Reynolds, 1992). Appendix A has a brief discussion of the Gaussian plume equation and the role of the dispersion coefficients.

Grass (with bushes, some trees)	4
1-2 m high vegetation	20
Trees (10-15m high)	40-70
Savannah scrub (trees, grass, sand)	40
Large city (Tokyo)	165

Recommendation: It is generally conservative to choose open country dispersion (or equivalently specify a z_o value of 3 cm) instead of urban or forest dispersion (z_o = 100 cm). It is recommended, however, that the analyst uses judgment based on site observation and published guidance to take credit for surface roughness effects in increasing puff and plume dispersion where appropriate. Ideally, consultation with the laboratory or site meteorology organization responsible for recording and maintaining site meteorological data is available to the analyst to assist in specifying this input and defending its use.

The ALOHA online help recommends using the dominant characteristic of the terrain that surrounds the postulated release and receptor distances of interest (NOAA, 1999b). Following this guidance, urban or forest terrain would be selected whenever more than 50% of the surrounding terrain is urban or forest. This recommendation is generally consistent with EPA guidance as defined in the Risk Management Program (RMP) (EPA, 1999). EPA considers the term rural to refer to terrain that is generally flat with few buildings or other obstructions (e.g., hills, trees). Conversely, EPA guidance recommends assuming urban conditions for a site area with many obstructions "even if it is in a remote location that would not usually be considered urban" (EPA, 1999).

Cloud Cover

This input parameter represents the proportion of the sky that is covered by clouds. It is expressed in tenths following the convention that is used by U.S. meteorologists. For example, 5 tenths corresponds to a sky that is half-covered by clouds. The allowable input range is from 0 (completely clear sky) to 10 (completely cloudy sky).

Cloud cover is a determining factor of atmospheric stability class. Since cloud cover and atmospheric stability are separate input parameters in ALOHA, input values entered for these two parameters should be consistent with one another. ALOHA primarily uses the cloud-cover input to estimate the amount of incoming solar radiation that is incident upon the puddle formed by a liquid spill (cloud cover is expected to also have an effect at night on the long wave radiation calculations and therefore a small effect on evaporation). Decreasing cloud cover during daytime allows for more heating of the puddle by the sun and a higher evaporation rate. The calculation uses this input for the release scenarios that involve a puddle forming on the ground (e.g., specified explicitly by user through puddle source or determined by ALOHA with a user-specified tank source). Although not used for scenarios that do not involve a puddle (e.g., direct source, pipe source), a value for the fractional cloud cover is still required by ALOHA.

Recommendation: The specification of fractional cloud cover should be consistent with the atmospheric stability class input. Stable and unstable atmospheric conditions are supported by

low cloud cover conditions. For daytime releases, some minimum amount of cloud cover may be necessary to support neutral (class D) atmospheric conditions.

A recommended conservative approach is based upon algorithms that are used in ALOHA to identify appropriate choices for atmospheric stability class based on the inputs for location, date and time, wind speed, surface roughness length, and cloud cover. Using the data entered for these other input parameters, ALOHA dims the stability class designations that it determines to be incompatible (and fills the associated selection bubble gray as shown in Figure 4-2) and leaves the other stability classifications available for selection (clear selection bubble).[15] A trial-and-error approach for specifying a conservative fractional cloud cover use with daytime puddle scenarios is outlined below.

- Following guidance that is in this document, determine the combination of atmospheric stability class and wind speed that is appropriate for the accident scenario to be analyzed and type of meteorological conditions (e.g., unfavorable, typical) to be assumed for the analysis.

- Completely enter data under the Site Data menu, which will include the inputs for location and date and time.

- Under the Set Up menu, start entering data under the Atmospheric Options submenu in the order that ALOHA prompts the user through the dialog boxes: wind speed; wind direction; measurement height for wind speed; and then ground roughness length.

- Enter 0 (tenths) for fractional cloud cover. Observe the section of dialog box pertaining to atmospheric stability class to see if the atmospheric stability class of interest for the scenario is identified by ALOHA as compatible with the other inputs. If so, continue with the data entry thus using 0 tenths as the fractional cloud cover for the calculation. If not, increase the fractional cloud cover by 1 (tenth) until the atmospheric stability class of interest for the scenario is identified by ALOHA as compatible.[16]

Air Temperature

The allowable input range for air temperature is -100 degrees F to 150 degrees F (-73 degrees C to 65 degrees C) (NOAA, 1999b). Air temperature is an input to the puddle heat-transfer algorithm that is used to determine the puddle temperature, from which the vapor pressure of the liquid chemical and the evaporation rate are determined for non-boiling liquids.

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[15] An override button allows the user to select any of the atmospheric stability classes that ALOHA has determined to be incompatible.

[16] If the atmospheric stability class of interest does not show up as compatible for any input value (0 to 10) for fractional cloud cover, check other input entries for correctness. The correctness check should include the date and time entries (note that if the user neglects to enter the date and time, ALOHA defaults to information supplied by the internal computer clock).

Recommendation: As discussed above, statistical analysis of site-specific, meteorological measurements is the preferred approach for specifying meteorological conditions. For air temperature, a reasonably bounding high temperature is recommended based on analysis of the site data. For example, Lazaro suggests the 95th percentile value of a five-year record of daily high temperatures for the warmest month of the year (Lazaro, 1997).

Stability Class

ALOHA uses data entered for date and time, wind speed, and cloud cover to identify stability classes that are compatible with the entered data and to automatically select one of the stability classes. ALOHA uses the table below for determining compatible stability classes (Turner, 1970; NOAA, 1999b).

Surface Wind	Day			Night	
Wind Speed	Incoming Solar Radiation			Cloud Cover	
[m/s]	Strong	Moderate	Slight	> 0.5	< 0.5
< 2	A	A-B	B	E	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
> 6	D	D	D	D	D

Notes for information above:

- Stability is D for completely overcast conditions during day or night.
- "Night" is the time period from 1 hour before sunset until 1 hour after sunrise.
- "Strong" solar radiation corresponds to clear skies with the sun high in the sky (solar angle greater than 60 degrees).
- "Slight" solar radiation corresponds to clear skies with the sun low in the sky (solar angle between 15 and 35 degrees).

Recommendation: As mentioned several times in this document, statistical analysis of site-specific, meteorological measurements is the preferred approach for specifying meteorological conditions. The determination of the meteorological conditions that correspond to the 50th and 95th percentile consequence results will require the simultaneous consideration of both atmospheric stability class and wind speed (ambient temperature may also be considered for scenarios that involve pool evaporation). In lieu of site-specific meteorological data, the following guidance is provided.

i) For ground-level (and nearly ground-level) releases that are neutrally buoyant, stable atmospheric conditions and low wind speeds represent generally accepted, unfavorable

meteorological conditions (i.e., F stability class and 1.5-m/s wind speed) (Hanna, 1996a; Lazaro, 1997). Stable atmospheric conditions and low wind speeds are also expected to produce unfavorable meteorological conditions for dense gas releases at ground level that are continuous (Hunter, 1993; Hanna, 1996a; Lazaro, 1997).

ii) For short-duration releases (i.e., puffs) of dense gases, unfavorable meteorological conditions may occur with neutral stability conditions and moderate wind speeds (Hanna, 1996a; Lazaro, 1997). With dense-gas puffs or plumes, it is recommended that a parametric study be performed among the various combinations of wind speed and atmospheric stability classes to determine unfavorable meteorological conditions for the receptor locations of interest.

iii) For elevated releases of neutrally buoyant gases, the atmospheric stability class associated with unfavorable meteorological conditions will be dependent upon the distance of the receptor from the source. At very close distances, the ground level concentration may be zero for stable conditions as the puff or plume simply passes overhead. Unstable atmospheric stability will result in the highest ground-level concentrations at close distances as high levels of turbulence will promote rapid dispersion of the puff or plume to the ground from its elevated release position. At receptor locations further downwind, neutral atmospheric buoyant conditions produce the highest ground-level concentrations with the Gaussian plume model. Even further downwind, the highest ground-level concentrations occur with stable atmospheric conditions as the puff or plume has traveled far enough downwind for the puff or plume to disperse enough to reach ground level. With elevated releases of neutrally buoyant gases, it is recommended that a parametric study be performed among the various combinations of wind speed and atmospheric stability classes to determine unfavorable meteorological conditions for the receptor locations of interest.

As mentioned above, accident analysis calculations under typical meteorological conditions may sometimes be performed. Atmospheric stability class D is the most common stability class for many DOE sites. This is due to the large number of combinations that can result in stability class D. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally associated with stability class D. A wind speed of 4.5 m/s together with atmospheric stability class D has been suggested to represent typical meteorological conditions (FEMA, 1989). This set of conditions is also consistent with a basis by chemical process industry for determining limits on chemical inventories, and is representative of most U.S. regions (CFR, 1992) and for radiological hazard categorization of DOE facilities (DOE, 1997).

Inversion Height

ALOHA prompts the user for an inversion height or to indicate that no inversion exists. ALOHA accept input values for the inversion height between 10 feet (about 3 meters) and 5,000 feet (about 1,524 meters) (NOAA, 1999b).

A dense-gas cloud generally remains close to the ground as it travels downwind. As a result, ALOHA assumes that dense-gas dispersion in unaffected by the presence of an inversion layer

(NOAA, 1999b). While this input is still required, ALOHA does not use the input value in the dense-gas dispersion calculations.

The presence of an inversion does restrict the upward dispersion of neutrally buoyant gases that is calculated by ALOHA. Increased ground-level concentrations may result due to the presence of the inversion.

The inversion layer height input that is used by ALOHA is frequently referred to as the mixing layer height. The mixing layer height varies throughout the day and throughout the seasons. During clear nights or early mornings when inversions are present, the mixed layer is relatively low, while during sunny days the mixing layer is much higher. The magnitude of these heights can be obtained from balloon soundings or from remote sensing techniques, such as acoustic or radar soundings. In the absence of such data, regional tables can be consulted.

Recommendation: Base mixing layer height on seasonal averages and day/night time of day. Apply archived site or laboratory meteorological data. If this is not available, use regional data as default input values, such as those of Holzworth (1972).[17] Since lower inversion heights can lead to higher downwind concentrations, it is appropriate for conservatism to specify an inversion height value that is reasonable, but skewed more towards the lower end of the observed or expected range.

Humidity

A number of chemicals are hygroscopic and react with moisture in the air. Transformations that result can have a pronounced impact on atmospheric transport and dispersion, but these effects are not modeled in ALOHA.

ALOHA takes relative humidity into account when it estimates the rate of evaporation from a puddle. Specifically, the relative humidity affects longwave radiation transfer between the atmosphere and the puddle (Reynolds, 1992). Relative humidity also plays a role in heavy gas dispersion computations. When the cloud is at a temperature that is different than that of the ambient air, less air is required to mix with the cloud to achieve thermal equilibrium when the relative humidity is high since water has a significantly higher heat capacity relative to dry air (Lazaro, 1997).

The relative humidity is expressed as a percentage and entered as a whole number that is between 0 and 100 (percent) inclusive.

Recommendation: Neither the ALOHA documentation nor the published literature in general supply much detail on the role of water vapor content on calculations of chemical evaporation and subsequent transport and dispersion. The CDCA WG recommends a value of 50% for the

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[17] The mean mixing heights for mornings in the continental United States range between approximately 200 m and 1200 m depending upon season and location (Holzworth, 1972). The mean mixing heights are higher for afternoons, ranging between 500 m and 4000 m (Holzworth, 1972).

relative humidity (Lazaro, 1997). In absence of other guidance, the use of a medium value for relative humidity seems reasonable. The user also has the option of using a value more representative of the site being analyzed. Another alternative is to perform a parametric study on the sensitivity of the results to relative humidity for the accident being analyzed. [18]

4.3.3 SOURCE

The ALOHA code allows for the source to be defined in one of four ways in order to model various accident scenarios. These are:

- Direct source
- Puddle source
- Tank source
- Pipe source.

Recall that for chemical accident analysis, the source term[19] defines the quantity released to the atmosphere for an instantaneous release or the release rate to the atmosphere for a continuous release. If the source term is already known through measurement or calculation, then the analyst uses the direct source option to enter a constant source term. Otherwise, the analyst characterizes the initial boundary conditions of the chemical with respect to the environment through the source configuration in order to provide ALOHA with the necessary information and data to calculate a time-dependent chemical release rate and physical state of the chemical upon release. The initial boundary conditions are defined through input specifications as delineated through the puddle, tank, or pipe source configurations.

Depending upon the source configuration specified, the analyst is prompted to supply a particular set of initial conditions such as temperature and storage pressure (if applicable), and the ALOHA code sets physical and thermodynamic properties based on these inputs and information in the ALOHA chemical database. The possible physical state of the chemical in its initial condition is identified in brackets below for each of the four source configurations. Brief overviews of the four source configurations are given first, followed by more detailed descriptions.

(1) Direct source {gas}: A point source is defined for this source configuration as either an instantaneous (duration of one minute or less) or a continuous release of gas into the

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[18] The primary author of this document did a limited parametric study on the role of relative humidity on the downwind concentration for evaporation from 10-m diameter puddles of hydrazine and chlorine. The study assumed meteorological conditions of F atmospheric stability and 1.5-m/s wind speed. The evaporation of hydrazine, which has relatively low volatility, produced a cloud that ALOHA modeled as neutrally buoyant. Chlorine, which is much more volatile and has a higher molecular weight, produced a cloud that ALOHA modeled as a heavy gas. In each case, the downwind concentration at 100 m that was calculated by ALOHA varied less than 2% as relative humidity varied from 0% to 100%. Slightly higher concentrations occurred with the higher values of relative humidity.

[19] ALOHA uses the label "source strength" in place of "source term".

atmosphere. For an instantaneous release, the total amount of gas that is released is specified. For a continuous release, the release rate and duration are specified (up to one hour). In either case, a ground level or elevated release is specified. Also, the analyst identifies the release as undergoing neutrally buoyant dispersion or dense-gas dispersion. The analyst makes this determination based on calculation of the Richardson number (Ri), as described later (Equations 4.1 and 4.2).[20]

(2) Puddle source {liquid}: This source configuration represents evaporating or boiling liquid from a pool or puddle of a spilled chemical. The analyst specifies the liquid quantity and the puddle surface area as well as liquid temperature, ground temperature, and ground type. The ALOHA code uses these inputs together with chemical properties from the ALOHA chemical database to calculate the time-dependent evaporation rate (non-boiling conditions) or vaporization rate (boiling conditions).

(3) Tank source {gas, liquid, or liquefied gas}: In this source configuration, the ALOHA code calculates the discharge rate of the gas, liquid, or two-phase flow from a hole in a tank. The analyst specifies the tank dimensions, quantity stored, storage temperature (and storage pressure if a gas), and hole characteristics (size, shape, and location). For gases, vapors and aerosols that remain suspended in air upon exiting the tank, the calculated time-dependent discharge rate defines the release rate to the atmosphere. For liquid that is released from a tank and falls to the ground, additional calculations, besides the discharge rate from the tank, are needed to define the release rate to the atmosphere that occurs through evaporation or boiling. The spilled liquid will pool on the ground. Transient puddle development is modeled by ALOHA. The time-dependent evaporation rate (non-boiling conditions) or vaporization rate (boiling conditions) is calculated by ALOHA using essentially the same algorithms as used in the puddle source configuration.

(4) Pipe source {gas}: This source configuration represents gas discharges from a long pipe either (i) connected to a very large reservoir or (ii) disconnected from a source. Gas temperature and pressure are specified along with pipe dimensions (length and diameter) and relative surface roughness (i.e., smooth or rough).

Guidance for each source term configuration follows.

Direct Source

The direct source algorithm is used when the emission rate of the gas is known or calculated from manual calculations or another computer code. The emission rate remains constant throughout the duration of the release (up to one hour). The direct source is also the only option for modeling elevated releases.

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[20] For source configurations other than direct, the user inputs sufficient data to allow ALOHA to calculate the Ri number and to make a determination to model the release as neutrally buoyant or dense gas.

With the direct source, the analyst should specify the release as undergoing neutrally buoyant dispersion or dense-gas dispersion (see Section 4.3.4 for additional discussion). The analyst makes this determination based on calculating the Ri number at the source (Ri_o), which is a relative measure of the potential energy of the cloud with respect to the mechanical turbulent energy of the atmosphere. Dense-gas behavior can potentially occur for gases with densities greater than air or with a chemical cloud with sufficient aerosol content such that the bulk cloud density is greater than that of the ambient air. Dense-gas behavior is more likely to occur with higher release rates and lower wind speeds. It is recommended that the analyst use the methodology used internally by the ALOHA code for other source configurations as a guide.

For source algorithms other than direct, the airborne release quantity or rate is calculated by the ALOHA code and used internally by ALOHA to determine Ri_o. The ALOHA code uses the following definitions of Ri_o for instantaneous and continuous releases, respectively.

For an instantaneous release (Reynolds, 1992):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_i}{\rho_a \times A_o \times u_*^2} \qquad (4\text{-}1)$$

Where,

$\rho_a \equiv$ Ambient air density

$\rho_o \equiv$ Released chemical density at source

$Q_i \equiv$ Instantaneous volumetric release

$A_o \equiv$ Ground area of the source

$u_* \equiv$ Friction velocity

For a continuous release (Reynolds, 1992):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_c}{\rho_a \times D_o \times u_{10} \times u_*^2} \qquad (4\text{-}2)$$

Where,

$Q_c \equiv$ Continuous volumetric release rate

$D_o \equiv$ Scale dimension of the source

$U_{10} \equiv$ Mean wind speed at a height of 10 m

The friction velocity is equal to about 5% to 10% of the mean wind speed at the height of 10 m (Hanna, 1996a). The ALOHA code basis is 6.25% ($u_* = u_{10}/16$) (Reynolds, 1992). For a ground level release, the length scale parameter D_o represents the initial width or diameter of the cloud

or plume before mixing with and transport by ambient air.[21] For a release out of a stack, D_o would represent the diameter of the stack (neglecting any boundary layer effects that would reduce the effective diameter of the jet or plume leaving the stack). For releases from evaporative or boiling pools, D_o is set equal to the pool diameter.

The criteria used by ALOHA for neutral-gas and dense-gas dispersion is as follows (Reynolds, 1992).

- $Ri_o \leq 1$ For neutral-gas dispersion
- $Ri_o > 1$ For dense-gas dispersion

It should be noted that an absolute threshold value does not actually exist. Dense-gas effects may begin to appear for Ri_o values less than one and become more pronounced as Ri_o is increased. It should also be noted that alternative definitions of Ri_o and corresponding dense-gas dispersion criteria are found in published literature (Hanna, 1996a).

Guidance for each parameter required by ALOHA for the direct source follows.

Source Strength Units

For the user's convenience, the source term may be entered on either a mass or volume basis. A variety of units (both metric and British) are available.

Source Duration

The source duration is specified as either instantaneous or continuous. A continuous release refers to any duration lasting longer than a minute. ALOHA assumes an instantaneous release to last one minute. Therefore, an instantaneous release is equivalent to a one-minute continuous release (e.g., specifying an instantaneous release of two kilograms is equivalent to specifying a continuous release of two kilograms per minute for a one-minute duration).

Recommendation: The recommendation below for source strength covers both source duration and source strength.

Source Strength

For an instantaneous release, the total quantity (mass or volume) released into the air is entered in the units specified by the source strength units chosen. For a continuous release the mass or volumetric release rate is specified as well as the duration in units of minutes. The allowable

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[21] Since D_o is not part of the input for the direct source, ALOHA does not have all the information to calculate Ri_o. For other source configurations D_o is either specified by user or calculated by ALOHA from the other input supplied.

input range for the duration is between 1 and 60 minutes. For the amount released, the allowable range is between 0 and 1,000,000,000, regardless of the units (NOAA, 1999b).

Recommendation: Conservatively specify release rate and duration. Calculated downwind concentrations are proportional to the release rate. So, the release rate should be conservatively estimated on the high side if there is some uncertainty or variability with its value. Note that for a given release rate, the calculated downwind concentrations generally increase as duration is increased (as the duration time increases, however, downwind concentrations become increasingly insensitive to further increases in duration).

Source Height

Only with the direct source may an elevated release be specified, such as would occur with a stack discharge. Furthermore, the release must be neutrally buoyant (i.e., Gaussian dispersion) release for an elevated release to be modeled. ALOHA will allow the user to specify a source height for a heavy gas, but the transport and dispersion calculations will be based on a ground level release.[22] This is consistent with the tendency of the heavy gas to slump to the ground.

Recommendation: The most conservative approach is to always assume a ground-level release. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

NRC Regulatory Guides 1.111 and 1.145 define a true "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977; NRC, 1983). It is recommended that the analyst enter the stack height only when this criterion is met of 2.5 times the height of adjacent structures. Otherwise, the release should be treated as ground level, or alternatively, a reduced effective release height can be determined (Hanna, 1982).

The identification of adjacent structures must take into account the extent of influence that the building has on the flow field in its vicinity. The wind flow that is directly over the top of the building is entrained downward into the wake cavity. The extent of the wake cavity downwind, as measured from the lee face of the building, can range from 2.5 times as great as the building height (H_b) to approximately 10 H_b for buildings that have large width-to-height ratios (Hanna, 1982). The wake cavity is marked by increased turbulence levels that decay progressively as a function of distance from the building. For releases from stacks not meeting the criterion of 2.5 times the height of adjacent solid structures, the effects of downward-directed entrainment into the wake cavity serve to increase ground-level concentrations above what would be observed in the absence of the building. The term downwash is frequently used to collectively describe these

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[22] The output text will echo the source height that was entered even though the dense-gas transport and dispersion calculations were based on a ground-level release.

effects. An accepted practice by the EPA is to assume that downwash effects can influence plumes that are released from stacks that are located in the range of 2 L upwind to 5 L downwind of building, where L is the lesser of the building height or projected width (EPA, 1995).

Physical State of Chemical

This input is only required when volume source strength units are chosen. Gas or liquid is entered to reflect the physical state of the stored chemical. ALOHA uses this input to convert the volume source strength to one of mass.

Chemical Storage Temperature

This input is only required whenever volume source strength units are chosen. ALOHA uses this input to convert the volume source strength to one of mass.

Recommendation: Usually chemicals are stored in tanks at ambient temperature. If the chemical is known to be stored at a different temperature, then that temperature should be entered.

Pressure of Stored Gas

This input is only required whenever volume source strength units are chosen, and the stored chemical is a gas. ALOHA uses this input to convert the volume source strength to one of mass.

Recommendation: When the user enters a pressure that is above ambient pressure, ALOHA responds with a warning that the user may want to consider modeling the scenario with either the tank or pipe source configuration models. Only a constant release rate can be considered with the direct source configuration. With the tank or pipe source configuration models, ALOHA will calculate a time-dependent release rate that takes into consideration the drop in source pressure that may occur as gas discharges from the tank or pipe.

Puddle Source

The puddle source algorithm is used when it is desired to calculate the time-dependent evaporation rate (non-boiling conditions) or vaporization rate (boiling conditions) of a known quantity of spilled chemical liquid that has pooled on the ground. Catastrophic failure of a storage vessel is an example of a scenario that could quickly progress to a puddle source configuration. The source term is proportional to the pool surface area, which is defined by the presence of a berm (or similar type barrier) or by assuming that the liquid spreads to some uniform thickness (e.g., 1 cm). As part of the source term solution, the mass and energy conservation equations are solved. The heat transfer mechanisms that are accounted for include short-wave solar influx, net longwave radiation flux between the pool and the atmosphere,

ground-to-pool heat conduction, atmosphere-to-pool sensible heat flux[23], and latent heat flux[24] from evaporation or boiling vaporization (Reynolds, 1992) (Figure 4-3).

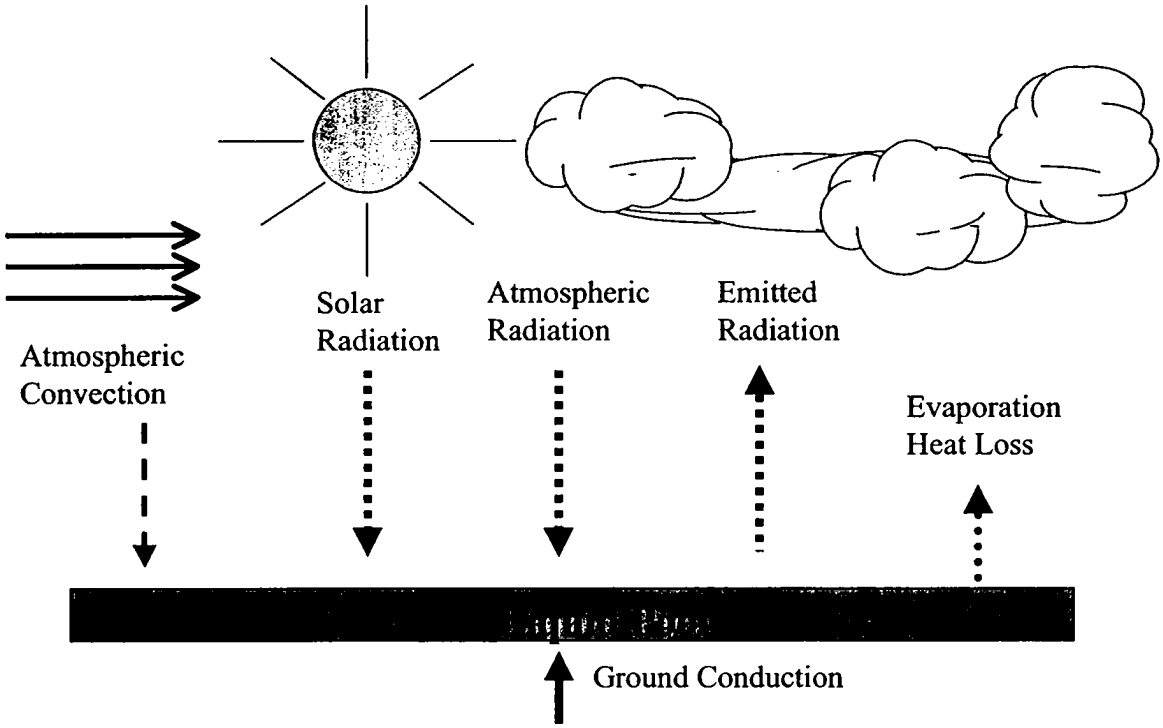

Figure 4-3. Heat Transfer Mechanisms with Puddle Source Configuration.

The Julian day, time of date, and global location (latitude and longitude) are inputs to the solar influx model (Raphael, 1962). The Stefan-Boltzman radiation law is the basis for the calculation of the net longwave radiation flux. The calculation of ground-to-pool heat flux uses the Fourier's law of heat conduction for transient, one-dimensional heat transfer of the pool in contact with a semi-infinite slab (representing the ground) of constant temperature (Carslaw, 1959). The pool temperature is assumed to be uniform. The analogy of mass transfer with heat transfer is the basis for the determination of the atmosphere-to-pool sensible heat flux. Brighton's steady-state solution of the advection-diffusion equation is the model for the evaporative mass transfer from the pool (Brighton 1985; Brighton, 1990). ALOHA assumes that the puddle grows thinner, while maintaining the same surface area, as the chemical material evaporates or boils. ALOHA considers all variables to be uniform throughout the puddle volume.

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[23] Sensible heat involves the release or absorption of thermal energy that is accompanied by a change in temperature.

[24] Latent heat is associated with phase change and involves the release or absorption of thermal energy with no change in temperature or pressure.

The liquid is non-boiling if the boiling point of the liquid (T_b) is greater than the ground temperature (T_g). The vapor pressure of the chemical at each time step determines the time-dependent evaporation rate (i.e., evaporative mass transfer) for non-boiling liquids and is a strong function of the puddle temperature (T_p). The sum of all the heat fluxes at each time step will either increase or decrease the internal energy of the puddle, and T_p will change proportionately to the change in internal energy.

If the boiling temperature of the liquid is less than the ground temperature, then the chemical vapor pressure is equal to the atmospheric pressure, and the liquid boils. The puddle temperature remains constant in time at the chemical boiling point. There is no change in the internal energy of the puddle as the evaporative heat flux balances the heat flux from the other heat flux sources. Thus, the net heat flux from these other sources at each time step determines the time-dependent vaporization rate. The term cryogenic refers to chemicals that have a very low boiling point, such that the ground-to-pool heat conduction is the dominant heat flux. ALOHA accounts for cooling of the ground beneath a cryogenic puddle.

Guidance for each parameter required by ALOHA for the puddle source follows.

Puddle Size I (Surface Area or Diameter)

This input (i.e., puddle surface area or diameter) and the next input (i.e., puddle volume, mass, or volume) together serve to characterize the quantity spilled and the physical dimensions of puddle that are necessary for evaporation calculations.

Either the surface area or diameter (for a circular puddle) is entered for the puddle-size I input. The input specification is straightforward if the spread of the puddle is constrained by the presence of the dike or similar structure that is being credited in the analysis. Topography can also play a similar role in confining the extent of liquid spreading. For puddle that forms from an unconstrained spill,[25] one usually considers the total volume spilled and assumes spreading occurs to some minimum depth. In this case, a preliminary calculation must be first performed by the analyst to calculate the surface area or diameter given the volume and depth specifications. The basic equations are given below that relate the puddle diameter (d), surface area (A), volume (V) and depth (Δh).

$$A = V/\Delta h$$

$$d = (4/\pi \times A)^{0.5}$$

In the sample calculation that is presented in Section 7.0, these equations are used to calculate the surface area and diameter of the puddle that is consistent with a 210-gallon spill that spreads to a 1-cm depth.

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[25] An unconstrained spill is analyzed when no barriers are present or have assumed to fail or when an unmitigated analysis is being performed in which no credit is being taken for the barriers that are present.

ALOHA assumes that the ground does not absorb any part of the spilled chemical. Moreover, the puddle diameter/surface area remains constant throughout the progression of the scenario (i.e., puddle grows thinner as liquid evaporates).

The allowable input range for the puddle area is between 20 square centimeters (3 square inches) and 31,400 square meters (37,500 square yards) (NOAA, 1999b). The allowable range for the puddle diameter is between 5 centimeters (2 inches) and 200 meters (220 yards) (NOAA, 1999b).

Recommendation: In an unmitigated analysis, no credit is taken for barriers and a puddle from an unconstrained spill is analyzed. Since the evaporation rate is proportional to the surface area, the analyst should make a conservative estimate of the maximum surface area or diameter that is reasonably conservative based on a maximum inventory and minimum puddle depth. The puddle-depth input is discussed below.

Puddle Size II (Volume, Mass or Depth)

This input in tandem with the puddle-size I input discussed above defines the total quantity of liquid spilled and completes the physical characterization of the puddle formed by a postulated spill. Either volume or mass (which equals the volume times the chemical liquid density) or depth (which equals the volume divided by surface area) is specified here.

The allowable input range for the volume is between 0.1 liter (0.026 gallon) and 10,000 cubic meters (2,640,000 gallons) (NOAA, 1999b). The depth must be between 1/2 centimeter (1/5 inch) and 100 meters (110 yards) (NOAA, 1999b)[26]. ALOHA accepts input values for mass between 1/10 kilogram (0.22 pound) and 100 metric tons (110 tons) (NOAA, 1999b).

Recommendation: It is recommended that a minimum depth of one centimeter be conservatively specified for an unmitigated spill analysis (EPA, 1987; Brereton, 1997).[27] As discussed above, the analyst should consider the maximum inventory in determining the volume spilled to form the puddle. This volume together with the one-centimeter depth should be used to calculate either the puddle surface area or puddle diameter that is needed for the puddle-size I input that is discussed above.

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[26] Note that the ALOHA user's manual (NOAA, 1999a) indicates that ALOHA will accept a minimum depth of 1/4 centimeter (1/10 inch), but when a user tries to input such a low value, ALOHA responds with an error dialog box stating that the depth must be at least 1/2 centimeter (1/5 inch).

[27] The 1-cm puddle depth is commonly used and suggested by EPA guidance (Brereton, 1997; EPA, 1987). Brereton (1997) notes that the 1-cm depth is somewhat arbitrary and recommends future development of an approach with more technical basis, such as one that would consider liquid physical properties (e.g., surface tension, viscosity) and ground surface properties (e.g., surface roughness).

Ground Type

Ground type influences the amount of heat energy transferred from the ground to an evaporating puddle. ALOHA offers four choices for ground type:

- Default: unwetted soil not covered by rock or concrete
- Concrete: concrete, cement, asphalt, or otherwise paved surfaces
- Sandy: sandy, dry soil
- Moist: sandy, moist soil

Recommendation: Heat is transferred most readily from a default or concrete ground into a puddle and least readily from sandy ground (NOAA, 1999b). The more heat energy that is transferred into the puddle, the higher the evaporation rate. The analyst should specify the ground type that most closely describes the area where the puddle has formed or choose a conservative ground type (e.g., default or concrete). If there is uncertainty or variability with the ground type, the user of course has the option of performing a parametric study on the sensitivity of the results to the ground-type input to aid in the specification of a conservative input.

Ground Temperature

The ground temperature also influences the amount of heat energy transferred from the ground to an evaporating puddle. The allowable input range for ground temperature is between -30 degrees C (-22 degrees F) and 64 degrees C (147 degrees F).

Recommendation: The best option is to make a specification based on statistical analysis of measurements of ground surface temperature (consistent with recommendation given in this document for air temperature). If these data are note available, the ground temperature should be set equal to the air temperature (Brereton, 1997; EPA, 1993).

Initial Puddle Temperature

The evaporation rate from a puddle is strongly dependent upon its temperature, increasing with increasing temperature. ALOHA assumes the initial temperature to be the uniform throughout the puddle volume (NOAA, 1999b). ALOHA accepts input that is between the liquid's freezing point and less than 9,937 degrees F (5,502 degrees C) (NOAA, 1999b). When the user specifies an initial puddle temperature that is above the normal boiling point of the liquid, ALOHA sets the temperature to the boiling point (NOAA, 1999b). It is expected that a boiling puddle will rapidly cool to its boiling point. ALOHA alerts the user that it is making this temperature adjustment.

Recommendation: The analyst should specify a liquid temperature that is consistent with the either the storage/operating temperature or the ambient temperature.

Tank Source

The tank source algorithm is used when it is desired to calculate the time-dependent source term when the chemical is stored in a tank that develops a leak. The chemical inventory of the tank can be a gas, liquid or liquefied gas.

- Gas Inventory: For gases, the time-dependent discharge rate from the tank is calculated using one-dimensional, compressible flow equations. The gas discharge rate quantifies the source term and is primarily a function of storage pressure and hole characteristics (size, shape, and location). The flow is either choked or unchoked at each time step depending upon the ratio of the tank pressure to atmospheric pressure and the critical pressure ratio for sonic flow. ALOHA takes into account the reduction in driving pressure and the temperature drop that occurs due to adiabatic expansion as the gas leaves the tank. ALOHA assumes that the heat flux through the tank walls has a negligible effect on the gas temperature. If the leak is through a short pipe or valve connect to the tank, frictional losses are neglected, simplifying the problem to that of a leak through an orifice-like hole in the tank. The leak stops once the pressure in the tank reaches atmospheric (i.e., enough gas is left in the tank to maintain atmospheric pressure).

- Liquid Inventory: Liquids leak from a tank at a time-dependent rate that is proportional to the size of the hole and described by Bernoulli's equation. The driving pressure is the sum of the vapor space pressure (set equal to the vapor pressure of the chemical) and the hydrostatic pressure of the column of liquid above the hole. The discharge coefficient is set to a value of 0.61 (Reynolds, 1992). As liquid leaves the tank, liquid evaporates or air ingested to maintain the vapor space pressure (Evans, 1993). Liquid leaks until the liquid level in the tank drops below the level of the hole. The temperature in the tank at each time step changes due to the net effect of evaporative heat loss and heat transfer through the tank walls.[28] The liquid that discharges from the tank falls to the ground to form a pool that may initially grow in size depending upon the evaporation or vaporization rate in comparison to the liquid discharge rate. ALOHA allows a minimum depth of 0.5 cm to be achieved and restricts spreading to maintain this minimum depth while spreading occurs (NOAA, 1999b). The puddle spreads until the evaporation rate or vaporization rate balances the spreading rate. At this point, the puddle surface area remains constant and grows thinner (0.5-cm minimum depth no longer imposed) as the chemical material evaporates or boils, consistent with the algorithms for the puddle source configuration. The puddle-source algorithms are the basis for determining the time-dependent rate at which the chemical evaporates or boils. The puddle energy balance includes an additional term that accounts for the energy due to any temperature difference between the liquid entering the puddle from the tank and the puddle itself.

- Liquefied Gas Inventory: The term "liquefied gas" refers to a chemical substance that is a vapor at atmospheric pressure and temperature, but is stored as a liquid. The chemical substance in storage may be either cooled (i.e., refrigerated) at ambient pressure or

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[28] ALOHA assumes 1-cm thick steel walls.

pressurized (i.e., compressed) at ambient temperature to achieve and maintain the liquid state. The refrigerated liquefied gas situation is conceptually straightforward and the easier of the two situations to model. A refrigerated liquefied gas is modeled as a liquid discharging from tank that forms a boiling puddle on the ground.

The model for the compressed liquefied gases must consider additional phenomena that can be quite complex. The various phenomena that may occur are briefly discussed followed by a discussion of the simplifications that ALOHA applies to the problem. Compressed liquefied gases may change from the liquid to vapor state in the tank as the pressure drops (i.e., flash boiling), at the exit from the tank in the form of a jet spray (i.e., two-phase flow), or on the ground through boiling. All three vapor-forming mechanisms may occur in one accident. Flash boiling (or flashing) occurs as the sudden depressurization results in the tank liquid being temporarily in the superheated condition (i.e., with excess latent heat as a result of being a liquid at a temperature above its boiling point). The internal excess heat rapidly vaporizes the liquid to vapor. The flashed vapor rapidly expands and fragments surrounding liquid into fine droplets that create a foam mixture that fills the tank. The greater the superheat, the smaller are the diameter of the liquid droplets. Liquid droplets that leave the tank in the jet-spray discharge may turn to vapor through flash boiling (as jet expansion outside the tank results in a further pressure reduction) or through general boiling as the atmospheric air externally exchanges energy with the droplet. If any liquid reaches the ground, a boiling puddle will form on the ground. ALOHA conservatively assumes, however, that all droplets leaving the tank are vaporized, so that no puddle is formed (only vapor and droplets that vaporize before reaching the ground exit the tank).

In calculating the mass discharge rate, ALOHA uses different algorithms to model the jet-spray discharge depending upon whether the leak is a simple hole in the tank or is at the end of a short length of pipe. In each case, ALOHA assumes that the tank contents form a uniform two-phase mixture.[29] For a simple hole, ALOHA uses a modified version of Bernoulli's equation in which the uniform two-phase mixture assumption is used to determine of the hydrostatic pressure. The density of the two-phase mixture is conservatively based on the liquid density, resulting in an over-estimation of the mass discharge rate. For a short pipe, the mass discharge rate is based on homogeneous nonequilibrium and homogeneous equilibrium models (Henry, 1971; Fauske, 1985; Leung, 1986; Fauske; 1988). The length of pipe is set to 0.1 m, which is conservative for longer pipes since mass discharge rates decrease slightly with increasing pipe length.[30] ALOHA tracks the amount of liquid and vapor remaining in the tank after each time step, and the leak stops once the pressure in the tank reaches atmospheric and hydrostatic pressure has dropped to zero (liquid level has reached bottom of hole) (Evans, 1993). The temperature in the tank is set

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[29] The uniform two-phase mixture completely fills the tank unless the criterion set by ALOHA for the maximum allowable quality (ratio of mass of vapor to total mass) is exceeded.

[30] The choice of 0.1-m pipe length is judicious since the homogeneous nonequilibrium model approximately reduces to the homogeneous equilibrium model as the length of the pipe approaches 0.1 m. It should also be noted that the homogeneous nonequilibrium model with zero pipe length reduces to the modified Bernoulli's equation that is used in ALOHA for the simple hole case (Reynolds, 1992).

at or above the boiling point at each time step (ALOHA considers the net effect of vaporization heat loss and heat transfer through the tank walls at each time step).

Guidance for each parameter required by ALOHA for tank source follows.

Tank Type/Orientation

ALOHA models three tank types.

- Horizontal cylinder
- Upright cylinder
- Sphere

Recommendation: Choose the type that best approximates the type of tank being analyzed.

Tank Size

For a sphere, the diameter or volume of the tank is to be entered. Here, volume refers to the total capacity of the tank and not to the volume of chemical in the tank. For a cylinder, values for two of the following three parameters are to be entered: diameter, length, and volume. ALOHA will compute and display values for the remaining dimension not entered for the sphere or cylinder. The allowable range for tank diameter is between 20 centimeters (about 0.7 feet) and 1,000 meters (3,280 feet) (NOAA, 1999b). Tank length must be between 50 centimeters (about 1.7 feet) and 1,000 meters (3,280 feet) (NOAA, 1999b).

Physical State of Chemical

ALOHA provides three input options for physical state of the chemical.

- Tank contains liquid
- Tank contains gas only
- Unknown

ALOHA uses this input to support the determination of the quantity of chemical in the tank and its rate of discharge from the tank.

Recommendation: ALOHA provides the following guidance (NOAA, 1999b).

- Tank contains liquid – appropriate if there is any liquid in the tank, even if it's just a small amount
- Tank contains gas only – appropriate when the tank contains only gas, with no liquid present
- Unknown – appropriate when uncertain about physical state of the chemical

Mass of Chemical in Tank

This input is only required if the physical state of the chemical is unknown. ALOHA uses this input along with the temperature input (discussed next) and the chemical properties to determine the physical state of the chemical. The mass entered must be greater than zero but less than 100,000 tons (200,000,000 pounds or 90,720,000 kilograms) (NOAA, 1999b).

Recommendation: Since the liquid discharge rate increases with increasing mass, the mass should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Chemical Storage Temperature

The storage temperature of a chemical within a tank determines its physical state (gas, liquid, or solid) and the pressure within the tank. These variables are important factors in estimating the rate of discharge from the tank.

If the chemical is identified as a gas and the temperature entered is below the chemical's normal boiling point, ALOHA will tank respond with a warning that the chemical is not a gas. The user should then consider that the chemical is in the liquid state if a check verifies that the correct inputs have been entered.

ALOHA will alert the user if storage temperature entered exceeds both the chemical's boiling point and the ambient air temperature. This warning, however, will not impede the analysis. The allowable input range is between than -459 degrees F (-273 degrees C) and 9,937 degrees F (5,503 degrees C) (NOAA, 1999b).

Recommendation: Usually chemicals are stored in tanks at ambient temperature. If the chemical is known to be stored at a different temperature, that temperature should be entered.

Mass or Pressure of Stored Gas

This input is only required if the physical state of the chemical is a gas. The input will take one of three forms.

- Tank pressure
- Mass of gas in the tank
- Volume of gas in the tank at standard temperature and pressure

If the pressure is entered, ALOHA will calculate the mass (or volume) and show its value in the space reserved for the mass (or volume) input in the dialog box.

ALOHA also checks to ensure that the chemical is a gas based upon the inputs of tank size, chemical storage temperature, and tank pressure (or equivalently chemical mass or volume). If the tank pressure is not high enough to liquefy the gas, ALOHA will respond with a warning that

the chemical is not a gas. The user should then consider that the chemical is in the liquid state if a check verifies that the correct inputs have been entered.

The mass entered must be greater than zero but less than 10,000 tons (20,000,000 pounds or 9,720,000 kilograms) (NOAA, 1999b). The allowable input range for pressure is between 1.1 atmospheres (836 millimeters of mercury, 16.2 pounds per square inch, or 111,458 pascals) and 68 atmospheres (51,680 millimeters of mercury, 1,000 pounds per square inch, or 6,890,100 pascals) (NOAA, 1999b). The pressure must be at least 1.1 atmospheres for ALOHA to calculate any gas release from the tank (NOAA, 1999b). The release stops once the pressure in the tank reaches atmospheric (i.e., not all the gas leaves the tank as some remains in the tank to maintain atmospheric pressure inside).

Recommendation: Since the gas discharge rate increases with increasing pressure (or mass), the pressure (or mass) should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Mass or Volume of Stored Liquid

This input is only required if the physical state of the chemical is a liquid. The input will take one of three forms.

- Mass of liquid and vapor in the tank
- Volume of liquid in the tank
- Percent of tank volume that is filled with liquid

After an entry is made for one of the above parameters, ALOHA calculates values for the other two parameters and displays their values in the dialog box.

The mass entered must be greater than zero but less than 10,000 tons (20,000,000 pounds or 9,720,000 kilograms) (NOAA, 1999b). The volume cannot exceed the tank capacity nor can the percent full exceed 100%.

Recommendation: Since the liquid discharge rate increases with increasing mass (or volume of liquid), the mass (or volume of liquid) should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Shape of Leak Opening

ALOHA offers the choice of rectangular opening or circular opening.

Recommendation: Choose the shape that best approximates the opening that is postulated for the scenario.

Size of Leak Opening

The diameter is to be entered for a circular opening and the length and width for a rectangular opening. The diameter of a circular opening must be at least 0.1 centimeter (0.04 inch) (NOAA, 1999b). The length of a rectangular opening must be at least 1 centimeter (0.4 inch) and its width must be at least 0.1 centimeter (0.04 inch) (NOAA, 1999b).

The area of the opening must less than the circular cross-sectional area of the tank or 10% of the total tank surface area, whichever is smaller (NOAA, 1999b). If the rupture area is larger than this, then the release must be modeled as a direct source or puddle source as directed below (NOAA, 1999b).

- The direct-source configuration is to be used with a gas inventory or if the tank is pressurized and a two-phase discharge is expected, such as the case with a liquefied gas inventory. The total chemical mass should be instantaneously released.

- The puddle-source configuration should be used with a liquid inventory. The total chemical mass should comprise the puddle.

Recommendation: Since the liquid or gas discharge rate increases with increasing leak size, the leak size should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

Type of Leak Opening

ALOHA offers the choice of a leak through a hole opening directly in the tank wall or through a short pipe or valve that extends at least 10 centimeters (4 inches) from the wall of the tank.

Recommendation: Hole type does not make a difference for a pure-gas discharge or for a pure liquid leak (NOAA, 1999b). For the liquefied gas release, ALOHA accounts for the friction generated as the two-phase mixture of liquid and gas flows through the valve or short pipe. As a result, higher release rates are calculated with the hole opening. The hole opening is thus recommended for conservative results unless the case for the valve or short-pipe opening can be adequately defended for the postulated scenario.

Height of Leak Opening

This input is not required if the physical state of the chemical is a gas. ALOHA allows this input to be expressed as either the distance from the tank bottom or percent way up to the top of the tank (once a value is entered for one of these parameters, ALOHA calculates the value for the other parameter and displays it in the dialog box).

For a pure liquid release, ALOHA uses this input to determine whether or not the hole site is above or below the liquid level in the tank. Liquid will spill from the hole until enough liquid drains from the tank to drop the liquid level below the hole (NOAA, 1999b). Liquid that spills to the ground forms a pool.

Recall that for the liquefied gas case, ALOHA assumes that a uniform two-phase mixture fills the tank (Reynolds, 1992). A mixture gas and droplets leave the tank, but the droplets are assumed to evaporate before reaching the ground (i.e., no puddle forms) (Reynolds, 1992). In general, the leak stops once the pressure in the tank drops to atmospheric and hydrostatic pressure has dropped to zero (liquid level has reached bottom of hole) (Evans, 1993). If the hole is at the bottom of the tank, however, the entire mass of the inventory is assumed to exit the tank (i.e., even the mass that would be expected to remain in the tank once the pressure reached atmospheric is conservatively assumed to exit the tank) (Evans, 1993).

Recommendation: The quantity of liquid that spills to form a puddle on the ground for the pure liquid case increases with lower leak opening heights, which results in higher evaporation rates for a puddle that forms from an unconstrained spill. Moreover, the hydrostatic pressure, which increases with increasing distance between the liquid surface and the hole, establishes the driving force for the discharge rate. Therefore, the height of the leak opening should be conservatively estimated on the low side if there is some uncertainty or variability with its value. The same approach of conservatively estimating the height of the leak opening on the low side should also be used for the liquefied gas case even though different phenomena come into play.

Surface Ground Type and Temperature

This input is only required if the physical state of the chemical is a liquid. For a liquid spill, a puddle will form on the ground, and ALOHA will calculate the evaporation rate from the puddle.

Recommendation: Follow the guidance given for the puddle source.

Maximum Puddle Diameter or Area

This input is only required if the physical state of the chemical is a liquid. Like for the puddle source, the specification is straightforward if the spread of the puddle is constrained by the presence of the dike or similar structure that is being credited in the analysis. When the spill is assumed to be unconstrained for the tank discharge case, ALOHA offers the option of choosing "unknown" for the maximum puddle diameter or area. ALOHA assumes that an unconstrained puddle will spread until the depth reaches 0.5 cm (about 0.2 inch). Note that this is conservative with respect to the recommended value of 1.0 cm given above for the unconstrained spread of a puddle source.

The allowable input range for the puddle area is between 20 square centimeters (3 square inches) and 31,400 square meters (37,500 square yards) (NOAA, 1999b). The allowable range for the puddle diameter is between 5 centimeters (2 inches) and 200 meters (220 yards) (NOAA, 1999b).

Recommendation: Follow the guidance given for the puddle source and let the puddle spread unconstrained for unmitigated accident analysis.

Pipe Source

The pipe source configuration represents gas discharges from a long pipe either (i) connected to a large-capacity reservoir (ii) closed off at its unbroken end.[31] The length-to-diameter ratio of the pipe must be at least 200 (if not, an ALOHA warning suggests that analyst use the tank source configuration). ALOHA assumes that the flow of gas through the pipe is isothermal, except for the last 200 pipe diameters. A balance between frictional heating and expansion cooling will result in isothermal flow. Gas moving through the last section of pipe is expected to expand adiabatically. Based on the user input of either rough or smooth for the inside walls of the pipe, ALOHA calculates a friction factor. The rupture area may be a size up to the cross-sectional area of the pipe.

ALOHA models the initial flow as choked for both cases of a large-reservoir source and a closed-off source. The initial flow rate is a function of rupture area, initial pressure, initial temperature, and the specific heat ratio of the gases. The flow is essentially steady for the large-reservoir source. For the closed-off source, the pressure will drop and the mass flow rate is reduced as gas empties from the pipe.

Guidance for each parameter required by ALOHA for the puddle source follows.

Pipe Diameter

ALOHA uses the inside pipe diameter to predict the discharge rate from a ruptured pipeline. The allowable input range is between 1 centimeter (0.4 inches) and 10 meters (32.8 feet) (NOAA, 1999b).

Recommendation: Since the gas discharge rate increases with increasing pipe diameter, the pipe diameter should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

Pipe Length

ALOHA uses the pipe length to predict the discharge rate from a ruptured pipeline. The allowable input range is between 200 times the pipe diameter and 10 kilometers (6.2 miles) (NOAA, 1999b). If the pipe is shorter than 200 times its diameter, then the analyst should consider modeling the release using the tank source configuration.

Recommendation: Since the gas discharge rate increases with decreasing pipe length, the pipe length should be conservatively estimated on the low side if there is some uncertainty or variability with this input.

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[31] The pipe source configuration does not support liquid discharges from pipes. In some instances, it may be possible to model liquid releases from a pipe using the tank source configuration, given that the pipe diameter is at least 8.4 inches (20 centimeters) and the length is no longer than 3,280 feet (1000 meters) (NOAA, 1999a).

Pipe Scenario (Unbroken End State)

ALOHA can model two different types of scenarios for a gas pipeline leak. The two types of scenarios differ in the state of the unbroken end.

- The unbroken end is closed off (e.g., shut-off valve), so a finite amount of gas is in the pipeline section. As gas is discharged at the broken end, the pressure drops and the discharge rate slows over time. The release occurs over a finite period of time

- The unbroken end is connected to a very large, essentially infinite, reservoir. Pressure and discharge rate remain essentially constant, and the release occurs for an indefinite period of time.

Recommendation: Use the model that best describes the scenario that is being analyzed.

Pipe Roughness

ALOHA uses the pipe surface roughness to predict the discharge rate from a ruptured pipeline. The rougher the pipe, the more friction as the gas flows through the pipe. Friction creates energy losses that result in lower discharge rates. ALOHA offers the two choices of surface roughness under the labels of smooth pipe and rough pipe. Examples of a rough pipes are those that have inner surfaces that have rusted or been corroded. Smooth pipes include new metal pipes, glass pipes and plastic pipes.

Recommendation: Since the gas discharge rate is higher with a smooth pipe, the smooth pipe should be conservatively used if there is some uncertainty or variability with this input.

Pipe Pressure

ALOHA uses the pipe pressure to predict the discharge rate from a ruptured pipeline. The allowable input range is between twice the ambient air pressure and 680 atmospheres (10,000 pounds per square inch) (NOAA, 1999b).

Recommendation: Since the gas discharge rate increases with increasing pipe pressure, the pipe pressure should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

Temperature of Chemical in the Pipe

ALOHA uses the temperature of the chemical in the pipe to predict the discharge rate from a ruptured pipeline. The allowable input range is between the boiling point of the chemical and 1,535 degrees C (2,795 degrees F) (NOAA, 1999b).

Recommendation: ALOHA recommends that the temperature be set to the ambient temperature if unknown (NOAA, 1999a; NOAA, 1999b). This seems reasonable, especially when one considers that the results are not expected to be real sensitive to the temperature input. The user

always has the option of performing a parametric study on the effect of chemical temperature to aid in the specification of a conservative input.

Hole Size

ALOHA uses the hole size to predict the discharge rate from a ruptured pipeline. This input is only required for the scenario involving the closed-off unbroken end. For the scenario involving the infinite reservoir, ALOHA assumes that the pipe is completely sheared off, such that the hole diameter equals the pipe diameter. For scenario involving the closed-off unbroken end, an area for the hole can be specified up to the area corresponding to the pipe diameter.

Recommendation: Since the gas discharge rate increases with hole size, the pipe pressure should be conservatively estimated on the high side if there is some uncertainty or variability with this input.

4.3.4 COMPUTATIONAL PREFERENCES

Under the computational preferences, ALOHA allows a couple of miscellaneous options that affect the computations to be changed from default values.

Dispersion Model

ALOHA presents three choices.

- Let model decide (default condition)
- Use Gaussian dispersion only
- Use heavy gas dispersion only

ALOHA generally makes a determination of whether the heavy gas dispersion model is to be used on the basis of the source Ri number has discussed previously. In order to calculate the source Ri number, the following chemical property data are required (NOAA, 1999b).

- Chemical name
- Molecular weight
- Normal boiling point
- Gas density, with a reference temperature and pressure
- Gas heat capacity (constant pressure), with a reference temperature and pressure
- Critical temperature and pressure or vapor pressure at 1 atmosphere with a reference temperature

If any of the above items are missing in the database library for the chemical of interest, ALOHA will calculate downwind concentrations using the Gaussian dispersion model.

Recommendation: The analyst generally should allow the ALOHA algorithms to determine which dispersion model to use (default condition) with the one exception as noted below for the direct source configuration. As stated above, ALOHA generally makes this determination on the basis of the source Ri number. Assuming the chemistry property data listed above is available in the database library, ALOHA has the information to calculate the source Ri number for the puddle, tank, and pipe source configurations. ALOHA cannot calculate the source Ri number for the direct source configuration, however, since the necessary length scale or area dimension is not supplied. For the direct source configuration, ALOHA apparently makes a determination solely on the molecular weight of the gas or vapor released. It is better if the analyst calculates the source Ri number when using the direct source configuration and then chooses the appropriate dispersion model. This is the recommended approach. In some cases, the analyst may judge it appropriate to calculate results with both models and use the more conservative of the two sets of results.

Dose Exponent

ALOHA defines the dose as "the concentration of pollutant at a specified location (to which people may be exposed), taken to a power, and multiplied by the period of time that it is present." The power "n" in this definition is referred to as the dose exponent.

Recommendation: For accident analysis work, human health evaluation guidelines, such as ERPGs and TEELs, are based on concentration limits and not dose limits. Therefore, doses calculated by ALOHA are not used. The ALOHA documentation states that its dose results are of limited use and only for use by someone trained in toxicology. The following is an excerpt from the user's manual and online help (NOAA, 1999a; NOAA, 1999b).

> *Dose information is difficult to interpret because the effects of most toxic chemicals on people are poorly understood. If you don't know the appropriate dose exponent to use for a particular chemical, or can't consult with a specialist who can advise you on the correct exponent to use and help you to interpret ALOHA's results, AVOID USING ALOHA'S DOSE CALCULATIONS. Instead, use information from ALOHA's footprint and concentration plots and your own knowledge of a chemical to make response decisions.*

4.4 Input Recommendations for Display Parameters

In general, the submenus that are included under the Display menu are concerned with the output options that are largely a matter of personal preference. An input of technical importance to the analysis, however, is found in the Options submenu. Here, an ERPG or TEEL value can be entered as the LOC value.

Options (TEEL or ERPG input)

The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The ERPGs are estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to

adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

> ***ERPG-1**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*
>
> ***ERPG-2**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*
>
> ***ERPG-3**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

Like the ERPGs, the TEELs are a collection of chemical-specific concentrations corresponding to varying levels of health effects (Craig, 2001). TEELs have been developed since ERPGs are available for only a limited number of chemicals. The TEELs are comprised of (a) Emergency Response Planning Guideline (ERPG) values for all chemicals for which ERPGs have been published and surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values), and (b) Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) values for all chemicals for which PEL-TWA values have been published and surrogate PEL-TWA values for chemicals for which PEL-TWA values have not been published (i.e., the TEEL-0 values) (Craig, 2001). PEL-TWA values are developed by the Occupational Safety & Health Administration (OSHA) for use in limiting worker exposures to airborne chemicals (CFR, 1999). Most people are not expected to experience any adverse health effects to accident exposures at the TEEL-0 level (Craig, 2001).

Recommendation: The DOE has not provided definitive evaluation guidelines for chemical exposures, so the specific use of ERPGs and TEELs in accident analysis remains an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001).

5.0 SPECIAL CONDITIONS FOR USE

ALOHA is a public domain code that is part of a system of software that is known as the Computer-Aided Management of Emergency Operations (CAMEO) that was developed to plan for and respond to chemical emergencies. This document does not specifically address application issues related to emergency response or emergency preparedness/planning.

Even though ALOHA was not developed specifically for safety analysis applications, it is also widely used throughout the DOE complex for this purpose and has been designated for the DOE Safety Software Toolbox to support 10 CFR 830 safety analysis. This document serves as a guide for prudent implementation of the ALOHA code for the purpose of modeling source term and consequence phenomenology supporting safety basis documentation. The user, however, must still demonstrate that ALOHA is being used within its domain of applicability and that site/laboratory procedures governing use of safety analysis software are being followed.

6.0 SOFTWARE LIMITATIONS

This section discusses limitations and areas of improvement of ALOHA. Section 6.1 summarizes technical limitations of Version 5.2.3 of ALOHA. Section 6.2 provides a summary of the outcome of the SQA gap analysis.

6.1 ALOHA Issues

The limitations of a computer code must be discussed in the context of its intended use. The limitations of ALOHA that are discussed in Table 6-1 below relate to both its use in general and specifically for safety analysis applications (recall that ALOHA was developed to plan for and respond to chemical emergencies).[32]

Table 6-1 ALOHA Limitations

ALOHA Limitation	Comment
Results are less reliable for conditions of low wind speed or very stable atmospheric conditions.	Issue of general concern to atmospheric transport and dispersion codes.
Results have high uncertainty very close to the source.[33]	Issue of general concern to atmospheric transport and dispersion codes. ALOHA shows average concentrations that are based on laws of probability and meteorologists' knowledge of atmospheric phenomena (NOAA, 1999a).

[32] Differences exist in the computational capabilities that are needed for a safety analysis calculation compared to those that are needed by people responding to a chemical accident. For example, the direction that a chemical puff or plume is traveling is of utmost importance to an emergency responder, since this information is crucial if efficient evacuation procedures are to be implemented. Thus, the inability of ALOHA to model the response of plume segments to shifts in wind direction during the course of modeling an accidental chemical release is a code limitation that affects emergency response calculations. Safety analysis calculations, however, traditionally consider exposures to a hypothetical receptor that is stationed on the centerline of a plume that is invariant with time. Thus, the inability of ALOHA to model shifts in wind direction does not constitute a limitation in the context of safety analysis calculations.

[33] In some cases, ALOHA may actually calculate an outdoor concentration near the source of greater than 1,000,000 parts per million, which is physically impossible. Substances that are gases at ambient temperature and pressure have an ambient saturation concentration of 1,000,000 parts per million, or 100%. The following text is from a 5/20/1999 e-mail from ALOHA technical support that is related to this topic:

When using the direct source option, ALOHA does not simulate the effects of jets, or high pressure releases, rather it assumes that the dispersion is dominated by turbulent diffusion in the atmosphere. Depending on the specifics of the release, pressure driven diffusion may well dominate the near field region. The ALOHA direct source option starts with a point source containing all the pollutant and allows it to diffuse as it travels downwind. This model should not be interpreted as a representation of reality close to the source where pressure effects, jets, and near-field patchiness play significant roles. Close to the source ALOHA artificially compresses all the pollutant into a small volume (even using the ideal gas law, it should be obvious that as the volume shrinks, the concentration gets large). Obviously, when the reported mole fraction in the air is over 100% you are too close to the source for the model to be trusted.

Table 6-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA does not allow for one or more years of meteorological data to be input and processed so that statistical methods can be employed to determine the 50th percentile (median) or 95th percentile (unfavorable) concentration results.	ALOHA accepts a single input combination of atmospheric stability class and wind speed. The user is responsible for specifying an appropriate combination of atmospheric stability class and wind speed that will yield representative median or unfavorable concentration results. If one or more years of meteorological data are available, other atmospheric dispersions that can accept and process the meteorological data can be used to assist in these specifications. For example at SRS, meteorologists evaluated SRS data with another atmospheric and dispersion code for neutrally buoyant plumes and found that the meteorological conditions that correspond to 95th percentile consequences were associated with E stability class and 1.7-m/s wind speed for ground level releases (Hunter, 1993). Alternatively, an electronic worksheet may also be programmed to perform similar analysis. In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes (EPA, 1999). For dense gas releases, sensitivity studies are recommended to determine median and unfavorable meteorological conditions.
ALOHA does not model the initial momentum of the release.	ALOHA does not account for the initial plume rise from momentum effects. This approach is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release when plume depletion from deposition effects are ignored, as is done in ALOHA.

Table 6-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA does not account for the effects of fires or chemical reactions.	ALOHA does not account for the initial plume rise from buoyancy effects. This approach is conservative in accident analysis applications since the ground-level concentration will be less with an elevated release with respect to a ground-level release when plume depletion from deposition effects are ignored, as is done in ALOHA. Also, ALOHA does not model combustion or chemical reactions of any kind. When the user selects an air- or water-reactive chemical, ALOHA informs the user of the type of reaction and expected reaction products. For example, sulfur trioxide reacts with water to form sulfuric acid and heat. ALOHA does not account for resulting phenomena such as buoyancy from the heat. Specialty codes have been developed to consider scenarios in which modeling specific chemical reactions is important in assessing toxicological effects. For example, HGSYSTEM/UF6 has been developed to model releases of uranium hexafluoride (UF_6) from containers and the chemical and thermodynamic processes that result from interaction of UF_6 with water vapor in the air to form hydrogen fluoride (HF) (Hanna, 1996b).
ALOHA does not account for terrain steering effects.	A natural canyon or street canyon formed by large buildings can constrain the lateral dispersion of the puff or plume. Development of codes that are suitable for complex terrain and urban settings is an area of ongoing research.
ALOHA does not model dispersion effects associated with building wakes.	Since wake effects near the source tend to enhance dispersion that provides additional dilution, it is generally believed to be conservative to neglect these effects in estimating chemical concentrations at downwind locations for ground-level releases.

Table 6-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA does not model the evaporation of chemical constituents in a mixture or solution.[34]	The property information for chemicals in the ALOHA database is limited to pure chemicals. The vapor pressure of the chemical is a key parameter in establishing the evaporation rate. For a chemical constituent in solution, the vapor pressure of the chemical constituent (i.e., partial pressure) is a function of its concentration and temperature. The chemical database does allow new chemicals and their properties to be added to the database. In some versions of ALOHA (such as 5.2.3), the vapor pressure can be entered directly (along with the reference temperature for the vapor pressure value) or calculated on the basis of other input properties, namely, the boiling point, freezing point, critical pressure, and critical temperature.[35] Actual data for these properties for chemical constituents in solution are rare, however, especially data for critical pressure and critical temperature. While ALOHA accepts the direct input of vapor pressure, it still requires the above-mentioned property data for sources other than the direct source configuration (NOAA, 1999a). An approach has been used with success at Savannah River Site (SRS) for dilute acids (e.g., 70 weight percent nitric acid) that involves entering pseudo property values for the boiling point, freezing point, critical pressure, and critical temperature. These pseudo property values are set through trial and error so that the ALOHA chemical database calculates vapor pressures at the temperature range of interest that closely match the vapor pressures for the dilute acid as found in a reference book. The sample calculation in Section 7.0 includes evaporation rate calculations for nitric acid for both 100 weight percent and 70 weight percent solutions.

[34] ALOHA 5.3 (March 2004) models evaporation from a limited number of solutions.

[35] ALOHA also uses these properties to calculate liquid and gas density.

Table 6-1 ALOHA Limitations (continued)

ALOHA Limitation	Comment
ALOHA limits predictions to one hour after the release begins or to distances up to ten kilometers (6 miles).	With a wind speed of approximately 2.8 m/s, the leading edge of the puff or plume will travel a distance of approximately 10 km in one hour. The downwind extent of the puff or plume will be less for lower wind speeds. For example, the puff or plume will travel a distance of approximately 5.4 km for a wind speed of 1.5 m/s, which is commonly used for worst-case consequence calculations. Therefore, ALOHA is incapable of making concentration predictions for receptors beyond approximately 5.4 km for a wind speed of 1.5 m/s. Of course, if the concentration is less than the LOC concentration at the maximum computed ALOHA distance, the concentration will be even lower and below the LOC at distances even farther away. If concentrations need to be calculated beyond the maximum computed ALOHA distance, the analyst may have to perform a hand calculation using the Gaussian model for either a plume (Equation A-1) or a puff (Equation A-4). At these distances, the Gaussian model is appropriate since enough air has mixed with the puff or plume for it to be neutrally buoyant even if it started out as a dense-gas cloud.
ALOHA does not model processes that affect the dispersion of particles, such as deposition from gravitational settling	In the case of low concentrations of airborne particles, it is reasonable to neglect transport phenomena peculiar to particulate and to assume that the particles act as a passive scalar contaminant that follows the flow field (Hanna, 2002). Larger particles released in a puff or plume will fall to the ground due to gravitational settling. Smaller particles and even gases will deposit on ground surface elements (e.g., ground vegetation) through a process known as dry deposition. Dry deposition refers to chemical reactions and physical interactions between the contaminant (particle or gas) in the puff or plume and the ground surface elements that serve to remove the contaminant from the puff or plume.

A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report. The main changes to the program are as follows according to the code developer:

- Windows source code was updated to a 32-bit application
- Footprint output (i.e., concentration contour plot) can now be displayed with up to three level-of-concern concentrations) simultaneously.
- Evaporation algorithm was updated.
- Capability to model the evaporation from puddles of five aqueous chemical solutions was added.
- Chemical library was updated.

6.2 Outcome of Gap Analysis

A gap analysis of Version 5.2.3 of the ALOHA computer code has been completed (DOE, 2004). The gap analysis reviewed the program, practices, and procedures associated with development of ALOHA compared with NQA-1 based requirements as contained in U.S. Department of Energy, Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes (DOE, 2003a). It was determined that the ALOHA 5.2.3 code does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of the software for supporting safety analysis. Informed use of the code can be assisted by appropriate use of current ALOHA documentation prepared by NOAA and this ALOHA code guidance report for DOE safety analysts. Furthermore, while SQA improvement actions are recommended for ALOHA, no evidence has been found of programming, logic, or other types of software errors in ALOHA 5.2.3 that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

Of the ten SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), two requirements are met at an acceptable level, i.e., *Classification* (1) and *User Instructions* (7). A third requirement, *Configuration Control* (9), is partially met. Improvement actions are recommended for ALOHA to fully meet *Configuration Control* (9) criteria and the remaining seven requirements and are summarized in Table 6-2. This evaluation outcome is deemed acceptable because: (1) ALOHA is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of ALOHA is limited to those analytic applications for which the software is intended.

Table 6-2 — Summary of Important Exceptions, Reasoning, and Suggested Remediation

No.	Criterion [Section refers to Gap Analysis Report for ALOHA, (DOE, 2004)]	Reason Not Met	Remedial action(s)
1.	SQA Procedures/Plans (Section 4.2)	SQA Plans and Procedures were not available for the gap analysis.	SQA Plans and Procedures should be developed and made available for review.
2.	Requirements Phase (Section 4.3)	A Software Requirements Document does not exist for review. Thus, it was necessary to infer requirements from draft model description and user guidance documents.	A Software Requirements Document should be prepared and made available for review.
3.	Design Phase (Section 4.4)	A Software Design Document does not exist for review. Thus, it was necessary to infer the intent of the design from draft model description and user guidance documents.	A Software Design Document should be prepared and made available for review. As part of this effort, the draft NOAA theoretical description memorandum for ALOHA 5.0 (Reynolds, 1992), which is the main source for technical information, should be updated for recent upgrades, technically reviewed, and issued as final.
4.	Implementation Phase (Section 4.5)	Documentation to support the implementation is lacking.	A verifiable, written set of SQA plans and procedures including implementation, test case descriptions, and associated criteria related to design should be made available.
5.	Testing Phase (Section 4.6)	A Software Testing Report Document does not exist for review. The documentation of results from validation and benchmark activities are incomplete and in the form of summaries that are found at ALOHA websites.	A Software Testing Report Document should be prepared and made available for review.
6.	Acceptance Test (Section 4.8)	A verifiable, written set of SQA plans and procedures, which would include acceptance-testing documentation, is lacking.	Documented acceptance testing should be developed.

No.	Criterion [Section refers to Gap Analysis Report for ALOHA (DOE, 2004)]	Reason Not Met	Remedial action(s)
7.	Configuration Control (Section 4.9)	A Configuration Control process is in place at NOAA, but limited documentation was forwarded to allow a gap analysis to be performed.	While a Configuration Control process is apparently functional at NOAA, written documentation should be prepared and made available for review.
8.	Error Notification (Section 4.10)	An Error Notification and Corrective Action Report does not exist for review.	While a Software Problem Reporting system is apparently in place, written documentation should be provided to the Central Registry for verification of its effectiveness.

By order of priority, it is recommended that ALOHA software improvement actions be taken, especially:

1. Correcting known defects in the SQA process
2. Upgrading existing SQA documentation, and
3. Revising and developing new software documentation.

A new software baseline set of documents is recommended for ALOHA to demonstrate completion of the revision to software documentation item (above). The list of revised baseline documents includes:

- Software Quality Assurance Plan
- Software Requirements Document
- Software Design Document
- Test Case Description and Report
- Software Configuration and Control
- Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

It is estimated that a concentrated program to upgrade the SQA pedigree of ALOHA to be compliant with the ten criteria important for software development would require fourteen to sixteen full-time equivalent (FTE)-months. Technical review of the chemical databases associated with this software is assumed to have been performed, and is not included in the level-of-effort estimate.

A new version of ALOHA, namely ALOHA 5.3, was released in March 2004 just prior to the issuance of this report. It is recommended that this version be evaluated relative to the software improvement and baseline document recommendations, as well as the full set of SQA criteria

discussed in this report. If this version is found to be satisfactory, it should replace version 5.2.3 as the designated version of the software for the toolbox.

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7.0 SAMPLE CALCULATIONS: PUDDLE EVAPORATION

Problem Statement: A vessel at Anytown, USA stores 210 gallons of concentrated (> 90 wt%) nitric acid (HNO_3) at ambient pressure and temperature. A scenario is postulated in which the vessel ruptures catastrophically, and the 210 gallons of HNO_3 spill on the ground. Determine the following: (1) the maximum concentration at 100 meters downwind and compare with the ERPG-3 value of 78 ppm and (2) the maximum concentration at 2500 meters downwind and compare with the ERPG-2 value of 6 ppm.

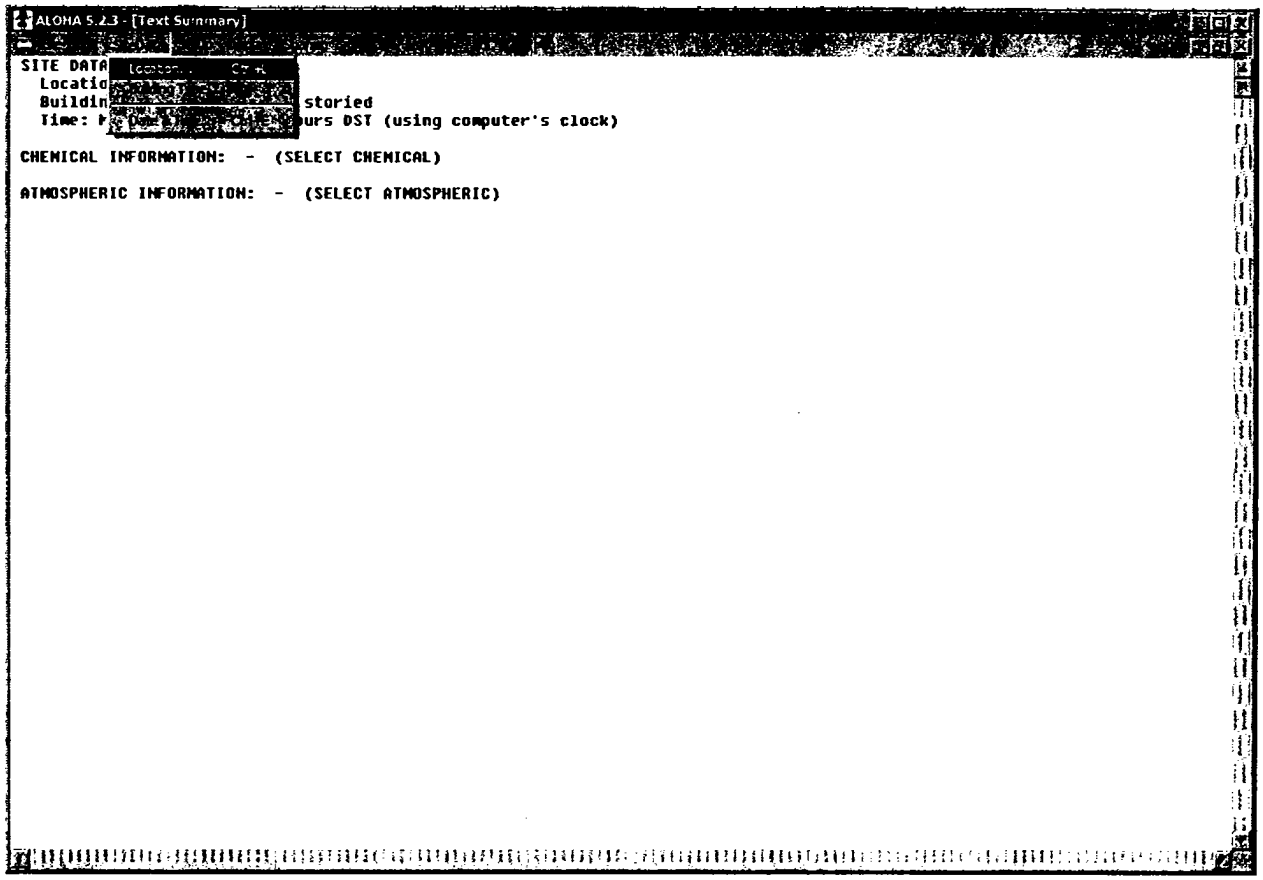
Analysis: The ALOHA chemical database contains properties for 100 wt% nitric acid since only pure chemicals, and not solutions, are part of the ALOHA 5.2.3 chemical library. New chemicals can be added to the database. As indicated in the body of the report, a dilute acid solution can be added as a new chemical if sufficient property information is available. For evaporation calculations from chemical pools, the vapor pressure is generally the controlling parameter. The table below shows the sensitivity of HNO_3 vapor pressure to the HNO_3 wt% at 30 °C (Perry, 1997).

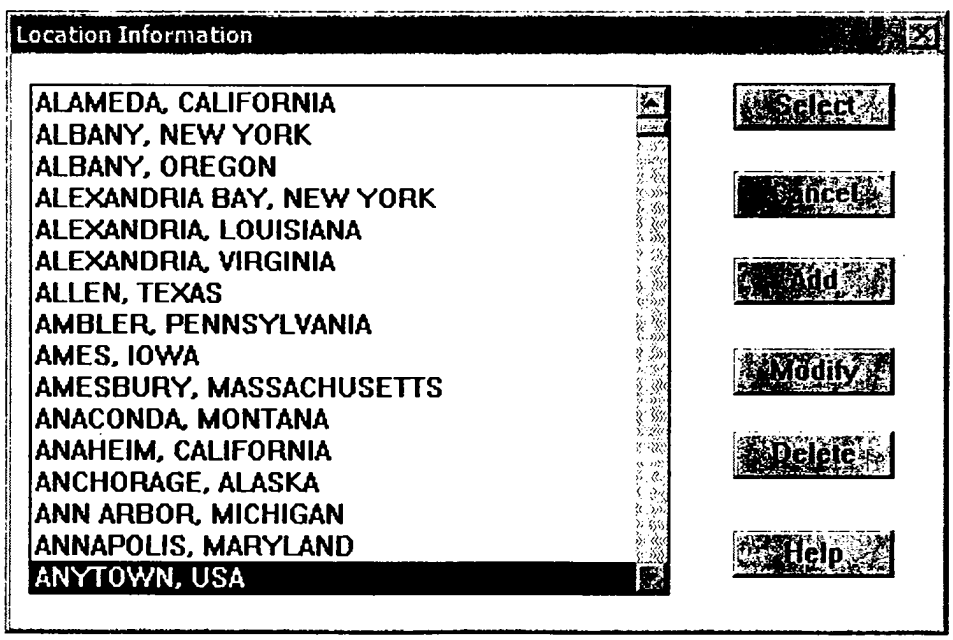
HNO_3 wt%	HNO_3 Vapor Pressure [mm Hg]
40	0.1
50	0.6
60	1.7
70	5.5
80	14
90	36
100	77

In this sample problem, we have assumed concentrated HNO_3 (>90 wt%) and will conservatively analyze the spill on the basis of 100 wt% HNO_3.

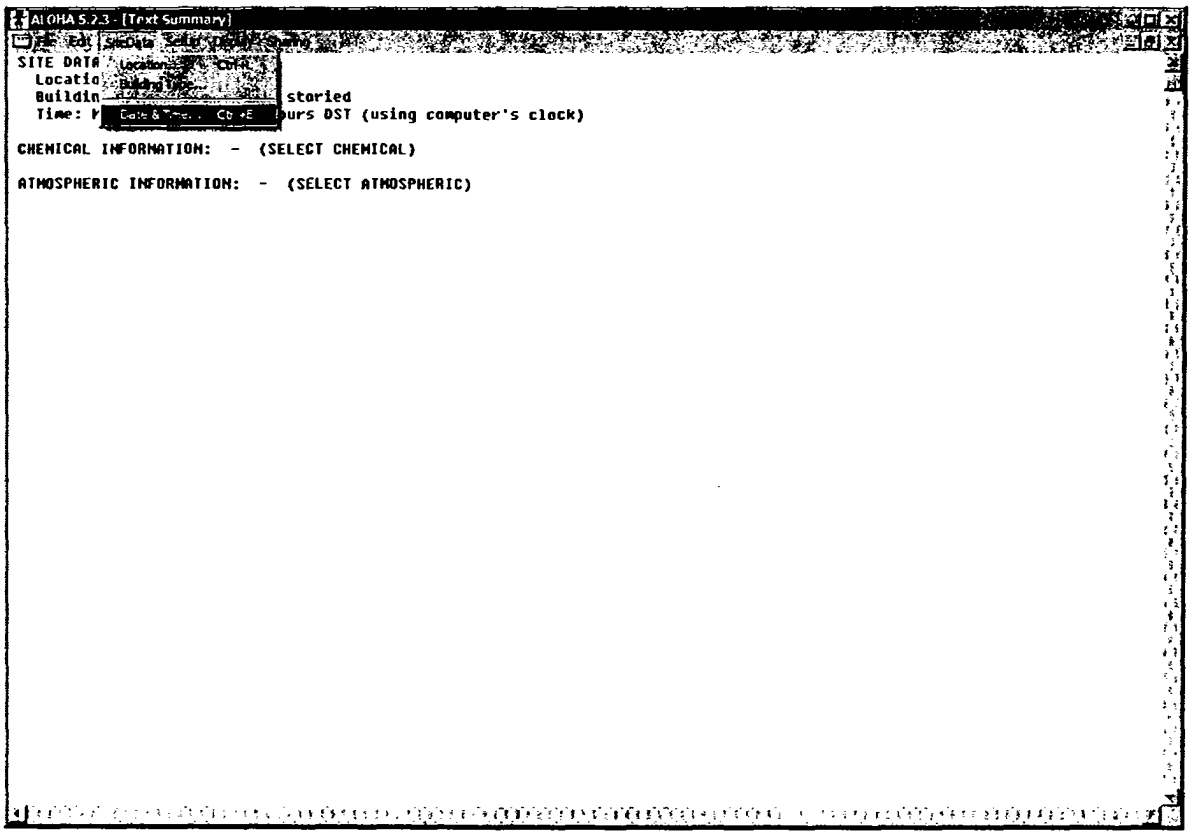
Site Data – Location and Building Type

The first step is specifying Anytown, USA as the location. Building Type is not a concern in the analysis since the receptor is assumed to be outdoors consistent with safety analysis practices.

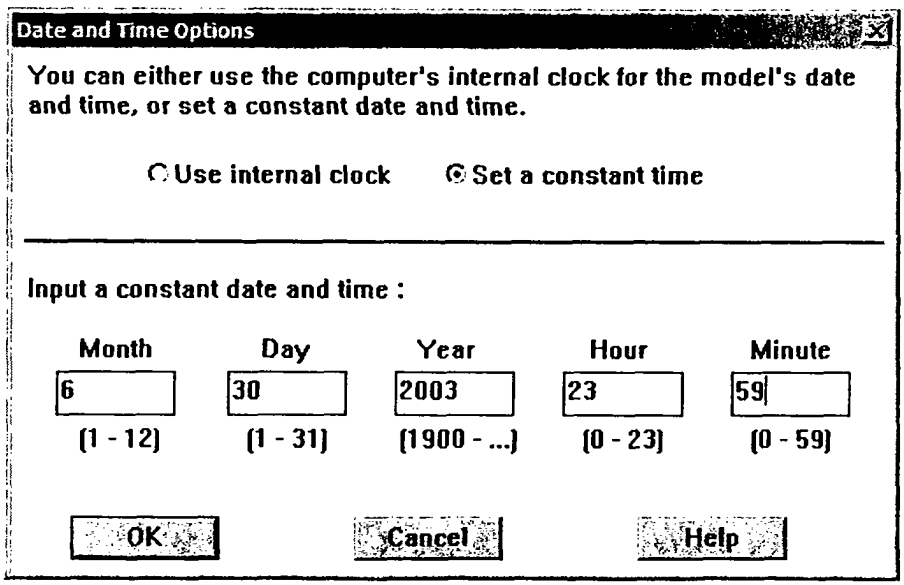

ALOHA 5.2.3 - [Text Summary]
SITE DATA
storied
urs DST (using computer's clock)
CHEMICAL INFORMATION: - (SELECT CHEMICAL)
ATMOSPHERIC INFORMATION: - (SELECT ATMOSPHERIC)


Location Information
ALAMEDA, CALIFORNIA
ALBANY, NEW YORK
ALBANY, OREGON
ALEXANDRIA BAY, NEW YORK
ALEXANDRIA, LOUISIANA
ALEXANDRIA, VIRGINIA
ALLEN, TEXAS
AMBLER, PENNSYLVANIA
AMES, IOWA
AMESBURY, MASSACHUSETTS
ANACONDA, MONTANA
ANAHEIM, CALIFORNIA
ANCHORAGE, ALASKA
ANN ARBOR, MICHIGAN
ANNAPOLIS, MARYLAND
ANYTOWN, USA
Select
Cancel
Add
Modify
Delete
Help

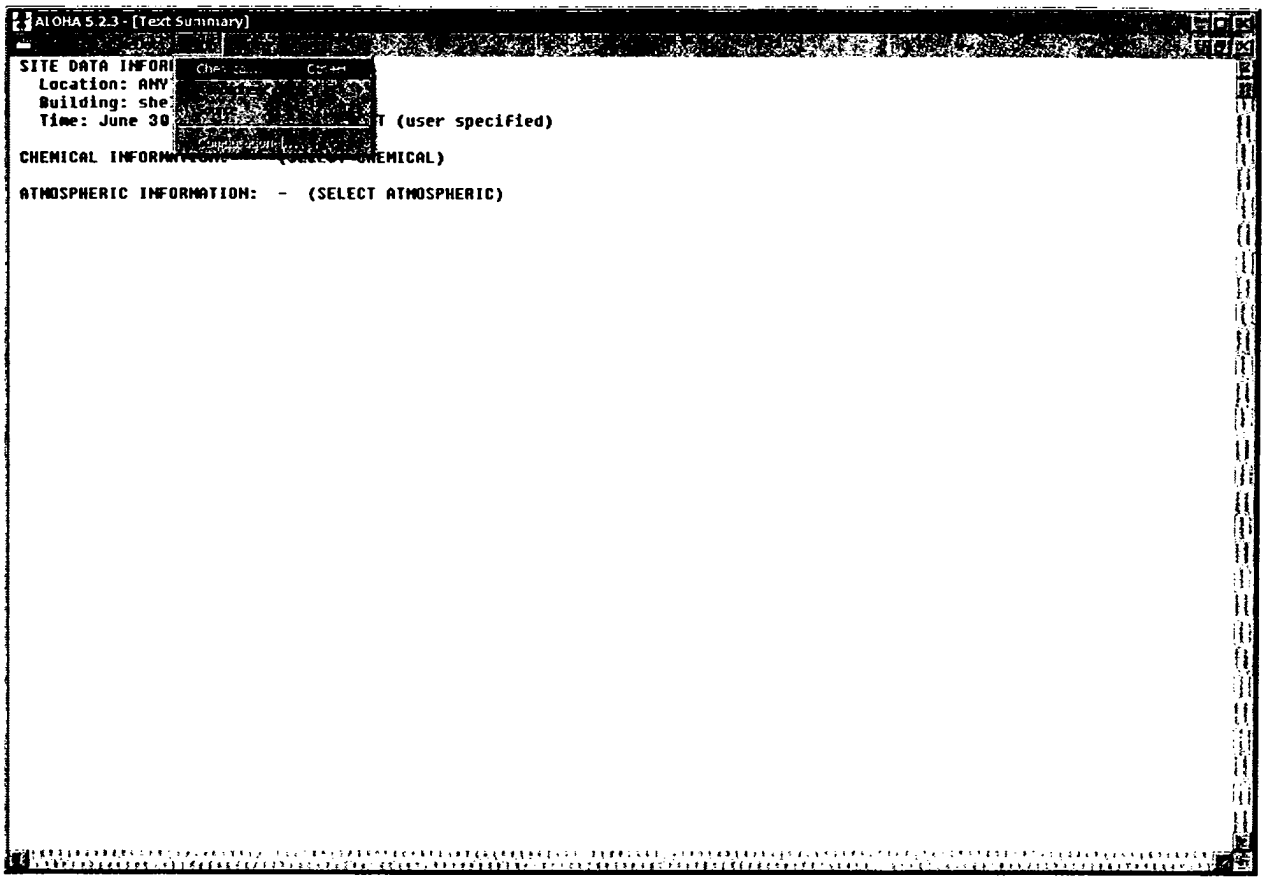
Site Data - Date and Time



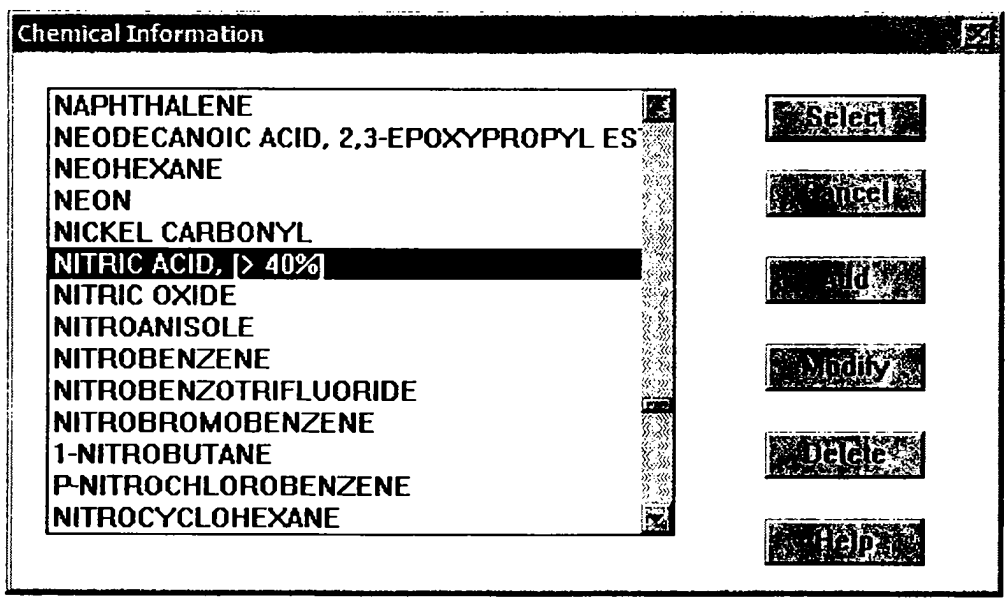
The analysis will be performed for worst-case meteorological conditions. A nighttime release (the time will be set at 23:59) under stable atmospheric conditions will be assumed. For a nighttime release, the date is unimportant (mid-summer day specified following recommendation in the body of the report).



Set Up – Chemical Information



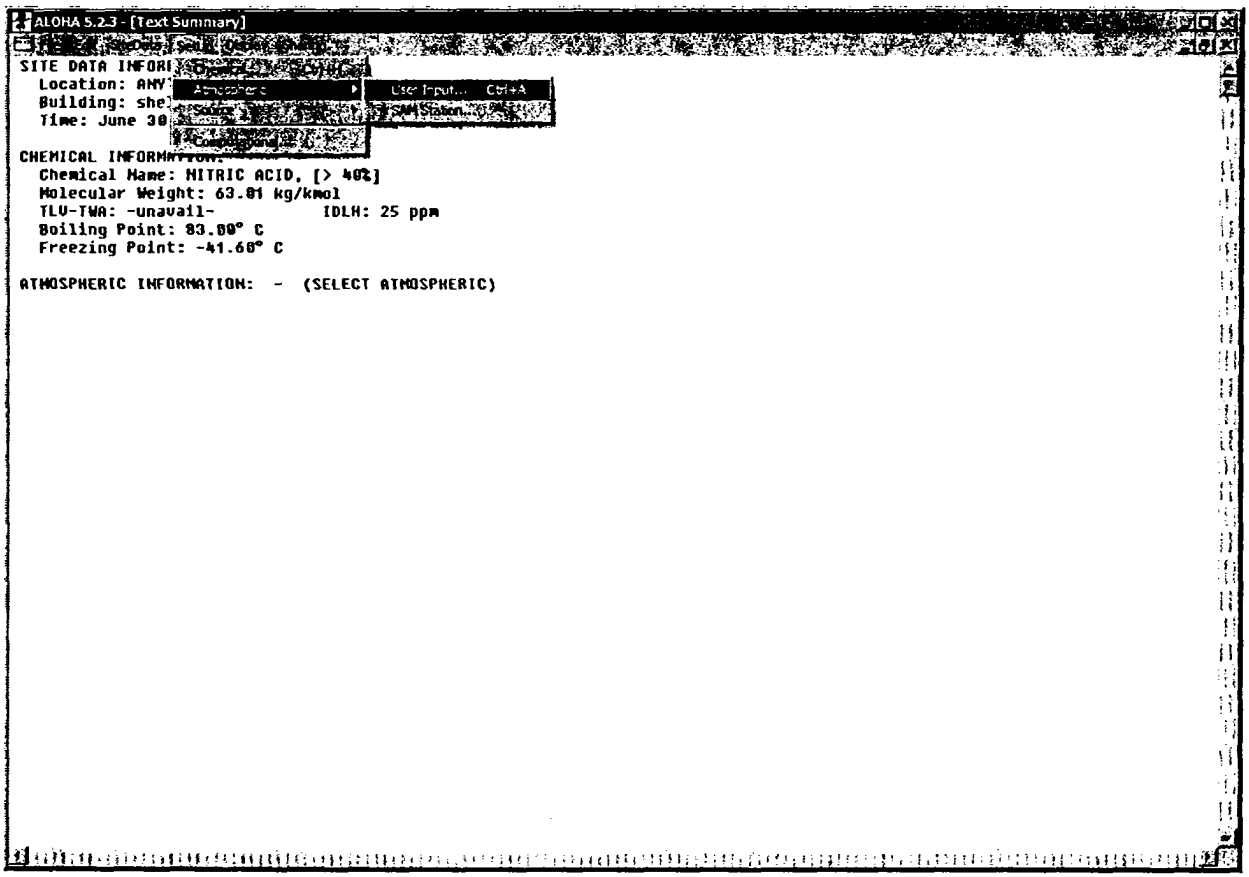
Nitric acid [>40%] is selected from the chemical database.



Once nitric acid is selected, chemical properties such as molecular weight, boiling point, and freezing point will appear on the Text Summary screen (shown in screen captures that follow after the chemical information is entered).

When atmospheric data is entered (e.g. air temperature), other data such as the vapor pressure at ambient temperature will appear. Specifically, ALOHA will determine a vapor pressure of 0.10 atmospheres at 29 °C, which is consistent with the 77 mm Hg cited above for the 100 wt% HNO_3 at 30 °C (Perry, 1997). The ambient saturation concentration is also given, which represents the maximum concentration in air that may be reached by vapor evaporating from a liquid pool (high ambient saturation concentration represents a strong capacity to displace air) (NOAA, 1999a).

Set Up – Atmospheric Options – User's Input

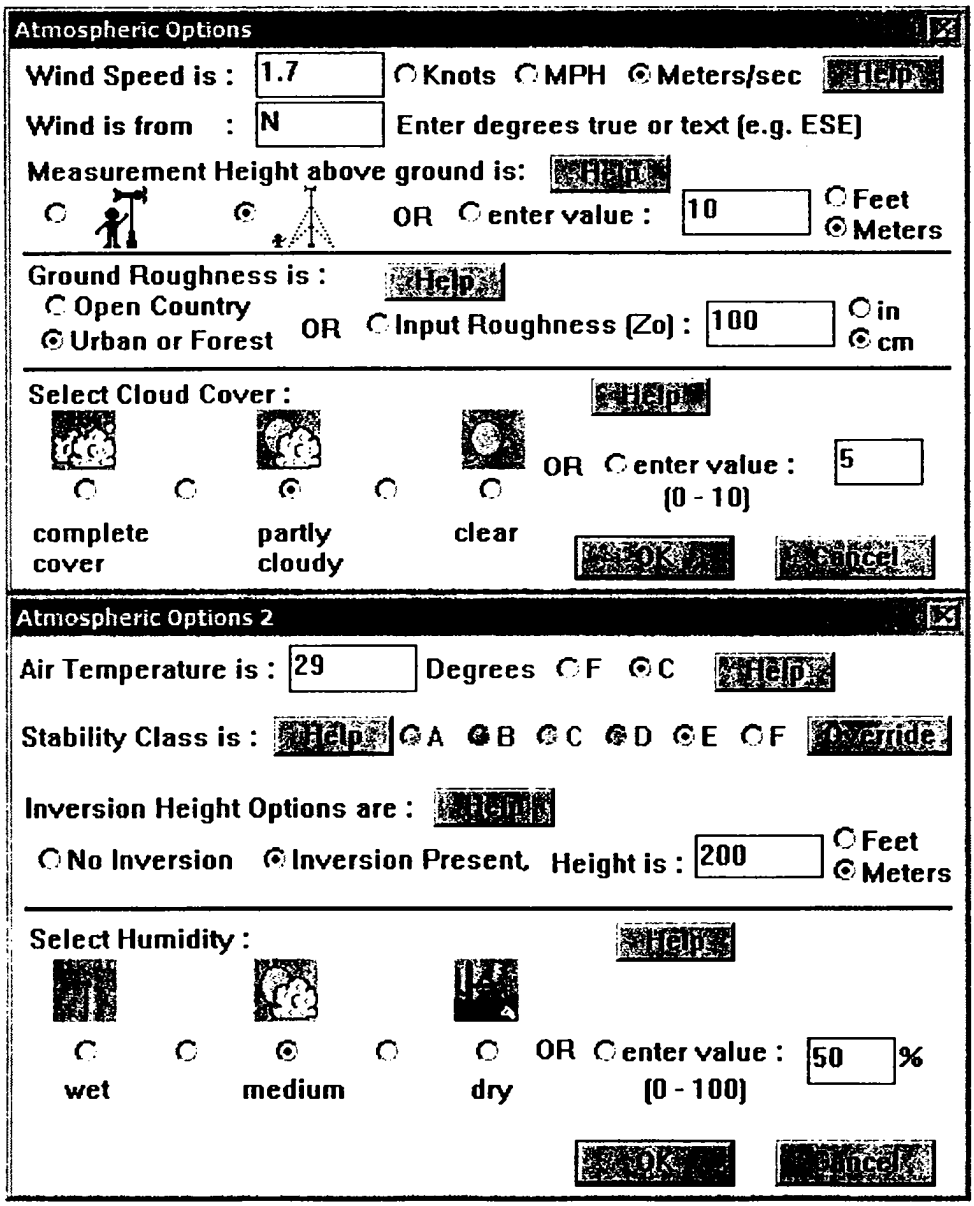


Atmospheric conditions are entered on two dialog boxes that appear on the screen sequentially. On the first screen, wind speed, wind direction, measurement height of wind speed, ground roughness, and cloud cover are entered. On the second screen, air temperature, stability class, inversion height, and humidity are then entered. Since the MW of nitric acid is greater than that of air, the potential exists for dense gas atmospheric transport.

For ground level releases of either neutrally buoyant and dense gas plumes, worst-case meteorological conditions are generally assumed to be associated with stable atmosphere and low wind speed. The meteorological conditions corresponding to 95th percentile consequences for both neutrally buoyant and dense gas plumes are taken to be E stability class and 1.7 m/s

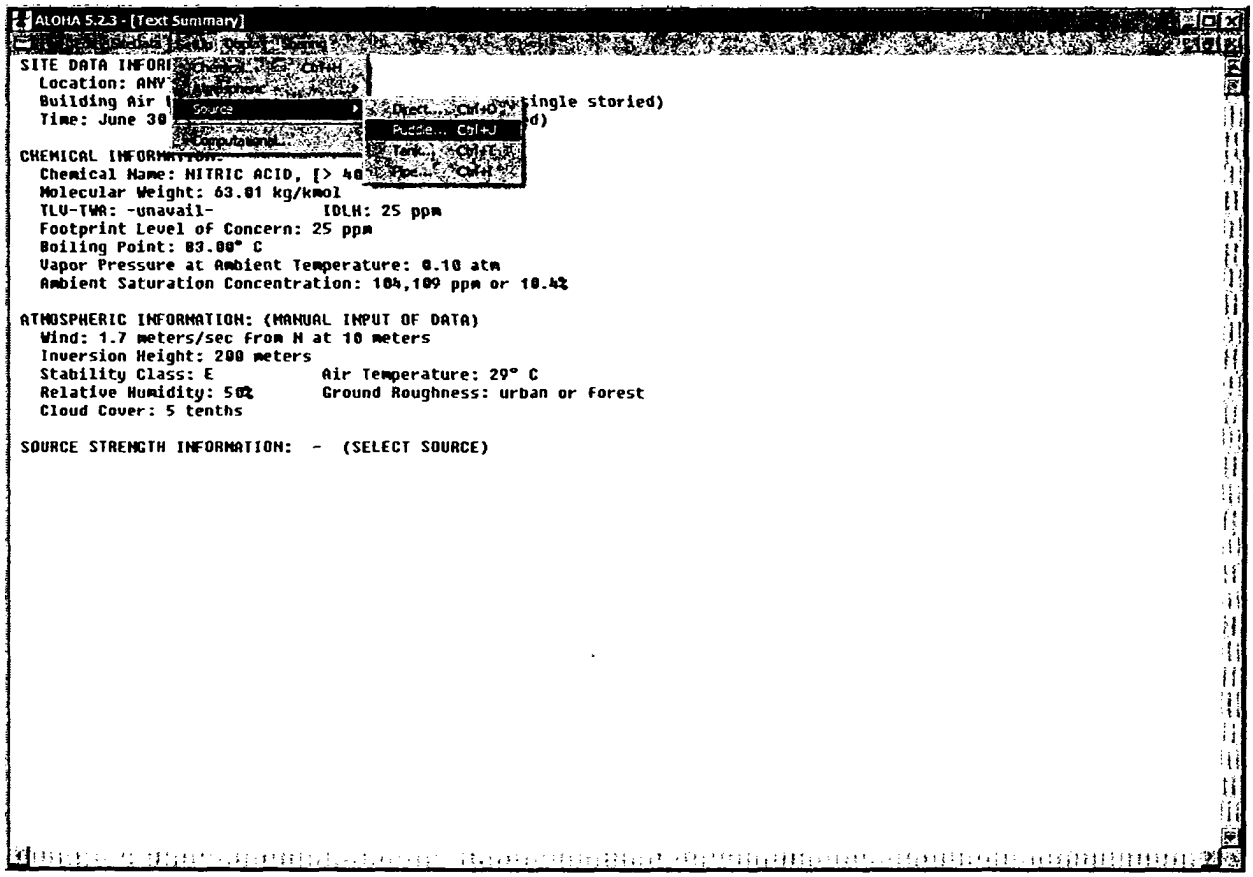
wind speed (corresponding to measurement height of 10 meter) for the purposes of this sample calculation based on assumed analysis of meteorological data that has been recorded for Anytown, USA. Moreover, the 95th percent highest air temperature is taken to be 29 °C. An inversion height of 200 m is conservatively used (Holzworth, 1972). The surface roughness length is another input that is site specific. In order to illustrate the sensitivity of the results to this input, calculations are performed for two input values, namely, 100 cm and 3 cm.

The calculated results are independent of wind direction, so any direction can be specified. Also for a nighttime (or early morning) release, which is consistent with the E stability class, the results will be largely independent of the amount of cloud cover. Humidity is specified at 50% as discussed in the body report (results are expected to be insensitive to humidity).



Note that based on location, time, wind speed, and cloud cover entries, ALOHA identifies stability classes E and F as compatible (other stability classes are filled grayed out).

Set Up – Source – Puddle



The catastrophic rupture of the vessel and subsequent spill of 210 gallons of concentrated HNO_3 is conservatively assumed to spill to the ground and spread unconfined to produce a circular puddle of 1-cm depth. The puddle source configuration is used to model this scenario. The puddle source data are entered on two dialog boxes that appear on the screen sequentially. The user characterizes the spill size in the first dialog box. The user then specifies ground boundary conditions as well as the initial puddle temperature in the second dialog box.

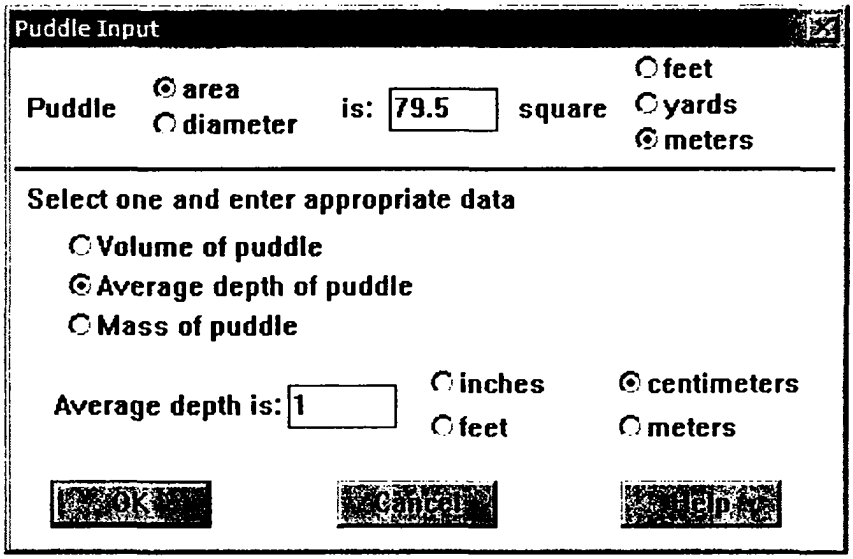
The analyst must first perform a preliminary calculation to determine the puddle diameter (d) or area (A) that is consistent with the 210-gallon volume (V) and 1-cm depth (Δh) specifications.

$$A\ [m^2] = V\ [m^3] / \Delta h\ [m] = (210\ [gal] \times 0.003785\ [m3/gal]) / (1\ [cm] \times 0.01\ [m/cm]$$

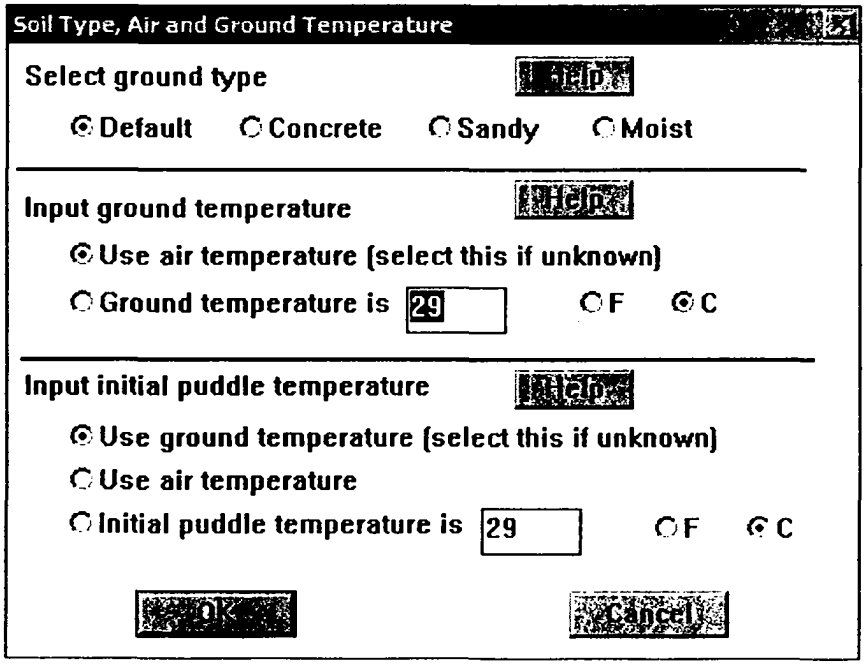
$$A\ [m^2] = 79.5\ m^2$$

$$d\ [m] = (4/\pi \times A\ [m^2])^{0.5} = (4/\pi \times 79.5\ [m^2])^{0.5} = 10.1\ m$$

The puddle-size dialog box that is shown below prompts the user for either the puddle area or puddle diameter. In this example, the user chooses to enter the puddle area of 79.5 m^2. Next, the user is prompted for ground boundary conditions.

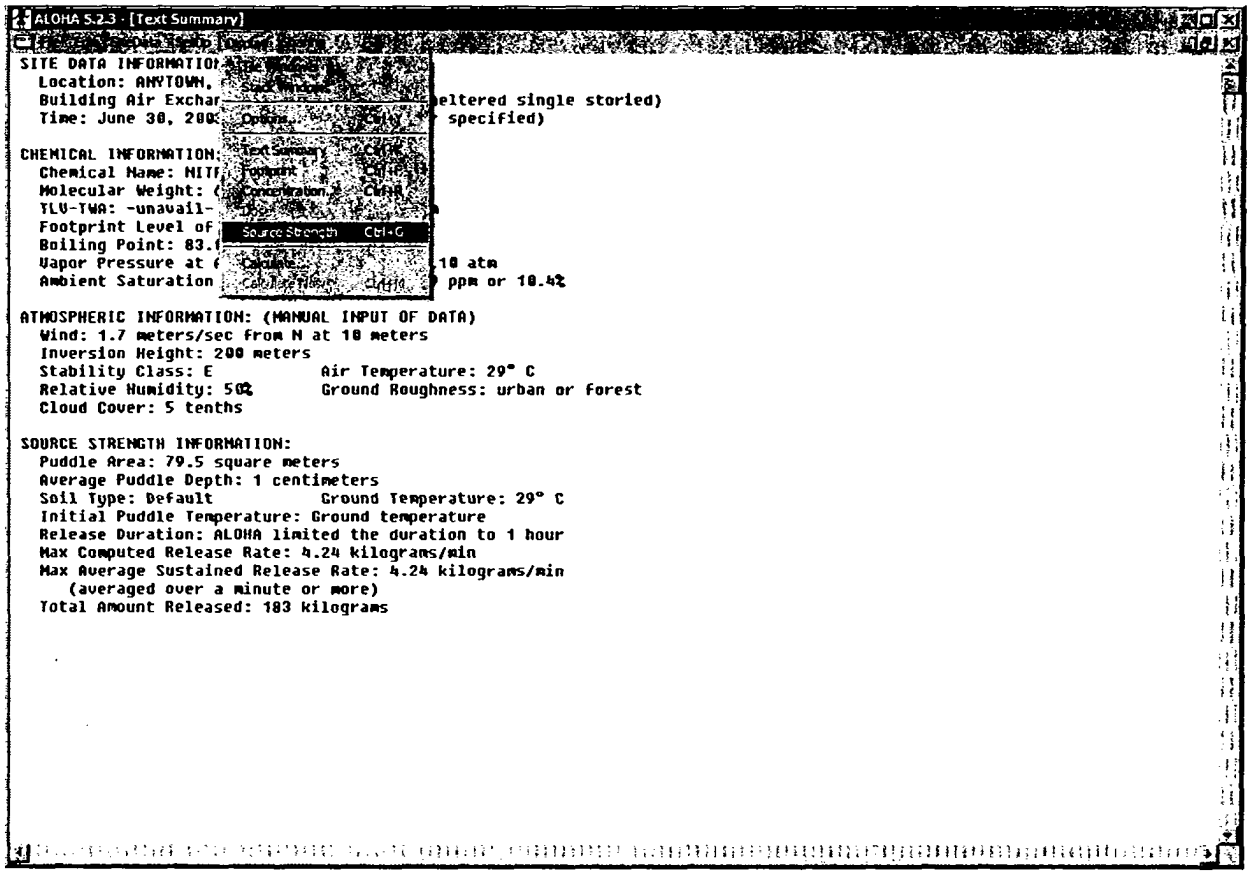


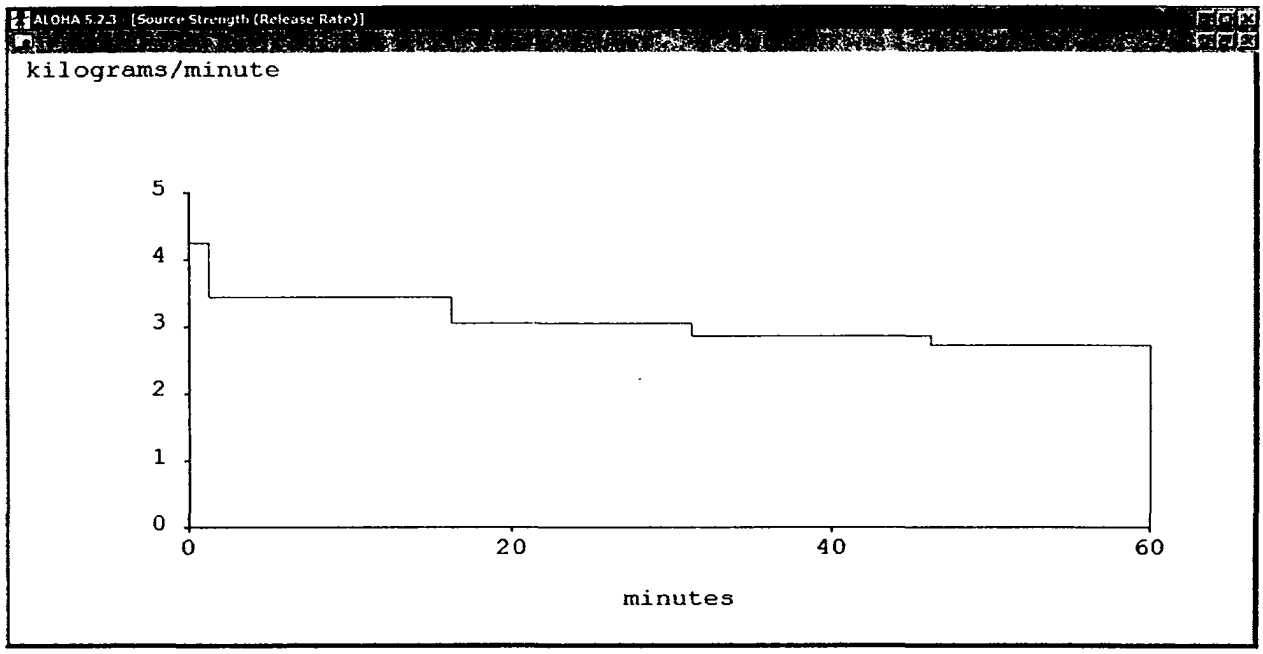
Since the problem statement does not specify a ground type, the default ground type is selected since it is expected to support the calculation of reasonably conservative evaporation rates. No information is available on the ground temperature, so the ground temperature is set equal to the air temperature (default specification). Since the problem statement indicates the HNO_3 is stored at ambient conditions and the ground temperature is assumed to be equal to the air temperature, the initial temperature of the puddle is set equal to the ground and air temperature of 29 °C.



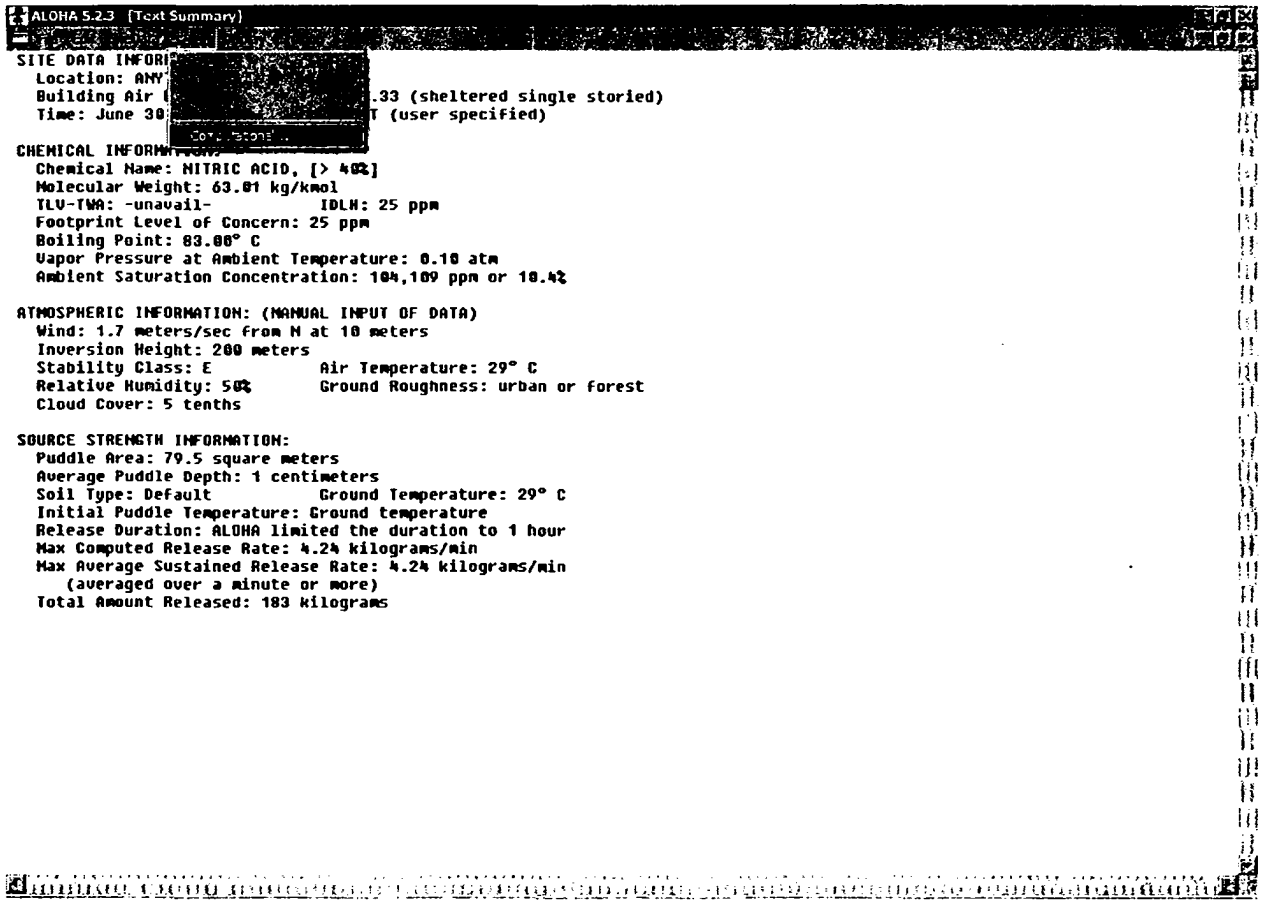
Following data entry above, the Text Summary screen now displays the maximum computed evaporation rate of 4.24 kilograms per minute. The maximum average sustained evaporation rate (over a minute or more) is also determined to be 4.24 kilograms per minute. ALOHA also determines the release to last more than one hour and that 183 kilograms are released in the first hour. The Text Summary screens that follow will display this information.

At this point, a graphical representation of the source strength (i.e., evaporation rate) as a function of time can be viewed. Note that the five averaging periods are clearly evident by the stair-step nature of the curve.

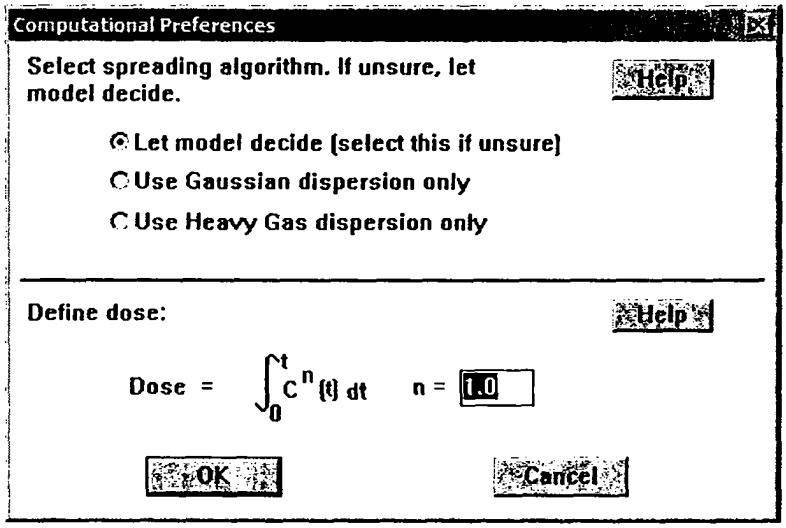




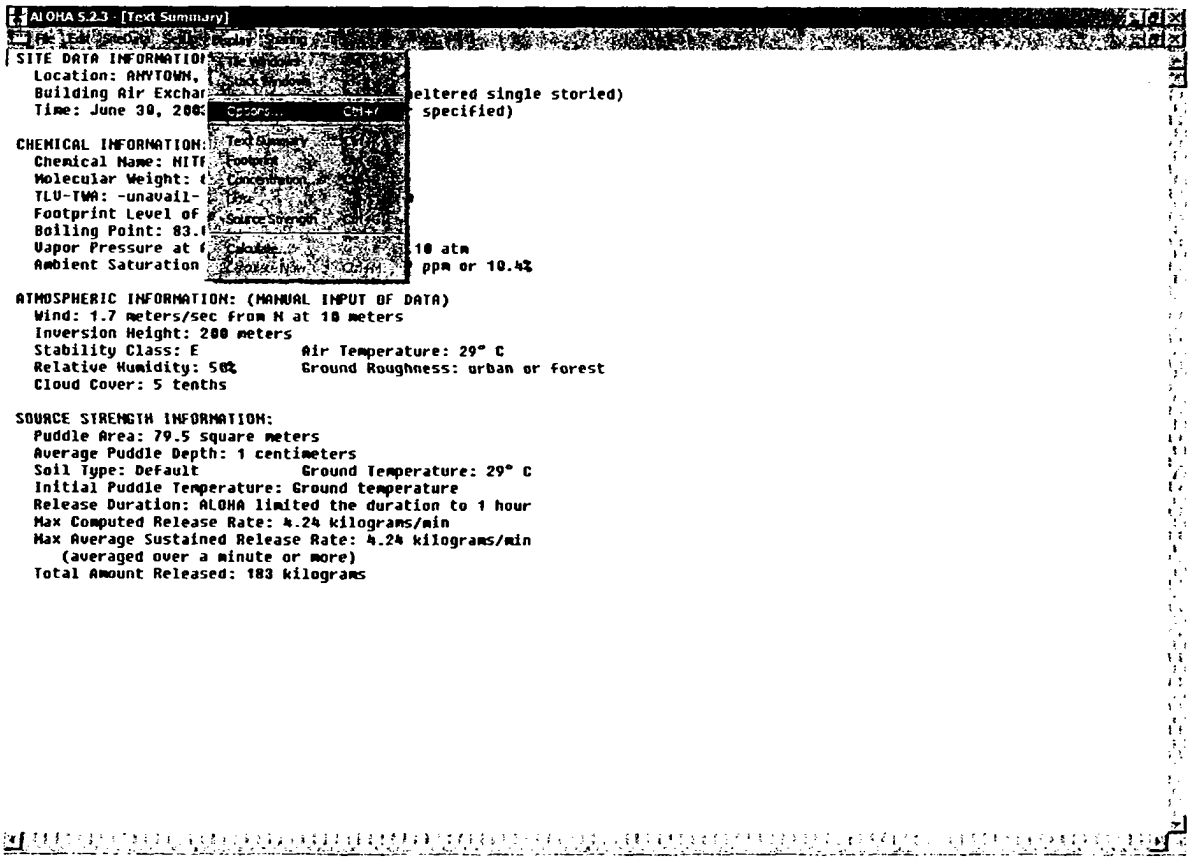
Set Up – Computational



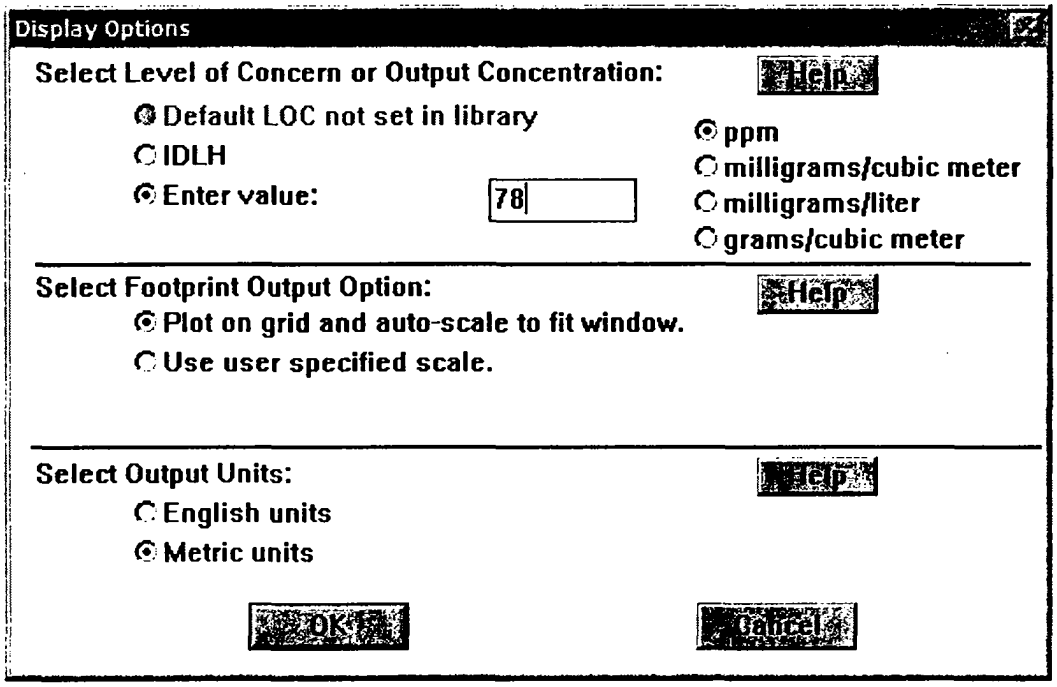
Here, the analyst indicates the recommended preference of letting ALOHA consider both heavy-gas and Gaussian dispersion models and to determine the appropriate model based on the source Ri number. Also under this submenu is the dose exponent input, which is not used in safety analysis since human health evaluation guidelines, such as ERPGs and TEELs, are based on concentration limits and not dose limits.



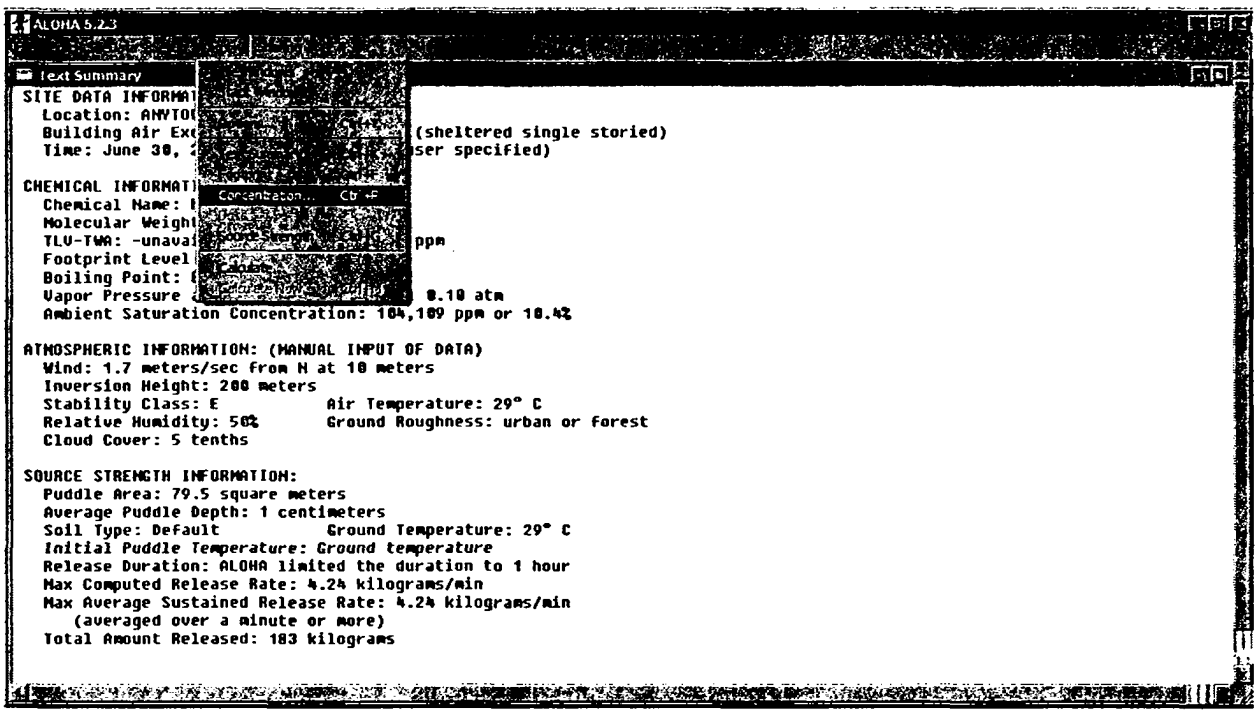
Display – Options



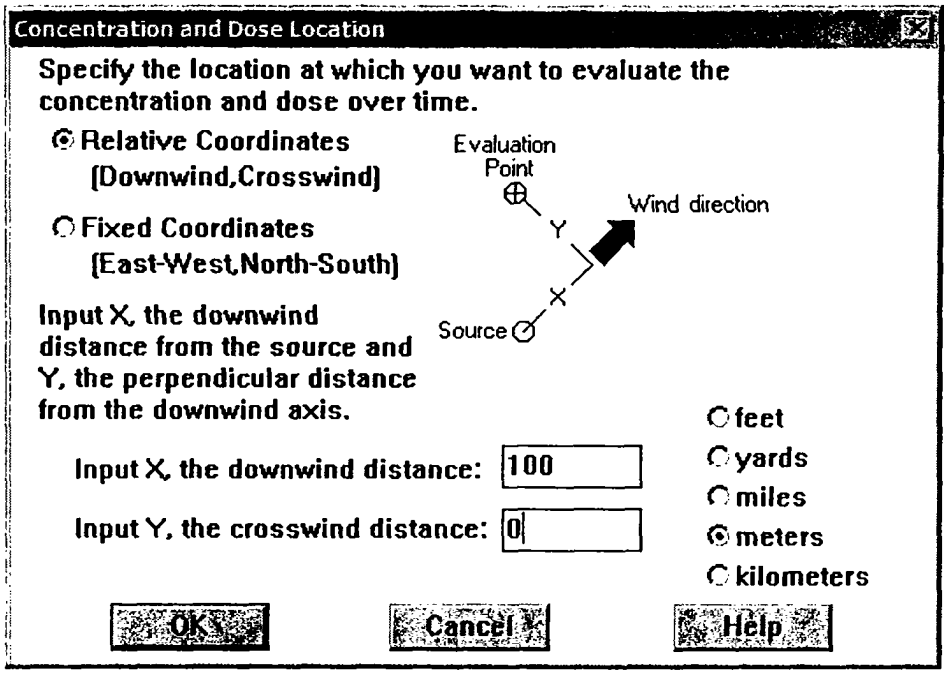
The ERPG-3 value of 78 ppm is entered as the LOC value.

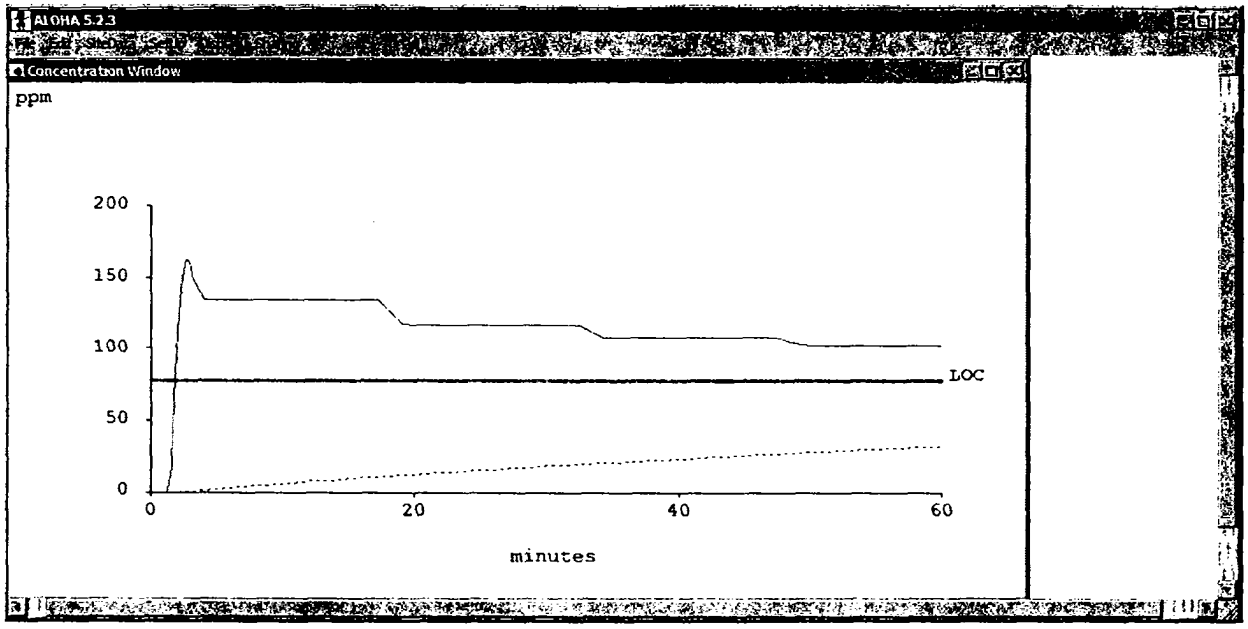


Display – Concentration



The concentration on the centerline (y =0) at 100 can now be determined and compared with ERPG-3 value of 78 ppm.



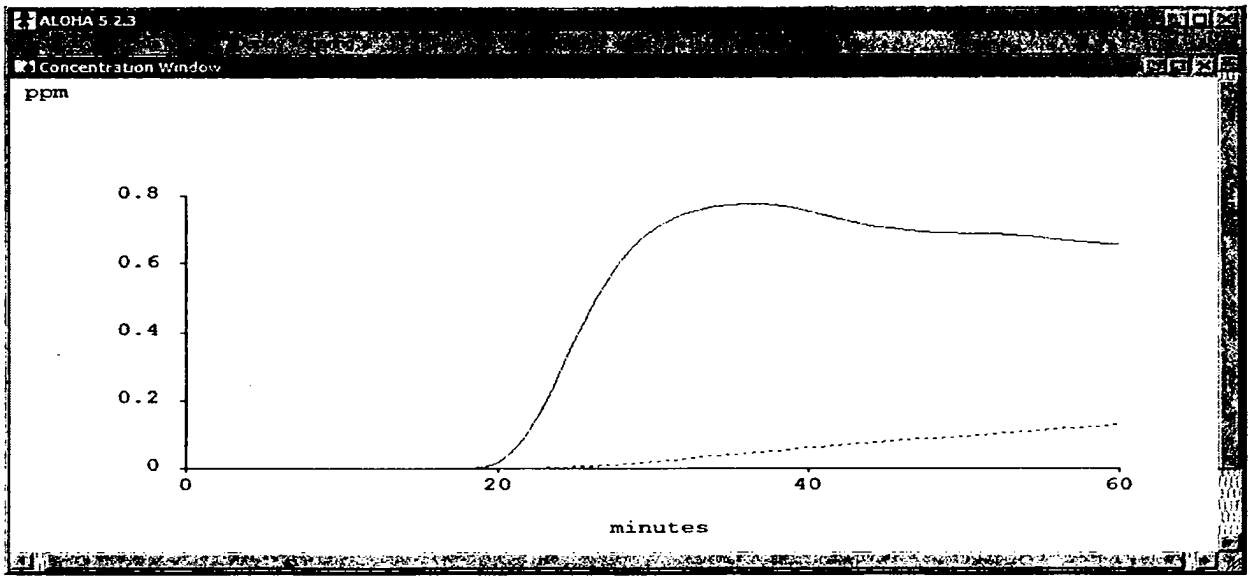


One can see from the concentration graph that it takes a few minutes for the plume (centerline concentration shown by solid, irregular line) to reach the receptor at 100 meters. Once the plume reaches the receptor, the receptor is exposed to concentrations in excess of 78 ppm (LOC line). (Note that the dotted line represents the estimated indoor concentration.)

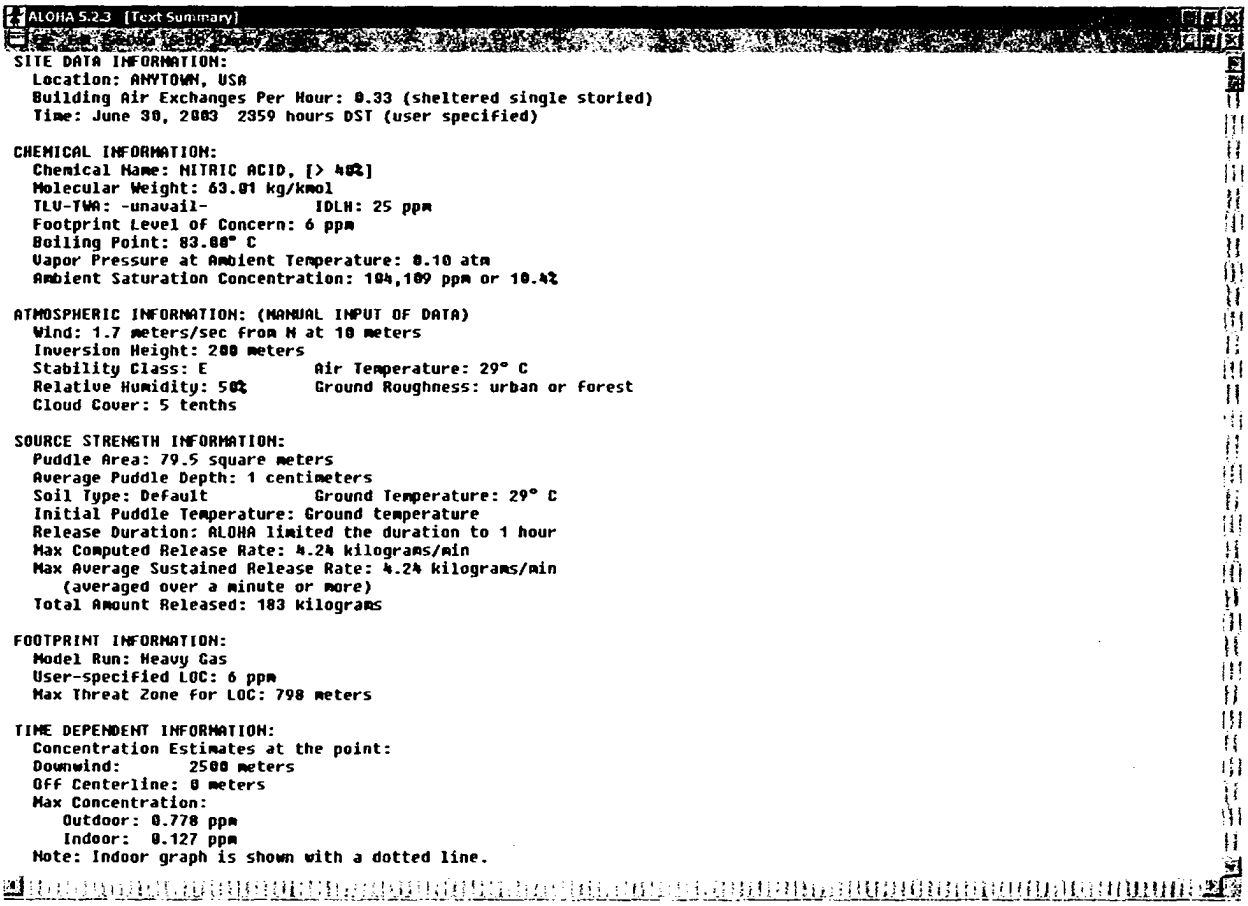
From the Text Summary screen next, the maximum concentration is given as 162 ppm. The Text Summary screen also indicates that ALOHA used the heavy gas dispersion algorithm to calculation the downwind concentration.

```
ALOHA 5.2.3 - [Text Summary]

SITE DATA INFORMATION:
  Location: ANYTOWN, USA
  Building Air Exchanges Per Hour: 0.33 (sheltered single storied)
  Time: June 30, 2003  2359 hours DST (user specified)

CHEMICAL INFORMATION:
  Chemical Name: NITRIC ACID, [> 40%]
  Molecular Weight: 63.01 kg/kmol
  TLV-TWA: -unavail-              IDLH: 25 ppm
  Footprint Level of Concern: 78 ppm
  Boiling Point: 83.00° C
  Vapor Pressure at Ambient Temperature: 0.10 atm
  Ambient Saturation Concentration: 104,189 ppm or 10.4%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)
  Wind: 1.7 meters/sec from N at 10 meters
  Inversion Height: 200 meters
  Stability Class: E              Air Temperature: 29° C
  Relative Humidity: 50%          Ground Roughness: urban or forest
  Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
  Puddle Area: 79.5 square meters
  Average Puddle Depth: 1 centimeters
  Soil Type: Default              Ground Temperature: 29° C
  Initial Puddle Temperature: Ground temperature
  Release Duration: ALOHA limited the duration to 1 hour
  Max Computed Release Rate: 4.24 kilograms/min
  Max Average Sustained Release Rate: 4.24 kilograms/min
     (averaged over a minute or more)
  Total Amount Released: 183 kilograms

FOOTPRINT INFORMATION:
  Model Run: Heavy Gas
  User-specified LOC: 78 ppm
  Max Threat Zone for LOC: 153 meters

TIME DEPENDENT INFORMATION:
  Concentration Estimates at the point:
  Downwind:       100 meters
  Off Centerline: 0 meters
  Max Concentration:
     Outdoor: 162 ppm
     Indoor:  32.2 ppm
  Note: Indoor graph is shown with a dotted line.
```

The second case of the problem statement involves calculating the maximum concentration at 2500 meters downwind and comparing it with the ERPG-2 value of 6 ppm. The details of changing the input data for this case are not shown since they involve steps similar to those already shown. The concentration graph for this second case is shown below.



One can see from the concentration graph that it takes approximately 20 minutes for the plume to reach the receptor at 2500 meters. The receptor at 2500 meters is not exposed to the maximum plume concentration until almost 20 minutes later. From the Text Summary screen shown next, the maximum concentration is given as 0.78 ppm.



```
ALOHA 5.2.3 [Text Summary]
SITE DATA INFORMATION:
  Location: ANYTOWN, USA
  Building Air Exchanges Per Hour: 0.33 (sheltered single storied)
  Time: June 30, 2003  2359 hours DST (user specified)

CHEMICAL INFORMATION:
  Chemical Name: NITRIC ACID, [> 40%]
  Molecular Weight: 63.01 kg/kmol
  TLV-TWA: -unavail-          IDLH: 25 ppm
  Footprint Level of Concern: 6 ppm
  Boiling Point: 83.88° C
  Vapor Pressure at Ambient Temperature: 0.10 atm
  Ambient Saturation Concentration: 104,109 ppm or 10.4%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)
  Wind: 1.7 meters/sec from N at 10 meters
  Inversion Height: 200 meters
  Stability Class: E          Air Temperature: 29° C
  Relative Humidity: 50%      Ground Roughness: urban or forest
  Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
  Puddle Area: 79.5 square meters
  Average Puddle Depth: 1 centimeters
  Soil Type: Default          Ground Temperature: 29° C
  Initial Puddle Temperature: Ground temperature
  Release Duration: ALOHA limited the duration to 1 hour
  Max Computed Release Rate: 4.2% kilograms/min
  Max Average Sustained Release Rate: 4.2% kilograms/min
     (averaged over a minute or more)
  Total Amount Released: 183 kilograms

FOOTPRINT INFORMATION:
  Model Run: Heavy Gas
  User-specified LOC: 6 ppm
  Max Threat Zone for LOC: 798 meters

TIME DEPENDENT INFORMATION:
  Concentration Estimates at the point:
  Downwind:       2500 meters
  Off Centerline: 0 meters
  Max Concentration:
     Outdoor: 0.778 ppm
     Indoor:  0.127 ppm
  Note: Indoor graph is shown with a dotted line.
```

The Text Summary screen also indicates that ALOHA used the heavy gas dispersion algorithm to calculation the downwind concentration. Sensitivity runs (not shown) were performed in which the wind speed was increased from the 1.7 m/s value. At 2.2 m/s wind speed, the transition from heavy gas to Gaussian plume dispersion occurred as determined by ALOHA.

If ALOHA is directed by the user to use the Gaussian plume model with the 1.7 m/s wind speed, the calculated concentration at 100 m is 169 ppm (compared to 162 ppm with the heavy gas model), and the calculated concentration at 2500 m is 0.61 ppm (compared to 0.78 ppm with the heavy gas model).

Recall that the above calculations were performed with a surface roughness length of 100 cm (urban environment). To demonstrate the sensitivity of the results to this input, the above cases were rerun with the surface roughness length set to 3 cm (rural environment) and the results are summarized below together with the results previously discussed for surface roughness length of 100 cm.

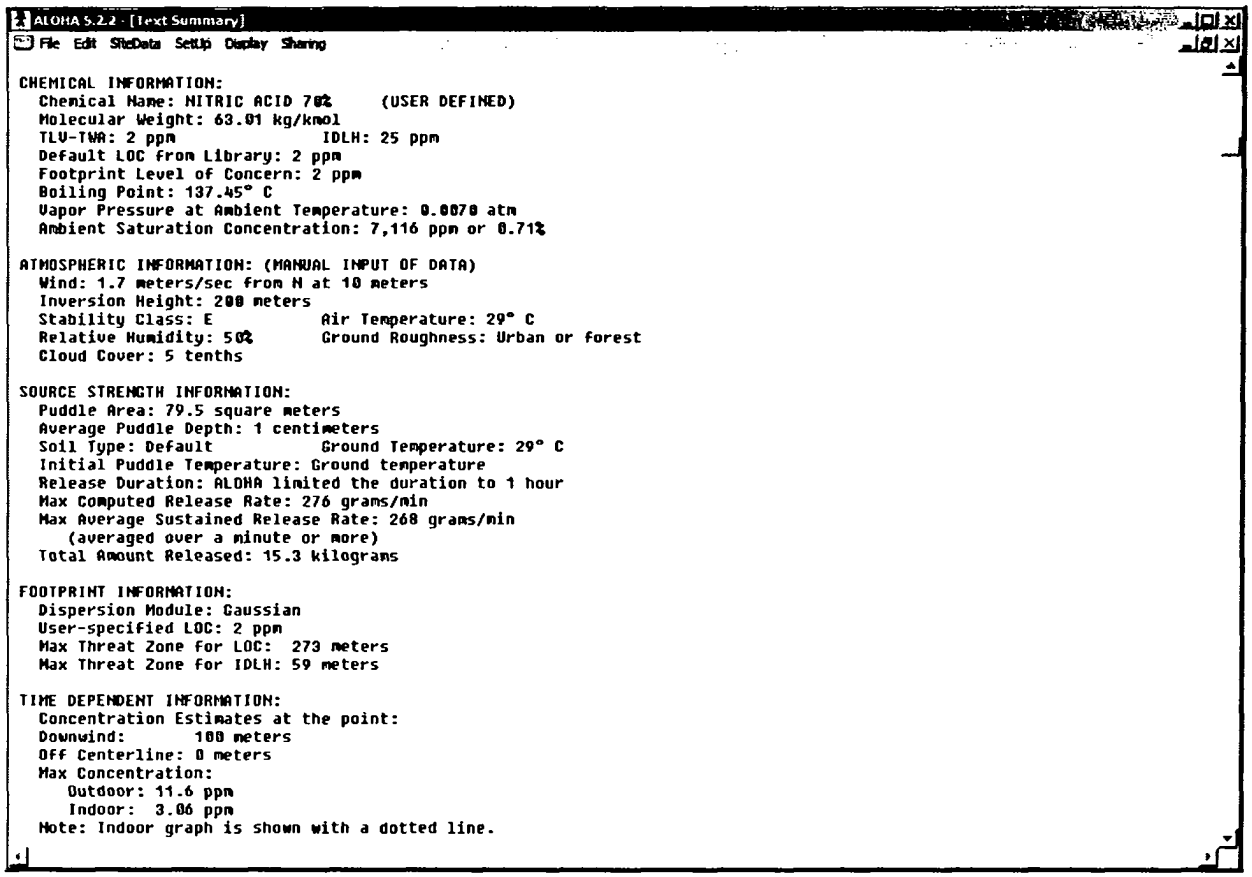
Comparison of Concentration Results with Surface Roughness Length Set to 3 cm and 100 cm.

Receptor at 100 m	**Heavy Gas Model Concentration [ppm]**	**Gaussian Model Concentration [ppm]**
3-cm surface roughness length	250	354
100-cm surface roughness length	162	169
Receptor at 2500 m	**Heavy Gas Model Concentration [ppm]**	**Gaussian Model Concentration [ppm]**
3-cm surface roughness length	1.1	1.0
100-cm surface roughness length	0.78	0.61

In all cases, the concentration results with the surface roughness length set to 3 cm were larger (up to a factor of 2 larger) than the corresponding results with the surface roughness length set to 100 cm.

Additional Analysis:

The maximum concentration at 100 meters downwind will now be calculated for an evaporative release from a 210-gallon puddle of 70 wt% HNO_3 and compared with the ERPG-3 value of 78 ppm. This additional calculation will highlight the large difference in evaporation rates between pure HNO_3 and 70 wt% HNO_3. The approach that has been developed at SRS for dilute acids that involves entering pseudo property values for the boiling point, freezing point, critical pressure, and critical temperature will be used. (Note that calculations are performed with an earlier version of ALOHA, namely 5.2.2, since the dilute acids were added to the chemical library of ALOHA 5.2.2. The minor differences between version 5.2.2 and version 5.2.3 are not expected to alter the calculations in any significant way.) Recall that these pseudo property values are set through trial and error so that the ALOHA chemical database calculates vapor pressures at the temperature range of interest that closely match the vapor pressures for the dilute acid as found in a reference book. From the table of HNO_3 vapor pressure at 30 °C as a function of weight percent shown earlier, the vapor pressure for HNO_3 70 wt% is 5.5 mm Hg (0.0072 atmospheres) compared to 77 mg Hg (0.10 atmospheres) for pure the HNO_3 (Perry, 1997). Therefore, a much lower evaporation rate and 100-m concentration can be expected since the vapor pressure for 70 wt% HNO_3 is approximately 7% of that for 100 wt% HNO_3. Results are shown below using the 100-cm surface roughness length and letting ALOHA decide upon the dispersion model (in this case, Gaussian model).



```
ALOHA 5.2.2 - [Text Summary]
File  Edit  SiteData  SetUp  Display  Sharing

CHEMICAL INFORMATION:
  Chemical Name: NITRIC ACID 70%     (USER DEFINED)
  Molecular Weight: 63.01 kg/kmol
  TLV-TWA: 2 ppm                IDLH: 25 ppm
  Default LOC from Library: 2 ppm
  Footprint Level of Concern: 2 ppm
  Boiling Point: 137.45° C
  Vapor Pressure at Ambient Temperature: 0.0070 atm
  Ambient Saturation Concentration: 7,116 ppm or 0.71%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)
  Wind: 1.7 meters/sec from N at 10 meters
  Inversion Height: 200 meters
  Stability Class: E            Air Temperature: 29° C
  Relative Humidity: 50%        Ground Roughness: Urban or forest
  Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
  Puddle Area: 79.5 square meters
  Average Puddle Depth: 1 centimeters
  Soil Type: Default            Ground Temperature: 29° C
  Initial Puddle Temperature: Ground temperature
  Release Duration: ALOHA limited the duration to 1 hour
  Max Computed Release Rate: 276 grams/min
  Max Average Sustained Release Rate: 268 grams/min
     (averaged over a minute or more)
  Total Amount Released: 15.3 kilograms

FOOTPRINT INFORMATION:
  Dispersion Module: Gaussian
  User-specified LOC: 2 ppm
  Max Threat Zone for LOC:  273 meters
  Max Threat Zone for IDLH: 59 meters

TIME DEPENDENT INFORMATION:
  Concentration Estimates at the point:
  Downwind:       100 meters
  Off Centerline: 0 meters
  Max Concentration:
     Outdoor: 11.6 ppm
     Indoor:  3.06 ppm
  Note: Indoor graph is shown with a dotted line.
```

Comparison of the 70 wt% HNO_3 results with the pure HNO_3 and results are summarized below.

	70 wt% HNO_3	**100 wt% HNO_3**
Vapor Pressure [atm]	0.0070	0.1
Vapor Pressure [mm Hg]	5.3	76
Vapor Pressure at 30 °C [mm Hg] (Perry, 1997)	05.5	77
Max. Computed Release Rate [kg/min]	0.276	4.24
Max. Concentration at 100 m [ppm]	11.6	162

Note that the maximum computed release rate and maximum concentration at 100 meters for the 70 wt% HNO_3 case are approximately 7% of the values calculated for the 100 wt% HNO_3 case, (recall vapor pressure proportional relationship was also 7%).

8.0 ACRONYMS & DEFINITIONS

Selected Terms and Definitions Used in Source Term, Atmospheric Transport and Dispersion, and Consequence Analysis

Acute Exposure Guideline Levels (AEGLs) – Threshold exposure limits for the general public above which acute exposure would be expected to lead to adverse effects of increasing severity for AEGL-1, AEGL-2, and AEGL-3. The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) is developing AEGLs to assist Federal and State agencies and private sector organizations with their need for short-term hazardous chemical exposure information in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h) and the three severity levels as defined below:

AEGL-1: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Advection – The transport of a fluid property by the bulk motion of the fluid, sometimes called convection in engineering terminology.[36]

Aerosol – Solid or liquid particles (droplets) that are suspended in a gas or vapor medium.

Atmospheric Stability Class – Characterization of the state of atmospheric turbulence. The different atmospheric stability classes typically used by meteorologist range from A for very unstable conditions to F (or sometimes G) for very stable conditions and account for differing levels of buoyant turbulence. High levels of buoyant turbulence are associated with unstable conditions.

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[36] Some of the definitions for atmospheric transport and dispersion terms are taken from the Chemical Dispersion and Consequence Assessment Working Group of the DOE-sponsored Accident Phenomenology and Consequence Methodology Evaluation Program (Lazaro, 1997).

Atmospheric Transport and Dispersion – The movement and dilution of a contaminant cloud under the influence of the prevailing wind flows and associated atmospheric turbulence.

Buoyant Turbulence – Atmospheric turbulence that is generated by solar heating of the ground and the formation of thermal updrafts.

Cloud – The volume that encompasses a chemical (contaminant) emission.

Dense Gas (Heavy Gas) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is greater than that of the ambient air (i.e., negatively buoyant cloud). In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind, and the cloud alters the atmospheric wind field in its vicinity. Dense-gas releases undergo what has been described in the literature as "gravitational slumping". Gravitational slumping is characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release.

Dilution – The reduction of the cloud concentration due to mixing with ambient air.

Dispersion – Spreading of the cloud boundaries due to atmospheric turbulence. Atmospheric, turbulent dispersion is the result of rapid and irregular fluctuations in wind components, such as velocity.

Dispersion Coefficients – A measure of the spreading of a contaminant cloud as it travels downwind. In Gaussian puff and plume formulations:

σ_x = longitudinal dispersion coefficient (function of downwind distance, x), representing the standard deviation of the concentration distribution in the downwind axis direction;

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction; and

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction.

Emergency Response Planning Guidelines (ERPGs) – Estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

> ***ERPG-1**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*
>
> ***ERPG-2**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*
>
> ***ERPG-3**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

Evaporation – Process by which molecules of a liquid come off the surface of a liquid and enter the vapor space.

Flashing – Sudden vaporization of a liquid as a result of the liquid undergoing a sudden change in pressure such that its temperature at the new pressure condition is above the boiling point.

Friction Velocity – A measure of the mechanical turbulence and a direct measure of the frictional forces of the wind in the boundary layer adjacent to the earth's surface. It can be thought of as the representing the consequences of Reynolds stresses, which cause velocity fluctuations to transport momentum.[36]

Gaussian Puff/Plume Model – A diffusion model for vapor or gas chemical releases to the environment in which the lateral and vertical distribution of the chemical concentration follow a normal or Gaussian distribution. Additionally in the puff model, the longitudinal distribution follows a normal or Gaussian distribution. A segmented Gaussian puff/plume model incorporates a computational approach in which the Gaussian puff/plume is spatially segmented into individual volume sources with each segment generating a concentration field.[36]

Inversion Layer – A region of air in which the temperature increases with increasing distance from the ground.[36] The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is often referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i.

Level of Concern (LOC) – Term used by ALOHA to refer to a concentration limit that is used for consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). Safety analysis work uses the emergency response planning guidelines (ERPGs) and temporary emergency exposure limits (TEELs) for assessing human health effects for both facility workers and the general public.

Liquefied Gas – A chemical substance that is a vapor at atmospheric pressure and temperature, but is stored as a liquid. The chemical substance in storage may be either cooled (i.e., refrigerated) at ambient pressure or pressurized (i.e., compressed) at ambient temperature to achieve and maintain the liquid state. Compressed liquefied gases may be subject to flashing as it discharges from its storage vessel.

Mechanical Turbulence – Atmospheric turbulence that is generated from the shear forces that result when adjacent parcels of air move at different velocities (i.e. either at different speeds or directions). Fixed objects on the ground such as buildings or trees increase the ground roughness and increase mechanical turbulence in proportion to their size.

Neutrally Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that occurs when the density difference between the chemical cloud and the ambient air is small. A neutrally buoyant cloud does not alter the atmospheric wind field. The term passive is used to describe the phenomenological characteristics associated with atmospheric transport and dispersion of the cloud as the cloud follows the bulk movements and behavior of the atmospheric wind flow.

Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) – Chemical concentration limits that are developed by the Occupational Safety & Health Administration for use in limiting worker exposures to airborne chemicals.

Plume – Term used to describe the form of the chemical cloud for a sustained or continuous release.

Plume Meander – Variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.

Positively Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is significantly less than that of the ambient air. A positively buoyant cloud behaves like a neutrally buoyant cloud with the added effect that the positive buoyancy produces upward forces that cause the puff or plume to rise.

Puff – Term used to describe the form of the chemical cloud for an instantaneous release or release of short duration.

Richardson (Ri) Number – Relative measure of the potential energy of the cloud with respect to the mechanical turbulence energy of the atmosphere. Potential energy is

associated with buoyancy forces that tend to suppress turbulence. Wind shear generates mechanical turbulence energy.

Source Term – The rate of release (may be time dependent), duration, and physical and energetic characteristics of hazardous material released to the environment. ALOHA uses the term source strength to refer to the time-dependent rate of vapor release to the environment.

Surface Roughness Length (z_o) – Measure of the amount of atmospheric mechanical turbulence that is induced by the presence of surface roughness elements such as vegetation and man-made structures.

Temporary Emergency Exposure Limits (TEELs) – Surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values) and surrogate Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) values for all chemicals for which PEL-TWA values have been published (i.e., TEEL-0 values).

Vapor – The gas produced from the evaporation of a liquid.

Vapor Pressure – The equilibrium pressure of the pure component vapor over the pure component liquid. When a chemical exists in a solution or mixture, the term partial pressure is generally used.

95th Percentile Consequence – A statistical method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to quantify the consequences for an airborne release conservatively taking into consideration the variability of meteorological conditions that may be present at the time of the release (NRC, 1983).[37] While this method was originally established for radiological releases, the concept easily extends to hazardous chemical releases. Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based χ/Q values calculated for a postulated release to downwind receptors at the site boundary that would result in a χ/Q values that is exceeded 5% of the time (based on hourly data over a period of one year or more).[38] Although the methods allows for variations in distance to the site boundary as a function of angular sectors to be taken into consideration in conjunction with the wind direction, assuming the minimum distance to the site

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[37] This method is prescribed in Appendix A to DOE-STD-3009-94 for consequence assessment to quantify the radiological dose that is received by the maximally exposed offsite individual (MOI) (DOE, 2000).

[38] Terminology that is sometimes unfortunately used in this context and that should be avoided is terms such as "95th percentile meteorology." The distribution and selection of the 95th percentile value are based on consequence results (e.g., χ/Q values) that are a function of meteorological parameters and not on the meteorological parameters themselves (e.g., wind speed).

boundary applies in all directions is a conservative implementation that is easily supported and that essentially makes the calculations sector independent. The site-specific meteorological data consist of (generally) hourly data of wind speed and atmospheric stability class at minimum (wind direction is also needed if sector-dependent distances to the site boundary are considered).

9.0 REFERENCES

AIHA (2002). *The AIHA Emergency Response Planning Guidelines and Workplace Environmental Exposure Level Guides Handbook*, American Industrial Hygiene Association (AIHA), AIHA Press, Fairfax, VA.

S. Brereton (1997), D. Hesse, D. Kalinich, M. Lazaro, V. Mubayi, and J. Shinn. *Final Report of the Accident Phenomenology and Consequence (APAC) Methodology Evaluation – Spills Working Group*, URLC-ID-125479, Lawrence Livermore National Laboratory (LLNL), Livermore, CA.

P. W. M. Brighton (1985). *Evaporation from a plane liquid surface into a turbulent boundary layer*, Journal of Fluid Mechanics, Vol. 159, 323-345.

P. W. M. Brighton (1990). *Further verification of a theory for mass and heat transfer from evaporating pools*, Journal of Hazardous Materials, Vol. 23, 215-234.

W. Brutsaert (1982). *Evaporation, into the Atmosphere: Theory, History, and Applications*, D. Reidel Publishing Company, Boston.

H. S. Carslaw (1959) and J. C. Jaeger. Conduction of Heat in Solids, Oxford University Press, London.

CFR (1992). *Process Safety Management of Highly Hazardous Chemicals; Explosives and Blasting Agents*; Final Rule, 29 CFR Part 1910, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

CFR (1999). Labor Chapter XVII—*Occupational Safety and Health Administration.* 29 CFR Part 1910.1000, Subpart Z—Toxic and Hazardous Substances, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

CFR (2001). *Nuclear Safety Management Rule*, 10 CFR Part 830, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

G. W. Colenbrander (1980). *A Mathematical Model for the Transient Behavior of Dense Gas Clouds*, 3rd International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Basel, Switzerland.

G. W. Colenbrander (1983) and J. S. Puttock. *Dense Gas Dispersion Behavior: Experimental Observations and Model Developments*, International Symposium on Loss Prevention and Safety Promotion in the Process Industries, Harrogate, England.

D. K. Craig (2001), J. S. Davis, P. W. Hoffman, L. G. Lee, and J. Prowse. *Toxic Chemical Hazard Classification And Safety Evaluation Guidelines For Use In Doe Facilities*, WSRC-MS-92-00206, Rev. 3, Savannah River Site, Aiken, SC.

DNFSB (2000). *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, Defense Nuclear Facilities Safety Board, Technical Report DNFSB/TECH-25, (January 2000).

DNFSB (2002). Defense Nuclear Facilities Safety Board, *Recommendation 2002-1, Quality Assurance for Safety-Related Software* , (September 2002).

DOE (1997). *Hazard Categorization and Accident Analysis Techniques for Compliance Order 5480.23, Nuclear Safety Reports*, U.S. Department of Energy, Washington, DC, DOE-STD-1027-92, Change Notice 1.

DOE (2002a). *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports*, DOE-STD-3009-94, Change Notice 2, U.S. Department of Energy, Washington, DC (April 2002).

DOE (2002b). *Selection of Computer Codes for DOE Safety Analysis Applications, Department of Energy*, National Nuclear Security Agency - Defense Programs Technical Report, (May 2002).

DOE (2003a). U.S. Department of Energy, *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes*, Revision 1, (November 2003).

DOE (2003b). U.S. Department of Energy, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1: Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, Report, (February 28, 2003).

DOE (2004). U.S. Department of Energy, *Software Quality Assurance Improvement Plan: ALOHA Gap Analysis*, Final (May 2004).

DOE/EH (2003). U.S. Department of Energy, *Designation of Initial Safety Analysis Toolbox Codes*, Letter, (March 28, 2003).

EPA (1987). *Technical Guidance for Hazards Analysis: Emergency Planning for Extremely Hazardous Substances*, PB93-206910, Environmental Protection Agency, Research Triangle Park, NC.

EPA (1993). *Guidance on the Application of Refined Dispersion Models for Hazardous/Toxic Air Releases*, EPA-454/R-93-002, U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA (1995). *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volume II – Description of Model Algorithms*, EPA-454/R-95-003b, U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA (1999). *Risk Management Program for Offsite Consequence Analysis*, EPA 550-B-99-0009, U.S. Environmental Protection Agency, Research Triangle Park, NC.

M. Evans (1993). *ALOHA User's and ARCHIE: A Comparison*, Report No. HAZMAT 93-2, Office of Ocean and Resources Conservation and Assessment of the National Oceanic and Atmospheric Administration (NOAA), Seattle, WA.

M. Evans (1994). *Quality Assurance of ALOHA*, Draft Report, Office of Ocean and Resources Conservation and Assessment of the National Oceanic and Atmospheric Administration (NOAA), Seattle, WA.

H. K. Fauske (1985). *Flashing flow: some practical guidelines for emergency releases*, Plant/Operations Progress, Vol. 4 (3), 132-134.

H. K. Fauske (1988) and M. Epstein. *Source term considerations in connection with chemical accidents and vapor cloud modeling*, Proceedings, International Conference on Vapor Cloud Modeling, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

FEMA (1989). *Handbook of Chemical Hazard Analysis Procedures*, (ARCHIE Manual), Federal Emergency Management Agency (FEMA), U. S. Department of Transportation (USDOT), and U.S. Environmental Protection Agency (USEPA) (1989), Washington, D.C.

S. R. Hanna (1982), G. A. Briggs, and R. P., Hosker, Jr. *Handbook on Atmospheric Dispersion*, DOE/TIC-11223, Technical Information Center, U.S. Department of Energy (DOE), Oak Ridge, TN.

S. R. Hanna (1996a), P. J. Drivas, and J. J. Chang. Guidelines for Use of Vapor Cloud Dispersion Models, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

S. R. Hanna (1996b), J. J. Chang and J. X. Zhang. *Technical Documentation of HGSYSTEM/UF6 Model*, prepared by Earth Technology Corporation, Concord, MA, for Lockheed Martin Energy Systems, Oak Ridge, TN.

S. R. Hanna (2002) and R.E. Britter. Wind Flow and Vapor Cloud Dispersion at Industrial and Urban Sites, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

J. A. Havens (1985) and T. Spicer. *Development of an Atmospheric Dispersion Model for Heavier-than-air Gas Mixtures*, Vol. 1, U.S. Coast Guard, Report CG-D-22-85, Washington, DC.

R. E, Henry (1971) and H. Fauske. *The two-phase critical flow of one-component mixture in nozzles, orfices, and short tubes*, Journal of Heat Transfer, May 1971, 179-187.

G. C. Holzworth (1972). *Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution Throughout the Contiguous United States*, EPA Report AP-101, Environmental Protection Agency, Research Triangle Park, NC, p. 109.

C. H. Hunter (1993). *Revised Onsite Meteorological data for Emergency Planning Hazards Assessments*, Savannah River Technology Center, Westinghouse Savannah River Company, SRT-ETS-931167.

J. S. Irwin (1979). *A Theoretical Variation of the Wind Power Law Exponent as Function of Surface Roughness and Stability*, Atmospheric Environment, Vol. 13, 191-194.

J. C. Leung (1986). *A generalized correlation for one-component homogeneous equilibrium choked flow flashing*, AIChE Journal, Vol. 32 (10), 1743-1746.

M. A. Lazaro (1997), K. Woodward, S. R. Hanna, D.J. Hesse, J. C. Huang, J. Lewis, and C. A. Mazzola. *Model Review and Evaluation for Application in DOE Safety Basis Documentation of Chemical Accidents – Modeling Guidance for Atmospheric Dispersion and Consequence Assessment*, ANL/EAD/TM-75, Environmental Assessment Division (EAD), Argonne National Laboratory (ANL), Argonne, IL.

A. D. Little (1988). *CHEMS-PLUS (Enhanced Chemical Evaluation Hazard Evaluation Methodologies) Reference Manual*, Version 1.0, Cambridge, MA.

NOAA (1998). *ALOHA Quality Assurance*, National Oceanic and Atmospheric Administration (NOAA), http://www.nwn.noaa.gov/sites/hazmat/cameo/alotech/quality.html.

NOAA (1999a) and EPA. *ALOHA User's Manual*, Office of Response and Restoration of the National Oceanic and Atmospheric Administration (NOAA) and Chemical Emergency Preparedness and Prevention Office (CEPPO) of the U.S. Environmental (EPA), Seattle, WA.

NOAA (1999b) and EPA. *ALOHA 5.2.3 Online Help*, Office of Response and Restoration of the National Oceanic and Atmospheric Administration (NOAA) and Chemical Emergency Preparedness and Prevention Office (CEPPO) of the U.S. Environmental (EPA), Seattle, WA.

NRC (1972). *Onsite Meteorological Programs*, U.S. Nuclear Regulatory Commission Regulatory Guide 1.23 U.S. Nuclear Regulatory Commission, Washington, DC.

NRC (1977). *Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water-Cooled Reactors*, Regulatory Guide 1.111, U.S. Nuclear Regulatory Commission, Washington, DC,

NRC (1983). *Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants*, Regulatory Guide 1.145, U.S. Nuclear Regulatory Commission, Washington, DC.

NRC (2003). *Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants*, U.S. Nuclear Regulatory Commission, Regulatory Guide 1.194, (June 2003), Washington, DC.

R. H. Perry (1997) and D. W. Green. Perry's Chemical Engineer's Handbook, 7th Edition, McGraw-Hill, N.Y.

J. M. Raphael (1962). *Prediction of temperature in rivers and reservoirs*, Journal of the Power Division, American Society of Chemical Engineers.

R. M. Reynolds (1992). *ALOHA Theoretical Description*, Draft Technical Memorandum NOS ORCA-65 Hazardous Materials Response and Assessment Division (HMRAD) of the National Oceanic and Atmospheric Administration (NOAA), Seattle, WA.

T. Spicer (1989) and J. A. Havens. *User's Guide for DEGADIS 2.1 Dense Gas Dispersion Model*, U.S. Environmental (EPA), EPA-450/4-89-019, Research Triangle Park, NC.

D.B. Turner (1970). *Workbook of Atmospheric Dispersion Estimates*, Report PB-191 482, Office of Air Programs, U.S. Environmental Protection Agency, Research Triangle Park, NC.

D. B. Turner (1994). *Workbook of Atmospheric Dispersion Estimates, An Introduction to Dispersion Modeling*, Lewis Publishers, Ann Arbor, MI.

A.H. Weber (1996) and C.H. Hunter, *Estimating Dispersion from a Tornado Vortex and Mesocyclone* (U), Savannah River Site, Aiken, SC, WSRC-TR-94-0386, Rev 2.

D. J. Wilson (1995). Concentration Fluctuations and Averaging Times in Vapor Clouds, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

APPENDIX A: ATMOSPHERIC TRANSPORT AND DISPERSION MODELS

The ALOHA code considers two classes of atmospheric transport and dispersion based upon the released chemical cloud density and how it affects the interaction of the chemical cloud with the atmospheric wind flow. For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, ALOHA treats the released chemical as being neutrally buoyant and as undergoing passive atmospheric transport and dispersion. If the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either passive or dense-gas type of atmospheric transport and dispersion. Dense gas behavior at the source is determined on the basis of the source Ri number having a value greater than one.[39]

The algorithms for both neutrally buoyant and dense-gas atmospheric transport and dispersion compute time-dependent, ground-level concentrations at a singular downwind location. In addition, ALOHA will generate a footprint plot that shows the area (in terms of longitudinal and lateral boundaries) where the ground-level concentration reached or exceeded the LOC during puff or plume passage.

ALOHA allows for meteorological data from a portable weather station to be captured and used in the atmospheric transport and dispersion calculations or for the user to manually input values for meteorological parameters that remain constant during the scenario duration. The ALOHA documentation refers to a portable weather station as a station for atmospheric measurements (SAM). The SAM samples wind speed and direction every two seconds. This capability is extremely useful for field use in emergency response situations. For safety analysis applications, however, the user analyzes a prescribed, hypothetical scenario and directly inputs the meteorological parameters that are necessary to perform the calculations.

NEUTRALLY BUOYANT MODEL

A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

Technical Background of Gaussian Dispersion Models

Time-averaged concentrations obtained from field studies of neutrally buoyant chemical releases are observed to follow Gaussian or bell-shaped distributions. The Gaussian plume and puff dispersion models that have been developed to predict the outcome of chemical releases that are represented by these field studies are well established and widely used. As the plume develops and moves downwind, it approximates a Gaussian distribution in both the crosswind (lateral) and

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[39] Definitions of source Ri number for continuous and instantaneous releases are given by Equations 4-1 and 4-2, respectively.

vertical directions. For continuous releases, the mean wind speed dilutes the chemical concentration but the longitudinal dispersion is negligible. As the plume moves downwind it gets progressively larger due to lateral and vertical dispersion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the longitudinal direction becomes more important. Accordingly, a puff is described by a three-dimension Gaussian equation.

The range of distances over which the Gaussian plume model should be used varies with conditions, but the model is considered generally applicable over the range of 100 m to 10 km and possibly beyond (Hanna, 1982). The basic form for the Gaussian plume model is given below beyond (Hanna, 1982).

$$\chi(x,y,z)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \quad \text{(A-1)}$$

where:

χ = atmospheric concentration [mg/m^3] for chemical releases

Q = source term release rate [mg/s] for chemical releases

x = downwind distance (relative to source location) [m]

y = crosswind distance (relative to plume centerline)[m]

z = vertical axis distance (relative to ground) [m]

H = effective release height (relative to ground) [m]

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction [m]

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction [m]

u = average wind speed[40] [m/s]

The last term accounts for reflection of the plume at the ground surface through adding an image source at distance H beneath the ground surface.

Note that the concentration is inversely proportional to the wind speed (i.e., greater initial dilution with higher wind speeds).[41] The concentration is also inversely proportional to the

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[40] Since the wind speed varies with distance above the earth's surface, the wind speed value in the Gaussian plume equation will ideally represent some average value over the plume depth, such as the wind speed at the plume centroid (center of mass). In practice, simpler specifications are made such as the wind speed at the effective release height or the wind speed at the height of 10 meters (Based on discussions with ALOHA technical staff, ALOHA uses either the wind speed at the release height or at 3 meters for release heights of 3 meters or less).

horizontal and vertical dispersion coefficients (i.e., higher dispersion enhances the dilution of the puff or plume). These dispersion coefficients are a measure of the effect of atmospheric turbulence in causing the plume to increasingly disperse in the lateral and vertical direction as the plume travels downwind. The dispersion coefficients account for the two sources of atmospheric turbulence, namely, mechanical turbulence and buoyant turbulence.

The horizontal and vertical dispersion coefficients, σ_y and σ_z, required in the Gaussian dispersion equation are obtained either from site-specific meteorological measurements (e.g., standard deviations of wind angles) or through established curves that are based on field experiments and the concept of atmospheric stability class. The averaging time over which the σ_y and σ_z parameters were determined in the field experiments establishes the averaging time for the time-averaged concentrations predicted by the Gaussian dispersion equation. Averaging time is important because greater apparent dispersion occurs with larger averaging time due to plume meander. Plume meander refers to variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.[42] The time-averaging effect on plume meander dispersion is generally accounted for by the following algebraic expression suggested by Gifford that relates the horizontal dispersion coefficient (σ_y) for the averaging time of interest (t_a) to a known reference horizontal dispersion coefficient ($\sigma_{y,ref}$) that is associated with a reference averaging time ($t_{a,ref}$) (Hanna, 1982).

$$\sigma_y = \sigma_{y,ref} \times \left(\frac{t_a}{t_{a,ref}} \right)^q \quad ; \qquad \text{(A-2)}$$

where, $q = 0.2$ for 3 minutes $< t_a <$ 1 hour

$q = 0.25$ to 0.3 for 1 hour $< t_a <$ 100 hours

Accounting for plume meander effects is typically done for radiological dose analysis, which can be concerned with radiological exposures that are integrated over times that may exceed the reference time for the set of $\sigma_{y,ref}$ values on which the Gaussian dispersion model is based. For chemical consequence analysis, toxic effect on human health can be immediate upon short-

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[41] Calm winds below 0.5 m/s are rare and generally not considered so that evaluating the Gaussian plume equation at a wind speed of zero is not an issue.

[42] In most engineering flow systems, the scales of turbulent motions are limited by the physical size of the system components (e.g., pipe diameter) so that time scales are on the order of seconds or minutes. For these systems, steady statistical averages can be achieved with reasonable sampling periods. Conversely, the range of spatial and time scales in the atmosphere is extremely large. As a consequence, observed statistics are not invariant with averaging time (i.e., one cannot obtain steady mean values since it is not possible to sample atmospheric parameters over a long enough time period) (Wilson, 1995).

duration exposures and the severity of the toxic effect may correlate more closely to concentration than to dose. Thus, an ideal chemical consequence analysis may, in some instances, be concerned with the peak concentrations that may last only a minute or even less. In practice, $\sigma_{y,ref}$ values developed for Gaussian dispersion codes are generally based on averaging times that range from 3 minutes to 1 hour. If the above correlation is be used to calculate (σ_y) for ($t_a < t_{ref}$), a prescribed minimum of t_a equal to 20 seconds has been recommended (Hanna, 1996a).

As the plume travels downwind, its vertical spread may be limited by the presence of an elevated temperature inversion layer. The temperature increases with increasing distance from the ground in the inversion layer. The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is typically referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i. The Gaussian dispersion equation can be modified to consider reflection from the elevated temperature inversion layer.[43] Reflection eventually results in a uniform concentration in the vertical direction (throughout the plume depth from ground to inversion layer boundary).

Determination of σ_y and σ_z from established, empirical curves is a common and acceptable practice. Each σ_y or σ_z curve represents a different atmospheric stability condition based upon the classification scheme first developed by F. Pasquill and later modified by F. A. Gifford. The different atmospheric stability classes range from A for very unstable conditions to F (or sometimes G)[44] for very stable conditions and account for differing levels of buoyant turbulence. High levels of buoyant turbulence are associated with unstable conditions.

The stability class is a function of both the amount of incoming solar radiation and the wind speed. High incoming solar radiation (as would occur on sunny days) and low wind speeds characterize unstable conditions (e.g. stability class A or B) and result in high levels of buoyant turbulence. Under unstable conditions, the air temperature of the atmosphere near the earth's surface declines rapidly with elevation. Warm parcels of air near the surface travel a long distance upward before cooling to the temperature of the air around it. As warmer air rises, the

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[43] The ground and the inversion layer boundary are treated as impenetrable and totally reflecting surfaces. Gaussian plume models such as ALOHA treat reflection through addition of mirror image sources both below the ground and above the inversion layer boundary. For reflection off the inversion layer boundary, an addition term is added to Equation (A-1) that is similar to the ground-reflection term with (z-H-$2z_i$) replacing (z+H). Additional terms can be added to account for multiple reflections off the ground and inversion layer boundary. Also at some point downwind (generally where σ_z approaches z_i), the value of the vertical dispersion coefficient, σ_z, in the Gaussian dispersion equation is typically limited to approximately z_i.

[44] ALOHA does not support the input of G stability class.

cooler air that is displaced sinks downward. Large-scale, convective motions develop that provide substantial vertical mixing. At the other end of the spectrum, stable atmospheric conditions (e.g., stability class E, F or G) can occur on clear nights with low wind speeds. The smaller atmospheric temperature gradient that occurs with stable atmospheric conditions limits upward convection and reduces vertical mixing. Neutral stability conditions (e.g., stability class C or D), tend to occur whenever wind speeds are high or with moderate wind speeds and cloud cover, and represent intermediate stability conditions that produce moderate levels of buoyant turbulence.

Original descriptions and conditions of occurrence given by Pasquill for each stability class are given below (Turner, 1994).

- A: Extremely Unstable (Strong superadiabatic). Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).
- B: Moderately Unstable (Moderate superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 3 to 5 m/s range to dim sunshine with wind speeds < 2 m/s.
- C: Slightly Unstable (Slight superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 5 to 6 m/s range to dim sunshine with wind speed in the 2 to 3 m/s range.
- D: Neutral (Adiabatic). Normally occurs with moderate to dim sunshine, cloudy conditions, and at night, with wind speeds > 3 m/s. It also occurs with very strong wind speeds on either sunny or cloudy days.
- E: Slightly Stable (Slight subadiabatic with or without inversion). Normally occurs at night or early morning with some cloud cover and with wind speeds in 2 to 5 m/s range.
- F: Moderately Stable (Moderate subadiabatic with inversion). Normally occurs at night or early morning with little cloud cover and with relatively low wind speeds (< 3 m/s).
- G: Extremely Stable (Strong subadiabatic with inversion). Normally occurs at night or early morning with very light to nearly zero wind speed.

Different set of dispersion coefficient curves have been established for rural environments and urban environments to account for the additional mechanical turbulence that is generated in urban settings by increased ground roughness due to building structures being taller and spaced closer together. A forest, however, can have a similar effect to that of buildings in increasing ground roughness. A surface roughness length (z_o) is typically used to characterize the amount of mechanical turbulence that is induced by the presence of surface roughness elements. A rule of thumb is that the surface roughness length is approximately one tenth the value of the height of the average surface roughness elements (Hanna, 2002). A surface roughness correction to σ_z is of the form $(z_o)^r$, where r is in the range of 0.1 to 0.25, with 0.2 being a commonly used value (Hanna, 1982; Hanna, 2002).

Recall that the atmospheric wind speed varies with distance from the ground (z). The wind speed (u) used in the Gaussian plume equation should ideally approximate the wind speed at the plume centroid (center of mass). Typically, the National Weather Service (NWS) measures wind speeds at 10 m (u_{10}). The following formula can be used to estimate the wind speed at other heights (Hanna, 1982).

$$u = u_{10} \times \left(\frac{z}{10}\right)^{p} \qquad \text{(A-3)}$$

The power-law exponent parameter (p) can be estimated on the basis of atmospheric stability class and general surface roughness characterization. An urban and rural set of power-law exponents that are found in the published literature are shown below (Hanna, 1982; Irwin, 1979).

Atmospheric Stability Class

	A	B	C	D	E	F
Urban	0.15	0.15	0.20	0.25	0.40	0.60
Rural	0.07	0.07	0.10	0.15	0.35	0.55

A puff model is used for instantaneous or near-instantaneous releases (Hanna, 1996a). For a puff, longitudinal dispersion also occurs.

$$\chi(x,y,z;t) = \frac{Q_T}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{x-x_o}{\sigma_x}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \qquad \text{(A-4)}$$

where:

Q_T = total source term [mg] for chemical releases

σ_x = longitudinal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the downwind axis direction [m]

x_o = $u \times t$; representing center of the puff in the longitudinal direction [m]

It is common practice to set σ_x equal to σ_y and to use the plume dispersion parameters[45] (Hanna, 1996a).

[45] The dispersion parameters for a puff release are known to be different than those for a plume release. Most dispersion models use plume dispersion parameters for both puff and plume releases due to the more extensive data available for plume releases (Hanna, 1996a).

ALOHA Application of Gaussian Dispersion Models

For direct source releases and pipe source releases in which the pipe is connected to a large-capacity reservoir, the airborne release rate remains steady. ALOHA calculates time-dependent airborne release rates for the other source cases. Recall that ALOHA calculates instantaneous release rates for up to 150 time steps. ALOHA then averages the release rates from the individual time steps over five averaging periods at most.[46] The five averaging periods are selected to most accurately portray the peak emissions. The five average release rates and associated duration for each (i.e., averaging periods) are inputs to the ALOHA algorithms for atmospheric transport and dispersion. ALOHA tracks the evolution of the mean concentration field of the five separate chemical clouds and calculates the concentration at a given time and location through superimposition.

ALOHA uses algebraic expressions for σ_y and σ_z that are a function of x and based on established σ_y and σ_z curves (based on data from field experiments). Recall that each σ_y or σ_z curve (and associated algebraic expression) reflects a specific atmospheric stability class and ground roughness condition (typically identified as either rural or urban[47]). Briggs developed the algebraic expressions that are incorporated into ALOHA. Briggs used a set of σ_y curves that reflect a 3-minute averaging time based on Prairie grass data.[48] ALOHA does not adjust σ_y for plume meander due to a different averaging time for the release. Following convention, σ_x is set equal to σ_y. Two sets of σ_z curves are used by ALOHA for rural and urban environments, respectively. The rural σ_z values reflect an averaging time of 10 to 15 minutes, and the urban σ_z values reflect a 1-hour averaging time (Reynolds, 1992).

DENSE GAS MODEL

A dense-gas cloud that is released to the atmosphere resists the influences of the hydraulic pressure field associated with the atmospheric wind and deflects the atmospheric wind around the cloud. Mixing occurs at the edges of the cloud. Unlike the Gaussian models used by the ALOHA code for neutrally buoyant transport and dispersion, the dense-gas set of equations used by ALOHA is too complicated to be presented and discussed in a condensed manner.[49] As a result, the approach taken in this report is to briefly highlight important phenomena associated with dense-gas transport and dispersion and summarize the historical background of the algorithms (Reynolds, 1992).

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[46] One minute is the minimum duration for an averaging period, so the number of averaging periods is less than five when the total release duration is less than five minutes.

[47] ALOHA uses the phrase "open country" in place of "rural" and "urban and forest" in place of "urban".

[48] Following a recommendation by the ALOHA Review Committee, the σ_y curves that were developed by Briggs for the urban environment were not used. Instead, the σ_y curves that were developed for rural environments (i.e., Prairie Grass data) are conservatively used for both rural and urban applications (Reynolds, 1992).

[49] The draft technical memorandum documents the 14 equations that ALOHA solves simultaneously to arrive at a solution for downwind concentration (Reynolds, 1992).

Initially, the cloud hugs the ground under the influence of its high density and spreads laterally similar to that of a liquid spill. The density distribution in the vertical direction of the slumping cloud is stably stratified, which inhibits turbulence and entrainment of air at the top of the cloud.[50] Dense-gas cloud dispersion is thus characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release. As the cloud travels downwind, enough air is entrained into the cloud that cloud density approaches that of the ambient air. The atmospheric transport and dispersion of the cloud then takes on the characteristics of that of a neutrally buoyant cloud. For small releases, this may take place as close as a few meters from the source (NOAA, 1999a).

The dense-gas dispersion model used by ALOHA is a simplified version of the DEGADIS dense-gas dispersion model (Havens, 1985; Spicer 1989). DEGADIS itself is an adaptation of the HEGADIS model that was developed by Shell Research (Colenbrander, 1980; Colenbrander, 1983). The ALOHA-DEGADIS algorithm incorporates simplifications that lessen input data needs and speed up computations (Reynolds, 1992). The ALOHA-DEGADIS model uses dispersion coefficients that are based on a five-minute averaging time. Benchmark tests show that the ALOHA-DEGADIS algorithm produces slightly conservative results (on the order of 10% higher peak concentrations) in comparison with DEGADIS results (Reynolds, 1992).

[50] If the temperature of the ground or air is higher than cloud, positive heat flow results, which reduces the cloud stability.

APPENDIX B: TORNADO DILUTION FACTOR

Atmospheric transport and dispersion of chemical material from the facility into the environment during a tornado can be modeled with a design basis accident dilution factor (Ψ/Q) designated for a specific class tornado and applied for the distance from the facility to the receptor. The Ψ/Q parameter (units of s/m^3) represents the time-integrated ground-level centerline air concentration normalized by the mass released and is analogous to the χ/Q value that is calculated from the Gaussian plume equation for neutrally buoyant releases as discussed in Appendix A. The Fujita scale is commonly used to categorize tornadoes. For most safety analysis applications, the tornado is assumed to be either Fujita - 2 (F2) or F3. Figure B-1 shows Ψ/Q values (s/m^3) as a function of downwind distance (km) for different mean translational speeds of the F2 tornado (Weber and Hunter, 1996). The consequence analysis should pick a maximum Ψ/Q for the assumed translational speed. For example, the translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers. The product of the maximum Ψ/Q value with the release rate of the chemical to the atmosphere yields the ground-level air concentration at the location of interest.

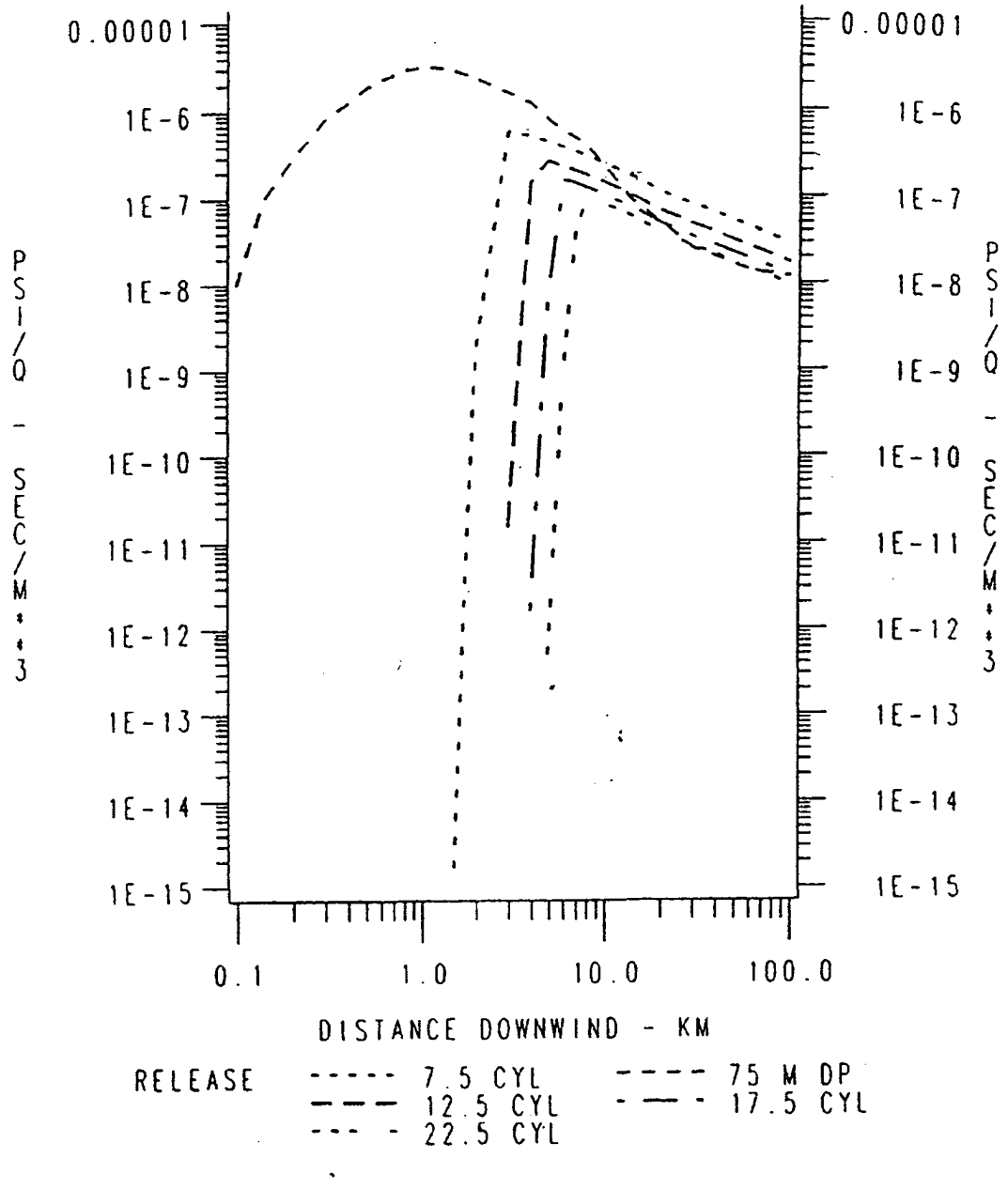

Figure B-1. The maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km) for different mean translational speeds from 7.5m/s to 22.5 m/s. The downdraft speed is 10 m/s and the height of the cylindrical mesocyclone is 3500 m (from Weber and Hunter, 1996).

APPENDIX C: DEVELOPMENTAL HISTORY OF ALOHA

From http://www.epa.gov/ceppo/cameo/request.htm

ALOHA 5.3 (March 2004)

- Can model up to three Levels of Concern (LOCs) for a single release
- Updated chemical library now includes TEELs, ERPGs, and AEGL LOCs
- Can now model evaporating puddles of five different chemical solutions

From http://response.restoration.noaa.gov/cameo/alohafaq/history.html

NOAA OR&R Home / Chemical Aids / CAMEO Toolkit / ALOHA History

ALOHA: An Evolutionary History

Over the years, ALOHA has changed and evolved. Here's a list of the most significant modifications to the program, from most to least recent:

ALOHA 5.2.3 (Summer 1999)

- ChemManager has been eliminated; changes to the chemical library now can be made from within ALOHA.
- Direct Source allows you to more easily model venting of an indoor puddle (by allowing you to enter release rate of an evaporating vapor at ambient pressure in volume units).
- ALOHA save files are now cross platform (files saved on a Macintosh can be used in Windows, and vice versa).
- A Fat Binary version was created for Macintosh users; there is no longer a math coprocessor version.
- The chemical library has been expanded, and a few chemicals have been removed.
- ALOHA now predicts the magnitude of the initial drop in release rate from ruptured pipes connected to large reservoirs.
- Bugs found in earlier versions were fixed.

- DIPPR[51] physical property values have been hidden from view, by request from DIPPR developers.

ALOHA 5.2.2 (Fall 1997)

- A problem in ALOHA 5.2.1 that prevented ALOHA from receiving SAM station data was corrected.

ALOHA 5.2.1 (Winter 1996)

- An erroneous value used in ALOHA 5.2 for the surface tension of ammonia was corrected. (The error caused overestimation of the rate of release of ammonia from a pressurized tank.)
- ALOHA was modified to correctly access weather data from a portable meteorological station when the data are "noisy" (noise in radio-transmitted data typically results from static caused by other electronic signals).
- The algorithm for predicting two-phase flow from a tank was refined.
- Tank and Puddle dialog boxes were modified to allow diked area to be specified as area or diameter.
- Additional LOC units options were added.
- ALOHA for Windows was modified so that it could open save files created in ALOHA 5.1 for Window.
- ALOHA for Windows was corrected to automatically load a chemical when you opened a record for a synonym for that chemical's name in CAMEO and then navigated to ALOHA.

ALOHA 5.2 (Fall 1995)

- ALOHA's heavy gas module was revised so that the heavy gas footprint is always ALOHA's best guess, rather than an overestimate. Previous versions overestimated heavy gas footprints for pressurized and/or short-duration releases.

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[51] The chemical database in ALOHA was compiled by Design Institute for Physical Properties Data and is known as the DIPPR database (NOAA, 1999a).

- The Direct Source module was modified to allow you to choose the duration of a continuous release, if it lasts for more than 1 minute and less than 1 hour.
- ALOHA was modified to automatically pick a stability class, once you have entered values for wind speed, cloud cover, and time of day; you no longer need to choose the class.
- ALOHA was modified to require the wind speed measurement height, and to adjust its computations accordingly. Previous versions expected wind speed to have been measured at a height of about 3 meters (about 10 feet).
- A horizontal line representing your Level of Concern (LOC) was added to the Concentration graph.
- BitPlot was replaced by MARPLOT for Windows.
- ALOHA's online helps, alerts and dialog boxes, and manual were extensively revised.
- New physical property information replaced older information in ALOHA's chemical library. A few chemicals were removed from the library, and new chemicals were added.
- Some of ALOHA's computations were refined as a result of testing. In particular, the equations used to predict puddle evaporation, two-phase flow, and heavy gas dispersion were modified.
- Bugs found in ALOHA 5.1 were fixed.

ALOHA 5.1 (Fall 1992)

- The first Windows version of ALOHA was released.
- Complex mapping functions were moved out of ALOHA into the new mapping program, MARPLOT.
- Footprints drawn on maps were modified to appear transparent rather than opaque.
- Carcinogen warnings were added to the chemical library.
- ALOHA's values for TLV-TWAs and IDLHs were updated to the latest published values.
- AlohaSpy was included, allowing you to archive ALOHA results.
- ALOHA's online helps, alert messages, and manual were revised and updated.

- ALOHA's equation describing subsonic flow of pure gas from a ruptured tank was revised.
- A problem with a few incorrect IDLH and/or TLV values in the chemical library was corrected.
- Internal checks were added, so that a physical property is estimated via a DIPPR equation only if temperature lies within the acceptable range (if temperature is above the range, the property value given for the maximum temperature is used, and if below the range, the value for the minimum temperature is used). Previously, checks were made only for negative values of a chemical property.
- The Heavy Gas module was modified to better interpolate between points where concentration is estimated.
- ALOHA was modified to recompute the footprint whenever building type or the dose exponent is changed.
- In the Display menu, the Concentration and Dose menu options were separated from each other.
- The "Conc & Dose" dialog box was modified to allow you to specify a location in either wind-relative or absolute coordinates.
- Internal memory management was improved. In particular, index files were added to speed access to ChemLib and CityLib.
- ALOHA's checks for inappropriate combinations of wind speed, cloud cover, and stability class were refined.

ALOHA 5.05 (Fall 1991)

- An ALOHA bug was repaired, allowing you to add cities in Arizona, Idaho, New Hampshire, New Mexico, Tennessee, Guam, and Wake Island to the location library.
- ALOHA was corrected to allow it to receive data transmitted from Weatherpak portable meteorological stations.
- ALOHA was modified to better load and handle large map files.
- ALOHA was corrected to accurately predict the rate of outflow through a large hole in a tank bottom.

ALOHA 5.0 (Fall 1990)

- ALOHA was rewritten in C.
- Time-dependent Gaussian and heavy gas dispersion algorithms were added.
- Source strength algorithms were added to predict releases from leaking tanks and ruptured gas pipelines.
- ALOHA was upgraded to predict infiltration of pollutant gases into buildings.

ALOHA 4.x and Earlier Versions

ALOHA was first written in Basic for the Apple II+ in the early 1980s as a passive gas plume model for in-house use by NOAA during emergency responses. It was rewritten in FORTRAN for the Apple Macintosh in the mid-1980s. A chemical property library, meteorological station serial port interface, and base-mapping were added at that time, and an energy-balance pool evaporation algorithm was added in the late 1980s.

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Revised: May 10, 2001
Office of Response and Restoration, National Ocean Service, National Oceanic and Atmospheric Administration

SEPARATION

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EPIcode Computer Code Application Guidance for Documented Safety Analysis

Final Report

U.S. Department of Energy
Office of Environment, Safety and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

June 2004

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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the EPIcode computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the EPIcode documentation provided by the code developer. EPIcode is one of six computer codes designated by the DOE Office of Environmental, Safety and Health as a toolbox code for safety analysis.

Suggestions for corrections or improvements to this document should be addressed to –

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EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications. The Emergency Prediction Information Code (EPIcode) is designated as one of the toolbox codes (EPIcode® is a registered trademark of Homann Associates, Inc.).

EPIcode may require completion of quality assurance improvement measures before meeting current SQA standards. In the interim period before these changes are completed, EPIcode is still considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available user's manual information.

The EPIcode guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

Use of the information contained here, although not ensuring correct use of EPIcode in each analytical context will minimize potential user errors and further standardize the use of EPIcode in appropriate regimes of applicability.

1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and in the variability of guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its Recommendation to DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the Board's concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include:

(i) identification of a suite of accident analysis software that is widely used in the DOE Complex, and

(ii) issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regime in accident analysis, default inputs, and special conditions for use.

Last year, safety analysis software for the DOE "toolbox" status was designated by the DOE Office of Environment, Safety and Health (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications*, (http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf), and includes Version 6.0 of the Emergency Prediction Information Code (EPIcode® is a registered trademark of Homann Associates, Inc.). Subsequently, Version 7.0 of EPIcode was released in September of 2003.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in the body of this report. This code-specific document will be maintained and updated until a minimum qualification software package is completed.

The contents of this report are applicable in the interim period until measures are completed to bring EPIcode into compliance with defined SQA standards. The primary objective of the guidance report is to provide information on the use of EPIcode for supporting DOE safety basis accident analysis. Specifically, the report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Overcoming known vulnerabilities and avoiding code errors
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications
- Default input value recommendations for site-independent parameters, and
- Citations of currently available SQA documentation.

Thus, this report is intended to complement existing EPIcode user's documentation. The latter tends to be much broader in coverage of the full range of capabilities of EPIcode and the spectrum of inputs that might be needed depending upon the application, but lack cohesive and targeted guidance for particular applications such as DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The EPIcode guidance document is written using the following format. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830 (CFR, 2001). More information follows on the scope and purpose of this document. The next major section is a summary description of EPIcode. A third section discusses applicable regimes for using EPIcode in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, succeeds this section. Following this discussion are sections on special conditions for use of the software and software limitations. A sample case is then provided, followed by acronyms and definitions, references, and appendices.

1.1 Background: Overview Of Toolbox Software In Context Of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software will in time be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as "toolbox" codes. Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

The EPIcode guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

1.3 Purpose

The EPIcode, while part of the toolbox collection of software, may still require SQA upgrades prior to meeting current established standards for software. However, until these EPIcode upgrades are completed so that EPIcode meets current established standards for software, EPIcode can be applied safely by following the guidance contained in this report is followed. Once SQA upgrades are finalized with EPIcode, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of EPIcode in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

Even though EPIcode was developed as a tool for emergency response and emergency preparedness/planning, it is also widely used throughout the DOE complex to support 10 CFR 830 safety analysis. Note that this guidance document does not specifically address application issues related to emergency response or emergency preparedness/planning.

It is recognized that other computer codes besides EPIcode exist that perform similar source term and downwind concentration calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for many accident analysis applications that involve chemical spills. The relative merits of using a different computer

program or using a hand calculation for a given application is a judgment that must be made by the analyst on a case-by-case basis.

The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program. As part of this program, the Chemical Dispersion and Consequence Assessment (CDCA) Working Group (WG) was established to address issues and evaluate methodologies in the CDCA domain. Other WGs were also established for other domains of safety analysis (i.e., fire analysis, explosion analysis, spill source term analysis, in-facility transport analysis, and radiological dispersion and consequence assessment). The CDCA WG (also referred to as WG 6) issued a report that identifies and evaluates methodologies and computer codes to support CDCA applications (Lazaro, 1997). Also of interest is the WG 3 report, which performed a similar function for source term analysis of spills (Brereton, 1997). In addition to code recommendations, both the Spills WG 3 report and the CDCA WG 6 report also provide a broad set of recommended "best practices" for modeling chemical releases to the atmosphere for safety analysis applications.

This report complements the WG 3 and WG 6 work to provide guidance and recommendations that are targeted to the use of the EPIcode to calculate source terms and downwind concentrations for safety analysis applications.[1]

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[1] The spills and CDCA working group reports did not specifically evaluate EPIcode as it limited its scope to public domain codes and thus did not consider proprietary codes such as EPIcode (Brereton, 1997; Lazaro, 1997). Since the EPIcode uses similar types of input data as other codes evaluated by the working groups to calculate chemical source term and downwind concentrations, much of the input guidance in the WG 3 and WG 6 reports can be applied to EPIcode as well.

2.0 SUMMARY DESCRIPTION OF EPICODE

This section provides a summary form description of the EPIcode. A brief overview is given with additional information to follow in other sections and appendices of the report to provide more in-depth coverage of topics such as the principles of source term development for analysis of accidents that involve chemical inventories, the interface with dispersion conditions in the atmosphere, and the overall assessment of toxicological exposure to receptors.

2.1 EPIcode Development

The version of EPIcode that is addressed by this report is Version 7.0 (released in September 2003). EPIcode was developed by Homann Associates, Inc., which maintains and upgrades the code. The code is commercially available from Homann Associates, Inc. The technical contact for EPIcode is the code author, Steven Homann (www.epicode.com or epicode@aol.com).

A history of its development is shown below (Mazzola, 1995; EPIcode, 2003):

- Version 3.0 (1988): First release beta test complete.
- Version 3.5 (1989): Incorporation of user input sampling time.
- Version 4.0 (1990): Incorporation of liquid spill model.
- Version 5.0 (1993): Incorporation of high-resolution graphics
- Version 6.0 (1996): Incorporation of fire and explosion models
- Version 7.0 (2003): Revised evaporation model[2] and fuel fire model

EPIcode Version 7.0 is a full 32-bit Microsoft™ Windows software package that will run on an IBM PC or compatible. Operating systems supported are Windows 95/98/00/NT and XP.

2.2 EPIcode Summary Description

EPIcode performs calculations for chemical source terms and resulting downwind concentrations. Source term calculations determine the rate at which the chemical material is released to the atmosphere, release height, release duration, and the form and properties of the chemical upon release. The term cloud is used in this document to refer to the volume that encompasses the chemical emission. In general, the released chemical may be a gas, a vapor, or

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[2] EPIcode has revised the spill model per EPA document "Risk Management Program Guidance for Offsite Consequence Analysis," United States Environmental Protection Agency, EPA 550-B-99-009, April 1999. Appendix D – Technical Background, pg. D-2 (EPA, 1999). The mass transfer coefficient of water is now assumed to be 0.67; the value of the factor that includes conversion factors, mass coefficient for water, and the molecular weight of water to the one-third power, originally 0.106, is now 0.284. The net result is an evaporation rate that is 2.68 times greater than previous versions of EPIcode.

an aerosol. The aerosol release may consist of either solid (e.g., fume, dust) or liquid (e.g., fog, mist, spray) particles that are suspended in a gas or vapor medium. Liquid particles are also referred to as droplets.

The analyst specifies the chemical and then either specifies the chemical source term rate or provides EPIcode with the necessary information and data to calculate a steady evaporation rate when the scenario involves a spill of a chemical liquid. Releases may be elevated either through discharge from a stack or as a result of plume rise from buoyancy or momentum effects.

Evolution of the mean concentration field of the chemical cloud is calculated through algorithms that model turbulent flow phenomena of the atmosphere. The prevailing wind flows and associated atmospheric turbulence serve to transport, disperse[3], and dilute the chemical cloud that initially forms at the source. For an instantaneous release or release of short duration, the chemical cloud will travel downwind as a puff. In contrast, a plume will form for a sustained or continuous release.

The wind velocity is a vector term defined by a direction and magnitude (i.e., wind speed). The wind direction and wind speed determine where the puff or plume will go and how long it will take to reach a given downwind location. For sustained or continuous releases, the wind speed has the additional effect of stretching out the plume and establishing the initial dilution of the plume (i.e., determines the relative proportion of ambient air that initially mixes with the chemical source emission). Atmospheric turbulence causes the puff or plume to increasingly mix with ambient air and grow (disperse) in the lateral and vertical direction as it travels downwind. Longitudinal expansion also occurs for a puff. These dispersion effects further enhance the dilution of the puff or plume. The two sources of atmospheric turbulence are mechanical turbulence and buoyant turbulence. Mechanical turbulence is generated from shear forces that result when adjacent parcels of air move at different velocities (i.e., either at different speeds or directions)[4]. Fixed objects on the ground such as trees or buildings increase the ground roughness and enhance mechanical turbulence in proportion to their size. Buoyant turbulence arises from vertical convection and is greatly enhanced by the formation of thermal updrafts that are generated from solar heating of the ground.

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[3] The term dispersion is sometimes used in the literature to describe the combined effects of advection (transport by the bulk motion of the wind flow) and turbulent diffusion (spreading) and other times, particularly in meteorological publications, to describe only the turbulent diffusion component. The latter, narrower sense is used in this document.

[4] Atmospheric flows experience a change in speed with height due to the friction of the earth's surface in slowing down the wind adjacent to it.

EPIcode considers the chemical cloud emission to be neutrally buoyant[5] and applies standard Gaussian puff and plume models as appropriate. A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow. Appendix A contains additional discussion on the role of atmospheric turbulence, wind speed, and other parameters on downwind puff or plume concentrations, especially as these parameters relate to the Gaussian transport and dispersion models.

In addition to the source term and downwind concentration calculations, EPIcode supports the use of concentration limits for the purpose of consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). When available, data for Immediately Dangerous to Life or Health (IDLH), Emergency Response Planning Guidelines (ERPGs), Temporary Emergency Exposure Limits (TEELs), and Acute Exposure Guideline Limits (AEGLs) have been incorporated into the chemical library of EPIcode as discussed in Section 4.1.

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[5] In the strictest sense, neutrally buoyant conditions exist when the density difference between the released chemical cloud and ambient air is small. A positively buoyant cloud is produced when the cloud density is significantly less than that of the ambient air. The positive buoyancy induces puff or plume rise that results in an effective elevated release that EPIcode can calculate with the necessary user-supplied inputs as discussed in Section 4.3.4. The Gaussian puff and plume models are used for both neutrally buoyant and positively buoyant releases.

3.0 APPLICABLE REGIMES

The objective of this section is to present a discussion of EPIcode applicability from two perspectives: (1) in terms of its overall function as a key step in accident analysis; and (2) noting the phenomenological regimes in which it provides an approximate model of dispersion in the environment and the resulting toxicological exposure to downwind individuals (receptors).

3.1 Overall Application in Safety Analysis

The EPIcode is in the toolbox under the area of applicability of chemical release and dispersion and consequence assessment. A code of this type of is used primarily to calculate the release rate to the atmosphere of a chemical involved in an accident scenario and the resulting instantaneous or time-averaged concentration of a chemical downwind from the accident. Because the DOE does not have an evaluation guideline for chemicals, the chemical concentration calculated is not used to distinguish safety-class designation for systems, structures, and components. A typical use of chemical consequence results is to confirm the selection of safety significant systems, structures, and components for worker protection.

Occasionally, chemical concentrations are used to help set limits on chemical inventory, and this may present more of a safety implication. When these code calculations are used to help set inventory limits, they have a direct effect on values used in technical safety requirements, and the quality of the calculation may be very important. Again, it is important to note that a hand calculation can often be used to verify this value.

In this context of setting limits on chemical inventory, analysts have generally applied the American Industrial Hygiene Association (AIHA) ERPGs[6] and TEELs[7] for the purpose of

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[6] The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The ERPGs are estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

> ***ERPG-1**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*
>
> ***ERPG-2**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*
>
> ***ERPG-3**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

assessing human health effects for both facility workers and the general public (Craig, 2001). Recently, another alternative has become available to analysts. The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) has been developing acute exposure guideline levels (AEGLs) to assist federal and state agencies and private sector organizations with their need for short-term hazardous chemical exposure information in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h).[8]

Since the DOE has not provided definitive evaluation guidelines for chemical exposures for use in DSAs, the specific use of ERPGs, TEELs, and AEGLs in accident analysis remains largely an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001). In some cases, surrogate values for inventory limits, such as Environmental Protection Agency (EPA) or Occupational Safety and Health Administration (OSHA) limits can also be used.

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[7] The temporary emergency exposure limits (TEELs) are another set of chemical-specific concentrations that correspond to varying levels of health effects (Craig, 2001). TEELs have been developed since ERPGs are available only for a limited number of chemicals. The TEELs consist of (a) ERPG values for all chemicals for which ERPGs have been published and surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values), and (b) Permissible Exposure Limit - TWA (PEL-TWA) values for all chemicals for which PEL-TWA values have been published and surrogate PEL-TWA values for additional chemicals (i.e., the TEEL-0 values) (Craig, 2001). PEL-TWA values are developed by the Occupational Safety & Health Administration (OSHA) for use in limiting worker exposures to airborne chemicals (CFR, 1999). Most people are not expected to experience any adverse health effects to accident exposures at the TEEL-0 level (Craig, 2001).

[8] The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) is developing AEGLs in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h) and three severity levels as defined below:

AEGL-1: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

3.2 Phenomenological Regimes of Applicability

The atmospheric transport and dispersion algorithms of EPIcode are based on the Gaussian models for puffs and plumes. These models are best suited for specific types of conditions. The chief phenomenological regimes for applying EPIcode include:

- Temporal regime – These models are best suited for "short" duration plumes, ranging from approximately several minutes to several hours.
- Spatial regime - The class of code also does not model dispersion close to the source (less than 100 meters from the source), especially where the influence of structures or other obstacles is still significant. Dispersion influenced by several, collocated facilities, within several hundred meters of each other should be modeled with care. Similarly, EPIcode should be applied with caution at distances greater than ten to fifteen miles, especially if meteorological conditions are likely to be different from those at the source of the release, or are likely to change in time during the release or during transport. Long-range projections of toxicological exposures are better calculated with mesoscale, regional models that are able to account for multiple weather observations.
- Terrain variability – Gaussian models are inherently flat-earth models, and perform best over regions of transport where there is minimal variation in terrain.
- Extreme weather – Gaussian models do not apply to extreme weather conditions such as tornadoes.
- Atmospheric transport and dispersion basis – The Gaussian models for atmospheric transport and dispersion, as used in EPIcode, were developed for and are directly applicable to neutrally buoyant releases in which the initial chemical cloud density is approximately equal to that of the ambient air. A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

  If the density of the initial chemical cloud is greater than that of the ambient air, however, then the possibility exists for dense-gas type of atmospheric transport and dispersion. As atmospheric air mixes with the cloud, dilution occurs that causes dense gas transport effects to essentially become negligible as the density of the plume mixture approaches that of the ambient air. All dense gas releases, therefore, eventually transition to transport and dispersion that is characteristic of a neutrally buoyant plume. So, the Gaussian models are frequently used when the receptors of interest are far from the source, even when the released cloud is likely to exhibit dense-gas behavior near the source.

  With dense-gas type of releases, the released cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind and alters the atmospheric wind field in its vicinity. Dense-gas behavior can potentially occur for gases with densities greater than air or with a chemical cloud with sufficient aerosol content such that the bulk cloud density is

greater than that of the ambient air. Dense-gas behavior is more likely to occur with higher release rates and lower wind speeds.

The basis for identifying the potential for dense-gas effects is the Richardson (Ri) number. The Ri number represents a relative measure of the potential energy of the cloud with respect to the mechanical turbulent energy of the atmosphere. The source Ri (Ri_o) number, above which dense gas transport effects are assumed important, is typically considered about 50 (Hanna, 1996).

- $Ri_o \leq 50$ For neutrally buoyant atmospheric transport and dispersion
- $Ri_o > 50$ For dense-gas atmospheric transport and dispersion

It should be noted that an absolute threshold value does not actually exist. Dense-gas effects may begin to appear for Ri_o values as low as one and become more pronounced as Ri_o is increased.

For an instantaneous release, the Ri_o is defined as follows (Hanna, 1996):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_i}{\rho_a \times D_o^2 \times u_*^2} \qquad \text{(Equation 3-1)}$$

Where,
- $\rho_a \equiv$ Ambient air density
- $\rho_o \equiv$ Released chemical density at source
- $Q_i \equiv$ Instantaneous volumetric release
- $D_o \equiv$ Scale dimension of the source
- $u_* \equiv$ Friction velocity

For a continuous release, the Ri_o is defined as follows (Hanna, 1996):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_c}{\rho_a \times D_o \times u_*^3} \qquad \text{(Equation 3-2)}$$

Where,
- $Q_c \equiv$ Continuous volumetric release rate

The friction velocity is equal to about 5% to 10% of the mean wind speed at the height of 10 m (Hanna, 1996). For a ground level release, the length scale parameter D_o represents the initial width or diameter of the cloud or plume before mixing with and transport by ambient air. For a release out of a stack, D_o represents the diameter of the stack (neglecting any boundary layer effects that would reduce the effective diameter of the jet or plume leaving the stack). For releases from evaporative or boiling pools, D_o is set equal to the pool diameter.

Note that alternative definitions of Ri_o and corresponding dense-gas dispersion criteria are found in published literature and used in atmospheric transport and dispersion codes.[9]

[9] For example, the Areal Locations of Hazardous Atmospheres (ALOHA) code substitutes "$u_{10} \times u_*^2$" for "u_*^3" in Equation 3-2, where u_{10} is the mean wind speed at a height of ten meters, and uses a critical Ri_o value of one (Reynolds, 1992).

4.0 INPUTS AND RECOMMENDATIONS

Input data on chemical properties, source configuration, and meteorological conditions in general factor into EPIcode calculations of downwind concentrations of released chemicals as a function of downwind distance. For a liquid spill of chemicals with a known vapor pressure, EPIcode algorithms calculate the evaporative release rate of the chemical into the atmosphere. For other release types, the user specifies the airborne release rate or equivalently the combination of the quantity released airborne and the release duration.

This section discusses and recommends input parameters needed to execute EPIcode. While emergency management applications can be supported with EPIcode, the emphasis here shall be on the type of inputs for supporting accident analysis in a DSA.

4.1 EPIcode Overview

The basic output that is produced by EPIcode is a table or graphical representation of downwind concentrations of released chemicals as a function of downwind distances. Example output including the concentration isopleth, tabular data, and X-Y plot, is shown in Figures 4.1 through 4.3, respectively, for a chlorine release.

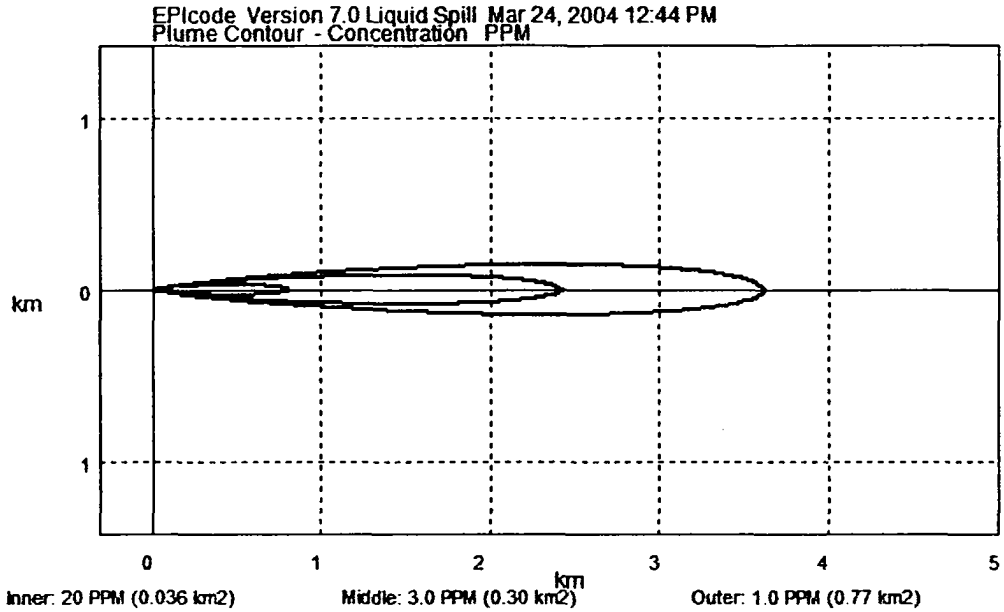

Figure 4-1. EPIcode Graphical Output – Contour Plot.

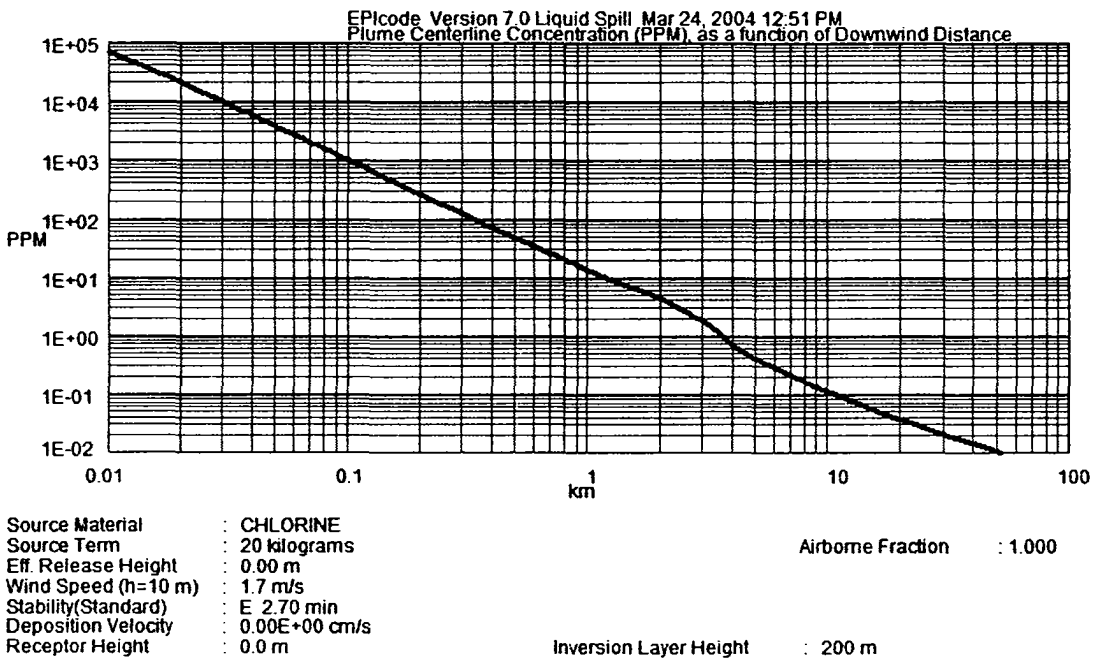

Figure 4-2. EPIcode Graphical Output – X-Y Plot.

```
EPIcode  Version 7.0 Liquid Spill
Mar 24, 2004 12:52 PM

Source Material            : CHLORINE
CAS Number                 : 7782-50-5
Source Term                : 20 kilograms
Spill Area                 : 1.36 m2
Spill Temperature          :25.0 deg C
Spill Vapor Pressure       : 5.74E+03 torr
Airborne Fraction          : 1.000
Evaporation Rate           : 124 gram/sec
Total Evaporation Time     : 2.7 minute
Physical Height of Spill   : 0 m
Wind Speed (h=10 m)        : 1.7 m/s
Distance Coordinates       : All distances are on the Plume Centerline
Stability Class (Standard) : E
Deposition Velocity        : 0.00E+00 cm/s
Receptor Height            : 0.0 m
Inversion Layer Height     : 200 m
Sample Time                :  2.70 min
Maximum Concentration      :  66,000   PPM
Max Concentration Distance : 0.010 km
ERPG-1                     : 1.000 PPM
ERPG-2                     : 3.000 PPM
ERPG-3                     : 20.00 PPM
Exceeds ERPG-1 Out To      : 3.60 km
Exceeds ERPG-2 Out To      : 2.40 km
Exceeds ERPG-3 Out To      : 0.80 km
```

DISTANCE	MAXIMUM CONCENTRATION		ARRIVAL TIME
km	(mg/m3)	(PPM)	(hour:min)
0.030	28,000	9,600	<00:01
0.100	2,900	990	00:01
0.200	770	260	00:03
0.300	350	120	00:05
0.400	210	71	00:06
0.500	140	47	00:08
0.600	98	34	00:10
0.700	74	26	00:12
0.800	59	20	00:13
0.900	48	16	00:15
1.000	40	14	00:17
2.000	13	4.3	00:34
4.000	1.9	0.66	01:08
6.000	0.82	0.28	01:43
8.000	0.47	0.16	02:17
10.000	0.32	0.11	02:52
20.000	0.10	0.036	05:44
40.000	0.040	0.014	11:28
60.000	0.024	0.0084	17:13
80.000	0.017	0.0060	22:57

Figure 4-3. EPIcode Tabular Output.

The first step in using EPIcode for chemical consequence analysis is to select the chemical. EPIcode 7.0 contains a library of over 2,000 toxic substances along with the associated exposure levels accepted by various professional organizations and regulatory agencies. These include the AIHA ERPGs, TEELs, and AEGLs. Typical units are milligram per cubic meter (mg/m^3) or parts per million (ppm). The DOE has not provided definitive evaluation guidelines for chemical exposures, so the specific use of exposure limits in accident analysis remains an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001).

The EPIcode library also contains information on substances that are listed in the Threshold Limit Values (TLVs) for Chemical Substances and Physical Agents and Biological Exposure Indices published by the American Conference of Governmental Industrial Hygienists (ACGIH).[10] IDLH data are also included when available.

Substance information is retrieved from the library by selecting the substance name or common synonym, U.S. Department of Transportation (DOT) Number, or Chemical Abstract Service (CAS) Number. Chemical property data in the library include molecular weight, specific gravity, boiling point, melting point and vapor pressure.

The user may add new chemicals to a user-defined chemical library and supply associated property, identification, and exposure limit data. Data in the EPIcode-supplied chemical library, however, cannot be altered. This prevents unintended corruption by the user of the EPIcode library, but a disadvantage of this setup is that data cannot be updated. For example, the user cannot readily update ERPG data when the ERPG data for a chemical is revised, as occasionally happens. A way to circumvent this limitation is to add the particular chemical to the user chemical library with the same information as in the EPIcode-supplied library, but with the updated ERPG data.

4.2 Input Recommendations for Source Term Parameters

EPIcode models five types of releases to the atmosphere:

- Term Release

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[10] The time-weighted average TLV (TLV-TWA), the short-term exposure limit TLV (TLV-STEL), and ceiling TLV (TLV-C) are defined as follows.

> ***TLV-TWA**: The time-weighted average concentration for a normal 8-hour workday and 40-hour workweek, to which nearly all workers may be repeatedly exposed, day after day, without adverse effect.*
>
> ***TLV-STEL**: The concentration to which workers can be exposed continuously for a short period of time without suffering from 1) irritation, 2) chronic or irreversible tissue damage, or 3) narcosis of sufficient degree to increase the likelihood of accidental injury, impair self-rescue or materially reduce work efficiency, provided that the daily TW is not exceeded.*
>
> ***TLV-C**: The concentration that should not be exceeded during any part of the working exposure.*

  - Surface Line Source
  - Elevated Line Source
  - Surface Area Source
  - Elevated Area Source
  - Point Source
- Continuous Release
  - Surface Line Source
  - Elevated Line Source
  - Surface Area Source
  - Elevated Area Source
  - Point Source
- Liquid Spill Release
- Fire Release
- Explosive Release

With the first two release types, the source may be modeled as a point, a line, or an area. With the line and areas source models, the cloud at the source location has a finite dimension in either one or two directions. The EPIcode algorithms translate each source dimension into a virtual source that is upwind of the actual source. Thus, credit is taken for initial distribution of the cloud in the form of an initial effective dispersion that lowers predicted cloud centerline concentrations particularly at short distances from the source (in comparison to modeling the release with a point source at the actual source location). This effect becomes increasing less significant as the plume travels further away from the source. The liquid spill release, fire release, and explosive release all employ area source models.

A term release differs from a continuous release in that it is of finite duration. As the release duration increases, the results from the term-release model approach that from the continuous-release model for equivalent specifications of release rates and other input variables. At the other end of the spectrum for term releases (i.e., releases of very short duration) is the instantaneous release. When the user specifies an instantaneous term release, EPIcode uses the puff model. For other term releases (i.e., non-instantaneous), EPIcode automatically selects the puff or plume equation at each downwind location based on the relative dimension of the cloud width with respect to the cloud length. When the cloud length is less than the cloud width, the puff equation is considered to be a more accurate model of the dispersion. Continuous releases are always modeled as plumes.

The airborne release rate to the atmosphere is established in one of three ways for the various types of releases:

- Specify source term rate directly – applicable to continuous release type

- Specify source term quantity and release duration – applicable to term release type; for fire and explosive release types, the quantity is specified by the user and EPIcode determines the release duration
- Let EPIcode calculate an evaporative release rate – applicable to liquid spill type release (when vapor pressure for chemical is known).

For specification of the source term rate or source term quantity, EPIcode accepts the input on a mass or volume basis (usually with a choice of units) at the preference of the user.

4.2.1 Source Term Rate

The user specifies this input signifying the rate at which the chemical substance is made airborne for continuous releases. The basis for the input can be measurement, but for DSA applications will likely be an external calculation. The latter can be the result of either a manual calculation or the output from another code. Note that for the liquid spill release, EPIcode internally calculates the airborne release rate and the release duration corresponds to the total time for all the liquid to evaporate.

Recommendation: Calculated downwind concentrations are proportional to the release rate. So, the release rate should be conservatively estimated on the high side if there is some uncertainty or variability with its value. In some scenarios, variability results from an unsteady source term rate. The use of a time-weighted average (TWA) is typically used in these situations. For example a peak 15-minute TWA is recommended for some situations as discussed in Section 4.4.2 (Craig, 2001).[11] Note that the analyst should normally specify the sample time input that is discussed later in Section 4.4.2 in a manner that is consistent with or conservative with respect to the release duration.

4.2.2 Source Term Quantity and Release Duration

The user specifies this input combination for term releases and fire releases. For these releases, the combination of source term quantity and release duration is used to establish the airborne release rate to the atmosphere. Note that for explosive releases, the user inputs the quantity released and EPIcode internally calculates the release duration.

The release duration also is used by EPIcode to determine whether the released cloud is best modeled as a puff or a plume. Recall that continuous releases are modeled as plumes and that the results from the term-release model approach that for the continuous-release model as the release duration increases. The basis for this input combination of source term quantity and release duration can be measurement, but for DSA applications will likely be an external calculation.

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[11] The peak 15-minute TWA is the highest rolling average over any 15-minute segment of the release period.

A zero value input for time duration signifies an instantaneous release (EPIcode automatically sets the release duration to 1 second). With an instantaneous release, EPIcode uses the puff model.

Recommendation: For plume releases, the source term quantity divided by the release duration defines the release rate, the recommendations above in Section 4.2.1 apply. Calculated downwind concentrations are proportional to the release rate for plumes (i.e., the same downwind concentrations will be calculated for various combinations of source term quantity and release duration that result in the same release rate). So, the release rate (through the input combination of source term quantity and release duration) should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Generally, the possibility of puff dispersion behavior exists for release durations of 10 minutes or less. For puff releases, the calculated downwind concentrations are proportional to the total quantity released and not to the release rate. For puff releases, it is important that the source term quantity be conservatively estimated on the high side if there is some uncertainty or variability with its value and the release duration then set accordingly. Generally for DSA applications, a duration of one minute is specified if the duration is less than one minute (Craig, 2001).

In many situations it may be difficult for the user to know apriori, whether EPIcode will model the release as a puff or plume. If this uncertainty exists, it may be practical for parametric runs to be performed to guide specifying the source term quantity and duration in a manner that maintains reasonable conservatism.

Note that the analyst should normally specify the sample time input that is discussed later in Section 4.4.2 in a manner that is consistent with or conservative with respect to the release duration.

4.2.3 Release Height

This input can reflect a physical stack height or the effective plume rise, from source momentum or buoyancy, or the combination of the two. The basis for the effective plume rise can be measurement, but for DSA applications will likely be an external calculation. Alternatively, the user has the option of supplying additional inputs and choosing to have EPIcode calculate the effective plume rise. The input specifications for the EPIcode plume rise option are discussed in Section 4.3.5.

Recommendation: With elevated plumes either from a stack or as a result of plume rise mechanisms, the separation of the plume centerline from the ground lowers the plume concentration that is observed at ground level. Thus, the most conservative approach generally is to assume a ground-level release. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be

drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

NRC Regulatory Guides 1.111 and 1.145 define a true "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977; NRC, 1983). It is recommended that the analyst enter the stack height only when this criterion is met of 2.5 times the height of adjacent structures. Otherwise, the release should be treated as ground level, or alternatively, a reduced effective release height can be determined (Hanna, 1982).

The identification of adjacent structures must take into account the extent of influence that the building has on the flow field in its vicinity. The wind flow that is directly over the top of the building is entrained downward into the wake cavity. The extent of the wake cavity downwind, as measured from the lee face of the building, can range from 2.5 times as great as the building height (H_b) to approximately 10 H_b for buildings that have large width-to-height ratios (Hanna, 1982). The wake cavity is marked by increased turbulence levels that decay progressively as a function of distance from the building. For releases from stacks not meeting the criterion of 2.5 times the height of adjacent solid structures, the effects of downward-directed entrainment into the wake cavity serve to increase ground-level concentrations above what would be observed in the absence of the building. The term downwash is frequently used to collectively describe these effects. An accepted practice by the EPA is to assume that downwash effects can influence plumes that are released from stacks that are located in the range of 2 L upwind to 5 L downwind of building, where L is the lesser of the building height or projected width (EPA, 1995).

The release height should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

4.2.4 Source Dimensions

For source configurations other than the point source and explosive release, EPIcode prompts the user for one or more source dimensions as indicated below.

- Line Source – horizontal dimension
- Area Source – horizontal dimension and vertical dimension
- Liquid Spill Source – spill area
- Fire Source – release radius

These input specifications are used to calculate upwind virtual point sources. For the fire source, the single input of the release radius is used to establish virtual sources for both the horizontal and vertical directions. Thus, credit is taken for the effective initial dispersion of a realistic source that has finite dimensions in comparison with the often-used conservative assumption of a point-source release at the source location. Note that for the explosive release, the input of explosive strength (see Section 4.2.6) is used to model initial vertical and horizontal dispersion and thus establish the virtual sources.

Also note that if the release is from a stack and the user desires to calculate the plume rise from momentum or buoyancy effects, the user is prompted to input the stack radius. This input is discussed separately in Section 4.3.5.

Recommendation: A source dimension should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

4.2.5 Fire Heat Emission Rate

For fires scenarios, the user may specify the effect release height from buoyancy effects or choose to have EPIcode calculate buoyant plume rise based upon the heat emission rate. The heat emission rate, in turn, may be directly specified by the user or calculated by EPIcode from user-supplied inputs of volume of fuel, fuel heat of combustion and burn duration.

Recommendation: In plumes arising from fire-related source terms, the user should exercise caution with codes such as EPIcode that use the Briggs model (Briggs, 1975). The Briggs model for accounting for sensible energy in a plume is valid for "open-field" releases. That is, the Briggs model is not applicable to situations in which the plume transport and dispersion can be influenced by buildings (and other obstacles). The presence of a building wake can inhibit plume rise, keeping the plume closer to the ground resulting in higher ground-level concentrations.

The most conservative assumption is generally not to credit plume rise from the sensible energy of fires and therefore to assume a non-buoyant release from ground level. In this situation, the release may be modeled as a term release with a surface-area or surface-line source or most conservatively with a point source. If the fire is well defined and sufficiently distance from buildings or similar obstructions such that the source term analysis can defend the amount of sensible energy, the temporal history, and the spatial distribution, then the fire release model may be used as part of the accident and consequence analysis. If the user chooses to input the heat emission rate, then it should be conservatively estimated on the low side if there is some uncertainty or variability with its value. Similarly, if the user alternatively inputs the combination of the volume of fuel, fuel heat of combustion and burn duration, then the volume of fuel and heat of combustion should be estimated conservatively on the low side and the burn duration on the high side in order to account for some uncertainties or variability with these specifications. Note that the burn duration is specified independently of the source term release duration, which is covered in Section 4.2.2.[12]

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[12] The source term release may not occur uniformly throughout the duration of the fire, with the possibility that the majority of the release occurs during a period that is a fraction of the total burn duration.

4.2.6 Explosion Strength

For explosion scenarios, the user is given the option of specifying the trinitrotoluene (TNT) equivalent of the explosion for the purpose of letting EPIcode approximate the initial effective plume rise and dispersion of the hazardous chemicals that are involved in the explosion.

Recommendation: Like the fire model, the explosion model was developed for "open-field" releases. The presence of buildings or other obstruction can inhibit plume rise with explosions (in a similar manner as with fires), keeping the plume closer to the ground resulting in higher ground-level concentrations. The most conservative assumption is not to credit plume rise from the explosion and therefore to assume a non-buoyant release from ground level. The burden is on the analyst to justify that the EPIcode explosion model is applicable for the scenario that is being analyzed and assign an appropriate TNT-equivalent value. If the analyst chooses to make use of the EPIcode explosion model and inputs the TNT-equivalent value to characterize the explosion strength, then it should be conservatively estimated on the low side to account for uncertainty or variability with its value.

4.2.7 Liquid Spill Release

For liquid spill scenarios, EPIcode prompts the analyst for inputs of total quantity of liquid that is spilled, surface area of pool that forms from the spill, the chemical vapor pressure and the liquid temperature. From these inputs, EPIcode calculates the evaporative release rate to the atmosphere and the duration of the release.

The evaporation rate is directly proportional to the vapor pressure and the surface area of the pool that forms from the spill. The depth determines the duration. For a pool that forms from an unconstrained spill,[13] one usually considers the total volume spilled and assumes spreading occurs to some minimum depth. The basic equations are given below that relate the puddle diameter (d), surface area (A), volume (V) and depth (Δh).

$$A = V/\Delta h \qquad \text{(Equation 4-1)}$$

$$d = (4/\pi \times A)^{0.5} \qquad \text{(Equation 4-2)}$$

Recommendation: The recommendation is given in multiple parts in order to account for the various component inputs that are needed to characterize the airborne release rate from the pool of a spilled chemical.

Total quantity spilled – A reasonably conservative estimate of the chemical inventory that is involved in the spill scenario should be specified. The specification of the quantity spilled

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[13] An unconstrained spill is analyzed when no barriers are present or have assumed to fail or when an unmitigated analysis is being performed in which no credit is being taken for the barriers that are present.

should be conservatively estimated on the high side if there is some uncertainty or variability with its value. Based on this input, EPIcode provides three recommended values for the surface area input that follows. These three surface-area recommended values are based on Equation 4-1 and pool depths of 1 cm, 1 mm, and 1 inch.

Surface area of the spill – For an unmitigated analysis, the surface area of the spill is to be consistent with the total quantity spilled and a spreading of the spill to some minimum depth. It is recommended that a minimum depth of one centimeter (10 mm) be conservatively specified for an unmitigated spill analysis (EPA, 1987; Brereton, 1997).[14] As discussed above, the analyst should consider the maximum inventory in determining the volume spilled to form the pool. That is, the specification of the volume spilled should be conservatively estimated on the high side if there is some uncertainty or variability with its value. This volume together with the one-centimeter depth should be used with Equation 4-1 to calculate the pool surface area.

For a mitigated analysis, the analyst may consider crediting the presence of a dike or similar structure to constrain the spill and specify the surface area accordingly. Topography can also play a similar role in confining the extent of liquid spreading.

Chemical vapor pressure and liquid temperature – The evaporation rate is directly proportional to the chemical vapor pressure, and the vapor pressure of the chemical constituent is a strong function of its temperature in the liquid state. The vapor pressure therefore should be conservatively estimated on the high side if there is some uncertainty or variability with its value. The specification of the liquid temperature should be consistent with the specification of the vapor pressure. In practice, the analyst will probably first consider the range of possible liquid temperatures, consistent with the storage/operating temperature or the environment temperature (see discussion in Section 4.3.5), and then specify the liquid temperature and its corresponding vapor pressure at that temperature.

4.3 Input Recommendations for Meteorological and Environmental Parameters

Once the source term is quantified, the next step is to characterize the meteorological and environmental conditions that will control the atmospheric transport and dispersion of the cloud of released material as it is carried by the wind away from the source. A comprehensive treatment of atmospheric dispersion is so complex that many approximations are needed to make it tractable. Since turbulence is random and chaotic, it cannot be parameterized and one must resort to empirical formulations. One early attempt to simplify the treatment of turbulence was to define atmospheric stability classes and associate a rate of lateral and vertical dispersion with each class as a function of downwind distance only. For continuous releases, the mean wind speed dilutes the chemical concentration but the longitudinal dispersion is negligible. As the

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[14] The 1-cm puddle depth is commonly used and suggested by EPA guidance (Brereton, 1997; EPA, 1987). Brereton (1997) notes that the 1-cm depth is somewhat arbitrary and recommends future development of an approach with more technical basis, such as one that would consider liquid physical properties (e.g., surface tension, viscosity) and ground surface properties (e.g., surface roughness).

plume moves downwind it gets progressively larger due to lateral and vertical dispersion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the longitudinal direction becomes more important.

Appendix A contains additional discussion on the role of atmospheric stability class, wind speed, and other parameters on downwind puff or plume concentrations, especially as these parameters relate to the Gaussian transport and dispersion models for neutrally buoyant releases. Input guidance on specifying these parameters for use in EPIcode is given below.

4.3.1 Terrain Factor (Dispersion Coefficient Set)

Different set of dispersion coefficient curves have been established for rural environments and urban environments to account for the additional mechanical turbulence that is generated in urban settings by increased ground roughness due to building structures being taller and spaced closer together. Also, the heat-retention capabilities of urban surfaces (e.g., concrete structures) can drive buoyant flows that increase dispersion.

Two sets of atmospheric dispersion coefficients are included in EPIcode that correspond to standard (rural) terrain or city (urban) terrain. The increased dispersion that is associated with city terrain generally leads to lower concentrations. In guidance for the Risk Management Program (RMP), EPA considers the term rural to refer to terrain that is generally flat with few buildings or other obstructions (e.g., hills, trees) (EPA, 1999). The EPA guidance recommends assuming urban conditions for a site area with many obstructions "even if it is in a remote location that would not usually be considered urban" (EPA, 1999).

Recommendation: It is generally conservative to choose the standard terrain dispersion coefficients. It is recommended, however, that the analyst uses judgment based on site observation and published guidance to take credit for surface roughness effects in increasing puff and plume dispersion where appropriate. Ideally, consultation with the laboratory or site meteorology organization responsible for recording and maintaining site meteorological data is available to the analyst to assist in specifying this input and defending its use.

4.3.2 Atmospheric Stability Class

In calculating puff or plume concentrations, both "unfavorable" and "typical" dispersion conditions are of special interest in accident analyses. For accident analysis consideration of the offsite receptor, unfavorable meteorology is ideally based on site data. In defining unfavorable meteorological conditions for chemical releases, it seems reasonable to follow the practices that are used for radiological consequence analysis. Unfavorable meteorology refers to the meteorology that coupled with the source term would lead to doses (or concentration exposures for chemicals) that are exceeded less than five percent of the time. The method should be conservative or consistent to the discussion in the NRC Regulatory Guide 1.145 (Position 3) (NRC, 1983) as summarized in Appendix A to DOE-STD-3009-94, CN2 (DOE, 2002a). The 95th percentile result of the distribution of doses (or concentration exposures for chemicals) to

the offsite receptor, accounting for variation in distance to the site boundary as a function of direction, is generally the consequence result of interest. The median or the 50th percentile result of the consequence distribution is usually the basis for typical meteorological conditions. The determination of the meteorological conditions that correspond to 50th and 95th percentile consequence results will require the simultaneous consideration of both atmospheric stability class and wind speed (the effect of ambient temperature on chemical vapor pressure may also be considered for scenarios that involve pool evaporation).

Meteorological variables such as wind speed and solar radiation affect both the evaporation rate and the amount of dilution of the puff or plume during atmospheric transport. Generally, these variables affect the evaporation rate and atmospheric dilution in opposite ways with regard to the effect produced on downwind concentrations. For example, higher wind speeds increase the evaporation rates, but also support greater dilution of the plume. Similarly, higher solar radiative influx and warmer temperatures also increase the evaporation rates, but typically support atmospheric conditions that are less stable and more dispersive. Meteorologists at Savannah River Site (SRS) studied these effects and concluded that the dominant influence of the meteorological variables generally occurs with atmospheric dispersion and dilution (Hunter, 1993). Higher downwind concentrations are associated with stable atmospheric conditions and low wind speeds (Hunter, 1993).

The size of the data set used in the meteorological assessments should be sufficiently large that it is representative of long-term meteorological trends at most sites. Meteorological data, qualified and meeting requirements of Regulatory Guide 1.23 (NRC 1972), available at most DOE sites should be applied that is representative of long-term trends. A five-year data set is desirable, but a one-year data set can be applied under the right circumstances.[15]

In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes for unfavorable dispersion conditions (EPA, 1999). As mentioned above, accident analysis calculations under typical meteorological conditions may sometimes be performed. Atmospheric stability class D is the most common stability class for many DOE sites. This is due to the large number of combinations that can result in stability class D. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally associated with stability class D. A wind speed of 4.5 m/s together with atmospheric stability D has been suggested to represent typical meteorological conditions (FEMA, 1989). This set of conditions is also consistent with a basis by chemical process industry for determining limits on chemical inventories, and is representative of most U.S. regions (CFR, 1992) and for radiological hazard categorization of DOE facilities (DOE, 1997).

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[15] In Regulatory Guide 1.194, this subject is discussed as follows: "The NRC staff considers five years of hourly observations to be representative of long-term trends at most sites. With sufficient justification of its representativeness, the minimum meteorological data set is one complete year (including all four seasons) of hourly observations." (NRC, 2003)

For elevated releases, the lofted plume must travel further downwind with stable atmospheric conditions before reaching the ground and exposing receptors to the hazardous contaminant. Therefore, neutral or even unstable stability conditions may produce the most unfavorable meteorological conditions for receptors close to the elevated release. In general, the atmospheric stability class associated with unfavorable meteorological conditions will be dependent upon the distance of the receptor from the source. At very close distances, the ground level concentration may be zero for stable conditions as the puff or plume simply passes overhead. Unstable atmospheric stability will result in the highest ground-level concentrations at close distances as high levels of turbulence will promote rapid dispersion of the puff or plume to the ground from its elevated release position. At receptor locations further downwind, neutral atmospheric buoyant conditions produce the highest ground-level concentrations with the Gaussian plume model. Even further downwind, the highest ground-level concentrations occur with stable atmospheric conditions as the puff or plume has traveled far enough downwind for the puff or plume to disperse enough so that the ground is exposed to higher-concentration regions of the puff or plume.

It should be noted that in the long run, site data is normally preferable over the default conditions for accident analysis. Meteorologists evaluated SRS data and found the specific meteorological conditions (i.e., atmospheric stability class and wind speed) that were associated with the 95th percentile results varied with release height and receptor distance (Hunter, 1993). For most facility distances to the offsite boundary, it was determined that E stability and the following wind speeds were associated with 95th percentile consequence results for neutrally buoyant plumes.[16]

- 1.7 m/s wind speed (release height 0 m – 10 m)
- 2.1 m/s wind speed (20-m release height), and
- 3.0 m/s wind speed (60-m release height).

For mitigated hazard analysis, DOE has not established guidance for evaluating the mitigative benefit of safety structures, systems, and components (SSCs). Both median statistical basis (i.e., 50th percentile) and 95th percentile bases have been applied to determine onsite receptor doses.

Recommendation: As discussed above, the preferred approach for specifying the atmospheric stability class and wind speed is statistical analysis of site-specific meteorological data. In absence of such data, the accident analysis may use generally accepted, default stability and wind speed combinations (e.g., F stability class and 1.5 m/s wind speed applied to a ground level release to represent unfavorable meteorological conditions). Guidance is complicated with elevated releases. With elevated releases of neutrally buoyant gases, it is recommended that a parametric study be performed among the various combinations of wind speed and atmospheric stability classes to determine unfavorable meteorological conditions for the receptor locations of interest. EPIcode has a useful feature that can aid in this process. When viewing the plume

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[16] The cited wind speeds reflect the value at the release height (at 10 m for the 0 m – 10 m release height range).

centerline concentrations graphically, the user has the option of requesting that EPIcode display results for each of the six stability classes simultaneously.

It should be noted that the specification of the deposition velocity and its effect on plume depletion also plays an important role in the consequence calculations and establishing unfavorable meteorological conditions. For example, if the deposition velocity is set to zero, the F stability class will always result in the maximum ground-level concentration for a ground level release. If the deposition velocity is set to 1.0 cm/s, however, the maximum ground level concentration at a given downwind location may be associated with another stability class, such as E stability class. The deposition velocity is discussed in Section 4.4.3.

4.3.3 Wind Speed

EPIcode accepts wind speeds in the range of 0.5 m/s through 50 m/s at a reference height of 2 m through 100 m. The height input parameter for the wind speed is discussed separately in the next section.

Recommendation: As discussed above, statistical analysis of site-specific, wind speed measurements is the preferred approach for specifying wind speed. The determination of the meteorological conditions that are associated with 50^{th} and 95^{th} percentile consequences will require the simultaneous consideration of both atmospheric stability class and wind speed (ambient temperature may also be considered for scenarios that involve pool evaporation).

In general, higher downwind concentrations (i.e., unfavorable meteorological conditions) are associated with lower wind speeds. In lieu of site-specific meteorological data, the following default wind speeds may be considered for each atmospheric stability class (Lazaro, 1997). It is recommended that a parametric study among the various combinations of wind speed and atmospheric stability classes be performed to gain useful insights about the role of wind speed and atmospheric stability class in determining unfavorable meteorological conditions.

	Atmospheric Stability Class					
	A	B	C	D	E	F
Default Wind Speed [m/s]	2.0	*	*	4.5	1.5	1.5

* Lazaro (1997) does not specify default wind speeds for B and C stability classes. The 2.0 m/s default wind speed value that is specified for A stability class would seem to be a reasonably conservative choice based on information presented in Appendix A.

4.3.4 Wind Speed Height

EPIcode accepts at a reference height from 2 m through 100 m. EPIcode algorithms, however, use the wind speed at the effective release height (2 m if the effective release height is 2 m or less). EPIcode accounts for the variation of wind speed with distance from the earth's surface as caused by friction using the basic power-law formula that is represented by Equation A-3 in

Appendix A. Therefore, EPIcode needs the height that is associated with the wind speed that is entered.

Recommendation: The input for this parameter must be consistent with the wind speed input (that was discussed above). If the value for wind speed that is input into EPIcode is based on site measurements at a known height, then that height should be input. Typically, the National Weather Service (NWS) measures and reports wind speeds at 10 meters. When using the generally accepted, default combination of F stability class and 1.5 m/s wind speed or the equivalent for analysis of ground-level releases of neutrally buoyant plumes, specifying a 10-meter measurement height is expected to yield a more conservative result than that obtained from specifying a 2-meter measurement height. With a 10-meter measurement height specification, EPIcode will calculate a wind speed at 2 meters that is less than 1.5 m/s for use in the Gaussian plume model, and the Gaussian plume model predicts downwind concentrations that are inversely proportional to wind speed as shown in Appendix A.

4.3.5 Stack Height / Effective Plume Rise

If the release is from a stack and additional information is available on the stack diameter, effluent temperature, and discharge velocity, EPIcode can calculate an effective release height that takes into account plume rise mechanisms. Plume rise can occur from either momentum effects or buoyancy effects (Briggs, 1969; Briggs, 1975). EPIcode calculates plume rise from each effect separately and chooses the larger of the two results.

Recommendation: With elevated plumes either from a stack or as a result of plume rise mechanisms, the separation of the plume centerline from the ground lowers the plume concentration that is observed at ground level. Thus, the most conservative approach generally is to assume a ground-level release. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

NRC Regulatory Guides 1.111 and 1.145 define a true "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977; NRC, 1983). It is recommended that the analyst model an elevated release only when this stack-height criterion is met of 2.5 times the height of adjacent structures. Otherwise, the release should be treated as ground level, or alternatively, a reduced effective release height can be determined (Hanna, 1982). Issues related to the identification of adjacent structures were discussed in Section 4.2.3 and should be followed. Also, the stack height should be conservatively estimated on the low side if there is some uncertainty or variability with its value, consistent with the recommendation given in Section 4.2.3.

Additional recommendations are given in multiple parts in order to account for the various component inputs that are needed to characterize the plume rise from buoyancy or momentum effects.

Stack exit velocity – The basis for the input can be measurement, but for DSA applications will likely be an external calculation. The latter can be the result of either a manual calculation or the output from another code. Plume rise from momentum effects increase with increasing stack exit velocity. The stack exit velocity should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

Effluent temperature – The basis for the input can be measurement or external calculation. Plume rise from buoyancy effects increase with increasing effluent temperature. The effluent temperature should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

Environment temperature – Statistical analysis of site-specific, meteorological measurements is the preferred approach for specifying meteorological conditions, including the ambient air temperature. Plume rise from buoyancy effects decrease with increasing ambient air temperature. The ambient air temperature should be conservatively estimated on the high side in order to address variability with its value. For air temperature, a reasonably bounding high temperature is recommended based on analysis of the site data. For example, Lazaro suggests the 95th percentile value of a five-year record of daily high temperatures for the warmest month of the year (Lazaro, 1997).

Stack diameter – Plume rise from both buoyancy effects and momentum effects increase with increasing stack diameter. The stack diameter should be conservatively estimated on the low side if there is some uncertainty with its value.

4.4 Input Recommendations for Additional Parameters

The parameters that were discussed above in Section 4.2 (source term parameters) and in Section 4.3 (meteorological and environment parameters) are treated by EPIcode as scenario-specific parameters in the sense that there are no default values for these parameters (in the earlier Version 6.0 of EPIcode, EPIcode would prompt the user to input data for most of the parameters covered in Sections 4.2 and 4.3 as needed for a scenario). The parameters that are discussed in this section have preset default values that may be overwritten by user input: inversion layer height (5000 meters)[17], sample time (10 minutes), deposition velocity (0 cm/s for gases and vapors and 0.3 cm/s for solid particulates), and receptor height (1.5 meters).

[17] A 5000-m inversion layer height effectively translates to the specification of no inversion layer.

4.4.1 Inversion Layer (or Mixing Layer) Height

The inversion layer is a region of air in which the temperature increases with increasing distance from the ground (i.e., inverted temperature gradient). The elevation where this layer begins is referred to as the inversion layer height or the mixing layer height (as the layer of air between the earth's surface and the inversion layer is generally referred to as the mixed or mixing layer). In atmospheric transport and dispersion modeling, the inversion layer is assumed to act as a barrier to rising thermals of air from below and thus limit the extent of vertical mixing. The inversion layer height varies throughout the day and throughout the seasons. During clear nights or early mornings when inversions are present, the inversion layer is relatively low, while during sunny days the inversion layer is much higher. The magnitude of these heights can be obtained from balloon soundings or from remote sensing techniques, such as acoustic or radar soundings. In the absence of such data, regional tables can be consulted.

The default value in EPIcode is 5000 m.

Recommendation: The analyst should base mixing layer height on seasonal averages and day/night time of day through application of archived site or laboratory meteorological data. If this is not available, the analyst use regional data as default input values, such as those of Holzworth (1972).[18] Since lower inversion heights can lead to higher downwind concentrations, it is appropriate for conservatism to specify an inversion height value that is reasonable, but skewed more towards the lower end of the observed or expected range.

4.4.2 Sample (or Averaging) Time

Even with a steady, source-term release rate, downwind instantaneous concentrations of the hazardous chemical will vary with time due to the turbulent nature of atmospheric conditions. Moreover, the time-average concentration at a given downwind location will depend on the time interval over which the concentrations are averaged. This time interval is referred to as the sample or averaging time. The horizontal and vertical dispersion coefficients that are used by EPIcode are based on field measurements of puff and plume releases.[19] The sample time over which measurements were taken to establish these horizontal and vertical dispersion coefficients determines the averaging time for the time-averaged concentrations that are predicted by EPIcode through the Gaussian dispersion equations that make use of these dispersion coefficients.

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[18] The mean mixing heights for mornings in the continental United States range between approximately 200 m and 1200 m depending upon season and location (Holzworth, 1972). The mean mixing heights are higher for afternoons, ranging between 500 m and 4000 m (Holzworth, 1972).

[19] For releases other than continuous releases, EPIcode automatically selects the puff or plume equation at each downwind location based on the relative dimension of the cloud width with respect to the cloud length.

Averaging time is important because greater apparent dispersion resulting in lower centerline plume concentrations occurs with larger averaging time due to plume meander. Accounting for plume meander effects is typically done for radiological dose analysis, which can be concerned with radiological exposures that are integrated over times that may exceed the reference time for the set of dispersion coefficients for which the Gaussian dispersion model is based.

For chemical consequence analysis, toxic effect on human health can be immediate upon short-duration exposures, and the severity of the toxic effect may correlate more closely to concentration than to dose. Thus, an ideal chemical consequence analysis may, in some instances, be concerned with the peak concentrations that may last only a minute or so. In these cases, the use of a shorter averaging time allows for better characterization of these higher concentrations that may only span a short period of time.

In the Gaussian dispersion model, the effect of averaging time is typically addressed through a correction factor to the horizontal dispersion coefficient. A fuller discussion of this phenomenon and an empirical correction factor that has been developed to quantify its effect are found in Appendix A.

The default sample time, which is labeled "Max Sample Time", for a continuous release in EPIcode is 10 minutes, which corresponds to the experimental basis for the plume dispersion coefficients. For other release types (term, liquid spill, fire, and explosive releases), the sample time is also set to the "Max Sample Time" value if the "Override" box is checked on the "Setup" page. If the "Override" box is unchecked, the sample time is set to the lesser of the two values between the release duration and the "Max Sample Time" value. Recall that the release duration is specified by the user for term and fire releases and internally determined by EPIcode for liquid spill and explosive releases.

Recommendation: The sample or averaging time should reflect the exposure time that is associated with the toxic exposure guideline of interest and should generally be equal to or less than the release duration (EPA, 1999). For example, if the toxic exposure guideline is the 10-minute Acute Exposure Guideline Level (AEGL), then an averaging time of 10 minutes is appropriate when the release duration is 10 minutes or more and an averaging time equal to the release duration is appropriate when the release duration is shorter than 10 minutes.

Guidance for the use of TEELs and ERPGs in DOE applications make a distinction between chemicals that have toxic effects that are best characterized as being concentration dependent versus those that have toxic effects that are best described as being dose dependent (Craig, 2001). For dose-dependent chemicals, the toxic effects correlate to the total quantity of material to which an individual is exposed. For dose-dependent chemicals, the peak 15-minute TWA or peak 1-hour TWA may be justified with any release duration (Craig, 2001).

Concentration-dependent chemicals have fast-acting toxic effects that correlate more closely with exposure concentration than with the total quantity. Chemicals should be considered concentration dependent if it has been assigned a short-term exposure limit (STEL) or ceiling (C) value such as an OSHA PEL-STEL or PEL-C or ACGIH TLV-STEL or TLV-C (Craig, 2001). If the release duration is 15 minutes or greater, a peak 15-minute TWA of the source term rate is

recommended for use with TEEL or ERPG values for these chemicals (Craig, 2001). For release duration less than 15 minutes, the TWA should generally correspond to the release duration, with the minimum time basis for the TWA being one minute (Craig, 2001).

4.4.3 Deposition Velocity

Larger solid particles released in a puff or plume will fall to the ground due to gravitational settling. Smaller particles and even gases will deposit on ground surface elements (e.g., ground vegetation) through a variety of processes that can include chemical, biological, and physical interactions between the contaminant (particle or gas) in the puff or plume and the ground surface elements. Depletion of the contaminant in plume occurs as a result.

The EPIcode default value for deposition velocity is 0 cm/s for gases and vapors and 0.3 cm/s for solids.

Recommendation: The most conservative results are generally obtained with the deposition velocity set to zero. This assumption could lead to unrealistically large concentration predictions for particles, particularly at large distances downwind. The EPIcode default values of 0 cm/s for gases and vapors and 0.3 cm/s for solids are therefore generally recommended, although other values may be used with justification.

4.4.4 Receptor Height

The EPIcode default value is 1.5m.[20]

Recommendation: For non-buoyant, ground-level releases, a zero or near-zero specification is appropriate and generally conservative. An analyst would only want to conceivably consider a value significantly different from zero when the release is elevated (e.g., from stack or plume rise mechanism) and when a reasonable possibility exists for a receptor to be in an elevated position.

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[20] Note that for a ground level release and the default receptor height, the peak plume concentration at the receptor height occurs downwind of the release location (e.g., at a distance of approximately 50 m for F atmospheric stability class).

5.0 SPECIAL CONDITIONS FOR USE

EPIcode was developed as a tool to plan for and respond to chemical emergencies. This document does not specifically address application issues related to emergency response or emergency preparedness/planning.

Even though EPIcode was not developed specifically for safety analysis applications, it is also widely used throughout the DOE complex for this purpose and has been designated for the DOE Safety Software Toolbox to support 10 CFR 830 safety basis documents. This document serves as a guide for prudent implementation of the EPIcode for the purpose of modeling chemical source terms and consequence phenomenology applicable to safety documentation. The user, however, must still demonstrate that EPIcode is being used within its domain of applicability and that site/laboratory procedures governing use of safety analysis software are being followed.

6.0 SOFTWARE LIMITATIONS

This section discusses limitations and areas of improvement of EPIcode. Section 6.1 summarizes technical limitations of Version 7.0 of EPIcode. Section 6.2 provides a summary of the outcome of the SQA gap analysis.

6.1 EPIcode Issues

The limitations of a computer code must be discussed in the context of its intended use. The limitations of EPIcode that are discussed in Table 6-1 below relate to both its use in general and specifically for safety analysis applications (recall that EPIcode was developed to plan for and respond to chemical emergencies).[21]

Table 6-1 EPIcode Limitations

EPIcode Limitation	Comment
Results are less reliable for conditions of low wind speed or very stable atmospheric conditions.	Issue of general concern to atmospheric transport and dispersion codes.
Results have high uncertainty very close to the source.	Issue of general concern to atmospheric transport and dispersion codes.
EPIcode does not model dense gas releases.	The basis for identifying the potential for dense-gas effects is the Ri number. The dense-gas effects are more pronounced near the source of the release. As atmospheric air mixes with the cloud, dilution occurs that causes dense gas transport effects to essentially become negligible as the density of the plume mixture approaches that of the ambient air. All dense gas releases, therefore, eventually transition to transport and dispersion that is characteristic of a neutrally buoyant plume. So, the Gaussian models are frequently used when the receptors of interest are far from the source, even when the

[21] Differences exist in the computational capabilities that are needed for a safety analysis calculation compared to those that are needed by people responding to a chemical accident. For example, the direction that a chemical puff or plume is traveling is of utmost importance to an emergency responder, since this information is crucial if efficient evacuation procedures are to be implemented. Thus, the inability of EPIcode to model the response of plume segments to shifts in wind direction during the course of modeling an accidental chemical release is a code limitation that affects emergency response calculations. Safety analysis calculations, however, traditionally consider exposures to a hypothetical receptor that is stationed on the centerline of a plume that is invariant with time. Thus, the inability of EPIcode to model shifts in wind direction does not constitute a limitation in the context of safety analysis calculations.

EPIcode Limitation	Comment
	released cloud is likely to exhibit dense-gas behavior near the source.[22] The burden is on the analyst to justify the applicability of this approach to the specific analysis.
EPIcode does not account for terrain steering effects.	A natural canyon or street canyon formed by large buildings can constrain the lateral dispersion of the puff or plume. Development of codes that are suitable for complex terrain and urban settings is a general area of ongoing research.
EPIcode does not model dispersion effects associated with building wakes.	Since wake effects near the source tend to enhance dispersion for that provides additional dilution for non-buoyant ground-level releases, it is generally believed to be conservative to neglect these effects in estimating chemical concentrations at downwind locations for these types of releases. This is not true for elevated releases (e.g., elevated either through discharge from a stack or as a result of plume rise from buoyancy or momentum effects). For an elevated release, the puff or plume can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs. The effects of downward-directed entrainment into the wake cavity serve to increase ground-level concentrations above what would be observed in the absence of the building. Guidance in this document recommends modeling the release as non-buoyant from ground level in this situation.

[22] For a large ammonia release, the EPIcode user's manual maintains that dense gas effects are significant when the cloud concentration is approximately 5% (50,000 ppm) or more, and that EPIcode can provide reasonable estimates when the cloud concentrations approximately below 5% (50,000 ppm). At this concentration level, passive dispersion is the dominant transport and dispersion mechanism.

EPIcode Limitation	Comment
EPIcode does not allow for one or more years of meteorological data to be input and processed so that statistical methods can be employed to determine the 50^{th} percentile (median) or 95^{th} percentile (unfavorable) concentration results.	EPIcode accepts a single input combination of atmospheric stability class and wind speed. The user is responsible for specifying an appropriate combination of atmospheric stability class and wind speed that will yield representative median or unfavorable concentration results. If one or more years of meteorological data are available, other atmospheric dispersions that can accept and process the meteorological data can be used to assist in these specifications. For example at SRS, meteorologists evaluated SRS data with another atmospheric and dispersion code for neutrally buoyant plumes and found that the meteorological conditions that correspond to 95^{th} percentile consequence results were associated with E stability class and 1.7-m/s wind speed for ground level releases (Hunter, 1993). Alternatively, an electronic worksheet may also be programmed to perform similar analysis. In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes (EPA, 1999).

6.2 Outcome of Gap Analysis

A gap analysis of Version 7.0 of the EPIcode computer code has been completed (DOE, 2004). The gap analysis reviewed the program, practices, and procedures associated with development of EPIcode compared with NQA-1 based requirements as contained in U.S. Department of Energy, Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes (DOE, 2003a). It was determined that the EPIcode 7.0 does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of the software for supporting safety analysis. Informed use of the code can be assisted by appropriate use of current EPIcode documentation and this EPIcode guidance report for DOE safety analysts. Furthermore, while SQA improvement actions are recommended for EPIcode, no evidence has been found of programming, logic, or other types of software errors in EPIcode 7.0 that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

Of the ten SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), two requirements are met at an acceptable level, i.e., *Classification* (1) and *User Instructions* (7). Improvement actions are recommended for EPIcode to fully meet the remaining eight requirements and are summarized in Table 6-2. This evaluation outcome is deemed acceptable because: (1) EPIcode is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of EPIcode is limited to those analytic applications for which the software is intended.

Table 6-2 — Summary of Important Exceptions, Reasoning, and Suggested Remediation

No.	Criterion [Section refers to Gap Analysis Report for EPIcode, (DOE, 2004)]	Reason Not Met	Remedial action(s)
1.	SQA Procedures/Plans (Section 4.2)	SQA Plans and Procedures were not available for the gap analysis.	SQA Plans and Procedures should be developed and made available for review.
2.	Requirements Phase (Section 4.3)	A Software Requirements Document does not exist for review. Thus, it was necessary to infer requirements from draft model description and user guidance documents.	A Software Requirements Document should be prepared and made available for review.
3.	Design Phase (Section 4.4)	A Software Design Document does not exist for review. Thus, it was necessary to infer the intent of the design from draft model description and user guidance documents.	A Software Design Document should be prepared and made available for review.

No.	Criterion [Section refers to Gap Analysis Report for EPIcode, (DOE, 2004)]	Reason Not Met	Remedial action(s)
4	Implementation Phase (Section 4.5)	Documentation to support the implementation is lacking.	A verifiable, written set of SQA plans and procedures including implementation, test case descriptions, and associated criteria related to design should be made available.
5.	Testing Phase (Section 4.6)	A Software Testing Report Document does not exist for review.	A Software Testing Report Document should be prepared and made available for review.
6	Acceptance Test (Section 4.8)	A verifiable, written set of SQA plans and procedures, which would include acceptance-testing documentation, is lacking.	Documented acceptance testing should be developed.
7.	Configuration Control (Section 4.9)	A Configuration and Control Document does not exist for review.	A Configuration and Control Document should be prepared and made available for review.
8.	Error Notification (Section 4.10)	An Error Notification and Corrective Action Report do not exist for review.	While a Software Problem Reporting system is apparently in place, written documentation should be provided to the Central Registry for verification of its effectiveness.

By order of priority, it is recommended that EPIcode software improvement actions be taken, especially:

1. Correcting known defects in the SQA process
2. Upgrading existing SQA documentation, and
3. Revising and developing new software documentation.

A new software baseline set of documents is recommended for EPIcode to demonstrate completion of the revision to software documentation item (above). The list of revised baseline documents includes:

- Software Quality Assurance Plan
- Software Requirements Document
- Software Design Document

- Test Case Description and Report
- Software Configuration and Control
- Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

It is estimated that a concentrated program to upgrade the SQA pedigree of EPIcode to be compliant with the ten criteria discussed important for software development would require fourteen to sixteen full-time equivalent (FTE)-months.

7.0 SAMPLE CALCULATIONS

Problem Statement: A vessel at Anytown, USA stores 210 gallons of concentrated (> 90 wt%) nitric acid (HNO_3) at ambient pressure and temperature. A scenario is postulated in which the vessel ruptures catastrophically, and the 210 gallons of HNO_3 spill on the ground. Determine the following: (1) the maximum concentration at 100 meters downwind and compare with the ERPG-3 value of 78 ppm and (2) the maximum concentration at 2500 meters downwind and compare with the ERPG-2 value of 6 ppm.

Analysis: The EPIcode chemical database contains properties for 100 wt% nitric acid since only pure chemicals, and not solutions, are part of the EPIcode chemical library. New chemicals can be added to the library. As indicated in the body of the report, a dilute acid solution can be added as a new chemical if sufficient property information is available. For evaporation calculations from chemical pools, the vapor pressure is generally the controlling parameter. The table below shows the sensitivity of HNO_3 vapor pressure to the HNO_3 wt% at 30 °C (Perry, 1997).

Table 7-1 Vapor Pressure of Nitric Acid in Solution as a Function of Concentration

HNO_3 wt%	HNO_3 Vapor Pressure [mm Hg]
40	0.1
50	0.6
60	1.7
70	5.5
80	14
90	36
100	77

In this sample problem, we have assumed concentrated HNO_3 (>90 wt%) and will conservatively analyze the spill on the basis of 100 wt% HNO_3.

The following set of inputs are entered into the EPIcode:

- Chemical - Nitric acid (The default vapor pressure of 62 mm Hg is set for 25 °C; EPIcode will adjust the vapor pressure once the liquid temperature is enter as discussed below.)
- Type of release - Liquid spill
- Terrain factor - The terrain factor input is based on judgment taking into account site terrain characteristics. For the purposes of this sample calculation, calculations are performed first specifying rural terrain and then specifying city terrain in order to show the sensitivity of the results to this input parameter.

- Stability class - E stability (For neutrally buoyant plumes that are released at ground level, worst-case meteorological conditions are associated with stable atmosphere and low wind speed. The meteorological conditions that are associated with the 95th percentile consequence results for such releases as determined from assumed analysis of site data are taken to be E stability class and 1.7 m/s wind speed at measurement height of 10 meters for the purposes of this sample calculation.)
- Wind speed - 1.7 m/s
- Quantity spilled - 210 gallons
- Spill area - 79.5 m^2 (This area corresponds to a pool depth of 1 cm (10 mm). In the dialog box for this input, EPIcode provides recommended values of 79.5 m^2, 795 m^2 31.3 $m^2$and for pool depths of 1 cm, and 1 mm, and 1 inch respectively.)
- Liquid temperature - 29 °C (The 95th percent highest air temperature as determined from site data is assumed to be 29 °C for the purposes of this sample calculation. Here, the liquid temperature is assumed to be the same as the air temperature.)
- Vapor pressure - 77 mm Hg (This is the value calculated by EPIcode, based on the temperature above, and presented in a dialog box for acceptance or revision. After this entry, EPIcode provides the following source term results: evaporation rate of 83 g/s and time for total evaporation of 4.0 hours.)
- Inversion height - 200 m (An inversion height of 200 m is taken as worst-case based on regional data (Holzworth, 1972). The default value of 5000 m, or effectively no inversion layer, is thus overridden.)
- Receptor height - 0 m
- Sample time - 10 minutes (This is the EPIcode default value, which is generally appropriate for predictions of the desired peak 15-minute TWA concentrations as discussed in Sections 4.2.2 and 4.4.2.)
- Deposition velocity - 0 cm/s (This is the EPIcode default value for gases and vapors.)

The following results are obtained.

- Centerline concentration at 100 m - 430 ppm (> ERPG-3 value of 78 ppm)
- Centerline concentration at 2500 m - 1.8 ppm (< ERPG-2 value of 6 ppm)

Note: To show the effect of the terrain factor, the calculations were re-run with the city terrain factor specified. The centerline concentration results were significantly lower (by a factor of three or more) yielding results of 120 ppm at 100 m and 0.6 ppm at 2500 m.

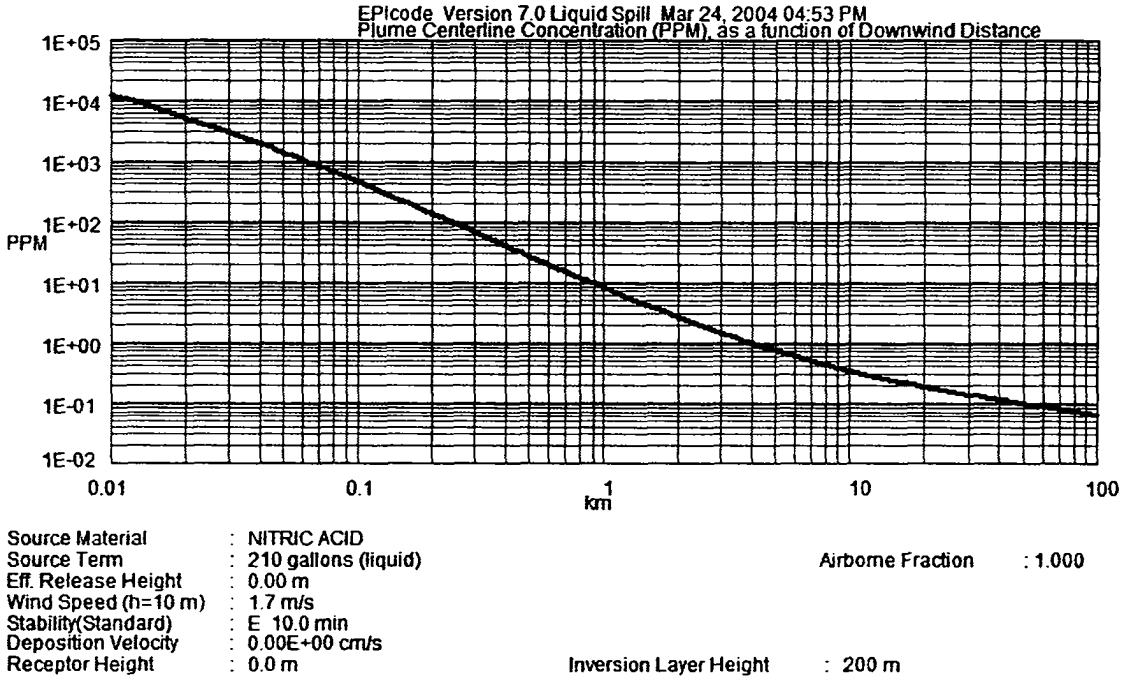

Figure 7-1. Epicode Sample Problem — Nitric Acid Concentration Versus Distance

Additional Analysis:

The maximum concentration at 100 meters downwind will now be calculated for an evaporative release from a 210-gallon puddle of 70 wt% HNO_3 in city terrain and compared with the ERPG-3 value of 78 ppm. This additional calculation will highlight the large difference in evaporation rates between pure HNO_3 and 70 wt% HNO_3. From the table of HNO_3 vapor pressure at 30 °C as a function of weight percent shown earlier in this section, the vapor pressure for HNO_3 70 wt% is 5.5 mm Hg (0.0072 atmospheres) compared to 77 mg Hg for pure the HNO_3 (Perry, 1997). Therefore, a much lower evaporation rate and 100-m concentration can be expected since the vapor pressure for 70 wt% HNO_3 is approximately 7% of that for 100 wt% HNO_3. The results will show that evaporation rate and predicted concentration at 100 meters for the 70 wt% HNO_3 case are approximately 7% of the values calculated for the 100 wt% HNO_3 case.

All inputs are the same as before except for the vapor pressure input.

Vapor pressure - 5.5 mm Hg

The following results are obtained.

- Evaporation rate - 6 g/s (compared to 83 g/s for 100 wt% HNO_3)
- Centerline concentration at 100 m - 31 ppm (< ERPG-3 value of 78 ppm and < 430 ppm calculated for 100 wt% HNO_3)

8.0 ACRONYMS & DEFINITIONS

Selected Terms and Definitions Used in Source Term, Atmospheric Transport and Dispersion, and Consequence Analysis

Acute Exposure Guideline Levels (AEGLs) – Threshold exposure limits for the general public above which acute exposure would be expected to lead to adverse effects of increasing severity for AEGL-1, AEGL-2, and AEGL-3. The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) is developing AEGLs to assist Federal and State agencies and private sector organizations with their need for short-term hazardous chemical exposure information in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h) and the three severity levels as defined below:

AEGL-1: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Advection – The transport of a fluid property by the bulk motion of the fluid, sometimes called convection in engineering terminology.[23]

Aerosol – Solid or liquid particles (droplets) that are suspended in a gas or vapor medium.

Atmospheric Stability Class – Characterization of the state of atmospheric turbulence.[24] The different atmospheric stability classes typically used by meteorologist range from

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[23] Some of the definitions for atmospheric transport and dispersion terms are taken from the Chemical Dispersion and Consequence Assessment Working Group of the DOE-sponsored Accident Phenomenology and Consequence Methodology Evaluation Program (Lazaro, 1997).

A for very unstable conditions to F (or sometimes G) for very stable conditions and account for differing levels of buoyant turbulence. High levels of buoyant turbulence are associated with unstable conditions.

Atmospheric Transport and Dispersion – The movement and dilution of a contaminant cloud under the influence of the prevailing wind flows and associated atmospheric turbulence.

Buoyant Turbulence – Atmospheric turbulence that is generated by solar heating of the ground and the formation of thermal updrafts.

Chi-over-Q (χ/Q) – For a chemical release into the atmosphere, this parameter represents the ratio of the airborne concentration of the chemical constituent in a cloud at given downwind location to the airborne release rate. The parameter provides a measure of dilution from atmospheric transport and dispersion processes at a given downwind distance.[25]

Cloud – The volume that encompasses a chemical (contaminant) emission.

Dense Gas (Heavy Gas) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is greater than that of the ambient air (i.e., negatively buoyant cloud). In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind, and the cloud alters the atmospheric wind field in its vicinity. Dense-gas releases undergo what has been described in the literature as "gravitational slumping". Gravitational slumping is characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release.

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[24] A comprehensive treatment of atmospheric dispersion is so complex that many approximations are needed to make it tractable. Since turbulence is random and chaotic, it cannot be parameterized and one must resort to empirical formulations. One early attempt to simplify the treatment of turbulence was to define atmospheric stability classes and associate a rate of lateral and vertical dispersion with each class as a function of downwind distance only. Although computations based on these stability classes provide only a rough approximation to reality, they have proved extremely useful and are still in use, although more accurate treatments are available. Wind direction variability and vertical temperature difference are the most common techniques that are employed.

[25] In practical terms, χ/Q values are time-averaged characterizations based generally on an average release rate over a specified time period and time-averaged dilution characterization of the atmospheric transport and dispersion effects. In the Gaussian plume model, the dispersion coefficients are empirically based on field observations over a given time period, referred to as the averaging time or sampling time. For releases of radiological material, χ/Q values are generally defined in an equivalent fashion as the ratio of the time-integrated airborne concentration in a cloud at a given downwind location to the total amount of material released.

Dilution – The reduction of the cloud concentration due to mixing with ambient air.

Dispersion – Spreading of the cloud boundaries due to atmospheric turbulence. Atmospheric, turbulent dispersion is the result of rapid and irregular fluctuations in wind components, such as velocity.

Dispersion Coefficients – A measure of the spreading of a contaminant cloud as it travels downwind. In Gaussian puff and plume formulations:

σ_x = longitudinal dispersion coefficient (function of downwind distance, x), representing the standard deviation of the concentration distribution in the downwind axis direction;

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction; and

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction.

Emergency Response Planning Guidelines (ERPGs) – Estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

***ERPG-1**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*

***ERPG-2**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*

***ERPG-3**: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

Evaporation – Process by which molecules of a liquid come off the surface of a liquid and enter the vapor space.

Friction Velocity – A measure of the mechanical turbulence and a direct measure of the frictional forces of the wind in the boundary layer adjacent to the earth's surface. It can be thought of as the representing the consequences of Reynolds stresses, which cause velocity fluctuations to transport momentum.[23]

Gaussian Puff/Plume Model – A diffusion model for vapor or gas chemical releases to the environment in which the lateral and vertical distribution of the chemical concentration follow a normal or Gaussian distribution. Additionally in the puff model, the longitudinal distribution follows a normal or Gaussian distribution. A segmented Gaussian puff/plume model incorporates a computational approach in which the Gaussian puff/plume is spatially segmented into individual volume sources with each segment generating a concentration field.[23]

Inversion Layer – A region of air in which the temperature increases with increasing distance from the ground.[23] The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is often referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i.

Mechanical Turbulence – Atmospheric turbulence that is generated from the shear forces that result when adjacent parcels of air move at different velocities (i.e. either at different speeds or directions). Fixed objects on the ground such as buildings or trees increase the ground roughness and increase mechanical turbulence in proportion to their size.

Neutrally Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that occurs when the density difference between the chemical cloud and the ambient air is small. A neutrally buoyant cloud does not alter the atmospheric wind field. The term passive is used to describe the phenomenological characteristics associated with atmospheric transport and dispersion of the cloud as the cloud follows the bulk movements and behavior of the atmospheric wind flow.

Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) – Chemical concentration limits that are developed by the Occupational Safety & Health Administration for use in limiting worker exposures to airborne chemicals.

Plume – Term used to describe the form of the chemical cloud for a sustained or continuous release.

Plume Meander – Variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.

Positively Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is significantly less than that of the ambient air. A positively buoyant cloud behaves like a neutrally buoyant cloud with the added effect that the positive buoyancy produces upward forces that cause the puff or plume to rise.

Puff – Term used to describe the form of the chemical cloud for an instantaneous release or release of short duration.

Richardson (Ri) Number – Relative measure of the potential energy of the cloud with respect to the mechanical turbulence energy of the atmosphere. Potential energy is associated with buoyancy forces that tend to suppress turbulence. Wind shear generates mechanical turbulence energy.

Source Term – The rate of release (may be time dependent), duration, and physical and energetic characteristics of hazardous material released to the environment.

Surface Roughness Length (z_o) – Measure of the amount of atmospheric mechanical turbulence that is induced by the presence of surface roughness elements such as vegetation and man-made structures.

Temporary Emergency Exposure Limits (TEELs) – Surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values) and surrogate Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) values for all chemicals for which PEL-TWA values have been published (i.e., TEEL-0 values).

Vapor – The gas produced from the evaporation of a liquid.

Vapor Pressure – The equilibrium pressure of the pure component vapor over the pure component liquid. When a chemical exists in a solution or mixture, the term partial pressure is generally used.

95th Percentile Consequence – A statistical method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to quantify the consequences for an airborne release conservatively taking into consideration the variability of meteorological conditions that may be present at the time of the release (NRC, 1983).[26] While this method was originally established for radiological releases, the concept easily extends to hazardous chemical releases. Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based χ/Q values calculated for a postulated

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[26] This method is prescribed in Appendix A to DOE-STD-3009-94 for consequence assessment to quantify the radiological dose that is received by the maximally exposed offsite individual (MOI) (DOE, 2000).

release to downwind receptors at the site boundary that would result in a χ/Q values that is exceeded 5% of the time (based on hourly data over a period of one year or more).[27] Although the methods allows for variations in distance to the site boundary as a function of angular sectors to be taken into consideration in conjunction with the wind direction, assuming the minimum distance to the site boundary applies in all directions is a conservative implementation that is easily supported and that essentially makes the calculations sector independent. The site-specific meteorological data consist of (generally) hourly data of wind speed and atmospheric stability class at minimum (wind direction is also needed if sector-dependent distances to the site boundary are considered).

[27] Terminology that is sometimes unfortunately used in this context and that should be avoided is terms such as "95th percentile meteorology." The distribution and selection of the 95th percentile value are based on consequence results (e.g., χ/Q values) that are a function of meteorological parameters and not on the meteorological parameters themselves (e.g., wind speed).

9.0 REFERENCES

AIHA (2002). *The AIHA Emergency Response Planning Guidelines and Workplace Environmental Exposure Level Guides Handbook*, American Industrial Hygiene Association (AIHA), AIHA Press, Fairfax, VA.

S. Brereton (1997), D. Hesse, D. Kalinich, M. Lazaro, V. Mubayi, and J. Shinn. *Final Report of the Accident Phenomenology and Consequence (APAC) Methodology Evaluation – Spills Working Group*, URLC-ID-125479, Lawrence Livermore National Laboratory (LLNL), Livermore, CA.

G. A. Briggs (1969). *Plume Rise*, U.S. Atomic Energy Commission, Division of Technical Information.

G. A. Briggs (1975). Chapter 3, "Plume Rise Predictions", in Lectures on Air Pollution and Environmental Impact Analysis, D. A. Haugen, ed., American Meteorological Society.

CFR (1992). *Process Safety Management of Highly Hazardous Chemicals; Explosives and Blasting Agents; Final Rule*, 29 CFR Part 1910, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

CFR (1999). Labor Chapter XVII—*Occupational Safety and Health Administration.* 29 CFR Part 1910.1000, Subpart Z—Toxic and Hazardous Substances, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

CFR (2001). *Nuclear Safety Management Rule*, 10 CFR Part 830, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

D. K. Craig (2001), J. S. Davis, P. W. Hoffman, L. G. Lee, and J. Prowse. *Toxic Chemical Hazard Classification And Safety Evaluation Guidelines For Use In Doe Facilities*, WSRC-MS-92-00206, Rev. 3, Savannah River Site, Aiken, SC.

DNFSB (2000). *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, Defense Nuclear Facilities Safety Board, Technical Report DNFSB/TECH-25, (January 2000).

DNFSB (2002). Defense Nuclear Facilities Safety Board, *Recommendation 2002-1, Quality Assurance for Safety-Related Software* , (September 2002).

DOE (1997). *Hazard Categorization and Accident Analysis Techniques for Compliance Order 5480.23, Nuclear Safety Reports*, U.S. Department of Energy, Washington, DC, DOE-STD-1027-92, Change Notice 1.

DOE (2000). U.S. Department of Energy, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, DOE Response to TECH-25, Letter and Report, (October 2000).

DOE (2002a). U.S. Department of Energy, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Reports*, DOE-HDBK-3010-94, Change Notice 2 (April 2002).

DOE (2002b). *Selection of Computer Codes for DOE Safety Analysis Applications, Department of Energy*, National Nuclear Security Agency - Defense Programs Technical Report, (May 2002).

DOE (2003a). U.S. Department of Energy, *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes*, Revision 1, (November 2003).

DOE (2003b). U.S. Department of Energy, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1: Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, Report, (February 28, 2003).

DOE (2004). U.S. Department of Energy, *Software Quality Assurance Improvement Plan: EPIcode Gap Analysis*, Final (May 2004).

DOE/EH (2003). U.S. Department of Energy, *Designation of Initial Safety Analysis Toolbox Codes*, Letter, (March 28, 2003).

EPA (1987). *Technical Guidance for Hazards Analysis: Emergency Planning for Extremely Hazardous Substances*, PB93-206910, Environmental Protection Agency, Research Triangle Park, NC.

EPA (1995). *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volume II – Description of Model Algorithms*, EPA-454/R-95-003b, U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPA (1999). *Risk Management Program for Offsite Consequence Analysis*, EPA 550-B-99-0009, U.S. Environmental Protection Agency, Research Triangle Park, NC.

EPIcode (2003). *EPIcode Version 7.0 User Documentation*, Online Help distributed with software package, Homann Associates, Inc. (September 2003).

FEMA (1989). *Handbook of Chemical Hazard Analysis Procedures*, (ARCHIE Manual), Federal Emergency Management Agency (FEMA), U. S. Department of Transportation (USDOT), and U.S. Environmental Protection Agency (USEPA) (1989), Washington, D.C.

S. R. Hanna (1982), G. A. Briggs, and R. P., Hosker, Jr. *Handbook on Atmospheric Dispersion*, DOE/TIC-11223, Technical Information Center, U.S. Department of Energy (DOE), Oak Ridge, TN.

S. R. Hanna (1996), P. J. Drivas, and J. J. Chang. Guidelines for Use of Vapor Cloud Dispersion Models, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

S. R. Hanna (2002) and R.E. Britter. Wind Flow and Vapor Cloud Dispersion at Industrial and Urban Sites, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

G. C. Holzworth (1972). *Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution Throughout the Contiguous United States*, EPA Report AP-101, Environmental Protection Agency, Research Triangle Park, NC, p. 109.

S. G. Homann (1996), *EPIcode User's Guide*, Version 6.0, Homann Associates, Inc., Fremont CA.

C. H. Hunter (1993). *Revised Onsite Meteorological data for Emergency Planning Hazards Assessments*, Savannah River Technology Center, Westinghouse Savannah River Company, SRT-ETS-931167.

J. S. Irwin (1979). *A Theoretical Variation of the Wind Power Law Exponent as Function of Surface Roughness and Stability*, Atmospheric Environment, Vol. 13, 191-194.

M. A. Lazaro (1997), K. Woodward, S. R. Hanna, D.J. Hesse, J. C. Huang, J. Lewis, and C. A. Mazzola. *Model Review and Evaluation for Application in DOE Safety Basis Documentation of Chemical Accidents – Modeling Guidance for Atmospheric Dispersion and Consequence Assessment*, ANL/EAD/TM-75, Environmental Assessment Division (EAD), Argonne National Laboratory (ANL), Argonne, IL.

C. A. Mazzola (1995) and R. P. Addis. *Atmospheric Dispersion Modeling Resources*, U.S. Department of Energy, Emergency Management Advisory Committee, Subcommittee on Consequence Assessment and Protective Actions.

NRC (1972). *Onsite Meteorological Programs*, U.S. Nuclear Regulatory Commission Regulatory Guide 1.23 U.S. Nuclear Regulatory Commission, Washington, DC.

NRC (1977). *Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water-Cooled Reactors*, Regulatory Guide 1.111, U.S. Nuclear Regulatory Commission, Washington, DC,

NRC (1983). *Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants*, Regulatory Guide 1.145, U.S. Nuclear Regulatory Commission, Washington, DC.

NRC (2003). *Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants*, U.S. Nuclear Regulatory Commission, Regulatory Guide 1.194, (June 2003), Washington, DC.

R. H. Perry (1997) and D. W. Green. Perry's Chemical Engineer's Handbook, 7th Edition, McGraw-Hill, N.Y.

R. M. Reynolds (1992). *ALOHA Theoretical Description*, Draft Technical Memorandum NOS ORCA-65 Hazardous Materials Response and Assessment Division (HMRAD) of the National Oceanic and Atmospheric Administration (NOAA), Seattle, WA.

D.B. Turner (1970). *Workbook of Atmospheric Dispersion Estimates*, Report PB-191 482, Office of Air Programs, U.S. Environmental Protection Agency, Research Triangle Park, NC.

D. B. Turner (1994). *Workbook of Atmospheric Dispersion Estimates, An Introduction to Dispersion Modeling*, Lewis Publishers, Ann Arbor, MI.

A.H. Weber (1996) and C.H. Hunter, *Estimating Dispersion from a Tornado Vortex and Mesocyclone* (U), Savannah River Site, Aiken, SC, WSRC-TR-94-0386, Rev 2.

D. J. Wilson (1995). Concentration Fluctuations and Averaging Times in Vapor Clouds, Center for Chemical Process Safety (CCPS), American Institute of Chemical Engineers (AIChE), N.Y.

Appendices

Appendix	Subject
A	Gaussian Models for Atmospheric Transport and Dispersion
B	Tornado Dilution Factor

APPENDIX A: GAUSSIAN MODELS FOR ATMOSPHERIC TRANSPORT AND DISPERSION

Two broad categories exist to characterize atmospheric transport and dispersion that are based upon the released chemical cloud density and how it affects the interaction of the chemical cloud with the atmospheric wind flow. For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, the cloud is characterized as neutrally buoyant and the atmospheric transport and dispersion as passive.[28] If the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either passive or dense-gas type of atmospheric transport and dispersion. Dense gas behavior at the source is determined on the basis of the source Ri number having a value greater than one.[29] This appendix discusses the atmospheric transport and dispersion of neutrally buoyant releases and the Gaussian models that are the basis for the equations used in EPIcode.

Time-averaged concentrations obtained from field studies of neutrally buoyant chemical releases are observed to follow Gaussian or bell-shaped distributions. The Gaussian plume and puff dispersion models that have been developed to predict the outcome of chemical releases that are represented by these field studies are well established and widely used. As the plume develops and moves downwind, it approximates a Gaussian distribution in both the crosswind (lateral) and vertical directions. For continuous releases, the mean wind speed dilutes the chemical concentration but the longitudinal dispersion is negligible. As the plume moves downwind it gets progressively larger due to lateral and vertical dispersion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the longitudinal direction becomes more important. Accordingly, a puff is described by a three-dimension Gaussian equation.

The range of distances over which the Gaussian plume model should be used varies with conditions, but the model is considered generally applicable over the range of 100 m to 10 km and possibly beyond (Hanna, 1982). The basic form for the Gaussian plume model is given below beyond (Hanna, 1982).

$$\chi(x,y,z)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \qquad \text{(Equation A-1)}$$

where:

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[28] A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

[29] Definitions of source Ri number for continuous and instantaneous releases are given by Equation 3-1 and Equation 3-2, respectively.

χ = atmospheric concentration [mg/m^3] for chemical releases

Q = source term release rate [mg/s] for chemical releases

x = downwind distance (relative to source location) [m]

y = crosswind distance (relative to plume centerline)[m]

z = vertical axis distance (relative to ground) [m]

H = effective release height (relative to ground) [m]

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction [m]

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction [m]

u = average wind speed[30] [m/s]

The last term accounts for reflection of the plume at the ground surface through adding an image source at distance H beneath the ground surface.

Note that the concentration is inversely proportional to the wind speed (i.e., greater initial dilution with higher wind speeds).[31] The concentration is also inversely proportional to the horizontal and vertical dispersion coefficients (i.e., higher dispersion enhances the dilution of the puff or plume). These dispersion coefficients are a measure of the effect of atmospheric turbulence in causing the plume to increasingly disperse in the lateral and vertical direction as the plume travels downwind. The dispersion coefficients account for the two sources of atmospheric turbulence, namely, mechanical turbulence and buoyant turbulence.

The horizontal and vertical dispersion coefficients, σ_y and σ_z, required in the Gaussian dispersion equation are obtained either from site-specific meteorological measurements (e.g., standard deviations of wind angles) or through established curves that are based on field experiments and the concept of atmospheric stability class. The averaging time over which the σ_y and σ_z parameters were determined in the field experiments establishes the averaging time for the time-averaged concentrations predicted by the Gaussian dispersion equation. Averaging time is important because greater apparent dispersion occurs with larger averaging time due to plume meander. Plume meander refers to variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged

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[30] Since the wind speed varies with distance above the earth's surface, the wind speed value in the Gaussian plume equation will ideally represent some average value over the plume depth, such as the wind speed at the plume centroid (center of mass). In practice, simpler specifications are made such as the wind speed at the effective release height or the wind speed at the height of 10 meters (EPIcode uses either the wind speed at the release height or at 2 meters for release heights of 2 meters or less).

[31] Calm winds below 0.5 m/s are rare and generally not considered so that evaluating the Gaussian plume equation at a wind speed of zero is not an issue.

centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.[32] The time-averaging effect on plume meander dispersion is generally accounted for by the following algebraic expression suggested by Gifford that relates the horizontal dispersion coefficient (σ_y) for the averaging time of interest (t_a) to a known reference horizontal dispersion coefficient ($\sigma_{y,ref}$) that is associated with a reference averaging time ($t_{a,ref}$) (Hanna, 1982).

$$\sigma_y = \sigma_{y,ref} \times \left(\frac{t_a}{t_{a,ref}} \right)^q \quad ; \qquad \text{(Equation A-2)}$$

where, $q = 0.2$ for 3 minutes $< t_a <$ 1 hour

$q = 0.25$ to 0.3 for 1 hour $< t_a <$ 100 hours

Accounting for plume meander effects is typically done for radiological dose analysis, which can be concerned with radiological exposures that are integrated over times that may exceed the reference time for the set of $\sigma_{y,ref}$ values on which the Gaussian dispersion model is based. For chemical consequence analysis, toxic effect on human health can be immediate upon short-duration exposures and the severity of the toxic effect may correlate more closely to concentration than to dose. Thus, an ideal chemical consequence analysis may, in some instances, be concerned with the peak concentrations that may last only a minute or even less. In practice, $\sigma_{y,ref}$ values developed for Gaussian dispersion codes are generally based on averaging times that range from 3 minutes to 1 hour. If the above correlation is be used to calculate (σ_y) for ($t_a < t_{ref}$), a prescribed minimum of t_a equal to 20 seconds has been recommended (Hanna, 1996).

As the plume travels downwind, its vertical spread may be limited by the presence of an elevated temperature inversion layer. The temperature increases with increasing distance from the ground in the inversion layer. The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is typically referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i. The Gaussian dispersion equation can be modified to consider reflection from

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[32] In most engineering flow systems, the scales of turbulent motions are limited by the physical size of the system components (e.g., pipe diameter) so that time scales are on the order of seconds or minutes. For these systems, steady statistical averages can be achieved with reasonable sampling periods. Conversely, the range of spatial and time scales in the atmosphere is extremely large. As a consequence, observed statistics are not invariant with averaging time (i.e., one cannot obtain steady mean values since it is not possible to sample atmospheric parameters over a long enough time period) (Wilson, 1995).

the elevated temperature inversion layer.[33] Reflection eventually results in a uniform concentration in the vertical direction (throughout the plume depth from ground to inversion layer boundary).

Determination of σ_y and σ_z from established, empirical curves is a common and acceptable practice. Each σ_y or σ_z curve represents a different atmospheric stability condition based upon the classification scheme first developed by F. Pasquill and later modified by F. A. Gifford. The different atmospheric stability classes range from A for very unstable conditions to F (or sometimes G)[34] for very stable conditions and account for differing levels of buoyant turbulence.

The stability class is a function of both the amount of incoming solar radiation and the wind speed (Turner, 1970; Turner, 1994). High incoming solar radiation (as would occur on sunny days) and low wind speeds characterize unstable conditions (e.g. stability class A or B) and result in high levels of buoyant turbulence. With unstable conditions, the air temperature of the atmosphere near the earth's surface declines rapidly with elevation. Warm parcels of air near the surface travel a long distance upward before cooling to the temperature of the air around it. As warmer air rises, the cooler air that is displaced sinks downward. Large-scale, convective motions develop that provide substantial vertical mixing. At the other end of the spectrum, stable atmospheric conditions (e.g., stability class E, F or G) can occur on clear nights with low wind speeds. The smaller atmospheric temperature gradient that occurs with stable atmospheric conditions limits upward convection and reduces vertical mixing. Neutral stability conditions (e.g., stability class C or D) that occur with high wind speeds or with moderate wind speeds and cloud cover, represent intermediate stability conditions that produce moderate levels of buoyant turbulence.

Original descriptions and conditions of occurrence given by Pasquill for each stability class are given below (Turner, 1994).

- A: Extremely Unstable (Strong superadiabatic). Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).
- B: Moderately Unstable (Moderate superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 3 to 5 m/s range to dim sunshine with wind speeds < 2 m/s.

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[33] The ground and the inversion layer boundary are treated as impenetrable and totally reflecting surfaces. Some Gaussian plume models such as ALOHA treat reflection through addition of mirror image sources both below the ground and above the inversion layer boundary (Reynolds, 1992). For reflection off the inversion layer boundary, an addition term is added to Equation (A-1) that is similar to the ground-reflection term. Additional terms can be added to account for multiple reflections off the ground and inversion layer boundary. Also at some point downwind (generally where σ_z approaches z_i), the value of the vertical dispersion coefficient, σ_z, in the Gaussian dispersion equation is typically limited to approximately z_i.

[34] EPIcode does not support the input of G stability class.

- C: Slightly Unstable (Slight superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 5 to 6 m/s range to dim sunshine with wind speed in the 2 to 3 m/s range.
- D: Neutral (Adiabatic). Normally occurs with moderate to dim sunshine, cloudy conditions, and at night, with wind speeds > 3 m/s. It also occurs with very strong wind speeds on either sunny or cloudy days.
- E: Slightly Stable (Slight subadiabatic with or without inversion). Normally occurs at night or early morning with some cloud cover and with wind speeds in 2 to 5 m/s range.
- F: Moderately Stable (Moderate subadiabatic with inversion). Normally occurs at night or early morning with little cloud cover and with relatively low wind speeds (< 3 m/s).
- G: Extremely Stable (Strong subadiabatic with inversion). Normally occurs at night or early morning with very light to nearly zero wind speed.

Different set of dispersion coefficient curves have been established for rural environments and urban environments to account for the additional mechanical turbulence that is generated in urban settings by increased ground roughness due to building structures being taller and spaced closer together. Also, the heat-retention capabilities of urban surfaces (e.g., concrete structures) can drive buoyant flows that increase dispersion.

A forest can have a similar effect to that of buildings in increasing ground roughness. A surface roughness length (z_o) is typically used to characterize the amount of mechanical turbulence that is induced by the presence of surface roughness elements. A rule of thumb is that the surface roughness length is approximately one tenth the value of the height of the average surface roughness elements (Hanna, 2002). A surface roughness correction to σ_z is of the form $(z_o)^r$, where r is in the range of 0.1 to 0.25, with 0.2 being a commonly used value (Hanna, 1982; Hanna, 2002).

Recall that the atmospheric wind speed varies with distance from the ground (z). The wind speed (u) used in the Gaussian plume equation should ideally approximate the wind speed at the plume centroid (center of mass). Typically, the National Weather Service (NWS) measures wind speeds at 10 m (u_{10}). The following formula can be used to estimate the wind speed at other heights (Hanna, 1982).

$$u = u_{10} \times \left(\frac{z}{10}\right)^p \qquad \text{(Equation A-3)}$$

The power-law exponent parameter (p) can be estimated on the basis of atmospheric stability class and general surface roughness characterization. An urban and rural set of power-law exponents that are found in the published literature are shown below (Hanna, 1982; Irwin, 1979).

	Atmospheric Stability Class					
	A	B	C	D	E	F
Urban	0.15	0.15	0.20	0.25	0.40	0.60
Rural	0.07	0.07	0.10	0.15	0.35	0.55

A puff model is used for instantaneous or near-instantaneous releases (Hanna, 1996). For a puff, longitudinal dispersion also occurs.

$$\chi(x,y,z;t)=\frac{Q_T}{(2\pi)^{3/2}\,\sigma_x\sigma_y\,\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{x-x_o}{\sigma_x}\right)^2\right]\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \quad \text{(Eq. A-4)}$$

where:

Q_T = total source term [mg] for chemical releases

σ_x = longitudinal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the downwind axis direction [m]

x_o = $u \times t$; representing center of the puff in the longitudinal direction [m]

It is common practice to set σ_x equal to σ_y. The dispersion parameters for a puff release are known to be different than those for a plume release (Hanna, 1996).[35].

[35] For convenience, some dispersion models use plume dispersion parameters for both puff and plume releases. More extensive data are available for plume releases (Hanna, 1996).

APPENDIX B: TORNADO DILUTION FACTOR

Atmospheric transport and dispersion of chemical material from the facility into the environment during a tornado can be modeled with a design basis accident dilution factor (Ψ/Q) designated for a specific class tornado and applied for the distance from the facility to the receptor. The Ψ/Q parameter (units of s/m^3) represents the time-integrated ground-level centerline air concentration normalized by the mass released and is analogous to the χ/Q value that is calculated from the Gaussian plume equation for neutrally buoyant releases as discussed in Appendix A. The Fujita scale is commonly used to categorize tornadoes. For most safety analysis applications, the tornado is assumed to be either Fujita - 2 (F2) or F3. Figure B-1 shows Ψ/Q values (s/m^3) as a function of downwind distance (km) for different mean translational speeds of the F2 tornado (Weber and Hunter, 1996). The consequence analysis should pick a maximum Ψ/Q for the assumed translational speed. For example, the translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers. The product of thus maximum Ψ/Q value with the release rate of the chemical to the atmosphere yields the ground-level air concentration at the location of interest.

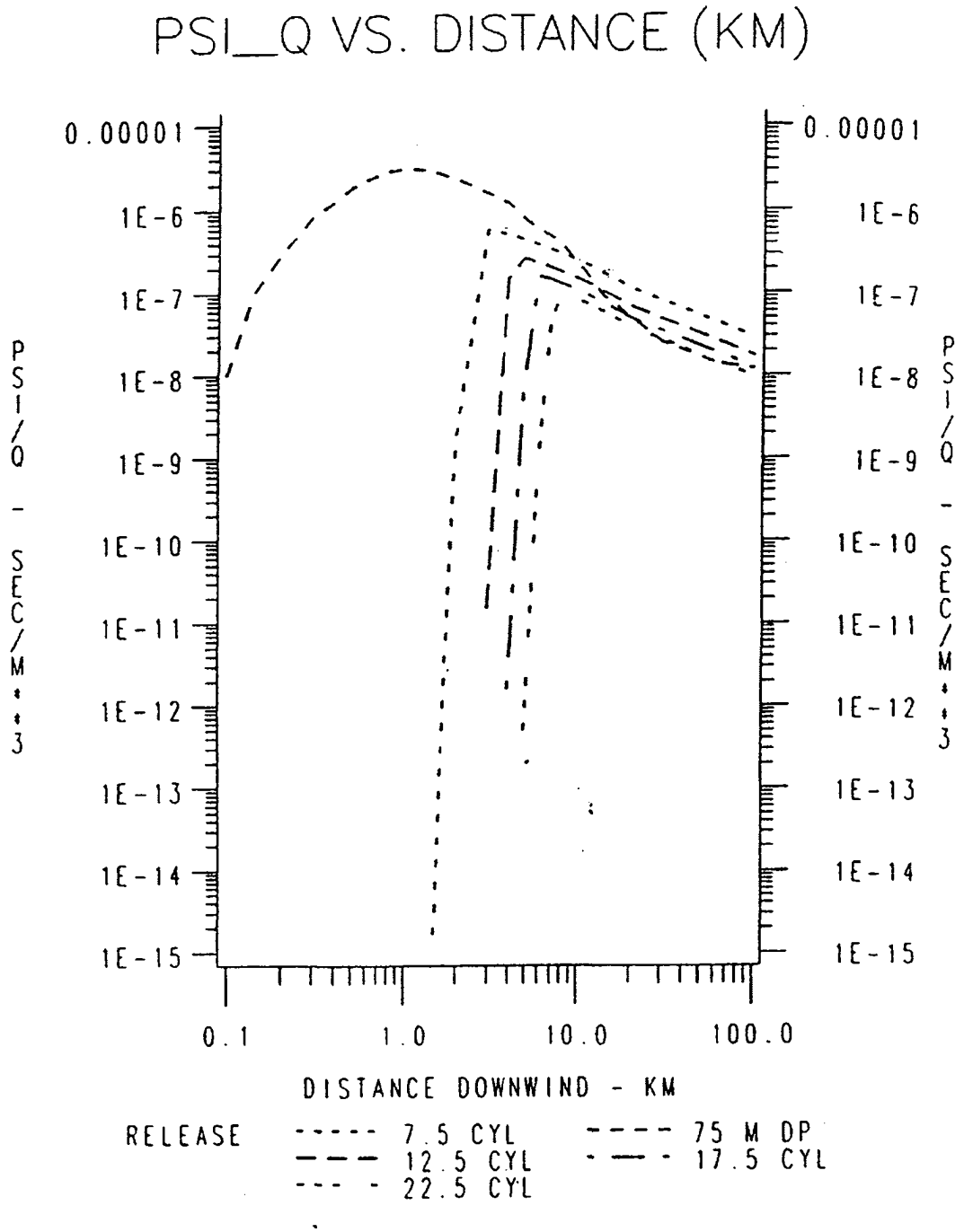

Figure B-1. The maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km). Applied for different mean translational speeds from 7.5m/s to 22.5 m/s. In this case, the downdraft speed is 10 m/s and the height of the cylindrical mesocyclone is 3500 m (from Weber and Hunter, 1996).

SEPARATION

PAGE

MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis

Final Report

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U.S. Department of Energy
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Foreword

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the MELCOR computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the MELCOR documentation provided by the code developer. MELCOR is one of six computer codes designated by DOE's Office of Environmental, Safety and Health as a toolbox code for safety analysis.

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Revision Status

Page/Section	Revision	Change
1. Entire Document	1. Final Draft for Review	1. Original Issue
2. Entire Document	2. Final Report	2. Changes due to Reviewer Comments

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MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis

Executive Summary

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in the February 28, 2003 *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities.* In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications. The MELCOR code is one of the designated toolbox codes.

The MELCOR code is likely to require completion of quality assurance improvement measures before meeting current SQA standards. In the interim period before these changes are completed, MELCOR is considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available user's manual information.

The MELCOR guidance report includes the following:

- Description of the software,
- Appropriate regimes and code limitations,
- Various models applicable for the evaluation of the leak path factor (LPF), and
- Several typical sample problems for leak path factor analyses.

Use of the information contained here, although not ensuring correct use of MELCOR in all analytical contexts, will minimize potential user errors and further standardize the use of MELCOR in appropriate regimes of applicability.

Following the introductory material, this report presents an overview of MELCOR use for Leak Path Factor evaluation. Various examples are given to cover a range of accident conditions.

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1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and the variability in guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, on September 23, 2002. As part of its Recommendation to the DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the Board's concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include:

(i) identification of a set of accident analysis software that is widely used in the DOE Complex; and,
(ii) issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regime in accident analysis, default inputs, and special conditions for use.

Safety analysis software for the DOE "toolbox" status was designated by DOE/EH in March 2003. The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications*, dated August 2002 (see http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf), and includes the Version 1.8.5 of MELCOR computer code.

The contents of this report are applicable in the interim period until measures are completed to bring MELCOR into compliance with defined SQA standards. The primary objective of the guidance report is to provide information on the use of MELCOR for supporting DOE safety basis accident analysis. Specifically, the purpose this report is to provide guidance on the use of MELCOR for Leak Path Factor analyses. The report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type Leak Path Factor (LPF) analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications when calculating LPF
- Modeling approach for various accident types
- Typical and default input value recommendations, and
- Citations of currently available SQA documentation..

This report is written to guide analysts in efficiently use MELCOR computer code to evaluate the Leak Path Factor for various accident conditions. In this area, this report is intended to complement existing MELCOR user's documentation. The existing user's documentation tends to be much broader in coverage of the full range of capabilities of MELCOR and the spectrum of inputs that might be needed depending upon the application. The existing documentation lacks cohesive and targeted guidance for particular applications such as LPF determination for DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The MELCOR LPF guidance document is written using the following set of sections. This first section contains an introduction and background providing an overview of appropriate software in the context of 10 CFR 830. More information follows on the scope and purpose of this document. The next major section is a summary description of MELCOR. A third section discusses applicable regimes for using MELCOR in performing accident analysis. A discussion on default inputs and input recommendations is provided, emphasizing appropriate inputs for DOE applications. This section is succeeded by a section on models and recommendations. Following this discussion are sections on special conditions for use of the software and software limitations. Several sample cases are then provided, followed by acronyms and definitions, references, and appendices.

1.1. Background: Overview Of Toolbox Software in Context of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software, may be viewed as appropriate computer software to be applied for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as "toolbox" codes. Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to software.

1.2. Scope

This document covers use of the MELCOR computer code for the evaluation of the Leak Path Factor for nonreactor nuclear facilities for various accident conditions. It includes a sample facility analyzed for seismic and fire induced release of aerosolized radioactive materials.

The MELCOR guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis related to LPF calculations
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Typical and default input value recommendations.

1.3. Purpose

The MELCOR code is part of the appropriate collection of software. Software Quality Assurance (SQA) concerns exist. Until MELCOR upgrades are completed so that MELCOR meets current established standards for software, MELCOR can be applied safety under the condition that the guidance contained in this report is followed. Once upgrades are finalized with MELCOR, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of MELCOR in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4. Applicability

In addition to MELCOR, other software exists for calculating the leak path factor and or analyzing the transport and deposition of hazard material in DOE nuclear facilities under postulated accident conditions. In some cases, manual or electronic spreadsheet calculations can be a preferred alternative to using a computer code for some accident analysis applications for simple geometries involving releases of radiological material. The relative merits of using different software or using a hand calculation for a given application is a judgment that must be made on a case-by-case basis.

The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program. As part of this program, the In-Facility Transport Working Group (WG) was established to address issues and evaluate methodologies in the leak path factor and in-facility transport domain. The WG issued a report that identifies and evaluates methodologies and computer codes to support safety basis calculations (Spore, 1996).

The WG report identified MELCOR as the best code for the analysis of in-facility transport when multidimensional effects are not significant. Significant benchmarking has also been performed with MELCOR especially with respect to its aerosol models. Finally as was noted in Section 1, MELCOR has been designated as a toolbox code for safety analysis DSA applications by DOE's Safety Analysis Software Group.

This report builds upon the APAC work to provide guidance and recommendations that are targeted to the use of MELCOR for leak path factor analysis of complicated flow situations in multi-cell, nuclear facilities. Specifically, the guidance is best suited for:

- Baseline, accident analysis calculations of the leak path factor
- Scoping analysis in the initial design of facilities, or backfit modifications of existing facilities
- Emergency management planning for workers, and
- Confirmatory calculations for evaluating mitigative and preventive safety controls.

2.0 SUMMARY DESCRIPTION OF THE MELCOR CODE

Leak Path Factor analysis can be performed by developing and applying physically realistic modeling utilizing the U. S. Nuclear Regulatory Commission generalized mass transport and thermal-hydraulics computer program MELCOR 1.8.5, (Gauntt, 2000). MELCOR was initially developed at the Sandia National Laboratory under the sponsorship of the USNRC to assess reactor severe accident conditions. Subsequently both NRC and the DOE have sponsored changes to the code. For example, modifications were made to a version of MELCOR to model K reactor severe accidents at the DOE operated Savannah River Site. For the last several years, MELCOR has been used in the DOE complex to model release of radioactive airborne material from non-reactor facilities and structures. The leakage is usually expressed as a fraction of the amount considered available for release and is termed the Leak Path Factor.

MELCOR is a fully integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. MELCOR estimates fission product source terms and their sensitivities and uncertainties in a variety of applications.

The MELCOR code is composed of a number of major modules, or packages, that together model the major systems of a reactor plant and its generally coupled interactions. Many of these models are not required for LPF analyses. Nevertheless, the user should be aware of the existence of the many modules. Reactor plant systems and their response to off-normal or accident conditions include:

1. Thermal-hydraulic response of the primary reactor coolant system, the reactor cavity, the containment, and the confinement buildings

2. Core uncovering (loss of coolant), fuel heat-up, cladding oxidation, fuel degradation (loss of rod geometry), and core material melting and relocation

3. Heatup of reactor vessel lower head from relocated fuel materials and the thermal and mechanical loading and failure of the vessel lower head, and transfer of core materials to the reactor vessel cavity

4. Core-concrete attack and ensuing aerosol generation

5. In-vessel and ex-vessel hydrogen production, transport, and combustion

6. Fission product release (aerosol and vapor), transport, and deposition

7. Behavior of radioactive aerosols in the reactor containment building, including scrubbing in water pools, and aerosol mechanics in the containment atmosphere such as particle

agglomeration and gravitational settling, and the impact of engineered safety features on thermal-hydraulic and radionuclide behavior

The various code packages have been written using a carefully designed modular structure with well-defined interfaces between them. This allows the exchange of complete and consistent information among them so that all phenomena are explicitly coupled at every step.

MELCOR modeling is general and flexible, making use of a "control volume" approach in describing the plant system. No specific nodalization of a system is forced on the user, which allows a choice of the degree of detail appropriate to the task at hand.

The various modules (or packages) available in MELCOR are listed in Table 2-1 to give a good understanding of the full capabilities of the computer code.

Table 2-1. MELCOR Modules

MELCOR Modules (or Packages) Available	
Module Name	**Description**
BH	Bottom Head. This model was developed by the Oak Ridge National Laboratory, and is an alternative to the lower plenum modeling in COR
BUR	Burn (Combustion) of Gases. Compares conditions within control volumes against criteria for deflagrations and detonations. Initiates and propagates deflagrations involving hydrogen and carbon monoxide. Calculates burn completeness and flame speed
CAV	Core-concrete Interactions. CORCON-MOD3 with enhanced sensitivity analysis and multi-cavity capabilities
CF	Control Functions. Evaluates user-specified "control functions" and applies them to define or control various aspects of the computation such as opening and closing of valves; controlling plot, edit, and restart frequencies; defining new plot variables, etc.
COR	Core Behavior. Evaluates the behavior of the fuel and other core and lower plenum structures including heatup, candling, flow blockages, debris formation and relocation, bottom head failure, and release of core material to containment
CVH	Control Volume Hydrodynamics. In conjunction with the FL package, evaluates mass and energy flows between control volumes

MELCOR Modules (or Packages) Available	
Module Name	**Description**
CVT	CVT - Control Volume Thermodynamics. Evaluates the thermodynamic state within each control volume for the CVH package. No users' guide is written for this package since no user input is required. However, a reference manual is written.
DCH	Decay Heat. Used by other packages to evaluate decay heat power associated with radionuclide decay
EDF	External Data Files. Controls the reading and writing of large external data files, in close interface with the Control Function and Transfer Process packages
EOS	Equation of State. The CVT, H2O, and NCG packages are stored as one block of code under this name
ESF	Engineered Safety Features. Models the thermal-hydraulics of engineered safety features that cannot be effectively modeled by building appropriate components or systems using the CVH, FL, HS, and CF packages. Currently, only the fan cooler model is included in ESF; the containment sprays are modeled in the SPR package
EXEC	Executive Package. Controls execution of MELGEN and MELCOR
FDI	Fuel Dispersal Interactions. Models ex-vessel debris relocation, heat transfer, and oxidation due to fuel-coolant interactions and high pressure melt ejection
FL	Flow Paths. Models, in conjunction with the CVH package, the flow rates of gases and liquid water through the flow paths that connect control volumes
H2O	Water Properties. Evaluates the water properties based on the Keenan and Keyes equation of state extended to high temperatures using the JANAF data. This set of routines is in the "EOS" code package. No user input is required
HS	Heat Structures. Models the thermal response of heat structures and mass and heat transfer between heat structures and control volume pools and atmospheres. Treats conduction, condensation, convection, and radiation, as well as degassing of unlined concrete

MELCOR Modules (or Packages) Available	
Module Name	**Description**
MP	Material Properties. Evaluates the physical properties of materials for other packages except for common steam and noncondensible gas properties (see H2O and NCG)
NCG	NonCondensible Gas Equation of State. Evaluates the properties of noncondensible gas mixtures using an equation of state based on the JANAF data. This set of routines is in the "EOS" code package
PAR	Passive Autocatalytic Hydrogen Recombiner. Includes general models for modeling hydrogen recombiners in the containment rooms
PROG	Part of MELGEN/MELCOR Executive package separated for computer library and link purposes
RN	Radionuclide Behavior. Models radionuclide releases, aerosol and fission product vapor behavior, transport through flow paths, and removal due to ESFs. Allows for simplified chemistry
SPR	Sprays. Models the mass and heat transfer rates between spray droplets and control volumes
TF	Tabular Functions. Evaluates user-selected "tabular functions" to define or control various aspects of the computation such as mass and energy sources; integral decay heat; plot, edit, and restart frequencies, etc.
TP	Transfer Process. Controls the transfer of core debris between various packages and the associated transfer of radionuclides within the RN package. In order to transfer core material between packages, some TP input is required, and is described in the COR, FDI, and CAV package Users' Guides
UTIL	Utility Package. Contains various utilities employed by the rest of the code.

All the modules described in Table 2-1 above are fully documented in the MELCOR documentation, (Gauntt, 2000). The assessments made on the various models are also documented and are also cited in (Gauntt, 2000). The user is encouraged to review their documentation to have a better understanding of the full capabilities of MELCOR.

Although this computer code was developed to model the progression of accidents in light water reactor nuclear power plants, the modeling capabilities of MELCOR are sufficiently flexible that

it can be applied to the analysis of nonreactor problems. MELCOR was originally conceived as a Probabilistic Risk Assessment code. The code is now viewed as a primary tool for source term calculations.

When performing LPF studies for nonreactor nuclear facilities the modules used are reduced (through input specification – the code activates modules based on the input card identification field) to those which will enable the modeling of the release and transport of aerosolized materials. The most common modules used for Leak Path Factor analyses are:

- Executive Package (EXEC).
- NonCondensible Gas Package (NCG)
- Control Volume Hydrodynamics Package (CVH)
- Flow Path Package (FL)

Appendix A. Heat Structures Package (HS)

- RadioNuclide Package (RN)
- Control Function Package (CF)
- Tabular Function Package (TF)

MELCOR is available for the UNIX workstation platform as well as the PC platform. The execution of MELCOR on a PC is very efficient and user friendly. While either platform may be used, simply because of ease of use the latter is recommended.

Figure 2-1 depicts a basic flowchart showing the steps required to successfully execute MELCOR.

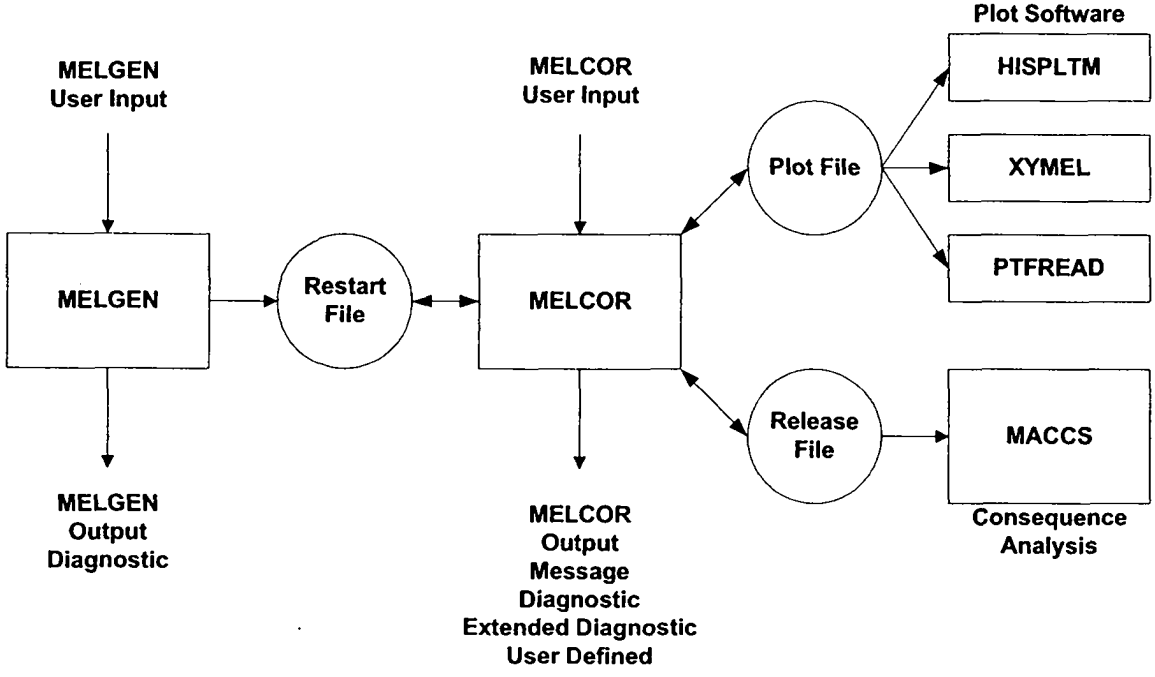

Figure 2-1. MELCOR Execution Flowchart

The user prepares an input data file which includes data for MELGEN and MELCOR. After running the two executables (MELGEN and MELCOR), all the output data files are created including a binary plot file (FILE.PTF) which can be used in one of three software packages provided to visualize the output graphically.

The plotting software distributed with MELCOR includes HISPLTM, XYMEL, and PTFREAD. The first package, HISPLTM, is an excellent plotting software package; however, it requires additional inputs (pre-planning by the user) in the main MELGEN/MELCOR input file to generate plots.

The two packages XYMEL and PTDREAD work very well and are recommended since they do not require any special inputs (as required for HISPLTM) in the main input file for MELGEN/MELCOR. These two latter packages work directly with the binary plot file generated by MELCOR. They provide for easy access to the various arrays the user desires to plot.

XYMEL software is equipped with a user-friendly interface and it allows the user to generate high quality plots via the XYMEL interface or by exporting that array to MS Excel.

PTFREAD is a MS Excel add-in (.XLA file) which is very simple to use and it can generate plots with the simplicity of a MS Excel interface.

The entire set of MELCOR documentation and additional information is available at the Sandia National Laboratory MELCOR website: http://melcor.sandia.gov/ .

3.0 APPLICABLE REGIMES IN ACCIDENT ANALYSIS

In accident analysis, the evaluation of the source term is an important step to assess the evaluation of the radiological consequences. The airborne source term is generally estimated using a five-component linear equation as reported in (DOE, 2002):

Source Term = MAR x DR x ARF x RF x LPF

Where:

MAR = Material-at-risk (curies or kg)
DR = Damage Ratio
ARF = Airborne Release Fraction
RF = Respirable Fraction
LPF = Leak Path Factor

A detailed discussion of the use of this formula in accident analyses is given in the MACCS guidance document and will not be repeated here, (DOE, 2003). See this guide for further detail.

With reference to a nonreactor nuclear facility (e.g., a building where forcing conditions could initiate releases of aerosolized radioactive materials), the LPF could be a critical component in the source term equation given above. The Leak Path Factor can be defined as the fraction of airborne radioactive material released, due to a forcing condition, as respirable particulate within the building that escapes via available pathways to the outside environment.

The MELCOR computer code is used to effectively evaluate the Leak Path Factor (LPF) component of the source term formula given above in mitigated design basis accident calculations as prescribed in DOE Std 3009 Rev 2, (DOE, 2002). For unmitigated analyses an LPF value of 1.0 is required by DOE Std. 3009.

4.0 DEFAULT INPUTS & RECOMMENDATIONS

The analysis of the Leak Path Factor for a facility (e.g., building) requires several front-end steps to be taken to assess the boundary of the problem as well as the modeling approximation approach.

When a facility (building) has to be analyzed it is important to gather the facility structural and architectural drawings. This first step is essential to model the facility with MELCOR.

MELCOR computer code uses a control volume approach, thus the facility (building) must be subdivided into control volumes (cells) connected by flow paths (flow junctions).

Depending on the type of accident condition, the facility is nodalized in different manners to properly model the event.

It is recommended to perform benchmark calculations to facility-specific operational test data when available to add confidence to the MELCOR analysis results.

4.1. Building Nodalization – Volumes and Flow Paths

In the case of a seismic-induced release, it is important to assess which structures within the facility will withstand the seismic event (i.e., walls, ceilings, etc.). When this assessment is made (e.g., by reviewing the structural analyses or discussing the subject matter with the structural engineering staff) the facility can be subdivided into cells formed by structures connected by flow paths. Any non-seismic (not seismically qualified) structure is not credited in the model (unless survival of the structure would increase the LPF).

One important aspect of this activity is to determine if the seismic event created penetrating cracks (or flow paths) though or around the qualified structures. This is important since these cracks provide a pathway for the released material to migrate to the outside environment. Furthermore it is of importance to evaluate possible pathways leading to the outside environment related to building penetrations (piping, ventilation ducts, electrical conduits, etc.).

The analyst must use good judgment in creating the various control volumes to assemble the facility nodalization model. It is recommended that the analyst keep the volumes within the same order of magnitude when possible. This helps by decreasing computational time. Very small volumes combined with larger volumes will increase the computational time since the small volumes will control the time-step advancement. If necessary, uniformity in nodalization can be achieved by combining smaller volumes. When nodalizing there is no specific rule to follow, the process is based on judgment acquired with experience. As a starting point for typical nodalization, Appendices C through G include input files demonstrating nodalization schemes that can act to steer the user in the correct direction.

The various flow paths to be used in a seismic event case are typically doors (normally closed or open, and doors opening/closing with a prescribed open area vs. time). Additional flow paths are the various penetrations mentioned above as well as any additional pathway within the building structure (section seams, joints, ducts, pipe chases, etc.) and pathways to the outside environment (failed vent lines, broken windows, severed pipes, roll-up doors, drains, etc.).

The ventilation system usually presents a challenge. If the ventilation system is seismically designed, an evaluation must be made to assess the various flows in and out of each cell. Generally it is not feasible to model the entire ducting system, but as explained later, fixed flows can be imposed to direct the ventilation flow where appropriate.

In the case of a fire-induced release an assessment has to be made to evaluate the various fire-rated walls. Once the analyst has knowledge of which structures will withstand the fire event, the steps discussed above still apply. That is, the analysts can build a nodalized model of the building under fire conditions with the appropriate initial and boundary conditions.

It has to be noted that the building model for a seismic event is not necessarily the same as the building model for a fire event. However, when an analysis has to be performed for a combined post-seismic and fire, the separate building seismic and fire models can usually be used without a significant alteration in nodalization or conditions. Examples in Appendices C to G illustrate typical problems for a model set up just for seismic, just for fire, and the combination of seismic and fire.

An important step for the Leak Path Factor analysis is the evaluation of the door gaps. In general we can assume that doors (single, double) have gaps all around the door frame. The gap under the door is generally wider. For the purpose of general analysis, gaps of about 0.00635 m (1/4 inch) average can be used all around the door(s) frames to evaluate the flow area. On a case-by-case basis door gaps can be smaller or bigger. The LPF results can be strongly dependent on these dimensions (especially for cases without forced ventilation) and correctly assessing these dimensions is important.

A facility walkdown is always recommended, to get information on doors gaps, etc. This is important since door sizes can vary or there can be non-standard doors. Table 4-1 shows some standard door clearances.

Table 4-1. Clearance Dimensions for Standard Steel Doors and Frames

Data from ANSI A250.8 -1998 SDI-100 "Recommended Specifications for Standard Steel Doors and Frames"	
Description	**Dimension**
Between door and head and jamb of frame	0.0032 m (1/8 inch)
Between bottom of door and sill	0.0191 m (3/4 inch)
Between face of door and door stop	0.00159 m (1/16 inch)

One more important aspect of the building modeling is to make an assessment of the emergency evacuation procedures (seismic and fire event). Facility personnel may crash through doors not normally used in order to exit in an emergency. Rescue personnel may enter to look for or

rescue injured individuals. Fire fighters may enter through non-standard doorways, and may drag hoses, or perform other emergency operations that change the flow paths available in the building. This assessment will enable the analyst to establish time-dependent operation of doors as input into the MELCOR analysis. This is critical for all the doors leading to the outside of the building. It is not uncommon, to find that the calculated LPF is dominated by the opening of a door if only for a short time.

The modeling of the environmental volumes is also important since these volumes will be used to compute the amount of aerosolized material escaped from the building enclosure, thus yielding the Leak Path Factor. The analyst can create as many environmental volumes as necessary. This volumes (cells) act as sources and sinks for the MELCOR analysis, thus they need to be large enough to maintain their environmental properties constant (e.g., pressure, temperature). It is generally recommended to set an environmental volume at each side of the building to input the appropriate pressure condition as dictated by the local wind. Additional environmental volumes can be set to model filtration systems, ventilation supply, or to monitor independently LPF contributions from different pathways to the outside environment. It is recommended large environmental volumes be used. A volume of 1.0E+10 m^3 is adequate.

Figure 4-1 shows a sketch outlining a typical building nodalization suitable for MELCOR analysis.

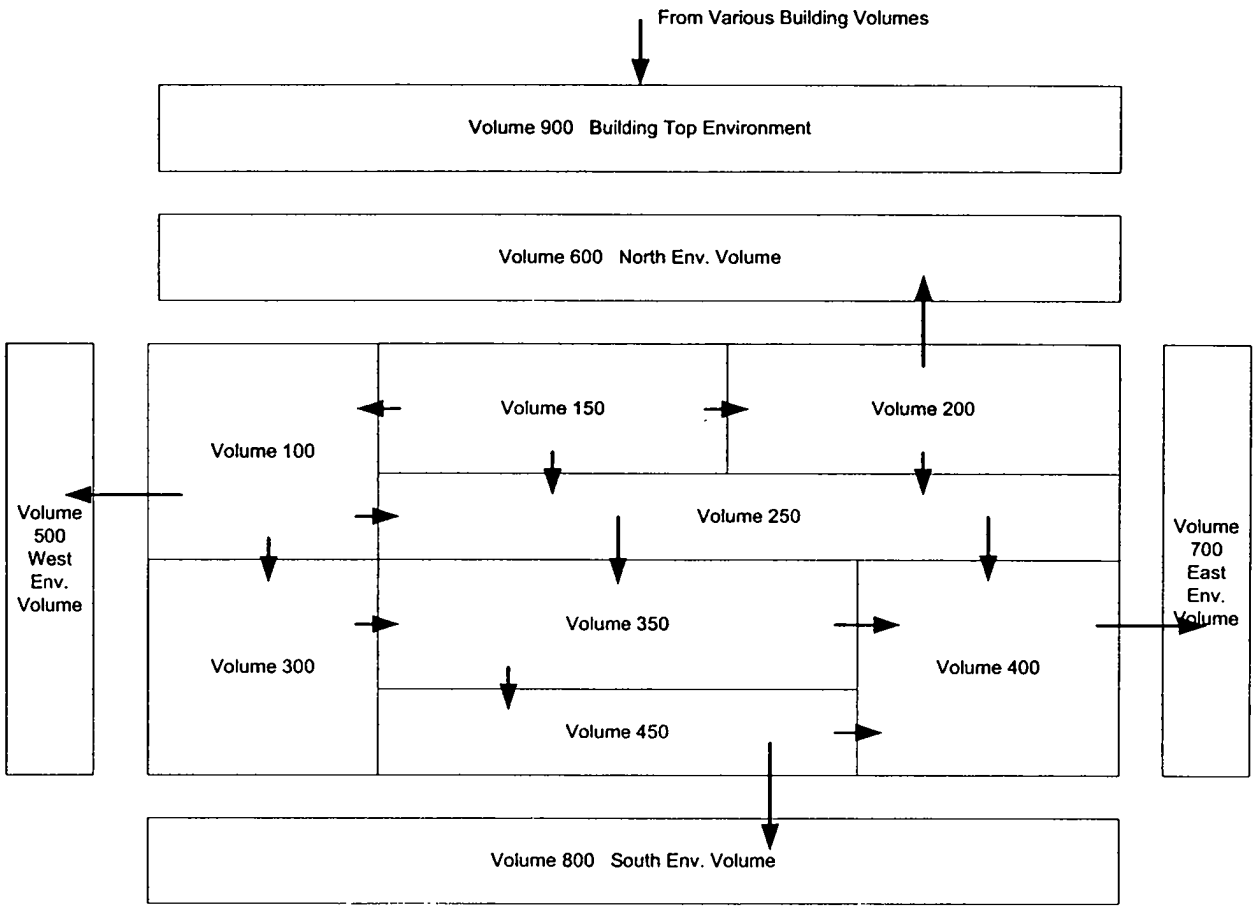

Figure 4-1. Typical Building Nodalization

The typical sketch depicted in Figure 4-1 will be useful when the Heat Structure module (HS) is used since it allows the analyst to easily associate the various heat structures for adjacent volumes when the heat transfer is modeled between building cells.

The analyst can also translate the sketch given in Figure 4-1 above into a basic building flow diagram to ease the various steps required to complete the MECOR flow modeling of the building.

Figure 4-2 shows a simple translation of the sketch given above into an effective flow model diagram to help the analyst in visualizing all the flow paths in a simpler representation.

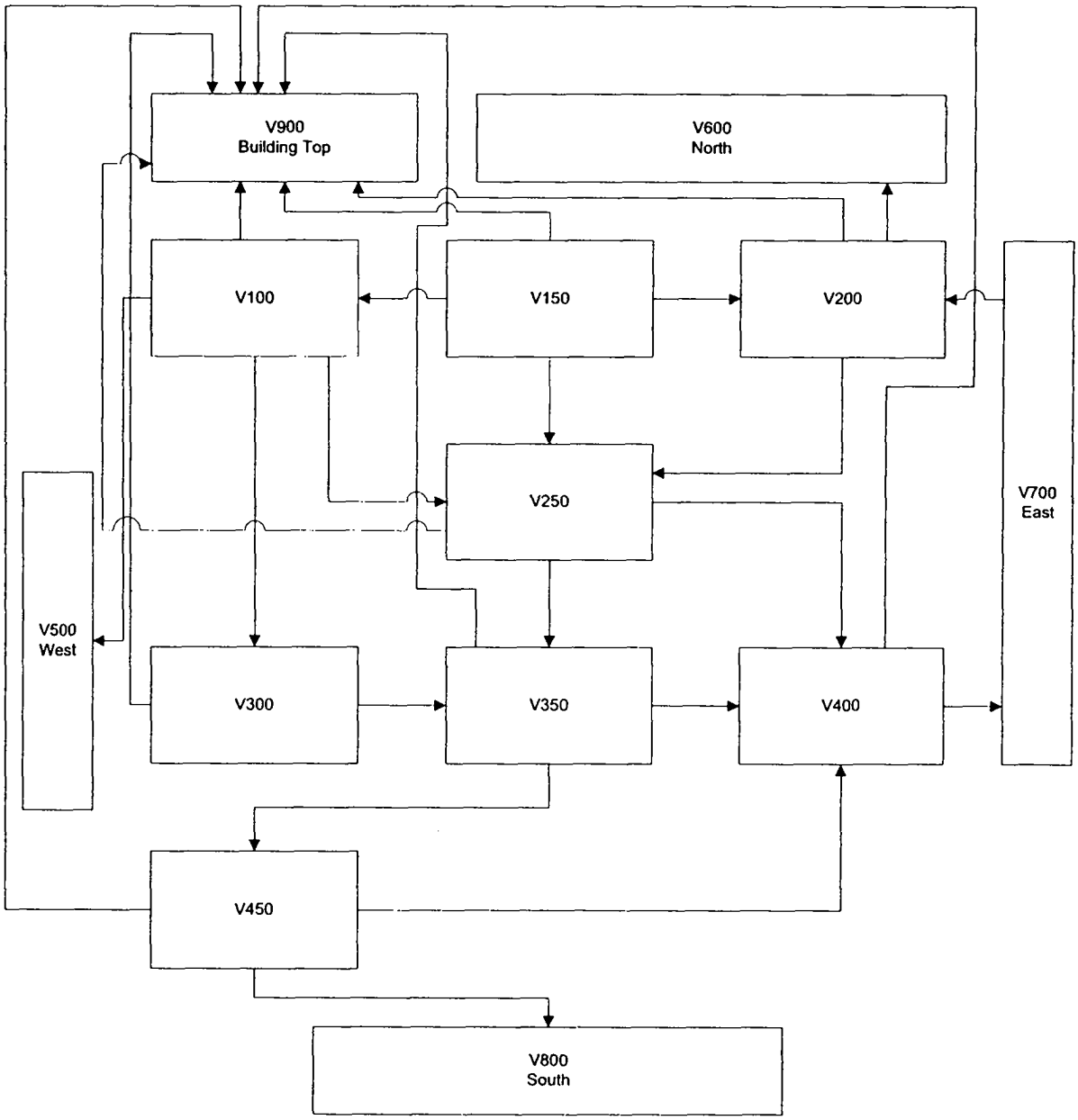

Figure 4-2. Typical Building Nodalization Flow Diagram

When two volumes (cells) are connected via a flow path like a pipe chase, or a long penetration (pipe-like), or any combination of small adjacent volumes, follow the instructions of the user's guide. Specifically, these flow paths should be lumped together into a single junction. MELCOR has a facility within the Flow Path Module (FL) that allows the user to model these flow paths with the piping segment input parameters.

4.2. Boundary and Initial Conditions

The equivalent wind pressure and temperature to be applied to the environmental volumes (boundary volumes) can be readily calculated. The analyst must have knowledge of the site meteorology. The parameters required are the wind speed and wind direction (the recommended wind speed is the same as used in the consequence analysis to maintain consistency). Once the wind speed, direction, and environmental temperatures are available, it is possible to evaluate the equivalent wind pressure to be applied to the environmental volumes.

The local air pressure due to wind condition is given by, (ASHRAE, 1977):

$$\Delta P = c_p \rho \frac{v^2}{2}$$

where:

c_p = Pressure coefficient
ρ = Local air density
v = Wind speed

Assuming a value for the wind speed of 2.24 m/s (5 mph), and using a pressure coefficient for a normal building from, (ASHRAE, 1977):

Table 4-2. Typical Building Wind Pressure Coefficients

Wind Pressure Coefficients	
Upwind Pressure Coefficient	0.7
Downwind Pressure Coefficient	-0.4
Side and Top of Building	-0.35

Using the above wind pressure coefficients and an assumed environmental volume temperature of 294.26 K (70 °F), and local air density of 1.2 kg/m^3, the resulting wind pressure is shown in Table 4-3.

Table 4-3. ΔP and Absolute Pressure on a Building

ΔP and Absolute Pressure for the Environmental Volumes—Normal Atmospheric Pressure set at 101352.9 Pa (14.7 psia), Wind speed 2.24 m/sec		
	ΔP Pa	Absolute Pressure[1] Pa
Upwind Side of Building	2.10	101355.00
Downwind Side of Building	-1.2	101351.69
Side and Top of Building	-1.051	101351.85

[1] Note that the 14.7 psia atmospheric pressure is an approximation and the user should use the site specific pressure

The absolute pressures and the reference temperature of 294.26 K (70 °F) are used as input in the environmental volumes initial conditions.

The values of the pressures given in Table 4-3 show that the actual pressure differentials across the building due to wind condition are very small, but large enough to promote the transport of aerosolized material within the building and finally to the outside environment. These pressures must be calculated on a case-by-case basis, and analyses should be performed by rotating the wind direction through the boundary volumes to assess the bounding LPF.

4.3. Aerosol Modeling

The MELCOR aerosol input to evaluate a Leak Path Factor is critical. The aerosol dynamics algorithms included in MELCOR are robust, however the analyst has to properly identify inputs to yield a consistent solution. It is very important to handle this part of the MELCOR input extremely carefully.

In many DOE facilities the major player is Pu oxide. For this particular material, when in a powder form, there is good information available for input into a MELCOR analysis. For other materials, parametric studies and various assessments may be required to analyze a leak path factor.

The MELCOR computer code input requires a distribution of aerosolized particles. The most-likely distribution is a lognormal since actual particle size typically extends through several orders of magnitude.

The lognormal distribution of aerosolized particles used by MELCOR (Probability Density Function, PDF) is

$$PDF = \frac{1}{\sqrt{2\pi}\, d_p \ln(\sigma)} e^{-\frac{1}{2}\frac{\ln^2(d_p/d_m)}{\ln^2(\sigma)}}$$

Where:

d_p is the distributed variable particle diameter,
d_m is the volume-equivalent mass median particle diameter, and
σ is the geometric standard deviation

When dealing with PuO_2 powders some experimental data are available from (Sutter, 1981). Table 4-4 reports an experimentally gained distribution from the above reference, which is specific to free fall spill in static air and it could represent a distribution in a seismic event.

Table 4-4. Oxide Powders Particle Size Distribution

Oxide Powders Particle Size Distribution Spill in Static Air Weight percent airborne 0.03% median (equivalent to ARF) Geometric Standard deviation = 2 (lognormal distribution) Particle size median = 8 μm (Aerodynamic Equivalent Diameter (AED))					
Particle Diameter Range μm AED		**Particle Diameter Range μm**		**Fraction in Range**	**Cumulative Fraction**
0.0	0.1	0.00	0.03	0.001	0.001
0.1	1.0	0.03	0.30	0.064	0.065
1.0	3.0	0.30	0.89	0.165	0.230
3.0	10.0	0.89	2.95	0.330	0.560
10.0	70.0	2.95	20.68	0.360	0.920
70.0	200.0	20.68	59.08	0.040	0.960
200.0	1000.0	59.08	295.40	0.030	0.990
> 1000.0		> 295.40		0.01	1.00

With the data given in Table 4-4 and using a theoretical density for the PuO_2 of 11.46E+3 kg/m^3, (CRC, 1986), the following discussion on the Aerodynamic Equivalent Diameter is given:

The aerodynamic equivalent diameter (AED) to be considered in the respirable range is ≤ 10 μm, and the D_{AED} specifically refers to an equivalent sphere with a density of 1 g/cm^3.

The particle Geometric Diameter D_g is related to the D_{AED} by the following equation described in (DOE, 2002):

$$D_{AED} = \left(D_g \left[\rho_p\right]^{0.5} \left[C_{C,e} / C_{C,a}\right]^{0.5}\right) / \alpha$$

Where:

ρ_p = Particle density (g/cm^3)
$C_{C,e}$ = Cunningham slip factor corresponding to volume equivalent diameter
$C_{C,a}$ = Cunningham slip factor corresponding to the aerodynamic equivalent diameter, and
α = Aerodynamic shape factor.

The Cunningham slip factor is related to the potential for particle impact with the mean free path of air molecules. Above the sub-micron size range, all particles impact with air molecules, and the ratio of Cunningham factors can be ignored. The aerodynamic shape factor is not typically known and is assumed to be 1. Therefore, D_{AED} may be estimated from D_g by simply multiplying D_g by the square root of the particle density. The maximum Aerodynamic Equivalent Diameter of 10 μm for Plutonium Oxide with a density of 11.46 g/cm^3 corresponds to a maximum geometric diameter of approximately 3 μm.

With this information and the PDF function given above, a lognormal distribution can be built.

Maximum aerosol particle diameter = 3 μm
Minimum aerosol particle diameter = 0.01 μm (this is an arbitrary minimum)
Volume-equivalent mass median particle diameter = 2.3 μm (8 μm AED)
Geometric standard deviation of the particle size distribution = 2 (95%)

With these data approximately 63% of the airborne particles distribution is smaller than 3 μm (10 μm Aerodynamic Equivalent Diameter) and are respirable.

Figure 4-3 shows the distribution as discussed above to be used as an initial aerosol distribution.

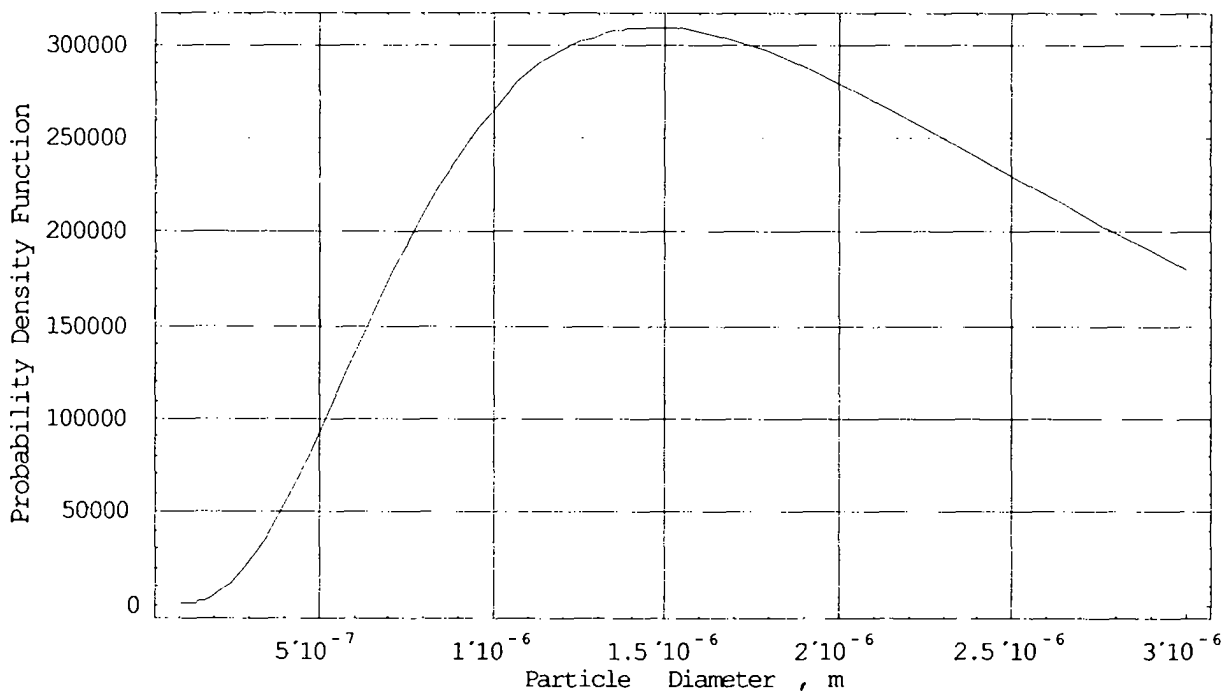

Figure 4-3. Lognormal Particle Diameter Distribution of PuO2

Note that the above distribution of aerosolized powders used as MELCOR input is all respirable (maximum aerosol particle diameter ≤ 10 μm AED). This is important since when combining the calculated LPF value in the source term five-component equation it results in consistency among the terms (the LPF is a multiplier of ARF x RF which is already all respirable).

If the analyst uses a distribution that extends beyond the 10 μm AED, the RF will be double counted, thus making the source term inconsistent.

Other experimental distributions for various events can be found in (Sutter, 1983, SNL, 1983, and Mishima, 1973).

If there is no experimental information available for the aerosolized material, parametric studies to assess possible distributions are recommended.

For conservatism, a material density of 1 g/cm^3 could be used. With this density the maximum respirable particle diameter is 10 μm geometric or 10 μm AED. From this a distribution can be built, but the volume-equivalent mass median particle diameter is not known. Figure 4-4 shows how the volume-equivalent mass median particle diameter changes the distribution.

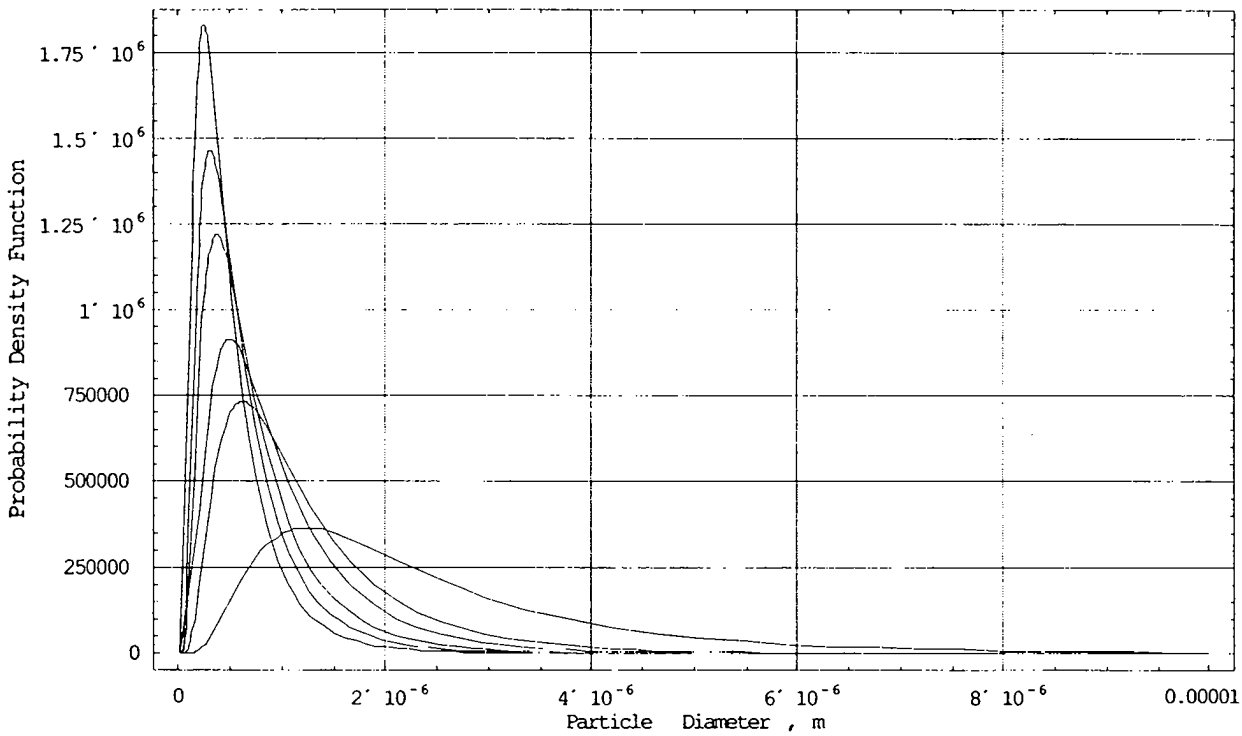

Figure 4-4. Volume-equivalent Mass Median Particle Diameter Influence on Lognormal Particle Distribution

This figure shows how the peak of the distribution shifts to the right for an increase of the volume-equivalent mass median particle diameter. The higher peak corresponds to a 0.5 μm volume-equivalent mass median particle diameter, and the lower peak to 5.0 μm. The intermediate values correspond to 1.0, 2.0, 3.0, and 4.0 μm respectively.

If a small volume-equivalent mass median particle diameter is chosen the LPF value will increase. It is evident that the determination of an appropriate volume-equivalent mass median particle diameter is quite complicated, and further studies would be required to properly justify an appropriate assumed analysis value of the volume-equivalent mass median particle diameter.

Figure 4-5 reports Figure 4-4 curves in semi-log scale to better render the curves.

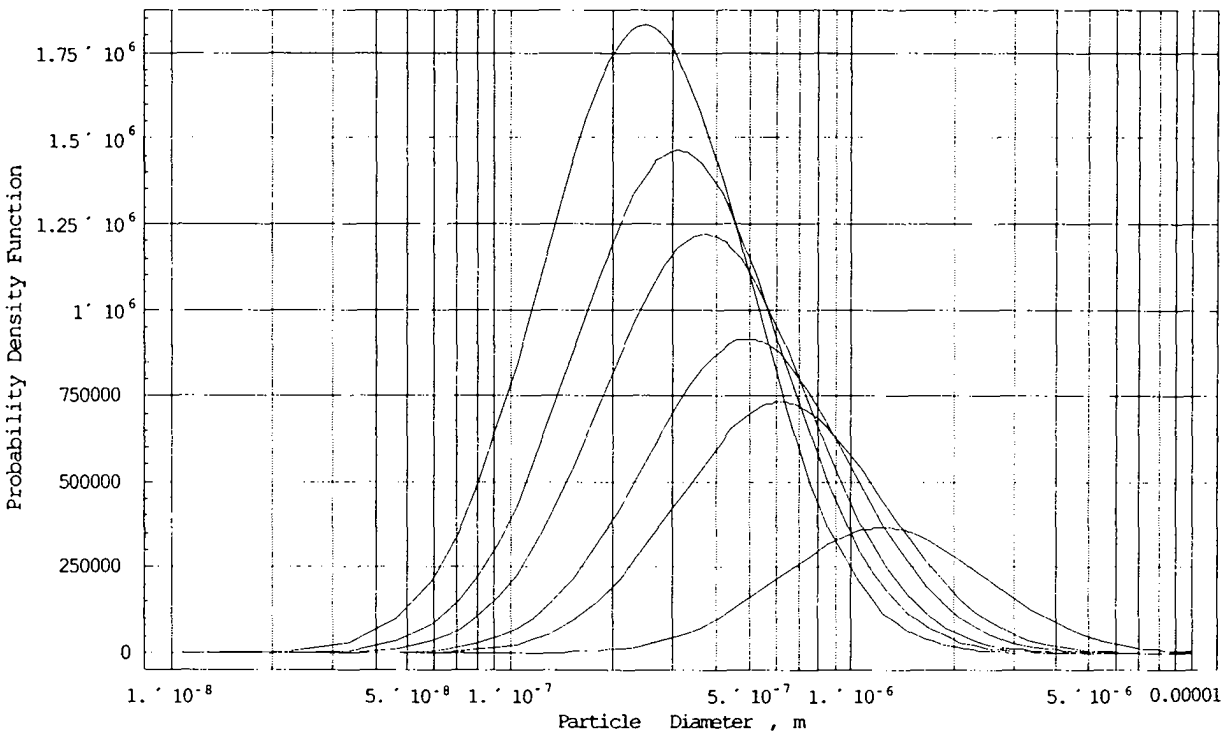

Figure 4-5. Volume-equivalent Mass Median Particle Diameter Influence on Lognormal Particle Distribution (Semi-log X-scale)

An additional MELCOR input is the amount of aerosolized material released in the facility (building). This input can be set as a tabular function (TF module) were the amount of material (kg) is input versus time.

Generally the analysis of the LPF can be performed prior to the establishment of the magnitude of the source term (MAR x DR x ARF x RF). That is, the aerosolized material released can be set conveniently to a unit weight (1.0 kg, or 1.0 g). This is a convenient way to easily express the LPF as a fraction of the released material, thus generalizing its definition to any amount of material actually released inside the facility.

A typical MELCOR input could be a triangular or rectangular normalized distribution as shown in the following Tables and Figures.

Table 4-4. Triangular Mass Spill Distribution

Triangular Mass Spill Distribution	
Time s	Spilled Mass kg
0.0	0.0
5.0	0.0
6.0	1.0
7.0	0.0
10.0	0.0

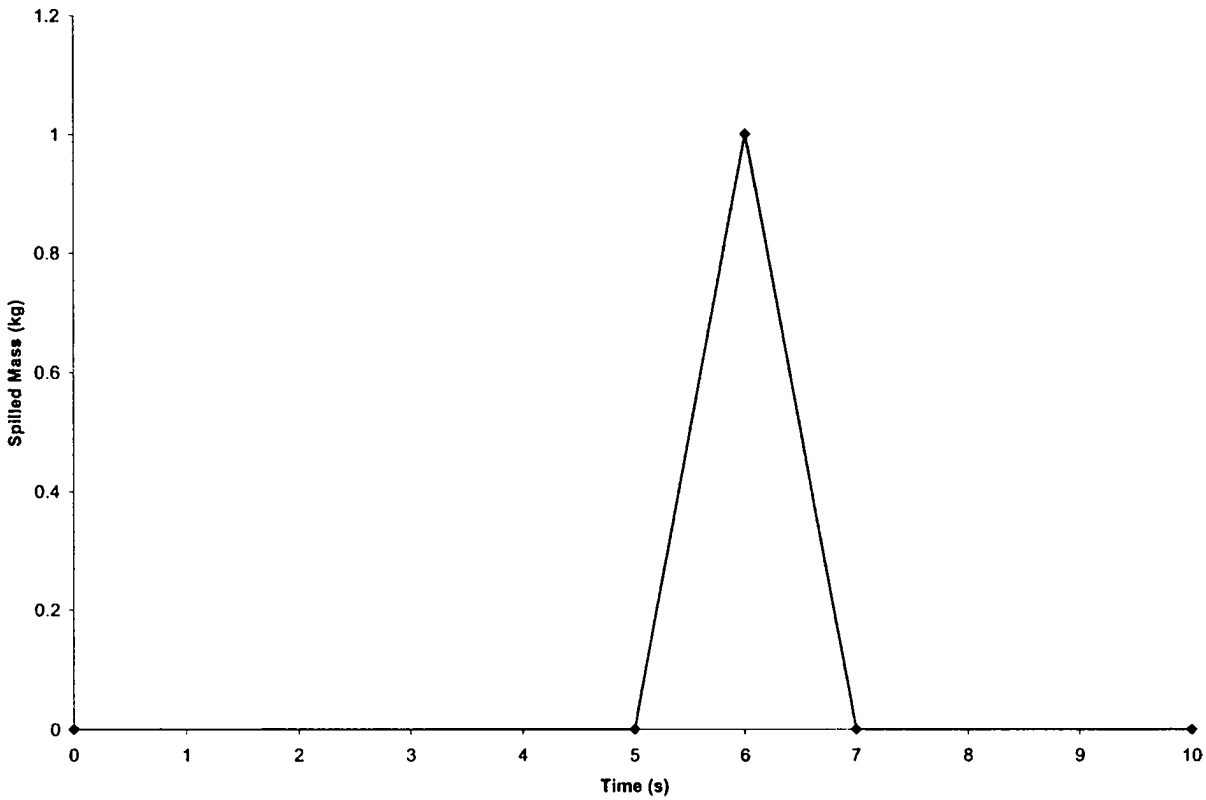

Figure 4-6. Triangular Spilled Mass versus Time Distribution

Table 4-5. Rectangular Mass Spill Distribution

Rectangular Mass Spill Distribution	
Time s	Spilled Mass kg
0.0	0.0
1.0	0.0
1.0	0.5
3.0	0.5
3.0	0.0
5.0	0.0

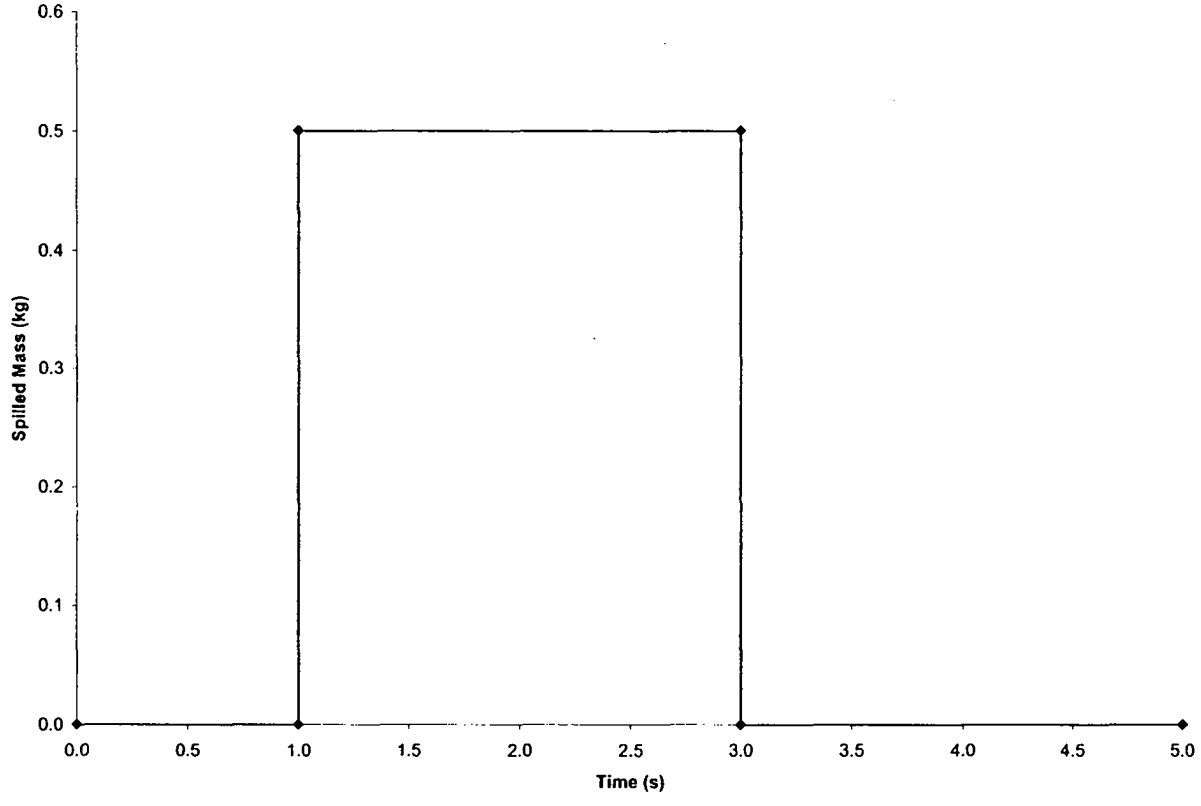

Figure 4-7. Rectangular Spilled Mass versus Time Distribution

One important aspect in the aerosol MELCOR input is the amount of material to be released as aerosol into a cell. The amount of aerosolized material initially present in a MELCOR cell contributes to the agglomeration (coagulation) of aerosol particles. If a large amount of material is present in a cell, the deposition of aerosol due to gravitational settling is enhanced. This is

important when the analyst does not know *a priori* the source term, and consequently, the LPF analysis must be performed with a nominal release of an aerosolized mass (1.0 kg, 1.0 g).

Figure 4-8 shows how the LPF value for a seismic case (aerosol released in static air) varies with increasing released masses; figure from (Polizzi, 2000), analysis performed using CONTAIN 2.0 computer code, (Murata, 1977).

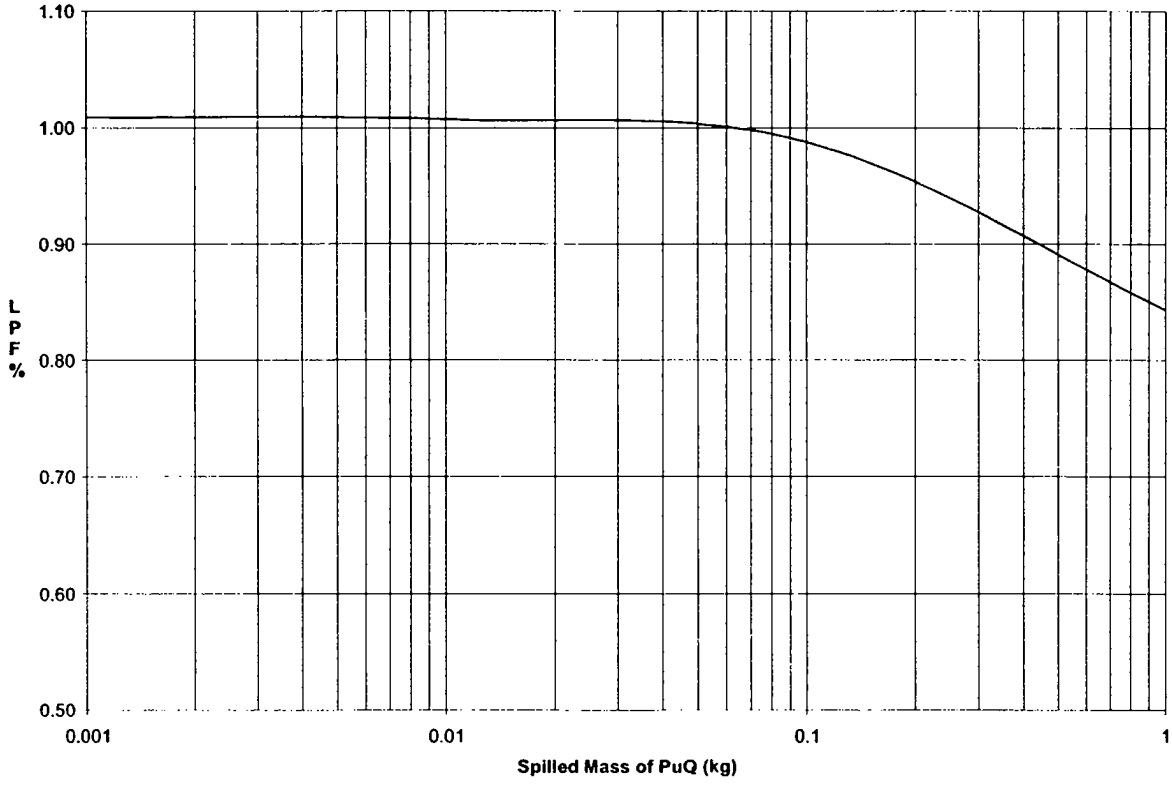

Figure 4-8. Influence of Released Mass on LPF

This figure is significant and the analyst should perform a similar sensitivity analysis for each unique LPF evaluation. The results given above cannot be generalized since the magnitude of the LPF variation with the released mass is specific to the initiating event, the forcing condition, etc. (e.g., in the case of a fire initiator, the variation of LPF with mass is most likely insignificant).

Unit mass releases are convenient and can be applied as already stated when the source term is not known. However, because of the mass effect indicated in Figure 4-8, if the analyst knows the actual source term injected into a volume, it is recommended the actual value be used.

In this situation with releases in multiple cells are taking place, and the actual source term in not yet available at the time of the LPF analysis, it is even more important to perform parametric studies. The interaction between initial source term in cells, flow between cells, and other phenomena may not be intuitive. Within the range of credibility, the user should vary the amount of release in various cells to assure the problem is fully understood, (Polizzi, 2002).

4.4. Fire Modeling

Melcor cannot explicitly model the physics of a fire. A fire can be approximately modeled in MELCOR by simply adding mass and energy into a cell(s). Adding energy to the systemgenerates pressure and temperature in the cell(s), which in turn acts as a forcing condition causing leakage of the aerosolized mass present in the cell(s).

The fire modeling is accomplished by using a combination of MELCOR Control Functions (CF) and Tabular Functions (TF) modules which will enable the analyst to input the fire model parameter in a tabular form.

A recommended approach to use when modeling a fire is to add into a cell(s) a rated mass of material such as water vapor or other gas at a rated enthalpy. (ie.g., add minimal mass at fictionally high but properly accounted for enthalpy) In this way, the mass can be minimized and the product of the two rated entities becomes the desired energy input into the system.

If the intent is to input a fire burning at 1.0 Mw for 30 minutes, Table 4-6 shows the rated mass and enthalpy to generate the fire.

Table 4-6. Typical Fire Input

Typical Fire Input			
Time	Mass	Enthalpy	Energy
s	kg/s	J/kg	W
0.0	0.0	0.0	0.0
300.0	0.0	0.0	0.0
600.0	0.001	1.0E+9	1.0E+6
2400.0	0.001	1.0E+9	1.0E+6
2700.0	0.0	0.0	0.0
5000.0	0.0	0.0	0.0

Figure 4-9 shows the typical fire as given in Table 4-6.

The correct intensity of the fire and duration will be dependent upon a specific fire analysis. Generally, the more intense the fire, the higher the LPF, and the longer duration the fire, the higher the LPF. However, this is not always true. The analysts should run parametric studies to assess the influence of the varying inputs to understand the specific problem and determine the appropriate LPF.

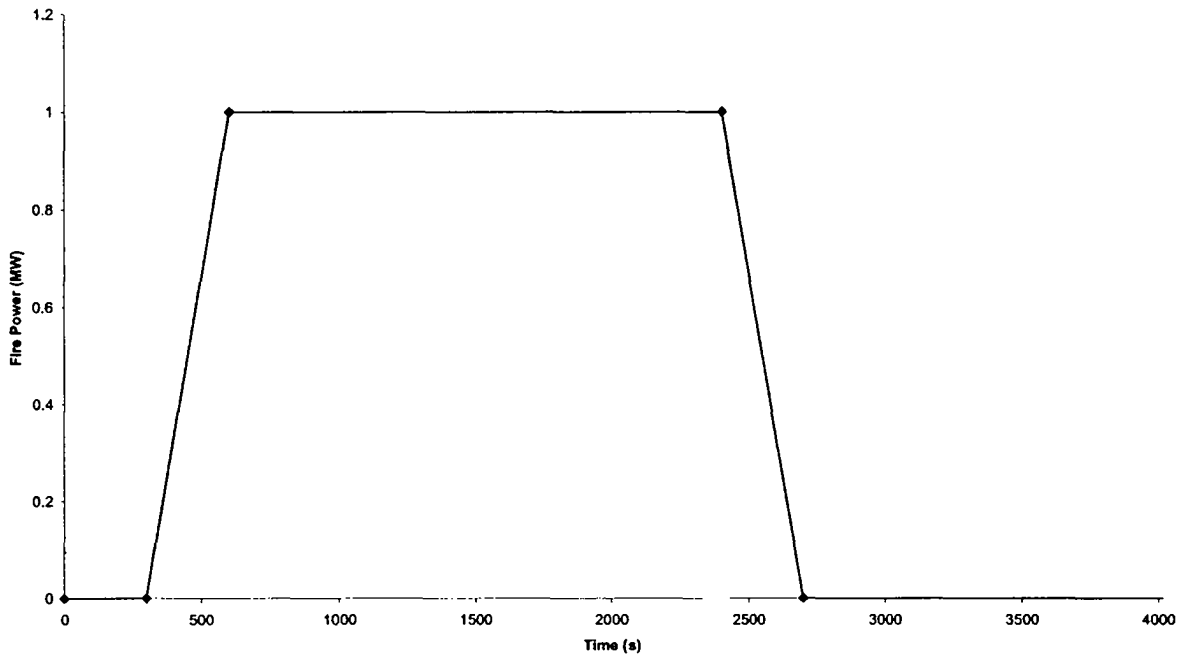

Figure 4-9. Typical Fire Input — Fire Power Versus Time

As mentioned above, MELCOR does not model the physics of the fire event, but uses an energy input to simulate the fire energy addition into a cell (volume). The actual fire analysis can produce the data required to model the fire. The fire analysis could produce a temperature profile vs. time in the room; the analysts can try to reproduce that profile by running MELCOR, predicting an energy input into the cell and then adjusting until the temperature profile is similar to the one originally calculated by the actual fire analysis.

It has to be noted that instead of using the method mentioned above, the analyst could use the potential energy due to the combustible material. This will generate unrealistically high temperature in the fire cells, but it should be conservative.

During the combustion process for most of the fires encountered in accident analysis, the production of combustion gases can be neglected. The dominant mechanism to transport aerosols out of the fire cell are the convective flows which are driven by density gradients in the fire compartment and hot gas expansion early in the fire.

4.5. Heat Structures Modeling

The heat structures models within MELCOR are required to define the heat transfer between the various heat structures present in each cell (volume) of the building model.

Each MELCOR cell will generally have a floor structure, a ceiling structure, and wall structures. In a MELCOR cell there could be various structures so that the heat transfer between adjacent

cells can be modeled. Generally speaking, structure heat transfer has little influence on the LPF. This is because ventilation and flow conditions tend to dominate the release, and usually, heat transfer to structures has little effect on the flows in the facility. (There may be exceptions to this general statement for unique analyses, for example, when a fire is on the cusp of causing a flow reversal to the outside environment and the heat sinks make the difference.)

When dealing with a seismic event (no fire) the maximum temperature variation is the difference between the building inside and outside. This difference does not play an important role in LPF determination because the heat transfer across the thickness of a wall, floor, or ceiling is second order to other leakage forcing functions (wind, ventilation).

In a case were there is forced ventilation, the heat transfer is second or third order in importance since the aerosolized mass transport from the building is quite fast and the heat transfer lags behind.

The MELCOR input for the heat structures is relatively straightforward and self-explanatory in the user's guide. See the users guide for detail.

The most important aspect of the heat structures modeling has more to do with the introduction of surface area for aerosol interactions than it does with heat transfer. Heat structure modeling introduces structures into the cells where the various aerosol deposition mechanisms will work by depositing aerosolized masses transported through the building. Thus, the user should pay attention to the heat structure surface area dimensions. (Especially horizontally facing upward) These dimensions are related to the amount of aerosolized masses that will be deposited. Gross error on the determination of these surface areas could negatively affect the values of the LPF.

Particular attention must be given when modeling the environmental volumes, when the LPF is calculated. In these external cells (environmental volumes), MELCOR collects all the aerosolized material transported out of the building. The user should model a fictitious structure for each of the volumes representing the outside environment (e.g., a floor structure with a nominal floor area of 0.001 m^2) so that practically all the aerosolized mass will be distributed in the cell volume and nothing deposited. This will enable the analyst to very simply account for the fraction of masses transported out of the building. See Section 7.0 for more detail.

Appendix A includes a brief description of the few steps required to execute MELCOR on a Personal Computer.

4.6. MELCOR Benchmarks

Few benchmark samples were executed with MELCOR to compare its results with the same samples nodeled with CONTAIN 2.0 computer code (Murata, 1977). In all cases the resulting LPF were basically identical. Appendix B shows the sample problems used for the benchmark and the resulting LPF.

5.0 SPECIAL CONDITIONS FOR USE OF SOFTWARE

The MELCOR code has many additional capabilities that generally are not used in standard DSA applications. The leak path factor is only an application of the code to utilize its robust aerosol dynamics models.

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6.0 SOFTWARE LIMITATIONS

The MELCOR compute code was developed to model the progression of accidents in light water nuclear power plants. The code is not ideally suited to analyze processes such as fluid flow in piping and ducting systems networks.

Because of the above limitation, when analyzing ventilation systems in buildings, the user should not model the ventilation ducts to credit deposition of aerosolized masses. The deposition, if any, will be generally negligible in comparison to the deposition in the rest of the building, the inclusion of such modeling will considerably increase the computational time, and the results will not be appreciably affected.

If the purpose of the MELCOR analysis is to understand the time-history of HEPA filters exposure to temperature (e.g., fire events), the inclusion the ventilation ducts model and heat structures in the ventilation control volumes is proper and necessary.

6.1. Outcome of Gap Analysis

A gap analysis of Version 1.8.5 of the MELCOR code has been completed (DOE, 2004). The gap analysis reviewed the program, practices, and procedures associated with development of MELCOR compared with NQA-1-based requirements as contained in U.S. Department of Energy, Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes, (DOE, 2003e). It was determined that MELCOR code does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of MELCOR for supporting safety analysis. Informed use of the software can be assisted by the current set of MELCOR reports (refer to Table 1-3), and the code guidance report for DOE safety analysts, *MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis*, (DOE, 2003f). Furthermore, while SQA improvement actions are recommended for MELCOR, no evidence has been found of programming, logic, or other types of software errors in MELCOR that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

Of the ten primary SQA requirements for existing software at the Level B classification ("important for safety analysis but whose output is not applied without further review"), five requirements are met at acceptable level, i.e., *Software Classification, Implementation Phase, User Instructions*, *Acceptance Test,* and *Configuration Control*; Requirements 1, 5, 7, 8, and 9 respectively. Improvement actions are recommended to meet SQA criteria for the remaining five requirements, and are summarized in Table 6-1. This evaluation outcome is deemed acceptable because: (1) MELCOR is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of MELCOR is limited to those analytic applications for which the software is intended.

By order of priority, it is recommended that MELCOR software improvement actions be taken, especially:

1. Correcting known defects in the SQA process
2. Upgrading existing SQA documentation
3. Providing training on a regular basis, and
4. Revising and developing new software documentation.

A new software baseline set of documents is recommended for MELCOR to demonstrate completion of the revision to software documentation item (above). The list of revised baseline documents includes:

- Updated Software Quality Assurance Plan
- Software Requirements Document (Specific to LPF)
- Software Design Document (Specific to LPF)
- Test Case Description and Report (Specific to LPF)
- Updated Software Configuration and Control
- Updated Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

Approximately two full-time equivalent years is conservatively estimated to upgrade MELCOR software to be compliant with NQA-1-based requirements for existing software. While most of this effort is logically to be used by the code developer, independent review of the end products is necessary.

A new version of MELCOR is planned for release in the future. It is recommended that this version be evaluated upon issue relative to the software improvement and baseline recommendations, as well as the full set of SQA criteria discussed in this report. If this version is found to be satisfactory, it should replace Version 1.8.5 as the designated version of the software for the toolbox.

Approximately one FTE-month per year would be needed to maintain a web-based error notification and corrective action process for MELCOR (Section 4.10). However, such a process has not been defined in depth for MELCOR and the other designated toolbox codes.

Table 6-1. Summary of Important Exceptions, Reasoning, and Suggested Remediation

No.	Criterion (Section refers to Gap Analysis Report for MELCOR, (DOE, 2004))	Reason Not Met	Remedial Action(s)
1.	SQA Procedures/Plans (Section 4.2)	SQA Plan and Procedures for Version 1.8.5 of MELCOR software were lacking components to match present day requirements. Portions of the existing version are out of date or are not currently followed.	As part of the new software baseline, the SQA Plan covering version 1.8.5 and successor versions of MELCOR should be provided to the Central Registry. SQA procedures that provide prescriptive guidance to the MELCOR software developers should be made available to a SQA evaluator for confirmatory review.
			Establish a written and approved SQA plan eliminating draft or non-compliant informal processes of development.
			Upgrade SQA program documentation, especially those procedures used for new features added in MELCOR that have an effect on modules that are typically used in LPF applications. Ensure prompt defect/error reporting.
2.	Requirements Phase (Section 4.3)	A Software Requirements Document for Version 1.8.5 of MELCOR is not available.	As part of the new software baseline for MELCOR, a Software Requirements Document should be prepared.
3.	Design Phase (Section 4.4)	A Software Design Document is not available. Thus, design information was not directly available. Instead, it was necessary to infer the intent of MELCOR design from model description and user guidance documents.	As part of the new software baseline for MELCOR, a Software Design Document should be prepared.
4.	Testing Phase (Section 4.6)	A Software Testing Report Document has not been produced for MELCOR, and therefore, test process and methodology could not be evaluated directly. Thus, testing process and methods had to be inferred from other information. Isolated validation studies have been previously documented for various phenomenological areas, including aerosol transport, which is the key area for LPF applications. While these studies promote confidence in the models for LPF applications, the necessary formality is lacking to make a complete evaluation.	As part of the new software baseline for MELCOR, a test case report should be prepared. An important part of the new baseline set of documentation should specifically address aerosol transport phenomena and LPF applications.

No.	Criterion (Section refers to Gap Analysis Report for MELCOR, (DOE, 2004))	Reason Not Met	Remedial Action(s)
5.	Error Notification (Section 4.10)	An Error Notification and Corrective Action Report process is in place at SNL, but limited documentation is available. Users are not necessarily notified of errors. Follow up with the notifying agent is not always guaranteed, and the impact is not always assessed and reported.	While a Software Problem Reporting system is in place at SNL, it requires revision to ensure affected users are notified, closure occurs with the originator, and impact determinations are completed promptly.

Reference: (DOE, 2004)

7.0 SAMPLE CALCULATIONS APPLYING SOFTWARE

This section of the document includes few sample problems covering several accident conditions of interest. These samples show how the various volumes, flow path, heat structure, and aerosolized material inputs are structured so that a user can easily modify them to fit their problems. The analyst will find a comprehensive discussion on the specific MELCOR modeling in the code user's and documentation guides, (Gauntt, 2000).

7.1. Building Seismic Event with Powder Spill

This sample problem involves a building surviving a seismic event. There is a spill of PuO_2 powder and the forcing condition driving the aerosolized material out of the building is the wind pressure only.

Figure 7-1 below is a simple model of a typical building that survives a seismic event.

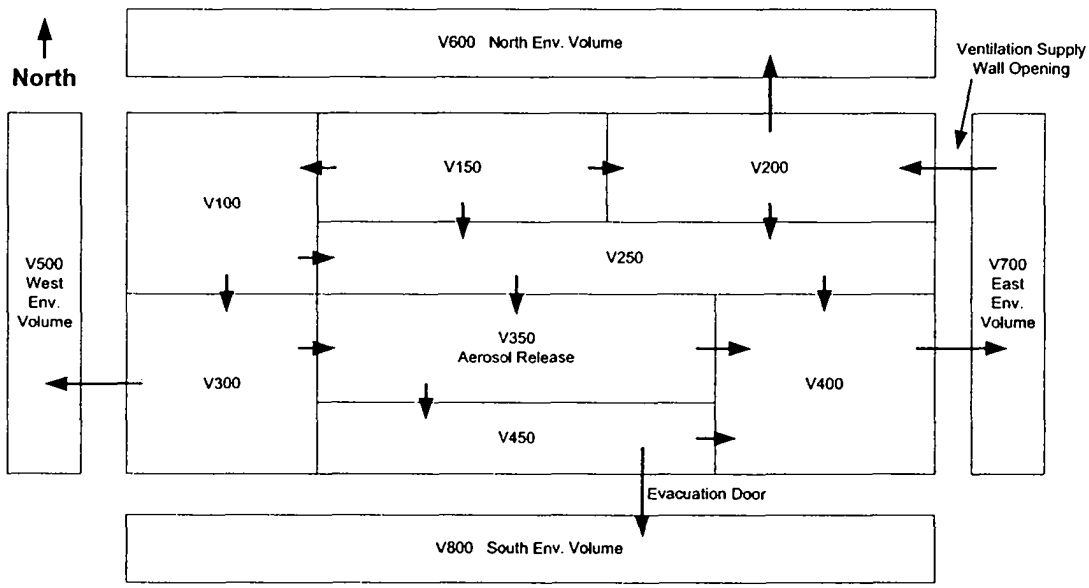

Figure 7-1. Seismic Problem — Building Simple Nodalization Model

In this sample problem the PuO_2 powder is spilled in volume 350, the wind speed used is 2.24 m/s (5 mph), and the wind direction is from East[2]. The building environmental temperature is arbitrarily selected to be uniform at 294 K (70 °F).

The volumes no. 500, 600, 700, and 800 are environmental volumes (external volumes) representing the four sides of the building.

[2] The user would have to analyze the worst wind direction. In this sample the East direction was arbitrary.

Table 7-1 gives the geometrical dimensions used for this simple model

Table 7-1. Seismic Problem Building Dimensions

Building Dimensions				
Volume No.	Length m	Width m	Height m	Volume m^3
100	15.2	18.3	4.0	1104.4
150	25.9	16.5	4.0	1689.7
200	25.9	16.5	4.0	1689.7
250	51.8	1.8	4.0	375.5
300	13.7	15.2	4.0	828.3
350	30.5	10.7	4.0	1288.4
400	21.3	13.7	4.0	1159.6
450	30.5	3.0	4.0	368.1
500	N/A	N/A	N/A	1.00E+10
600	N/A	N/A	N/A	1.00E+10
700	N/A	N/A	N/A	1.00E+10
800	N/A	N/A	N/A	1.00E+10

The pressure inside the building is assumed to be atmospheric, 101352.9 Pa (14.7 psia). The equivalent wind pressure, applied to the environmental volumes No. 500, 600, 700, and 800, is given it Table 7-2.

Table 7-2. Seismic Problem Environmental Volumes Pressure

Environmental Volumes Pressure		
Volume No.	Pressure Ps	Pressure psia
500	101351.6992	(14.69982)
600	101351.8493	(14.69984)
700	101355.0013	(14.7)
800	101351.8493	(14.69984)

A flow diagram of the building depicted in Figure 7-1 above is given in Figure 7-2, where the full connectivity of all cells is outlined.

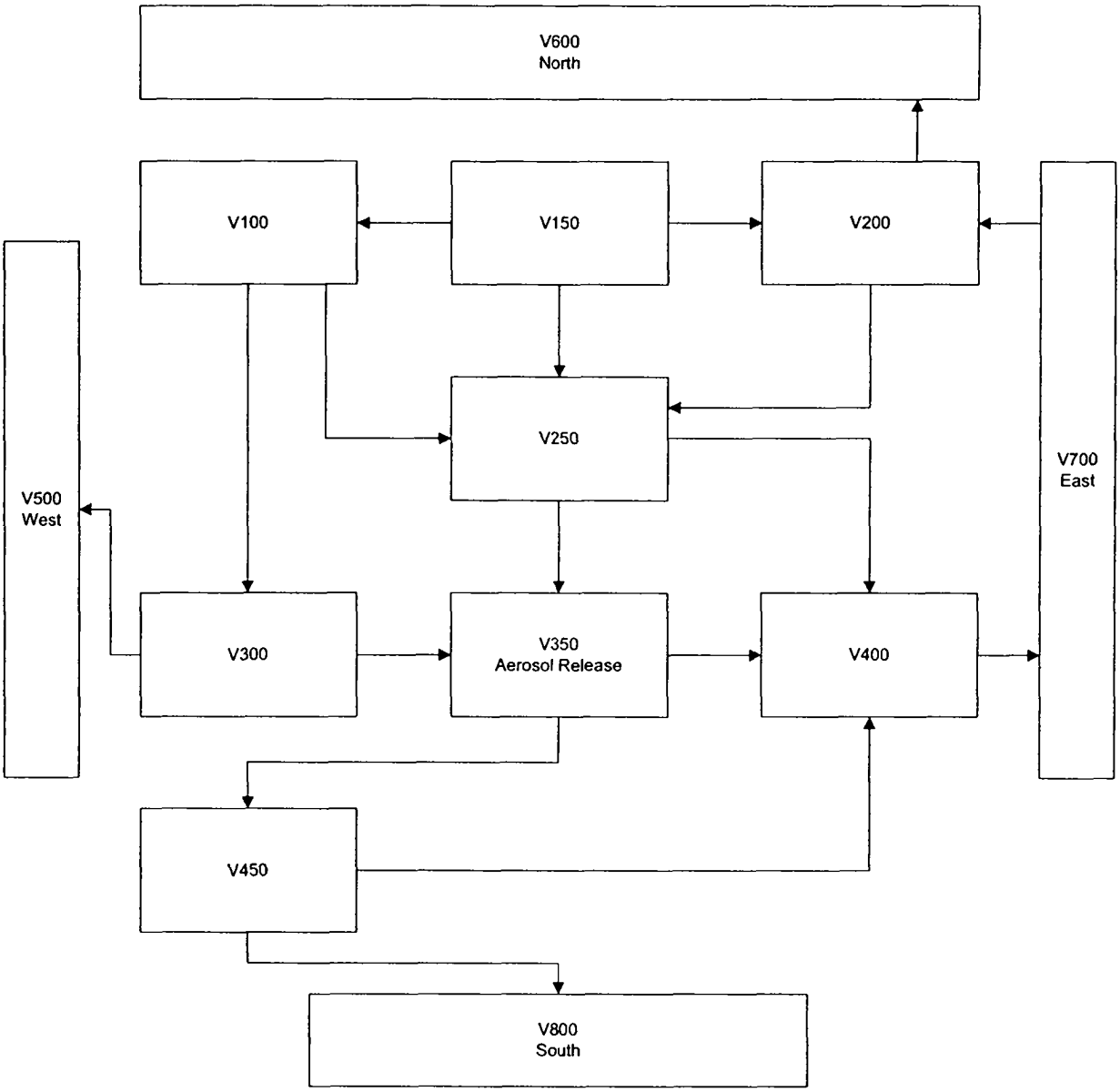

Figure 7-2. Seismic Problem — Building Simple Nodalization Flow Diagram

Note that the arrow directions in Figure 7-2 above represent a conventional positive direction of the flow. The MELCOR computer code will calculate the actual direction of the flow and will assign a new flow direction if the one assumed is not in the assigned conventional direction.

Table 7-3 includes a description of all the flow paths connecting the volumes shown in Figures 7-1and 7-2 above, including the flow path areas used in the analysis.

Table 7-3. Seismic Problem Volume Connectivity

Volume Connectivity				
Junction No. (Flow Path)	From Volume	To Volume	Flow Area m^2	Comments
110	100	300	0.0387	Single Pane Closed Door
115	100	250	0.0387	Single Pane Closed Door
120	150	100	0.0387	Single Pane Closed Door
125	300	350	0.0387	Single Pane Closed Door
130	150	250	0.0387	Single Pane Closed Door
135	150	200	0.0387	Single Pane Closed Door
140	200	250	0.0387	Single Pane Closed Door
145	250	350	0.0387	Single Pane Closed Door
150	250	400	0.0387	Single Pane Closed Door
155	350	400	0.0387	Single Pane Closed Door
160	350	450	0.0387	Single Pane Closed Door
165	450	400	0.0387	Single Pane Closed Door
170	300	500	0.0639	Double Pane Closed Door
175	200	600	0.0639	Double Pane Closed Door
180	400	700	0.0639	Double Pane Closed Door
185	450	800	Modulating Door (See Figure 7-3 Below)	Double Pane Closed Door
190	700	200	2.0	Ventilation Supply Wall Opening Due to Seismic Event

The modulating door (Junction No. 185) between volumes 450 and 800[3] is modeled by using a simple variable flow area to simulate the door opening to allow building evacuation. Figure 7-3 shows the time-history of the junction flow area used in the simulation.

[3] For simplicity this sample problem only opens one door. In actuality the user needs to model doors appropriately.

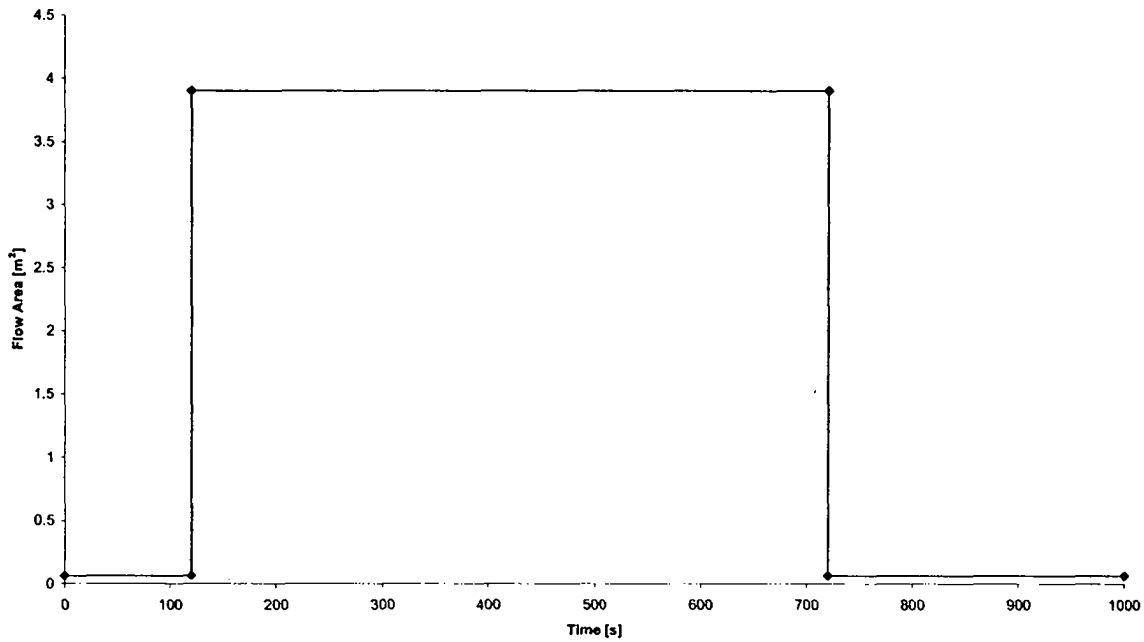

Figure 7-3. Seismic Problem — Modulating Door Representation (Model of Room Area versus Time)

The above shows how the door is initially closed with an associated flow area (Flow path area) equivalent to the area of the various gaps around the door. The full door flow area is used for a predetermined time until the door is re-closed and the area of the gaps is again in place.

The amount of material released in volume No. 350 due to the seismic event is set for simplicity to 1.0 kg and the lognormal distribution used is all respirable as described in paragraph 4.3:

Maximum aerosol particle diameter = 3 μm
Minimum aerosol particle diameter = 0.01 μm (this is an arbitrary minimum)
Volume-equivalent mass median particle diameter = 2.3 μm (8 μm AED)
Geometric standard deviation of the particle size distribution = 2 (95%)

The tabular function used to represent the initial aerosol release rate is shown in Figure 7-4 which is normalized to 1.0 kg of material released.

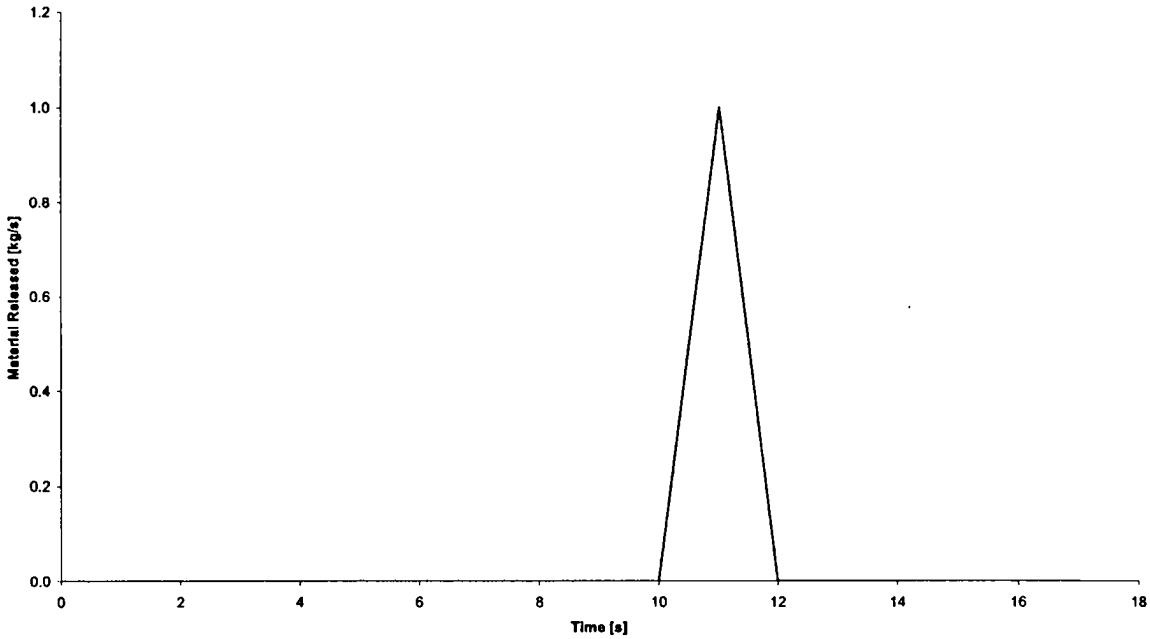

Figure 7-4. Seismic Problem Aerosol Material Release Rate in Volume No. 350

The definition of the heat structures is very simple as MELCOR input . The guidance given in the user's guide is extensive (recommended reading). The input data file given for this sample problem can be easily adapted as a template for other analyses. When defining the environmental volumes only one heat structure is recommended (nominal heat structure of 0.001 m^2) with a very small surface area. That is, when computing the amount of material released to the outside environment to evaluate the LPF, use of only one heat structure makes it easier to assess.

The MELCOR computer code is executed and the results are given in graphical form. The conventional output of the code includes information useful to monitor the entire code run. For the purpose of assessing the Leak Path Factor, the following is a typical set of results using the PTFREAD MS Excel Add-in.

Figure 7-5 shows the amount of aerosolized material (originally in volume 350) that has been transported out of the building into the environmental volumes 500, 600, 700, and 800.

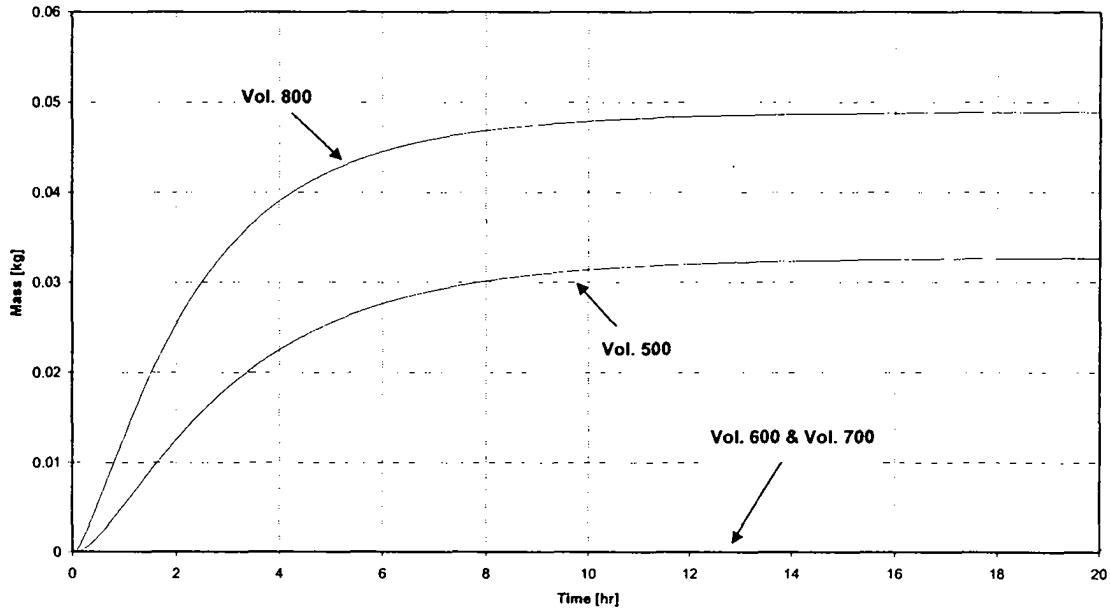

Figure 7-5. Seismic Problem Result — Aerosolized Material in Environmental Volumes

Figure 7-5 shows that the only environmental volumes containing aerosolized material are Vol. No. 500 and Vol. No. 800. The total amount of material transported out of the building is about 0.08 kg. The LPF can be expressed in percent of the material originally in volume 350. By manipulating the data used to generate Figure 7-5, the following Figure 7-6 represents the LPF of the building as percent of the material originally aerosolized in the building.

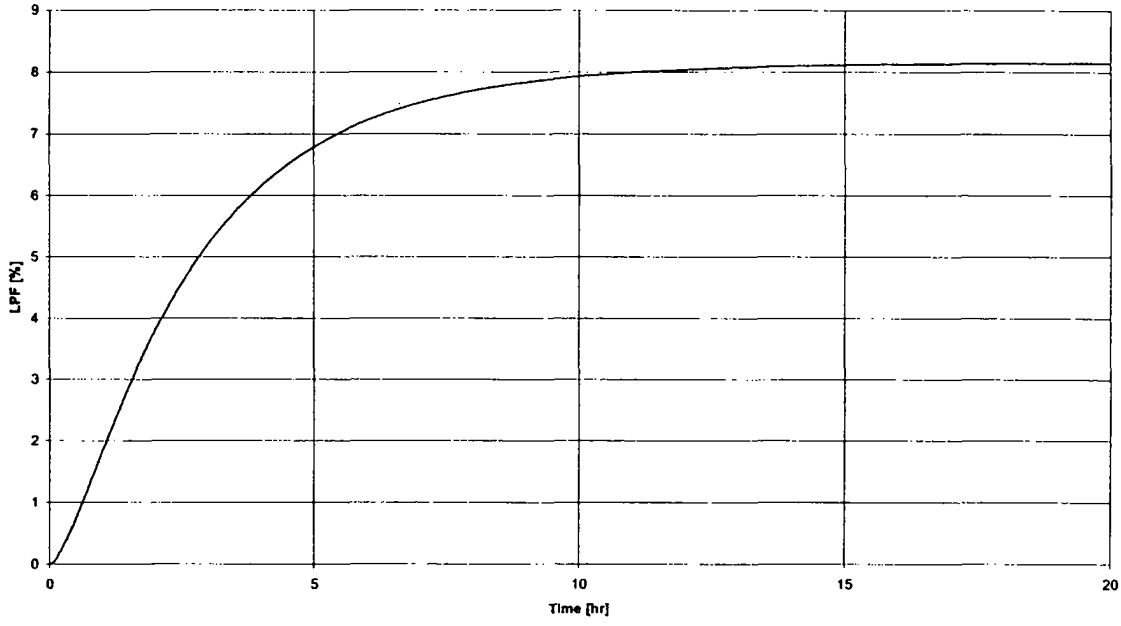

Figure 7-6. Seismic Problem Result — Total Building LPF

Additional data extracted from the MELCOR run is the amount of material deposited inside the building, Figure 7-7.

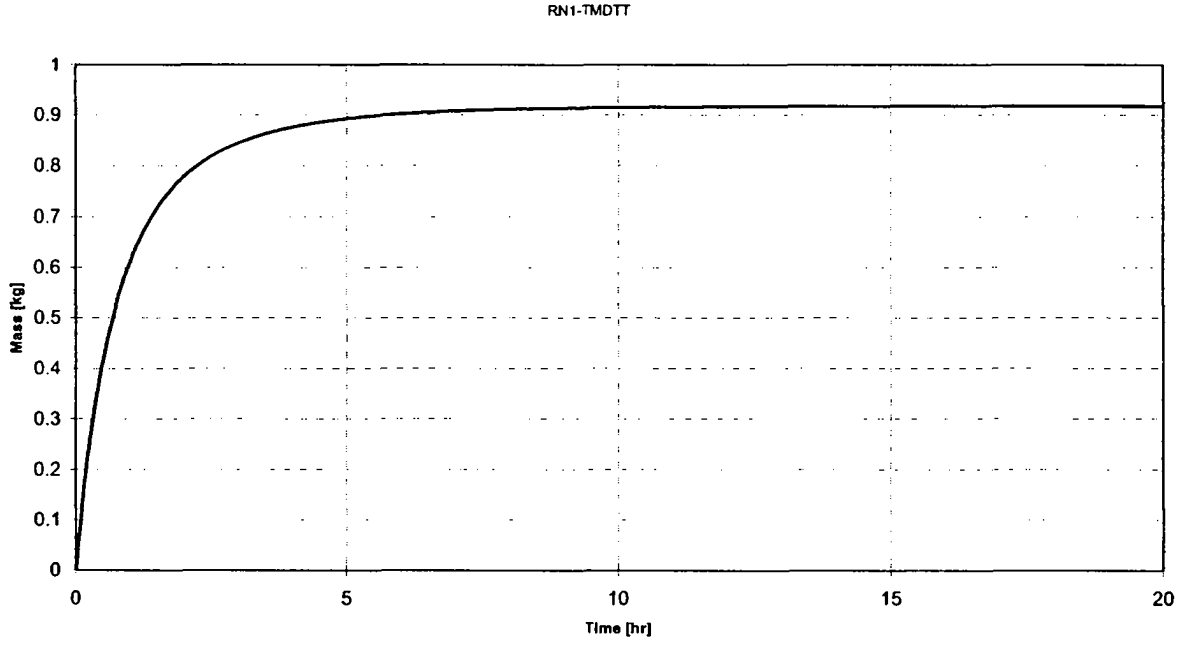

Figure 7-7. Seismic Problem Result — Material Deposited Inside Building

Figures 7-5 and 7-7 show that the mass of aerosol is conserved and the total mass (outside and inside the building) is equal to 1.0 kg, the original mass of material in volume no. 350.

In this particular sample problem the selected wind direction is from East. In general, the user should run MELCOR changing the direction of the wind to assess the most conservative results.

Appendix C includes the input data file used to execute the above sample problem.

7.2. Building Seismic Event with Powder Spill and Exhaust Ventilation Operating

This sample problem involves a building surviving a seismic event. There is a spill of PuO_2 powder in volume No. 350 and the exhaust portion of the ventilation network is operating using a filtration system. This sample problem is basically the same as in paragraph 7.1 above. An additional environmental volume (Vol. 900) is added to simulate the filtration system, and fixed flows are imposed out of each building cell to the volume representing the filtration system. The assumed filter system efficiency is set to 0.005.

Figure 7-8 is a simple model of the building, including the modification to accommodate the filtration system. In this model the ventilation supply is assumed to fail with the seismic event, leaving a wall opening in the East side of the building.

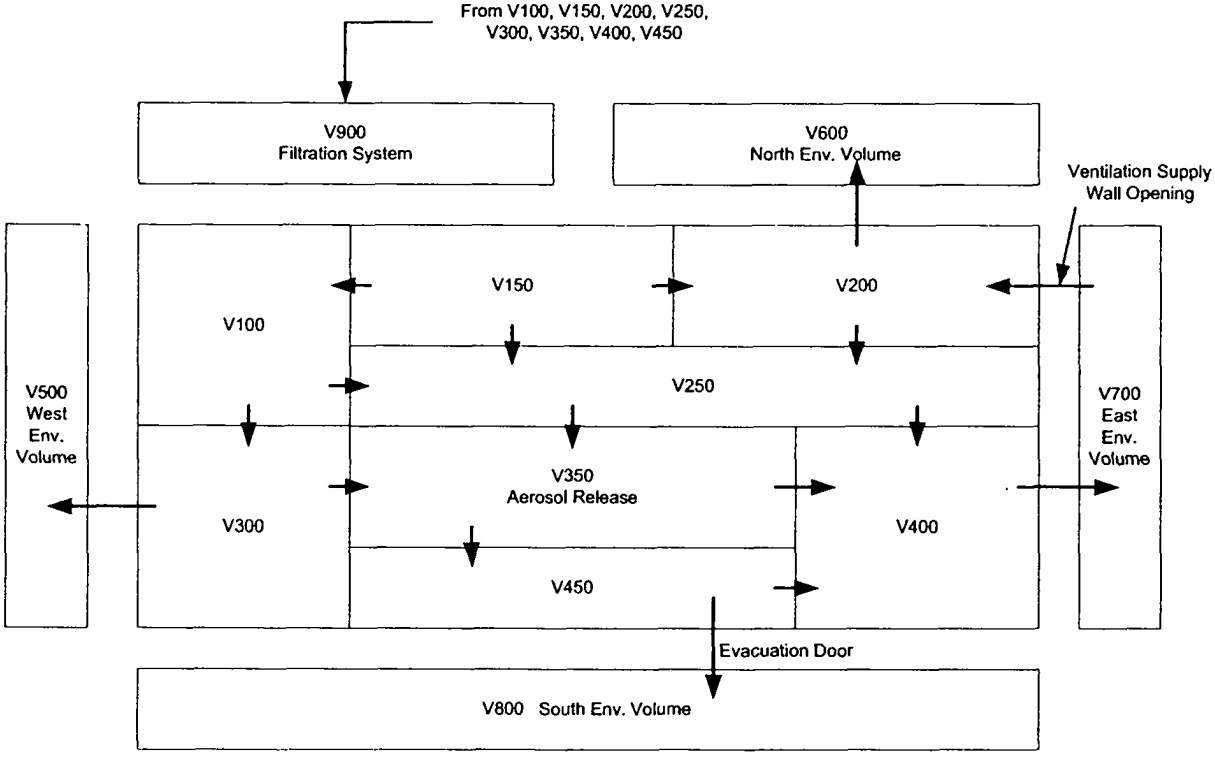

Figure 7-8. Building Nodalization for a Seismic Event with Exhaust Ventilation On

The assumed ventilation flows from each building cell to the system exhaust (Vol. No. 99) are listed in Table 7-4. The total exhaust flow is assumed to be 9.44 m^3/s (20,000 cfm), and the individual flows out to the exhaust are taken as proportional to the cell geometrical volume. An additional MELCOR run is also made using a total exhaust flow of 14.16 m^3/s (30,000 cfm). This latter flow data is shown in Table 7-5.

Table 7-4. Seismic Problem Ventilation Flows (9.44 m3/s)

Ventilation Flows - (9.44 m^3/s)		
From Volume	To Volume	Flow m3/s
100	900	1.226
150	900	1.876
200	900	1.876
250	900	0.417
300	900	0.919
350	900	1.430
400	900	1.287
450	900	0.409

Table 7-5. Seismic Problem Ventilation Flows (14.16 m3/s)

Ventilation Flows - (14.16 m^3/s)		
From Volume	To Volume	Flow m3/s
100	900	1.839
150	900	2.813
200	900	2.813
250	900	0.625
300	900	1.379
350	900	2.145
400	900	1.931
450	900	0.613

It is noted that when using fixed flows in MELCOR, as in this example, the actual input required by the code is a flow velocity. This is accomplished using the time-dependent flow path and a tabular function describing the fluid velocity. In this particular case a 1.0 m^2 reference flow area was used to yield the volumetric flow rate desired.

The model flow diagram given in the previous sample problem is modified to accommodate the changes made to the model for ventilation. The modified model flow diagram is shown in Figure 7-9.

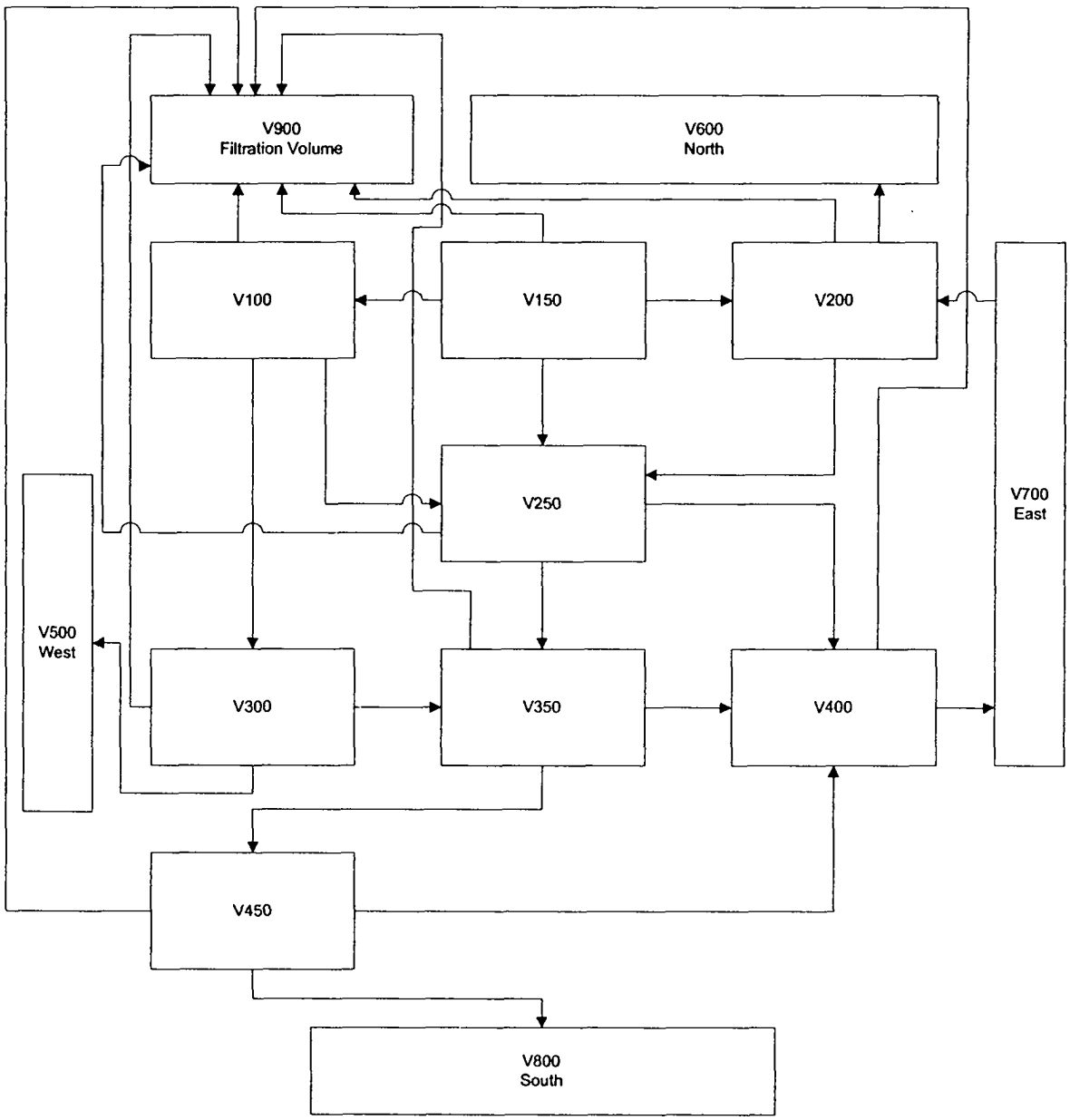

Figure 7-9. Seismic Problem (Ventilation On) —Building Nodalization Flow Diagram

Figure 7-10 shows the amount of aerosolized material (originally in volume 350) that has been transported out of the building into the environmental volumes. An analysis of the output shows that only volume No. 900 (the filtration system) receives aerosol.

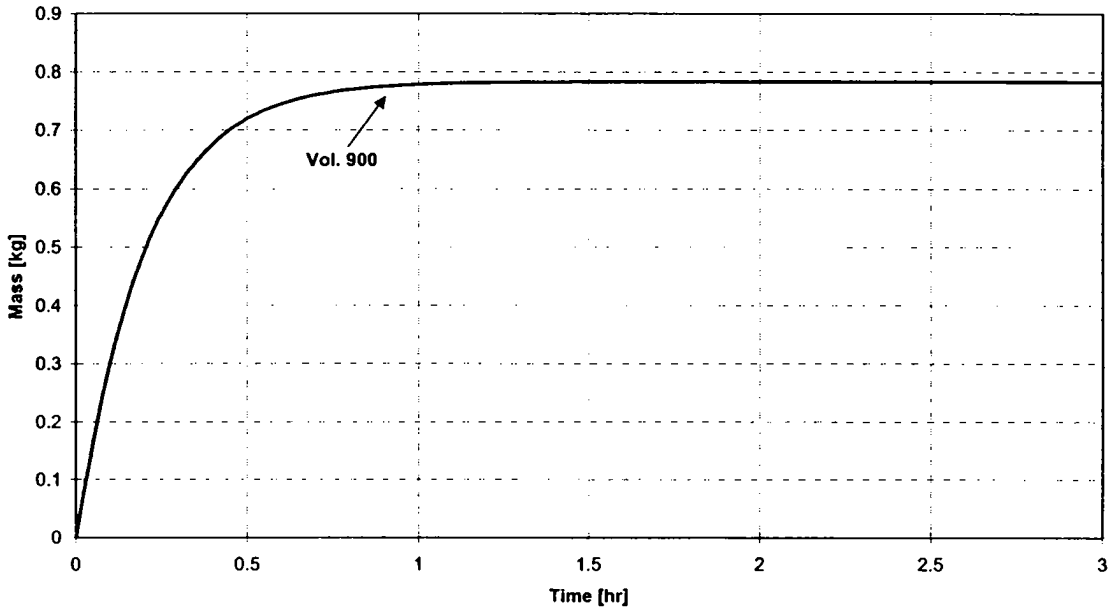

Figure 7-10. Seismic Problem Result (Ventilation On) —Aerosol Material in Volume Number 900

Figure 7-11 shows the amount of aerosol material deposited in the building.

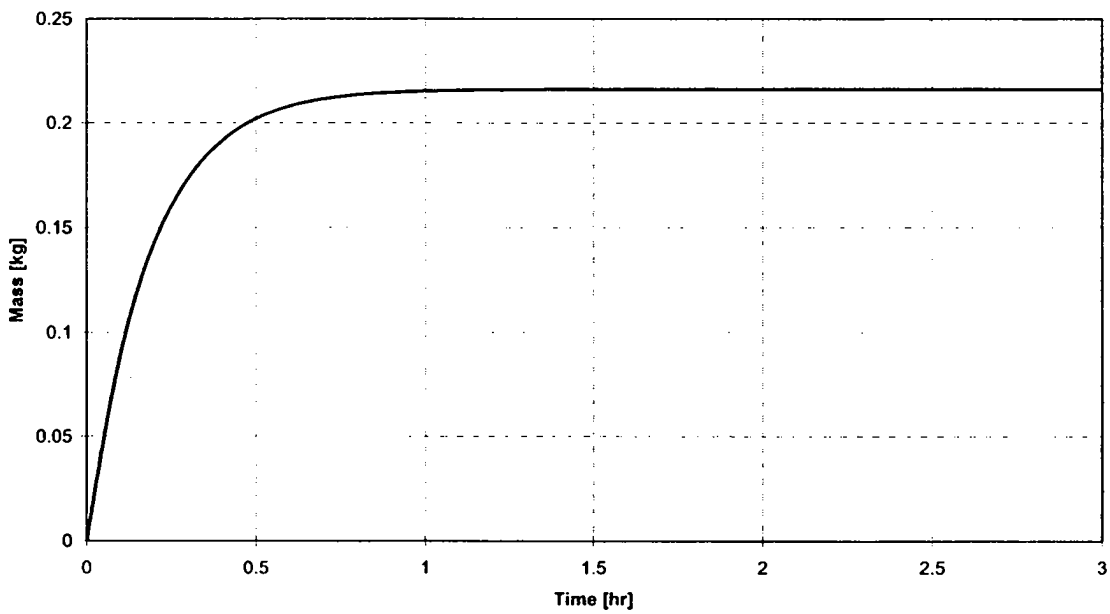

Figure 7-11. Seismic Problem Result (Ventilation On) —Aerosol Material Deposited Inside Building

The building LPF can be computed using Figure7-11 above multiplied by the filtration efficiency and expressing the results in percent of the material originally in volume No. 350.

Figure 7-12 shows the building LPF with a total ventilation flow of 9.44 m^3/s.

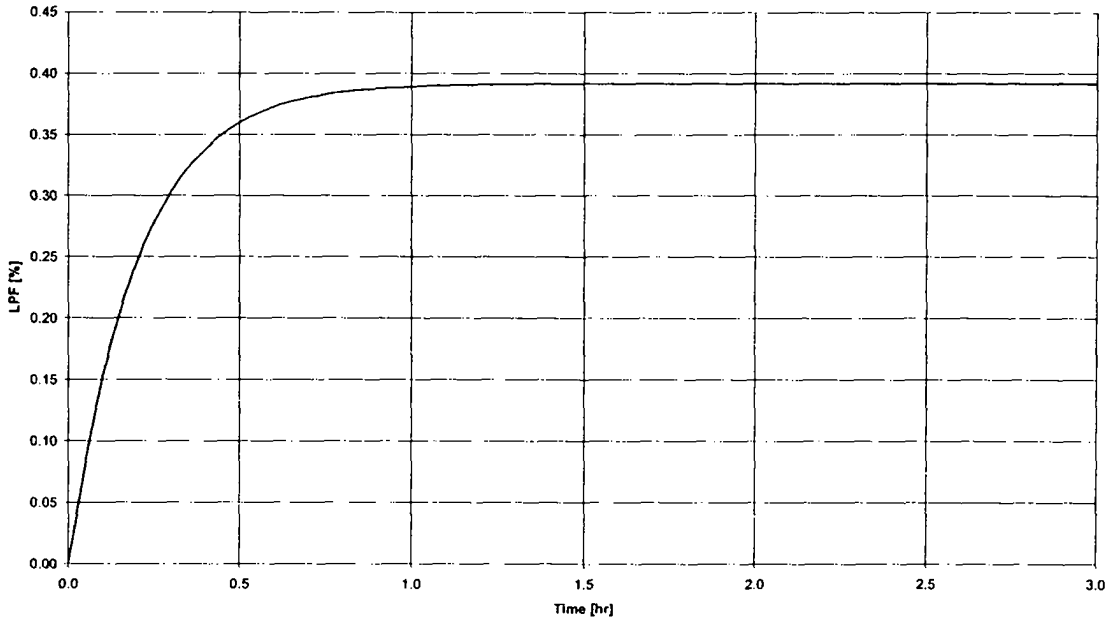

Figure 7-12. Seismic Problem Result (Ventilation On) —Building LPF (Total ventilation flow of 9.44 m3/s)

Figure 7-13 shows the building LPF with a total ventilation flow of 14.16 m^3/s.

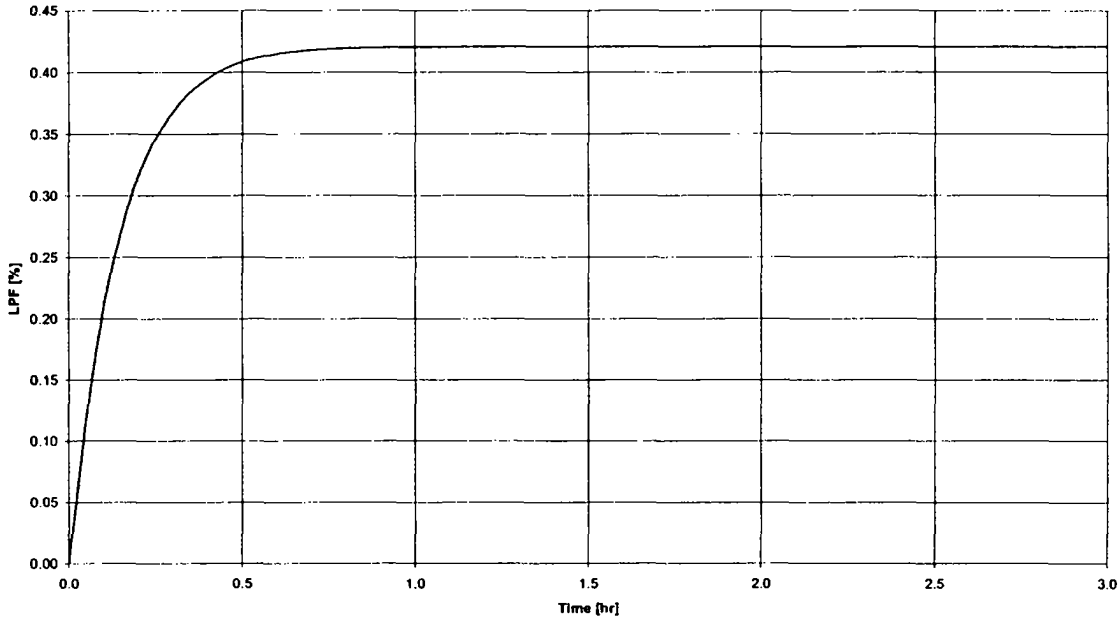

Figure 7-13. Seismic Problem Result (Ventilation On) —Building LPF (Total ventilation flow of 14.16 m3/s)

Appendix D includes the input data file used to execute this sample problem using a total ventilation flow of 9.44 m^3/s.

7.3. Building Seismic Event with Powder Spill and Post Seismic Fire

This sample problem is equal to the sample problem given in paragraph 7.1 with the addition of a fire in volume No. 360 (same volume where initially there is aerosolized material).

Figure 7-14 is a simple model of the building as previously shown in paragraph 7.1.

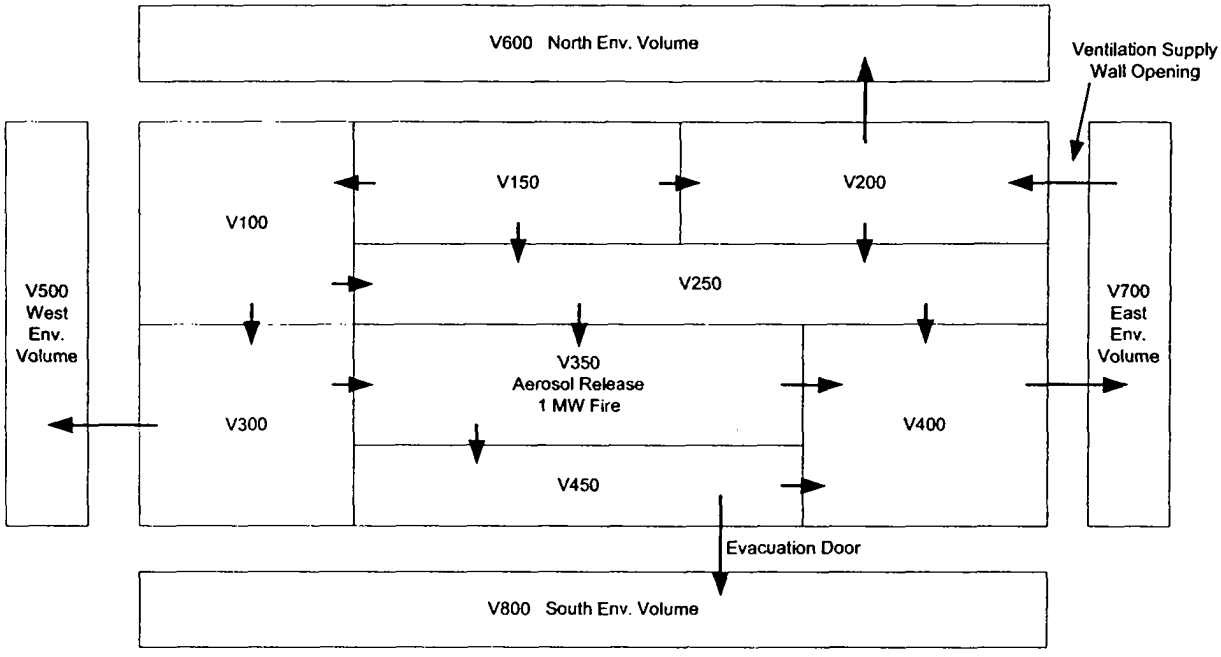

Figure 7-14. Fire Problem — Nodalization of Building with a Fire in Volume No. 350

The flow diagram for this model is identical to the diagram shown in Figure 7-2.

The fire input into this model is described in Table 7-6 and Figure 7-15.

Table 7-6. Fire Mass Enthalpy and Energy

Fire Input			
Time	Mass	Enthalpy	Energy
s	kg/s	J/kg	W
0.0	0.0	0.0	0.0
300.0	0.001	1.0E+9	1.0E+6
900.0	0.001	1.0E+9	1.0E+6
1200.0	0.0	0.0	0.0
5000.0	0.0	0.0	0.0

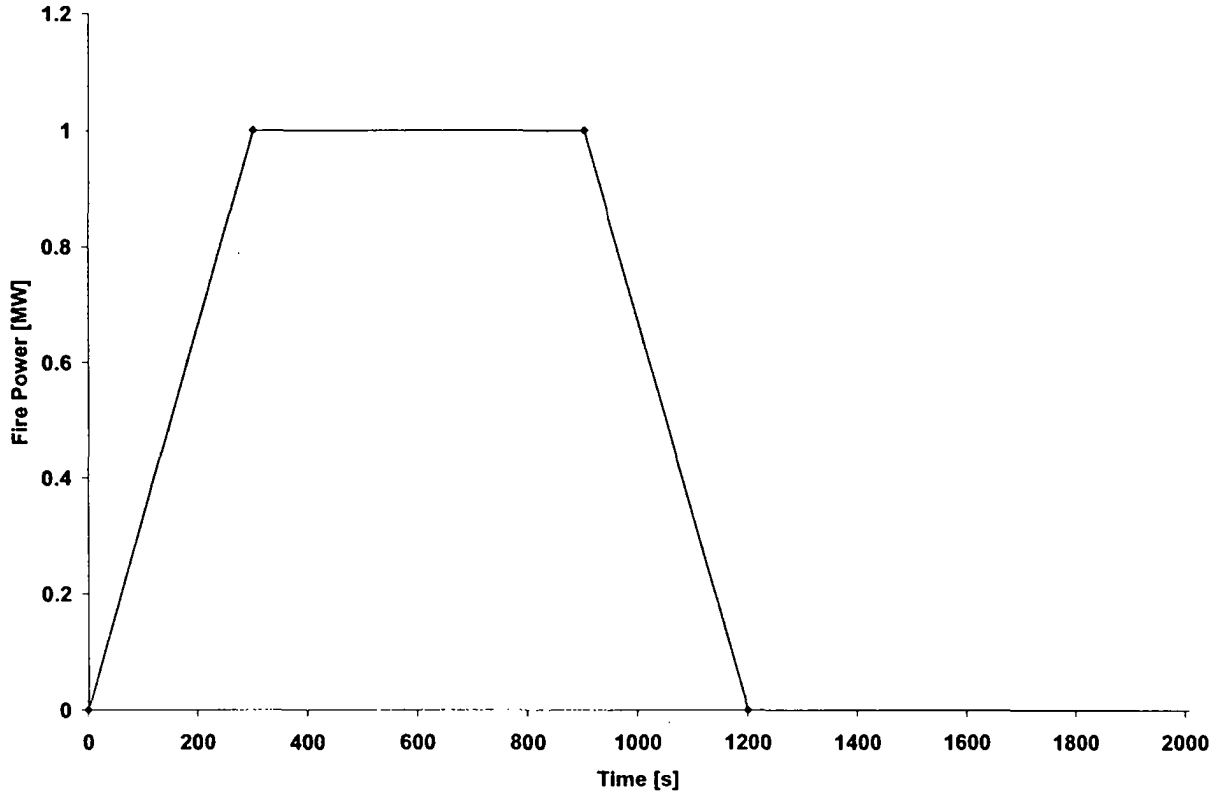

Figure 7-15. Fire Problem — Fire Power versus Time

The results of this sample problem are summarized in the following figures showing the amount of aerosol material transported out of the building, deposited in the building, and the LPF.

Figure 7-16 shows the contribution to the LPF from the four environmental volumes set outside the building. It is noted that in this problem the LPF results are higher since the fire stressor enhances the transport of aerosolized material outside the building.

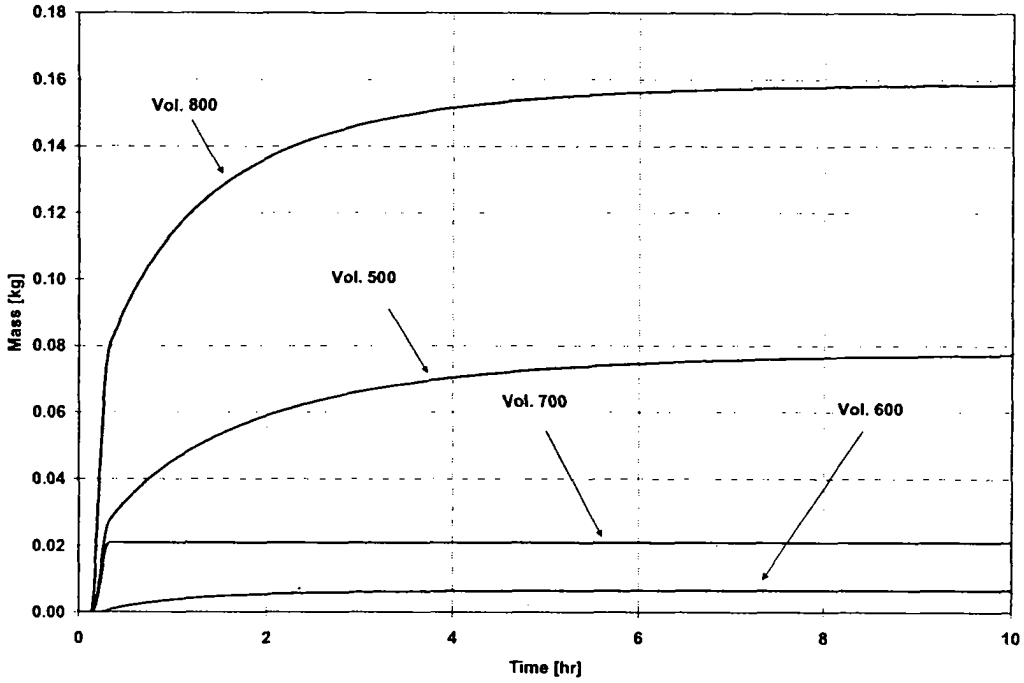

Figure 7-16. Fire Problem Result — Aerosolized Material in Environmental Volumes

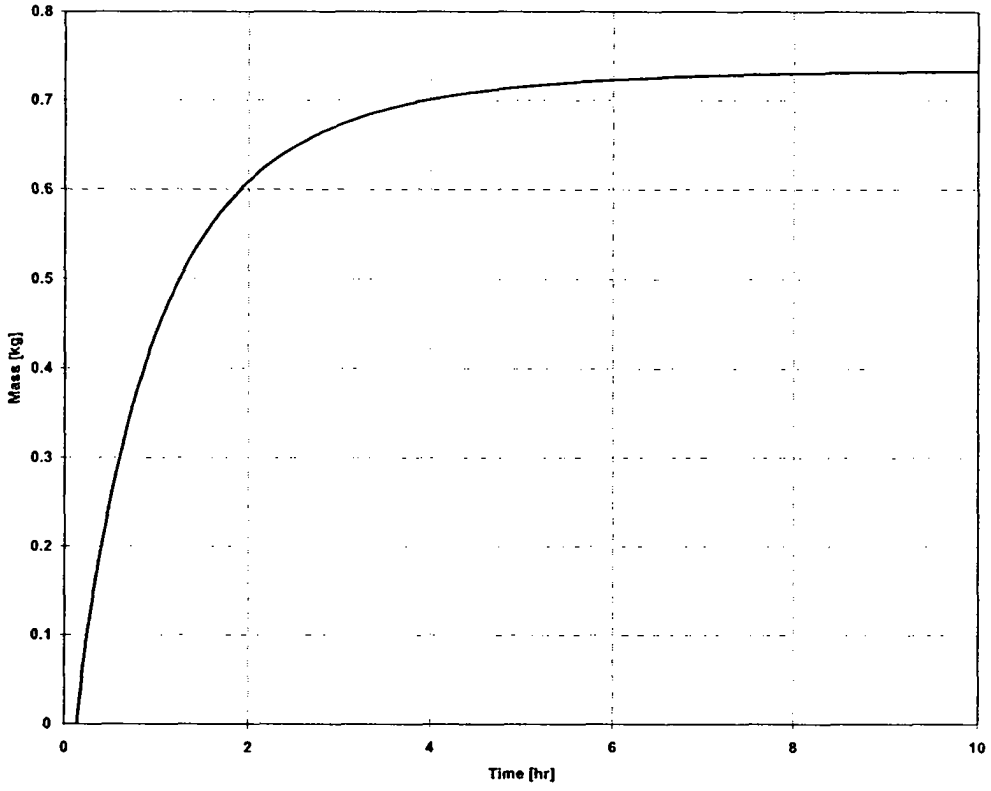

Figure 7-17. Fire Problem Result — Aerosol Material Deposited Inside Building

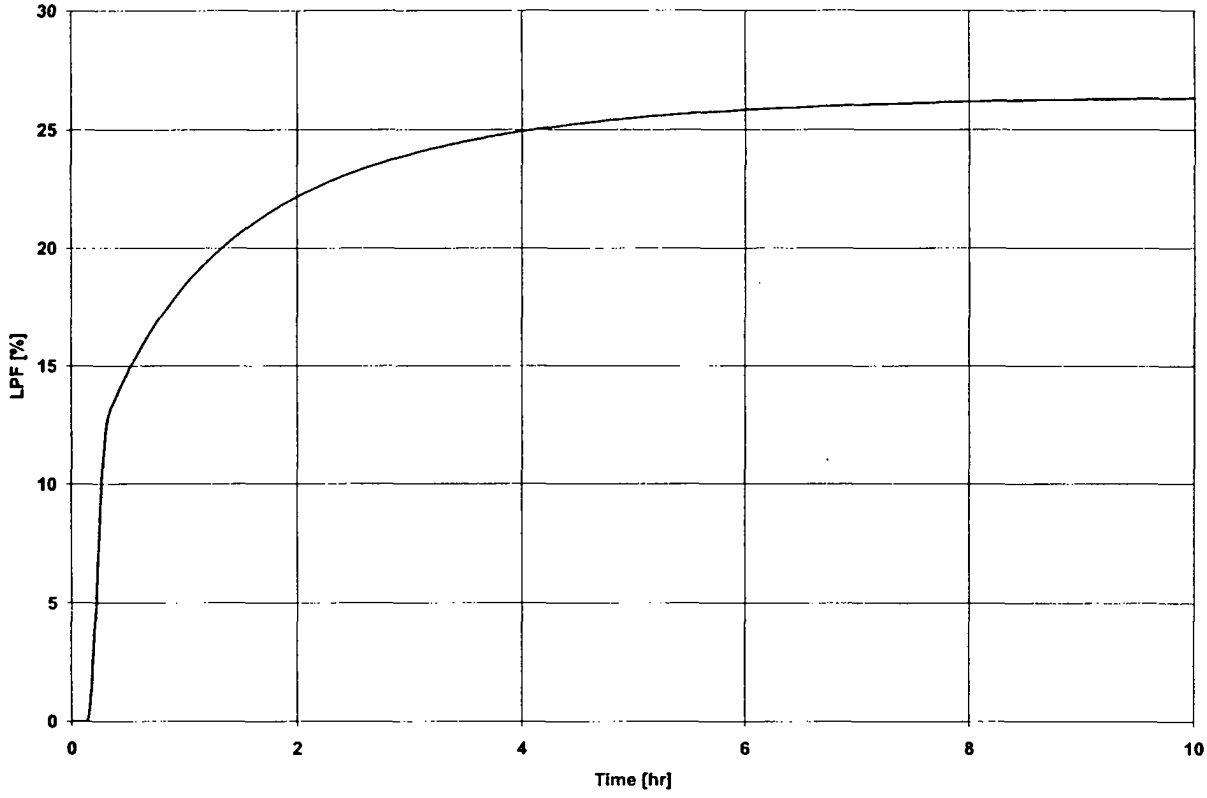

Figure 7-18. Fire Problem Result — Total Building LPF

Appendix E includes the input data file used to execute this sample problem.

7.4. Building Seismic Event with Powder Spill and Post Seismic Fire and Exhaust Ventilation

This sample problem is basically the same as reported in paragraph 7.2 except for the addition of the operation of the exhaust ventilation (total flow 14.16 m^3/s). The time at which the material spill occurs in volume No. 350 is also shifted in time (spill starts at 500 seconds and ends at 502 seconds).

The figures representing the building model and the building flow diagram are identical to those shown in figures 7-8 and 7-9 respectively.

The following figures show the results for this sample problem.

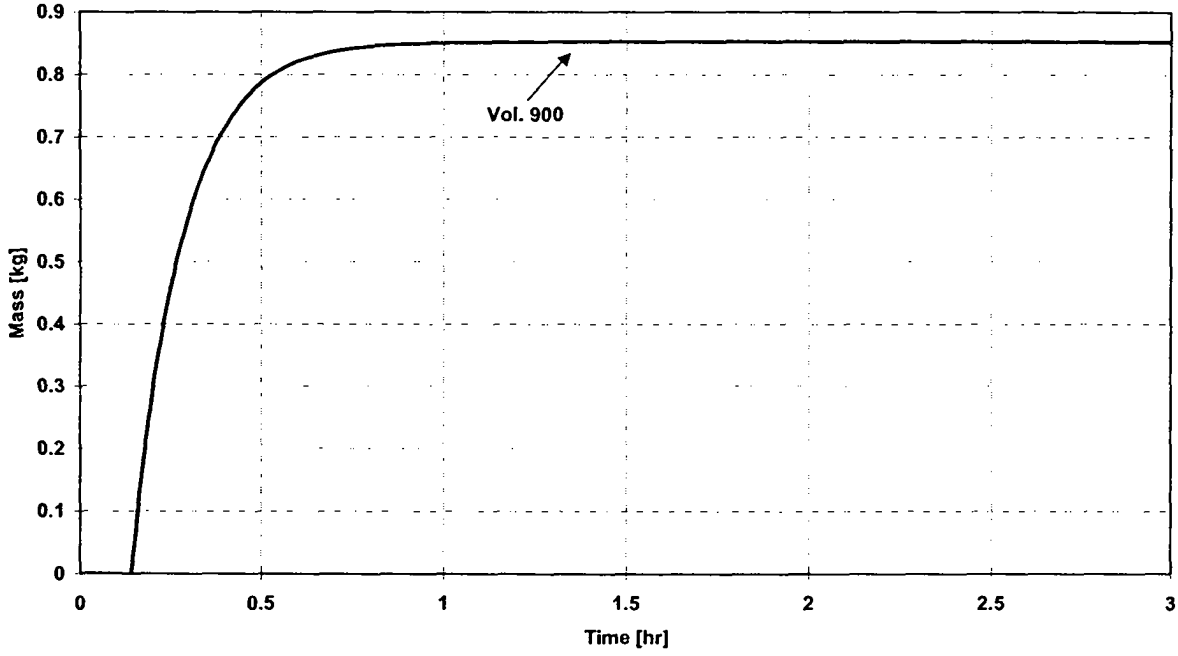

Figure 7-19. Fire Plus Seismic (Ventilation On) — Aerosol Material in Volume No. 900

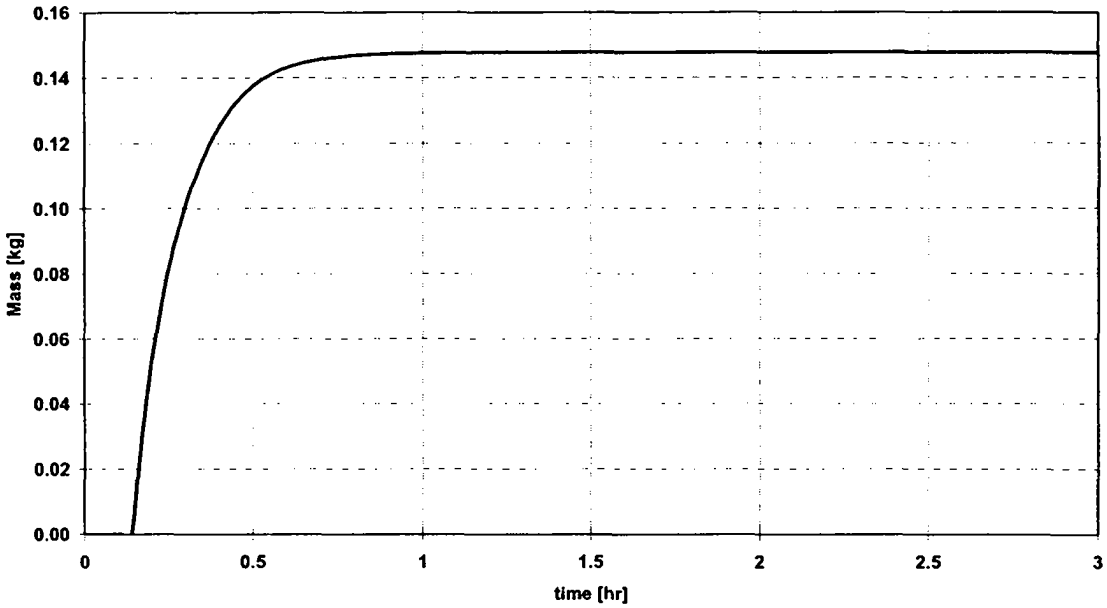

Figure 7-20. Fire Plus Seismic (Ventilation On) — Aerosol Material Deposited Inside Building

The LPF can be computed using Figure 7-19 above multiplied by the filtration efficiency and expressing the results in percent of the material originally in volume No. 350.

Figure 7-21 shows the building LPF with a total ventilation flow of 14.16 m^3/s.

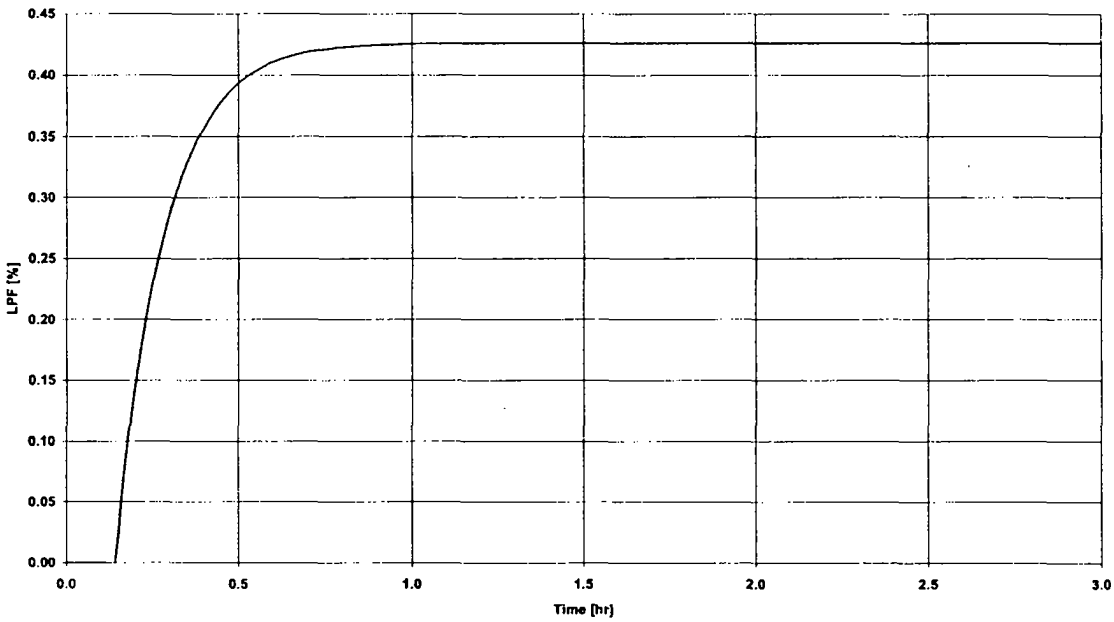

Figure 7-21. Fire Plus Seismic (Ventilation On) — Building LPF (Total ventilation flow 14.16 m3/s)

Appendix F includes the input data file used to execute this sample problem.

7.5. Building Seismic Event with Multiple Powder Spill

This sample problem is identical to the sample given in paragraph 7.1 with the exception that multiple spills are situated in the building after a seismic event. The total amount of aerosolized material released is 1.0 kg. Table 7-7 shows the distribution of the released material.

Table 7-7. Seismic Multiple Spill Problem Released Material Distribution Results

Distribution of Released Material	
Vol. No.	Released Material kg
200	0.3
250	0.4
350	0.3

Figure 7-22 is the same building model as given in paragraph 7.1 where the three volumes where the material is released are shown.

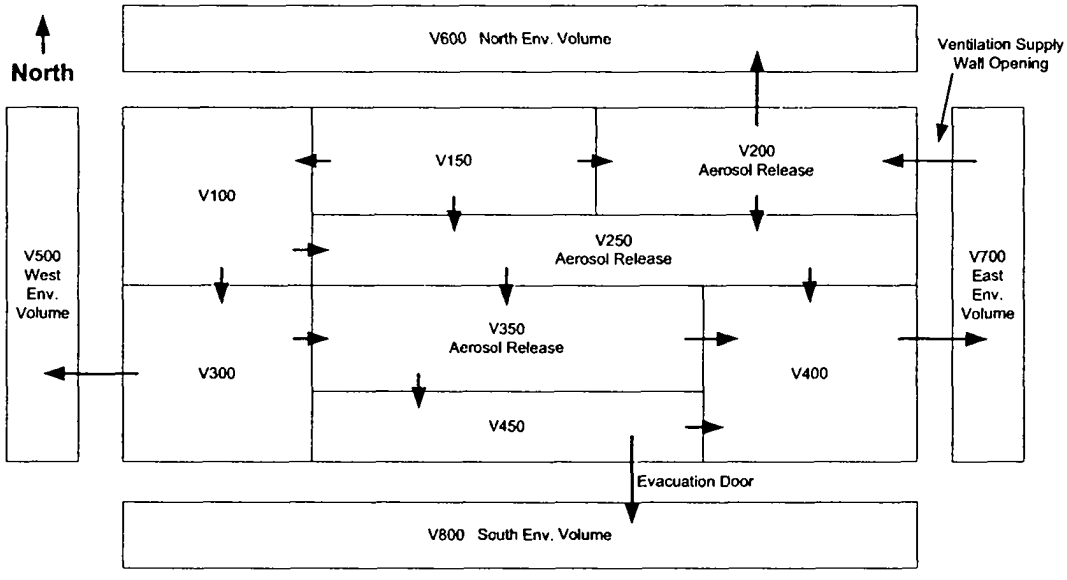

Figure 7-22. Seismic Problem With Multiple Spills — Building Nodalization

The building flow diagram used to build the MELCOR model is identical to the flow diagram reported in paragraph 7.1.

The results of this sample problem are summarized in the following figures.

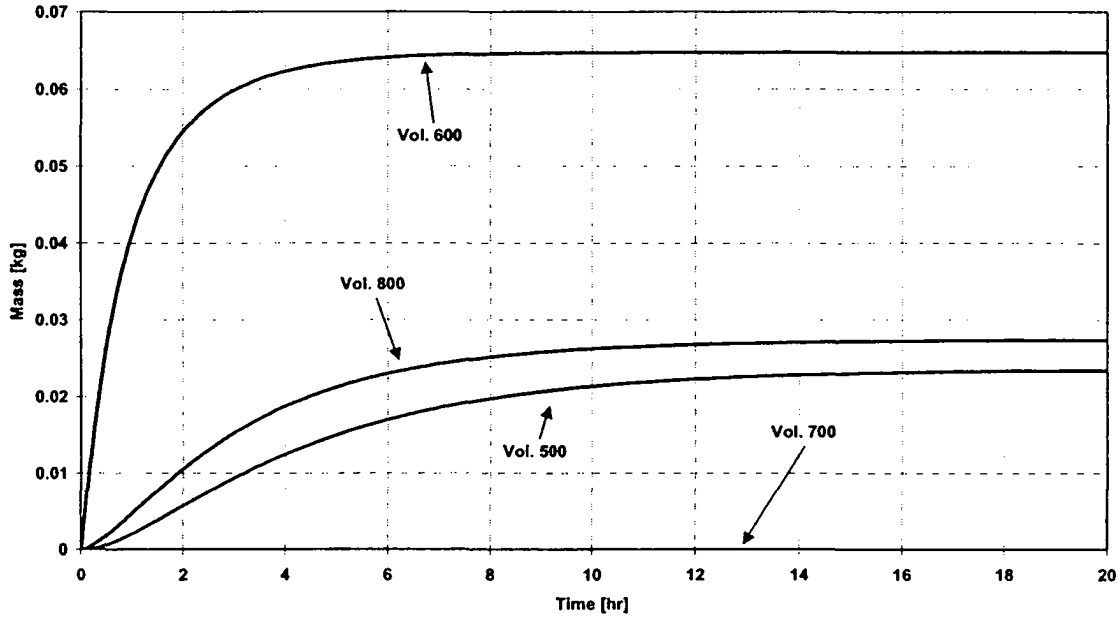

Figure 7-23. Seismic Problem With Multiple Spills — Aerosolized Material in Environmental Volumes

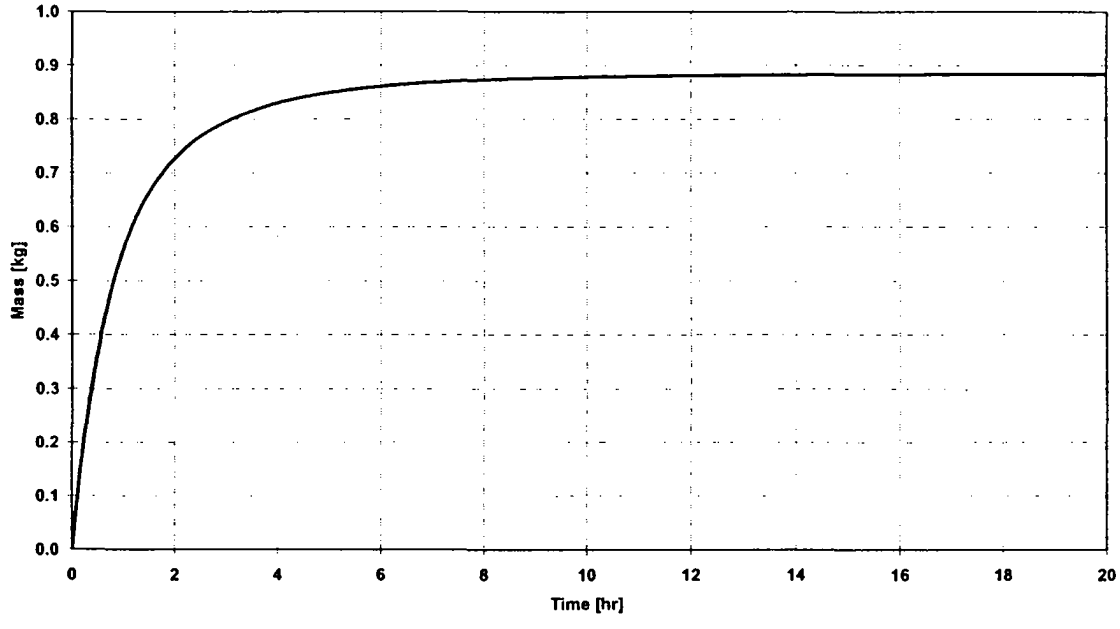

Figure 7-24. Seismic Problem With Multiple Spills — Material Deposited Inside Building

The building LPF is evaluated by summing the material contribution as shown in Figure 7-23 above and expressing the results in percent of the total material originally in volumes 200, 250, and 350.

Figure 7-25 represents the building LPF as a percent of the material originally aerosolized inside the building.

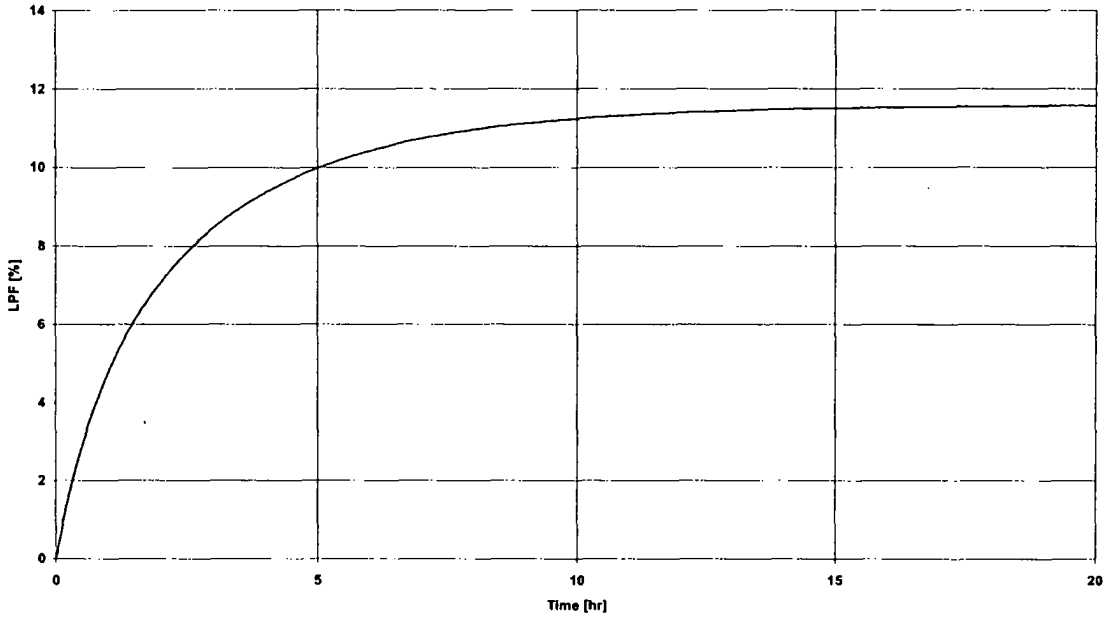

Figure 7-25. Seismic Problem With Multiple Spills — Building LPF

A parametric study is performed to assess the influence of the amount of aerosolized material on the LPF. The original inventory of aerosolized material of 1.0 kg is reduced a few orders of magnitude.

Table 7-8 shows the amount and distribution of released material used in the parametric study.

Table 7-8. Parametric Study Distribution of Released Material Used

Distribution of Released Material Used in Parametric Study				
Vol. No.	Released Material kg	Released Material kg	Released Material kg	Released Material kg
200	0.3	0.03	0.003	0.0003
250	0.4	0.04	0.004	0.0004
350	0.3	0.03	0.003	0.0003
Total	1.0	0.1	0.01	0.001

The resulting building LPF as a function of the Aerosolized released material is shown in the following Figure 7-26.

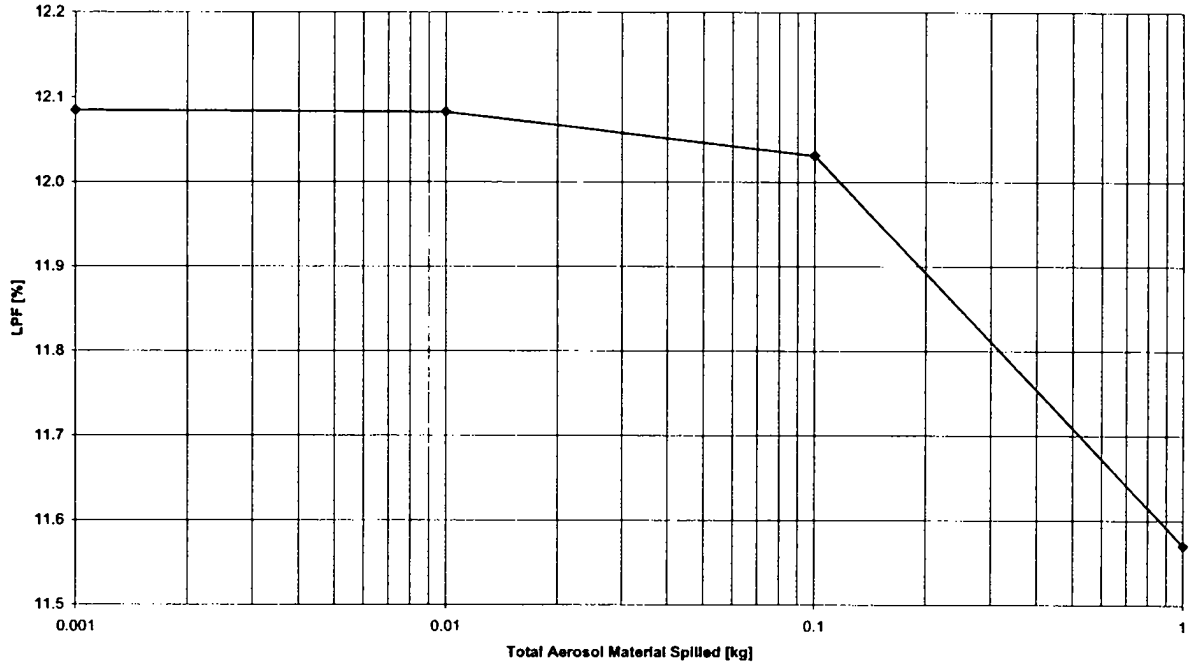

Figure 7-26. Influence of Released Material on LPF

Appendix G includes the input data file for this sample problem using a 1.0 kg total mass of released material.

8.0 ACRONYMS AND DEFINITIONS

Selected Terms and Definitions Used in Accident and Consequence Analysis & Software Quality Assurance

Gap Analysis — Evaluation of the Software Quality Assurance attributes of specific computer software against identified criteria.

Leak Path Factor (LPF) – Defined as the fraction of airborne radioactive material released, due to a forcing condition, as respirable particulate within the building that escapes via available pathways to the outside environment.

Aerodynamic Equivalent Diameter (AED) – Diameter of a sphere of density 1 g/cm that exhibits the same terminal velocity as the particle subject of the analysis.

Software — Computer programs, operating systems, procedures, and possibly associated documentation and data pertaining to the operation of a computer system. [IEEE Standard 610.12-1990, *IEEE Standard Glossary of Software Engineering Terminology*]

Toolbox Codes — A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and meeting minimum qualification standards. These codes shall be sufficiently verified and validated, and as such, applicable to support 10 CFR 830 DSAs. That is to say, the analysts using these codes do not need to present additional defense as to their qualification, provided that they are sufficiently qualified to use the codes and the input parameters are valid.

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9.0 REFERENCES

ASHRAE, 1977, Handbook of Fundamentals, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc, 1997.

CRC, 1986, Handbook of Chemistry and Physics, 67th Edition, CRC Press, 1986.

DOE 1994, U.S. Department of Energy, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities*, DOE-HDBK-3010-94, December 12, 1994.

DOE, 2002, U.S. Department of Energy, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Reports*, DOE-HDBK-3010-94, Change Notice 2, April 2002.

DOE, 2003, U. S. Department of Energy, *MACCS2 Computer Code Application Guidance for Documented Safety Analysis,* September 2003.

DOE, 2004, U.S. Department of Energy, *Software Quality Assurance Improvement Plan: MELCOR Gap Analysis*, Final.

Gauntt, 2000, Gauntt et al., *MELCOR Computer Code Manuals*, Version 1.8.5, NUREG/CR-6119 Rev. 2, SAND2000-2417/1, May 2000.

Mishima, 1973, J. Mishima, L. C. Schwendiman, F*ractional Airborne Release of Uranium (Representing Plutonium) During Burning of Contaminated Waste*, BNWL-1730, Battelle Pacific Northwest Laboratory, Richland, WA, April 1973.

Murata, 1977, K. Murata, et al., *Code Manual for CONTAIN 2.0: A Computer Code for Nuclear Reactor Containment Analysis*, NUREG/CR-6533, SAND 97-1735, December 1997.

Polizzi, 2000, M. Polizzi, N. Flouras, *Leak Path Factor Study at Savannah Rive Site*, Safety Analysis Working Group (SAWG) Workshop 2000, Santa Fe, NM.

Polizzi, 2002, L. M. Polizzi, K. R. O'Kula, D. C. Thoman, L*eak Path Factor Analysis for a Large, Multiple-Cell Nuclear Facility*, Safety Analysis Working Group (SAWG) Workshop 2002, Oak Ridge, TN.

SNL, 1983, *Transuranic Package Transporter, TRUPACT-1, SARP*, SAND 83-7077 (TTC-0338) Sandia National Laboratory, GA Technologies, San Diego, CA, November 1983.

Sutter, 1981, S. L. Sutter, J. W. Johnson, J. Mishima,, *Aerosols Generated by Free Fall Spill of Powders and Solutions in Static Air*, NUREG/CR-2139, Battelle Pacific Northwest Laboratory, Richland, WA, December 1981.

Sutter, 1983, S. L. Sutter, *Aerosols Generated by Releases of Pressurized Powders and Solutions in Static Air*, NUREG/CR-3093, Battelle Pacific Northwest Laboratory, Richland, WA, August 1983.

APPENDICES

Appendix	Subject
A	Steps to Run MELCOR
B	Benchmark Problems
C	Seismic Problem Input File
D	Seismic Problem (Ventilation Operating) Input File
E	Fire Problem Input File
F	Fire Plus Seismic (Ventilation Operating) Input File
G	Seismic Problem with Multiple Spills (Ventilation Operating) Input File

Appendix A. Steps to Run MELCOR

The user needs to follow a few simple steps to run MELCOR on a Personal Computer. The MELCOR package includes two executables: MELGEN and MELCOR.

1. Prepare an input data file with a text editor. The file name can be any, e.g., input.txt or sample1.inp, etc.

2. Open a Command Prompt Window in the folder where the input data file is located (this assumes the user has set environmental variables in Windows to have the MELGEN/MELCOR folder in the path.

3. Execute MELGEN input data file (MELGEN input.txt)

4. Execute MELCOR input data file (MELCOR input.txt)

5. Use the MS Excel Add-in to analyze the output file (.PTF) or use Xymel software

Appendix B. Benchmark Problems

Several benchmarks were performed to assess the LPF evaluation using MELCOR and CONTAIN.

The problems of interest are:

Seismic spill – no ventilation (wind-driven LPF)
Seismic spill – with ventilation
Spill with large fire and ventilation
Spill with small fire – no ventilation

The building layout used is shown in Figure B-1 and the MELCOR model block diagram is shown in Figure B-2

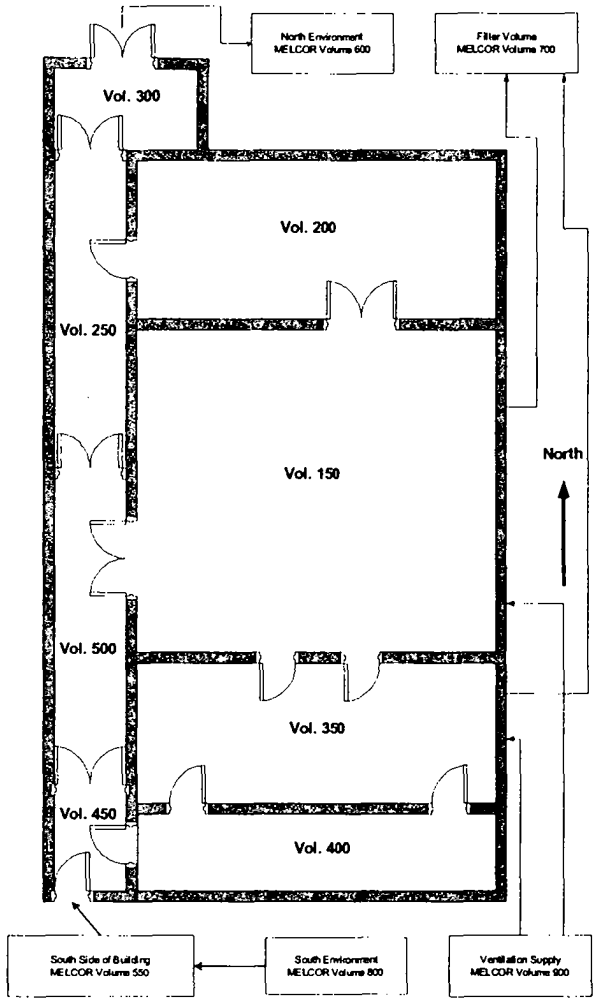

Figure B-1. Building Layout Used in Benchmark

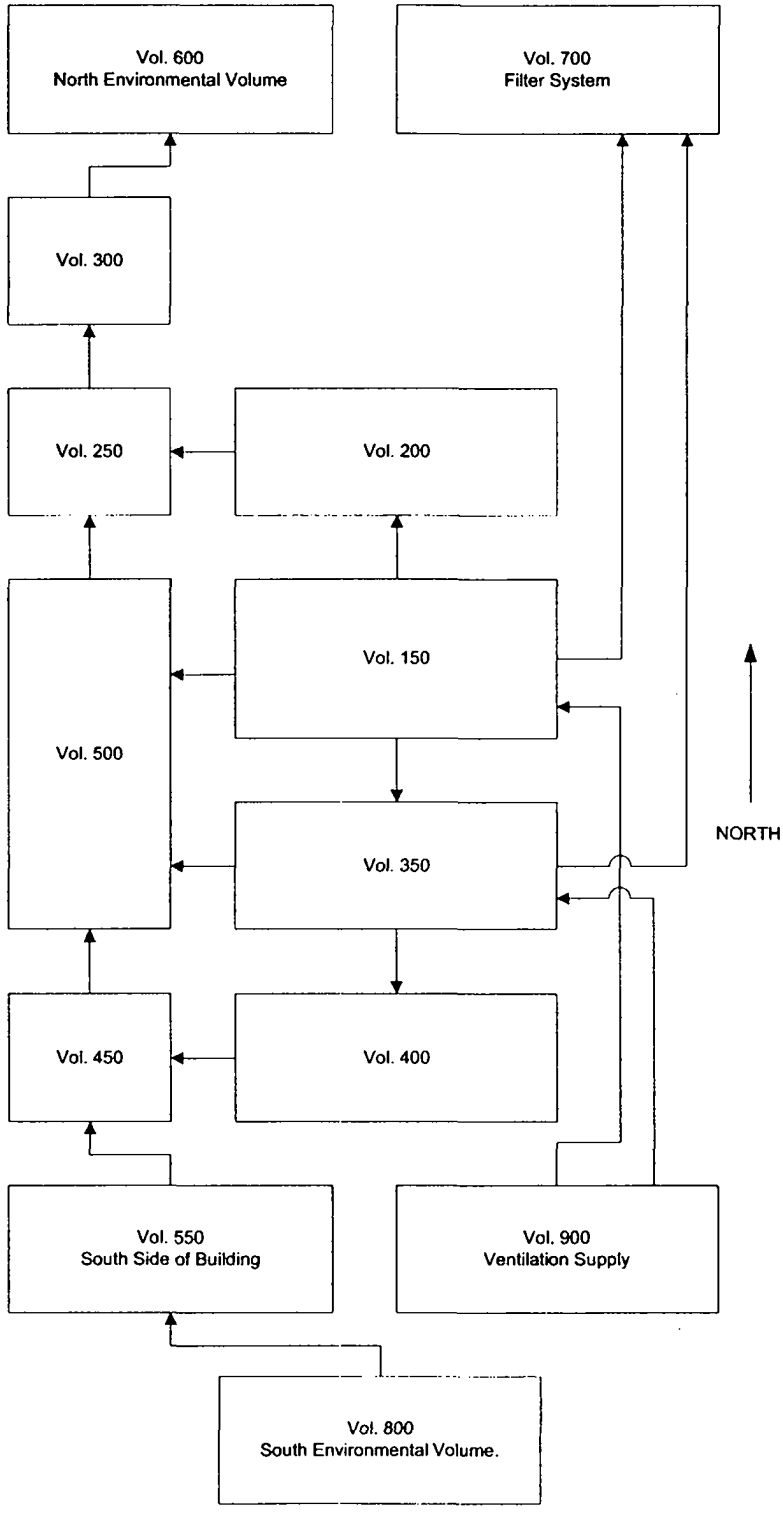

Figure B-2. MELCOR Model Block Diagram

Tables B-1 and B-2 show the dimensions of the various control volumes (cells) used in the analyses.

Table B-1. Volume Dimensions

Volume No.	Floor Area m^2	Height m	Volume m^3
150	96	4.0	384
200	8.	4.0	32
250	14.	4.0	56
300	8.	4.0	32
350	34	4.0	136
400	10.	4.0	40
450	6.	4.0	24
500	22	4.0	88
550	147	4.0	588
600	N/A	N/A	1.0E+10
700	N/A	N/A	1.0E+10
800	N/A	N/A	1.0E+10
900	N.A	N/A	1.0E+10

Table B-2. Flow Path Dimensions

From Vol.	To Vol.	Flow Area m^2
150	200	2.
200	250	2.
250	300	4.
150	350	0.0174
350	400	0.0174
350	500	0.0174
400	450	0.0087
450	500	0.0174
500	250	0.0174
550	450	0.0174
800	550	0.0174
300	600	4.

The analysis data used for the benchmark is as follows

Wind Speed 2.23 m/s (5 mph)
Wind from South
1 g of PuO2 spilled in Vol. 150 in 2.0 s (Fully aerosolized and all respirable)
Lognormal distribution of aerosolized material
Maximum aerosol particle diameter, 3 μm
Minimum aerosol particle diameter, 0.003 μm
Volume-equivalent mass median particle diameter, 2.3 μm
Geometric standard deviation of the particle size distribution, 2
Fire in Vol. 150
Ventilation flow from volume 150 to filters 0.93 m3/s
Ventilation flow from volume 350 to filters 0.21 m3/s
Vol. 150 Ventilation supply 0.71 m3/s
Vol. 350 Ventilation supply 0.14 m3/s
Filters efficiency 0.995
No cracks in the building structure

The large fire profile used in the analysis is shown in Figure B-3

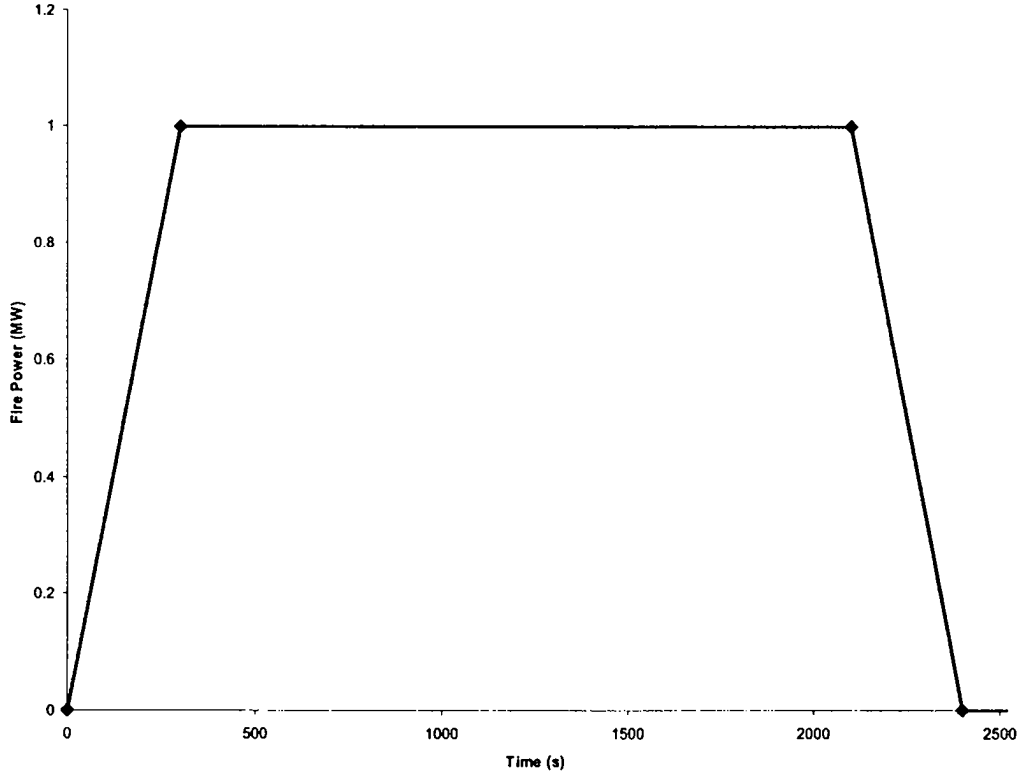

Figure B-3. Large Fire Profile

The small fire profile used in the analysis is shown in Figure B-4

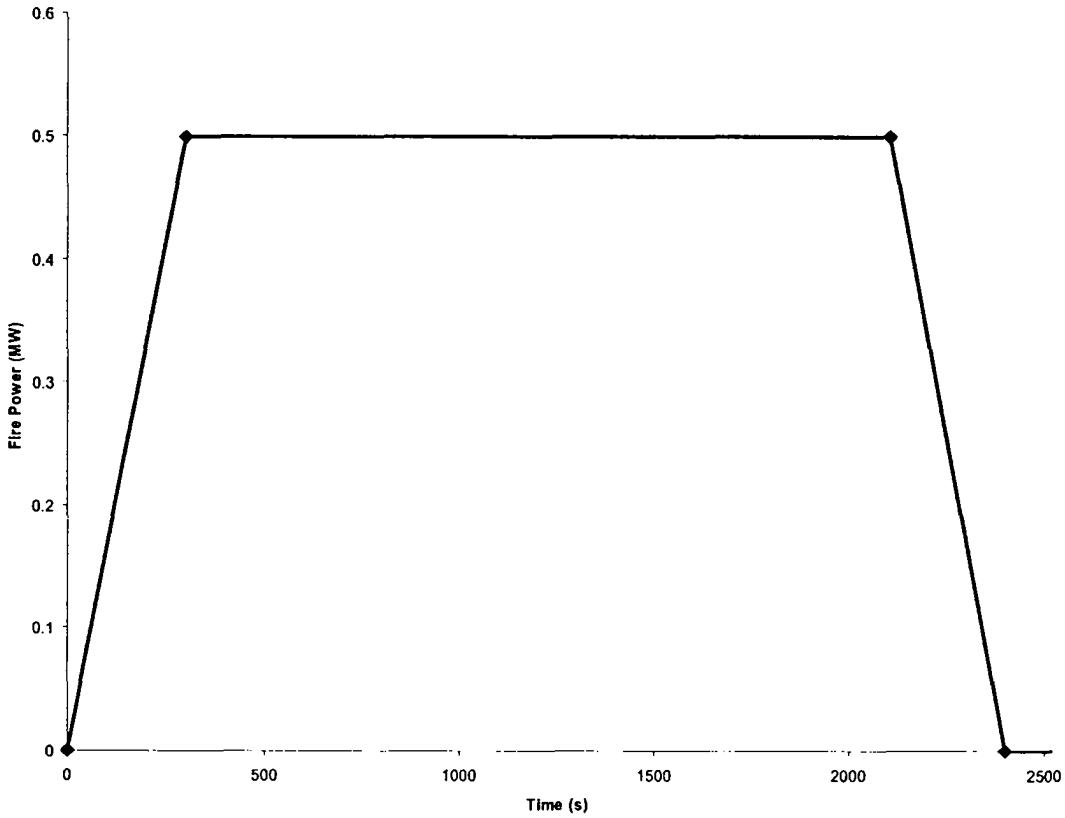

Figure B-4. Small Fire Profile

Benchmark Results

Seismic Spill – No ventilation

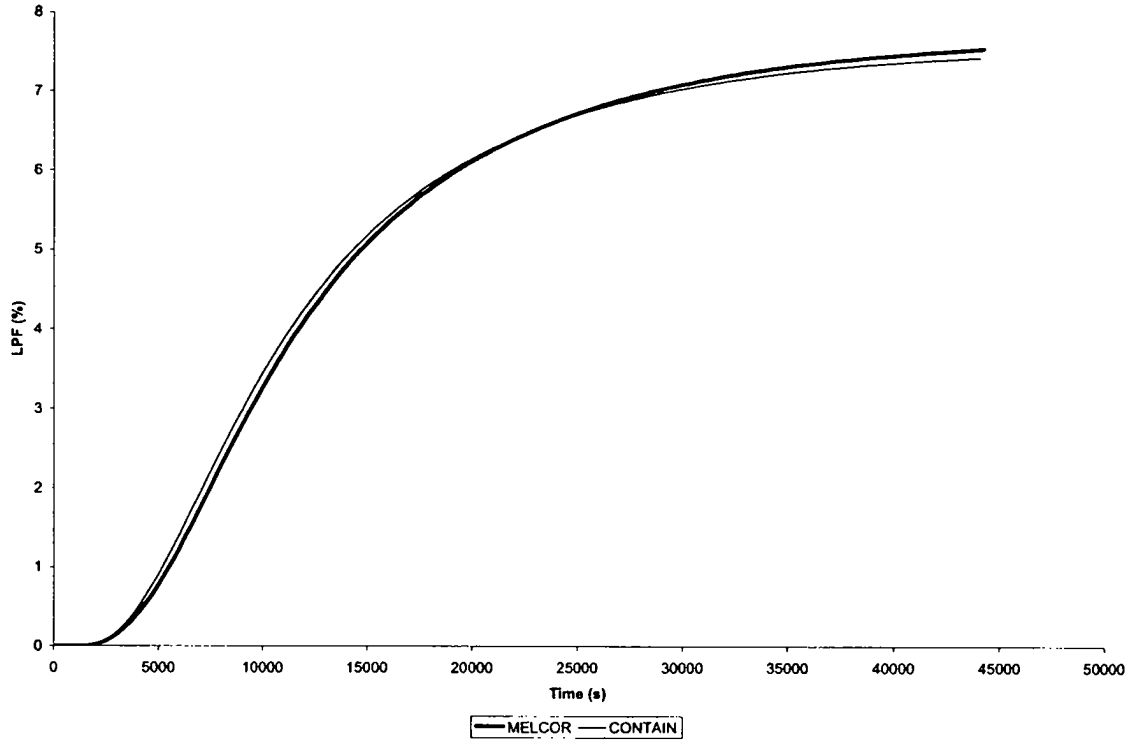

Figure B-5. Total LPF (Seismic Spill – No ventilation)

Seismic Spill – With ventilation

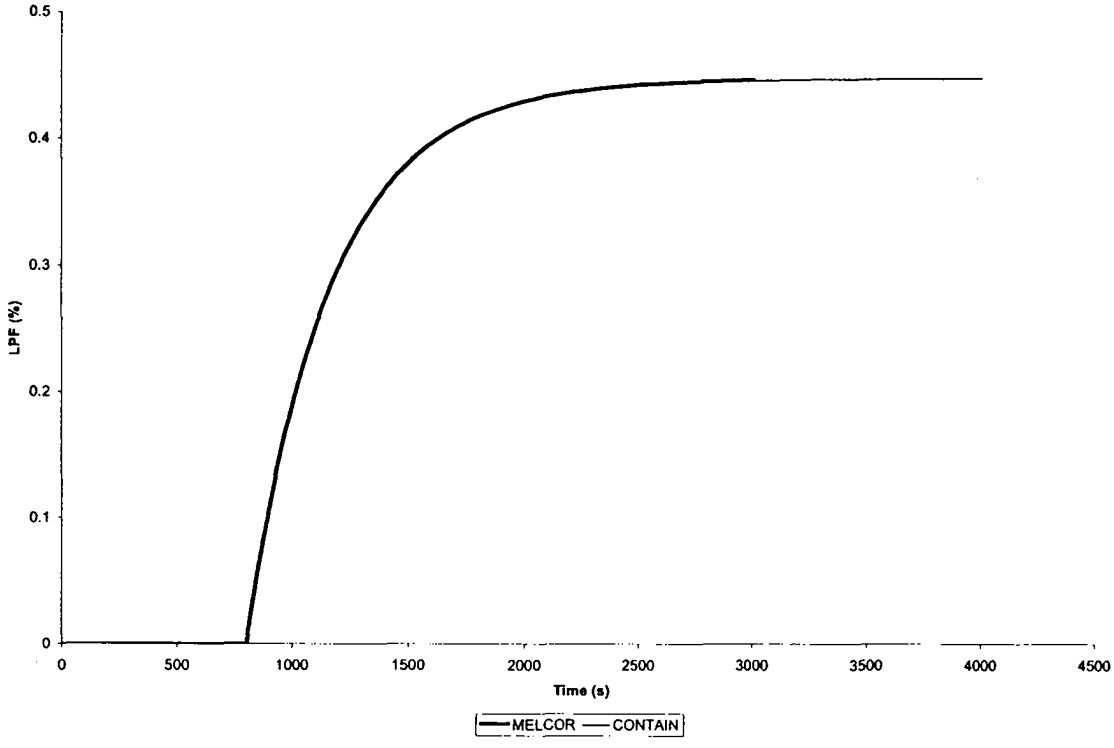

Figure B-6. Total LPF (Seismic Spill – With ventilation)

Spill With Large Fire and Ventilation

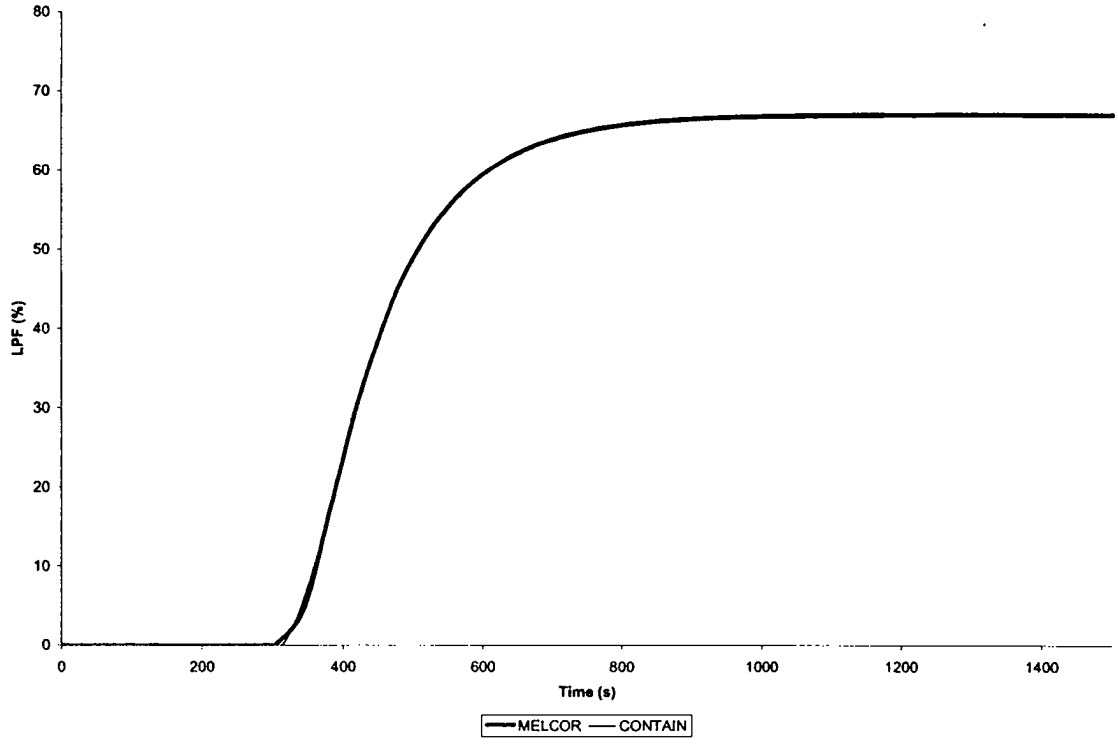

Figure B-7. Total LPF (Spill With Large Fire and Ventilation)

Spill With Large Fire and Ventilation – Predicted Temperature in Volume 150

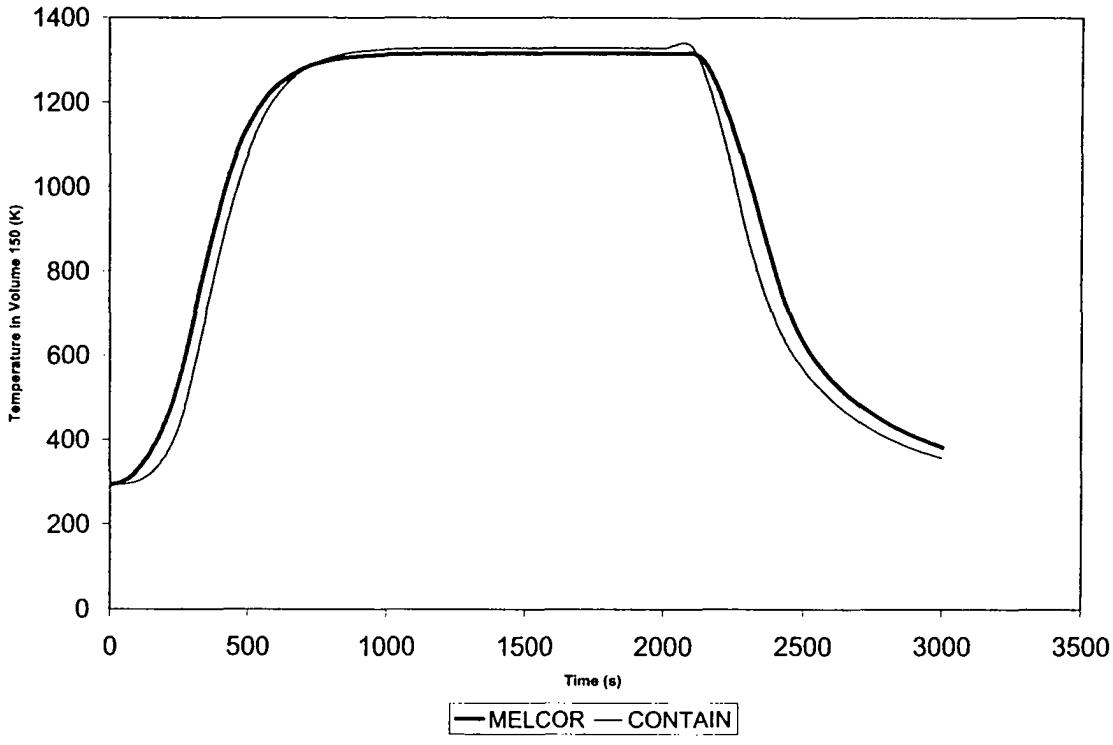

Figure B-8. Temperature in Volume 150 (Spill With Large Fire and Ventilation)

Spill with Small Fire – No Ventilation

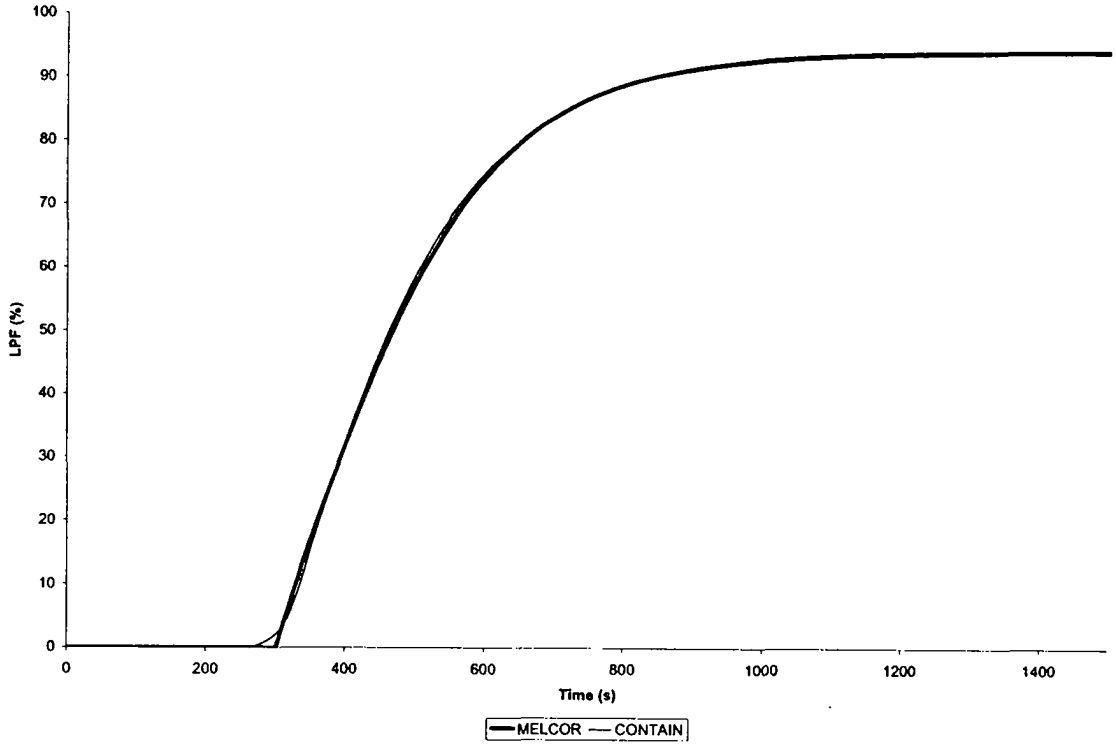

Figure B-9. Total LPF (Spill with Small Fire – No Ventilation)

Spill with Small Fire – No Ventilation - Predicted Temperature in Volume 150

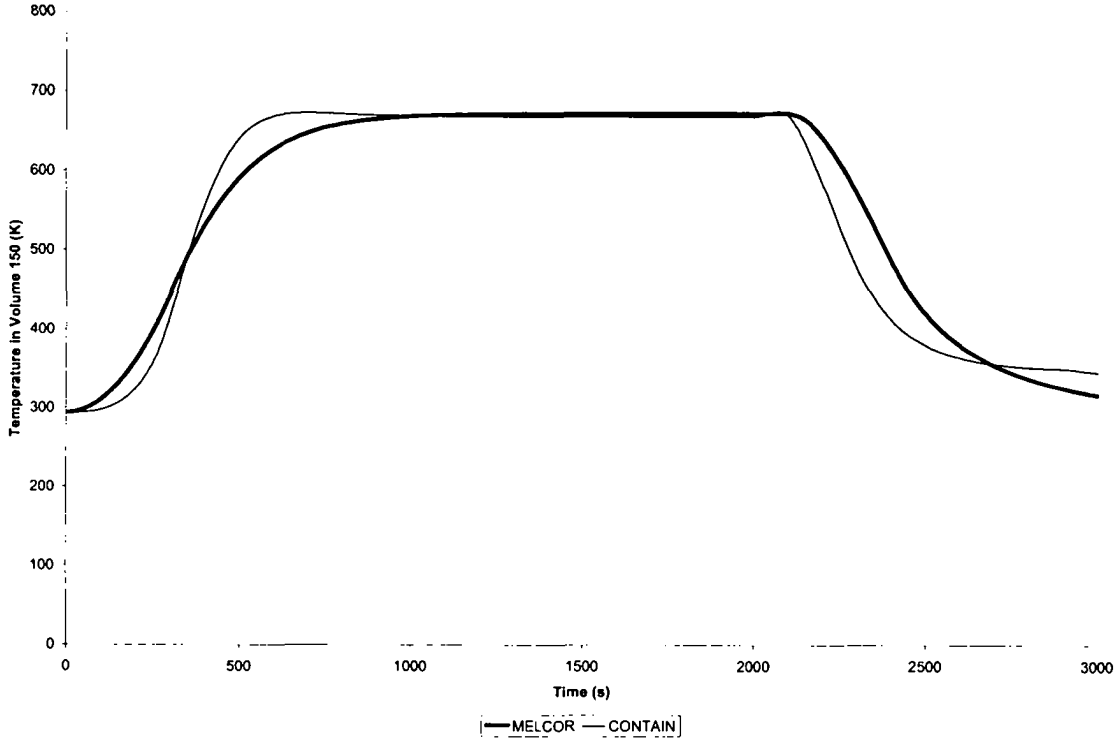

Figure B-10. Temperature in Volume 150 (Spill with Small Fire – No Ventilation)

Appendix C. Seismic Problem Input File

```
*EOR* MELGEN
*
**********************************
********** MELGEN INPUT **********
**********************************
* THE FOLLOWING CARD IS A TITLE CARD TO IDENTIFY THE INPUT
* DATA FILE AND OUTPUT RUN
TITLE     'TEST PROBLEM'
*
DTTIME    0.0001  * INITIAL TIME-STEP OF 1 MS
*
CRTOUT            * 80-COLUMN OUTPUT FORMAT
*
*********
* FILES *
*********
*  DEFINITION OF OUTPUT FILE NAMES
* THE USER CAN ASSIGN FILE NAMES AT HIS/HER DISCRETION
OUTPUTFILE   SAMPLEG.OUT
DIAGFILE     SAMPLEG.DIA
RESTARTFILE  SAMPLE.RST
*
*
* DEFINITION OF DEFAULT FLUID
* AIR DEFINITION - IN THIS PROBLEM THE DEFAULT FLUID IS
* DEFINED AS AIR 80% N2 AND 20% O2
NCG001    N2  4          * N2 IS MATERIAL NO. 4
NCG002    O2  5          * O2 IS MATERIAL NO. 5
* END AIR DEFINITION
**************************
* PRIMARY SYSTEM VOLUMES *
**************************
* FOR A TYPICAL LPF ANALYSIS THERE IS NO LIMITATION ON THE
* NUMBER OF CONTROL VOLUMES THE USER CAN SET IN THE ANALYSIS
*
* SEE THE CVHUSERGUIDE DOCUMENT FOR THE FOLLOWING INPUT DATA CARD
CV10000   ROOM100     2  1  1   * ROOM-100
*  VOLUME ENV. CONDITIONS
CV100A1   PVOL 101352.9          *  INITIAL PRESSURE IN PA
* NEXT INPUT CARD REPRESENTS THE CONTROL VOLUME INITIAL
* CONDITIONS
CV100A4 MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0 * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
* SEE THE CVHUSERGUIDE DOCUMENT FOR THE FOLLOWING INPUT DATA CARDS
CV100B1     0.0       0.0             * BOTTOM 0.0
CV100B2     4.        1104.4          * TOTAL VOLUME
*
*  THIS IS THE NEXT VOLUME (CELL) - COMMENTS AS ABOVE
CV15000   ROOM150     2  1  1   * ROOM-150
*  VOLUME ENV. CONDITIONS
CV150A1   PVOL 101352.9          * INITIAL PRESSURE
CV150A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV150B1     0.0       0.0         * BOTTOM AT 0.0
CV150B2     4.        1689.7      * TOTAL VOLUME
*
*
CV20000   ROOM200     2  1  1   * ROOM-200
CV200A1   PVOL 101352.9          * INITIAL PRESSURE
CV200A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV200B1     0.0       0.0         * BOTTOM AT 0.0
CV200B2     4.0       1689.7      * TOTAL VOLUME
*
*
CV25000   ROOM250     2  1  1   * ROOM-250
CV250A1   PVOL 101352.9          * INITIAL PRESSURE
```

```
CV250A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV250B1    0.0       0.0        * BOTTOM AT 0.0
CV250B2    4.0       375.5      * TOTAL VOLUME
*
*
CV30000   ROOM300     2  1  1   * ROOM-300
CV300A1   PVOL 101352.9         * INITIAL PRESSURE
CV300A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV300B1    0.0       0.0        * BOTTOM AT 0.0
CV300B2    4.0       828.3      * TOTAL VOLUME
*
*
CV35000   ROOM350     2  1  1   * ROOM-350
CV350A1   PVOL 101352.9         * INITIAL PRESSURE
CV350A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV350B1   0.0        0.0         * BOTTOM AT 0.0
CV350B2   4.0        1288.4      * TOTAL VOLUME
*
*
CV40000   ROOM400     2  1  1   * ROOM-400
CV400A1   PVOL 101352.9         * INITIAL PRESSURE
CV400A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV400B1   0.0      0.0          * BOTTOM AT 0.0
CV400B2   4.0      1159.6       * TOTAL VOLUME
*
*
CV45000   ROOM450     2  1  1   * ROOM-400
CV450A1   PVOL 101352.9         * INITIAL PRESSURE
CV450A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV450B1   0.0      0.0          * BOTTOM AT 0.0
CV450B2   4.0      368.1        * TOTAL VOLUME
*
*
****************************************
* ENVIRONMENTAL VOLUME - OUTSIDE CELLS *
****************************************
* THE EXTERNAL/ENVIRONMENTAL VOLUMES ARE USED TO COLLECT THE LPF DATA
CV50000   WEST-VOL500     2  1  1   * ENV-500 WEST
CV500A1   PVOL 101351.6992          * INITIAL PRESSURE
CV500A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV500B1   0.0      0.0          * BOTTOM AT 0.0
* FOR THE EXTERNAL/ENVIRONMENTAL VOLUMES A GEOMETRICAL VOLUME
* OF 1.0E+10 M3 IS ADEQUATE
CV500B2   4.0      1.0E10       * TOTAL VOLUME
*
*
CV60000   NORTH-VOL600     2  1  1   * ENV-600 NORTH
CV600A1   PVOL 101351.8493          * INITIAL PRESSURE
CV600A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV600B1   0.0      0.0          * BOTTOM AT 0.0
CV600B2   4.0      1.0E10       * TOTAL VOLUME
*
*
*  WIND FROM EAST AT 5 MPH
CV70000   EAST-VOL700     2  1  1    * ENV-700 EAST
CV700A1   PVOL 101355.0013          * INITIAL PRESSURE
CV700A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV700B1   0.0      0.0          * BOTTOM AT 0.0
CV700B2   4.0      1.0E10       * TOTAL VOLUME
*
*
CV80000   SOUTH-VOL800     2  1  1   * ENV-800 SOUTH
CV800A1   PVOL 101351.8493          * INITIAL PRESSURE
```

```
CV800A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV800B1   0.0     0.0          * BOTTOM AT 0.0
CV800B2   4.0     1.0E10       * TOTAL VOLUME
*
*
*
************************
* INTERNAL FLOW PATHS *
************************
* THE NEXT SET OF INPUT CARD ARE TYPICAL FLOW PATH (JUNCTION) DATA
* SEE THE FLUSERGUIDE DOCUMENT FOR EXTENDED DETAILS
*                        VOLUMES     JUNCTION ELEVATION
*                       FROM  TO     FROM    TO
FL11000   100-300       100   300    1.      1.
FL11001    0.0387       0.05   1.0            * AREA, LENGTH, OPEN FRACTION
*  NEXT CARD INCLUDES THE FORWARD AND REVERSE LOSS COEFFICIENT
FL11003    1.5    1.5                         * LOSS COEFFICIENTS
*  NEXT CARD INCLUDES THE FLOW AREA, FLOW PATH LENGTH, AND FLOW PATH
*  HYDRAULIC DIAMETER
FL110S0    0.0387       0.0508      0.0254    * A, L, HYD.DIAM.
*
*
*                        VOLUMES     JUNCT.ELEV.
*                       FROM  TO     FROM    TO
FL11500   100-250       100   250    1.      1.
FL11501    0.0387       0.05   1.0            * A, L, FRACTION OPEN
FL11503    1.5    1.5                         * LOSS COEFFICIENT
FL115S0    0.0387       0.0508    0.0254      * A, L, HYD.DIAM.
*
*
*                        VOLUMES     JUNCT.ELEV.
*                       FROM  TO     FROM    TO
FL12000   150-100       150   100    1.      1.
FL12001    0.0387       0.05   1.0            * A, L, FRACTION OPEN
FL12003    1.5    1.5                         * LOSS COEFFICIENT
FL120S0    0.0387       0.0508    0.0254      * A, L, HYD.DIAM.
*
*
*                        VOLUMES     JUNCT.ELEV.
*                       FROM  TO     FROM    TO
FL12500   300-350       300   350    1.      1.
FL12501    0.0387        0.05   1.0            * A, L, FRACTION OPEN
FL12503    1.5    1.5                         * LOSS COEFFICIENT
FL125S0    0.0387        0.0508    0.0254      * A, L, HYD.DIAM.
*
*
*                        VOLUMES     JUNCT.ELEV.
*                       FROM  TO     FROM    TO
FL13000   150-250       150   250    1.      1.
FL13001    0.0387       0.05   1.0            * A, L, FRACTION OPEN
FL13003    1.5    1.5                         * LOSS COEFFICIENT
FL130S0    0.0387       0.0508    0.0254      * A, L, HYD.DIAM.
*
*
*                        VOLUMES     JUNCT.ELEV.
*                       FROM  TO     FROM    TO
FL13500   150-200       150   200    1.      1.
FL13501    0.0387       0.05   1.0            * A, L, FRACTION OPEN
FL13503    1.5    1.5                         * LOSS COEFFICIENT
FL135S0    0.0387       0.0508    0.0254      * A, L, HYD.DIAM.
*
*
*                        VOLUMES     JUNCT.ELEV.
*                       FROM  TO     FROM    TO
FL14000   200-250       200   250    1.      1.
FL14001    0.0387       0.05   1.0            * A, L, FRACTION OPEN
FL14003    1.5    1.5                         * LOSS COEFFICIENT
FL140S0    0.0387       0.0508    0.0254      * A, L, HYD.DIAM.
*
*
```

```
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL14500   250-350      250   350     1.      1.
FL14501    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL14503    1.5    1.5                           * LOSS COEFFICIENT
FL145S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL15000   250-400      250   400     1.      1.
FL15001    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL15003    1.5    1.5                           * LOSS COEFFICIENT
FL150S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL15500   350-400      350   400     1.      1.
FL15501    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL15503    1.5    1.5                           * LOSS COEFFICIENT
FL155S0    0.0387      0.0508      0.0254       * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL16000   350-450      350   450     1.      1.
FL16001    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL16003    1.5    1.5                           * LOSS COEFFICIENT
FL160S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL16500   450-400      450   400     1.      1.
FL16501    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL16503    1.5    1.5                           * LOSS COEFFICIENT
FL165S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
**********************************
* FLOW PATHS FROM/TO EXTERNAL VOLUMES *
**********************************
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL17000    300-500     300   500     1.      1.
FL17001    0.0639      0.05    1.0              * A, L, FRACTION OPEN
FL17003    1.5    1.5                           * LOSS COEFFICIENT
FL170S0    0.0639      0.0508     0.0254        * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL17500   200-600      200   600     1.      1.
FL17501    0.0639      0.05    1.0              * A, L, FRACTION OPEN
FL17503    1.5    1.5                           * LOSS COEFFICIENT
FL175S0    0.0639      0.0508      0.0254       * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL18000   400-700      400   700     1.      1.
FL18001    0.0639      0.05    1.0              * A, L, FRACTION OPEN
FL18003    1.5    1.5                           * LOSS COEFFICIENT
FL180S0    0.0639      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       VOLUMES      JUNCT.ELEV.
*                      FROM  TO      FROM    TO
FL18500   450-800      450   800     1.      1.
FL18501    3.9     0.05    1.0              * A, L, FRACTION OPEN
```

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FL18503    1.5     1.5                    * LOSS COEFFICIENT
FL185S0    3.9     0.0508  1.6            * A, L, HYD.DIAM.
FL185V0    -1   251  251
* CONTROL FUNCTION TO USE TABULAR FUCTION 233
* SEE THE CFUSERGUIDE DOCUMENT FOR EXTENDED DETAILS
CF25100    'JUN CONROL' TAB-FUN 1  1.0  * TRIP ON TIME
CF25101    0.0
CF25103    233  * TAB FUNCTION NUMBER
CF25110   1.0  0.0  TIME
*  TAB FUNCTION NEXT
* SEE THE TFUSERGUIDE DOCUMENT FOR EXTENDED DETAILS
TF23300    'MOD DOOR'  6  1.0  0.
TF23310    0.0       0.0164
TF23311    120.      0.0164
TF23312    120.      1.0
TF23313    720.      1.0
TF23314    720.      0.0164
TF23315    200000.   0.0164
*
*  VENTILATION SUPPLY WALL OPENING
*                       VOLUMES     JUNCT.ELEV.
*                      FROM  TO     FROM    TO
FL19000   700-200      700   200    1.      1.
FL19001    2.0      0.05    1.0              * A, L, FRACTION OPEN
FL19003    1.5    1.5                       * LOSS COEFFICIENT
FL190S0    2.0    0.3048    2.0             * A, L, HYD.DIAM.
*
*
*
*
*************************
* HEAT STRUCTURES INPUT *
*************************
*
* SEE THE HSUSERGUIDE DOCUMENT FOR EXTENDED DETAILS
*
*
HS10001000   3       1                     * 3 NODES, RECTANGULAR GEOMETRY
HS10001001   'FLOOR 100'                   * STRUCTURE NAME
HS10001002   0.0   0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS10001100   -1      1       0.0           * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS10001101   0.3048     3                 * THIRD NODE NODE AT 0.3048 M
HS10001200   -1                           * DEFINE MATERIAL
HS10001201   'CONCRETE'     2             * 2 MESH POINTS
HS10001300   0                            * NO INTERNAL POWER SOURCE
HS10001400   0                            * ADIABATIC LOWER BC
HS10001600   1    100  EXT 0.0  0.0       * UPPER BC
*            AREA   CHAR.L  WIDTH          * EXTERNAL HEAT TRANSFER
HS10001700   278.7  20.0    20.0          * SUFRACE AREA M**2
*
HS10002000   3       1
HS10002001   'CEILING 100'
HS10002002   4.0    0.0                    * HEIGHT, HORIZONTAL
HS10002100   -1      1       0.0
HS10002101   0.3048     3
HS10002200   -1
HS10002201   'CONCRETE'      2
HS10002300   0
HS10002400   1    100  EXT 0.0  0.0
*            AREA   CHAR.L  WIDTH
HS10002500   278.7  5.0     5.0
HS10002600   0
*
HS10003000   3       1
HS10003001   'WALL 100'
HS10003002   0.0     1.0                   * BOTTOM AT 0.0 M, VERTICAL
HS10003100   -1      1       0.0
HS10003101   0.3048     3
HS10003200   -1
HS10003201   'CONCRETE'     2
HS10003300   0
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HS10003400   1       100    EXT    0.0    0.0
*            AREA    CHAR.L  WIDTH
HS10003500   265.7    3.0     3.0
HS10003600   1       300    EXT    0.0   0.0
*            AREA    CHAR.L  WIDTH
HS10003700   265.7    3.0     3.0
*
*
*
HS15001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS15001001   'FLOOR 150'                        * STRUCTURE NAME
HS15001002   0.0    0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS15001100   -1       1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS15001101   0.3048      3                     * THIRD NODE NODE AT 0.3048 M
HS15001200   -1                                 * DEFINE MATERIAL
HS15001201   'CONCRETE'      2                 * 2 MESH POINTS
HS15001300   0                                  * NO INTERNAL POWER SOURCE
HS15001400   0                                  * ADIABATIC LOWER BC
HS15001600  1     150  EXT 0.0  0.0           * UPPER BC
*            AREA    CHAR.L  WIDTH             * EXTERNAL HEAT TRANSFER
HS15001700   426.4  20.0     20.0              * SUFRACE AREA M**2
*
HS15002000   3       1
HS15002001   'CEILING 150'
HS15002002   4.0     0.0                        * BOTTOM NB
HS15002100   -1       1        0.0
HS15002101   0.3048      3
HS15002200   -1
HS15002201   'CONCRETE'       2
HS15002300   0
HS15002400   1     150  EXT 0.0  0.0
*            AREA    CHAR.L  WIDTH
HS15002500   426.4  5.0      5.0
HS15002600   0
*
HS15003000   3       1
HS15003001   'WALL 150'
HS15003002   0.0      1.0                       * BOTTOM AT 0.0 M, VERTICAL
HS15003100   -1       1        0.0
HS15003101   0.3048      3
HS15003200   -1
HS15003201   'CONCRETE'      2
HS15003300   0
HS15003400   1       150    EXT    0.0    0.0
*            AREA    CHAR.L  WIDTH
HS15003500   335.8    3.0     3.0
HS15003600   1       300    EXT    0.0   0.0
*            AREA    CHAR.L  WIDTH
HS15003700   335.8    3.0     3.0
*
*
*
HS20001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS20001001   'FLOOR 200'                        * STRUCTURE NAME
HS20001002   0.0    0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS20001100   -1       1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS20001101   0.3048      3                     * THIRD NODE NODE AT 0.3048 M
HS20001200   -1                                 * DEFINE MATERIAL
HS20001201   'CONCRETE'      2                 * 2 MESH POINTS
HS20001300   0                                  * NO INTERNAL POWER SOURCE
HS20001400   0                                  * ADIABATIC LOWER BC
HS20001600   1     200  EXT 0.0  0.0           * UPPER BC
*            AREA    CHAR.L  WIDTH             * EXTERNAL HEAT TRANSFER
HS20001700   426.4  20.0     20.0              * SUFRACE AREA M**2
*
HS20002000   3       1
HS20002001   'CEILING 200'
HS20002002   4.0     0.0                        * BOTTOM NB
HS20002100   -1       1        0.0
HS20002101   0.3048      3
HS20002200   -1
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HS20002201   'CONCRETE'      2
HS20002300   0
HS20002400   1    200  EXT 0.0  0.0
*            AREA   CHAR.L  WIDTH
HS20002500   426.4  5.0     5.0
HS20002600   0
*
HS20003000   3       1
HS20003001   'WALL 200'
HS20003002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS20003100   -1      1       0.0
HS20003101   0.3048     3
HS20003200   -1
HS20003201   'CONCRETE'     2
HS20003300   0
HS20003400   1      200   EXT   0.0   0.0
*            AREA   CHAR.L  WIDTH
HS20003500   335.8   3.0    3.0
HS20003600   1      300   EXT   0.0  0.0
*            AREA   CHAR.L  WIDTH
HS20003700   335.8   3.0    3.0
*
*
*
HS25001000   3       1                      * 3 NODES, RECTANGULAR GEOMETRY
HS25001001   'FLOOR 250'                    * STRUCTURE NAME
HS25001002   0.0   0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS25001100   -1      1       0.0            * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS25001101   0.3048     3                   * THIRD NODE NODE AT 0.3048 M
HS25001200   -1                           * DEFINE MATERIAL
HS25001201   'CONCRETE'     2              * 2 MESH POINTS
HS25001300   0                            * NO INTERNAL POWER SOURCE
HS25001400   0                            * ADIABATIC LOWER BC
HS25001600   1    250  EXT 0.0  0.0        * UPPER BC
*            AREA   CHAR.L  WIDTH          * EXTERNAL HEAT TRANSFER
HS25001700   94.8   20.0    20.0           * SUFRACE AREA M**2
*
HS25002000   3       1
HS25002001   'CEILING 250'
HS25002002   4.0     0.0                    * BOTTOM NB
HS25002100   -1      1       0.0
HS25002101   0.3048     3
HS25002200   -1
HS25002201   'CONCRETE'      2
HS25002300   0
HS25002400   1    250  EXT 0.0  0.0
*            AREA   CHAR.L  WIDTH
HS25002500   94.8   5.0     5.0
HS25002600   0
*
HS25003000   3       1
HS25003001   'WALL 250'
HS25003002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS25003100   -1      1       0.0
HS25003101   0.3048     3
HS25003200   -1
HS25003201   'CONCRETE'     2
HS25003300   0
HS25003400   1      250   EXT   0.0   0.0
*            AREA   CHAR.L  WIDTH
HS25003500   425.1   3.0    3.0
HS25003600   1      300   EXT   0.0  0.0
*            AREA   CHAR.L  WIDTH
HS25003700   425.1   3.0    3.0
*
*
*
HS30001000   3       1                      * 3 NODES, RECTANGULAR GEOMETRY
HS30001001   'FLOOR 300'                    * STRUCTURE NAME
HS30001002   0.0   0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS30001100   -1      1       0.0            * DEFINE NODE POSITIONS, FIRST AT 0.0 M
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HS30001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS30001200   -1                               * DEFINE MATERIAL
HS30001201   'CONCRETE'     2                 * 2 MESH POINTS
HS30001300   0                                * NO INTERNAL POWER SOURCE
HS30001400   0                                * ADIABATIC LOWER BC
HS30001600   1    300  EXT 0.0  0.0           * UPPER BC
*            AREA   CHAR.L  WIDTH             * EXTERNAL HEAT TRANSFER
HS30001700   209.   20.0    20.0              * SUFRACE AREA M**2
*
HS30002000   3       1
HS30002001   'CEILING 300'
HS30002002   4.0    0.0                       * BOTTOM NB
HS30002100   -1      1       0.0
HS30002101   0.3048     3
HS30002200   -1
HS30002201   'CONCRETE'      2
HS30002300   0
HS30002400   1    300  EXT 0.0  0.0
*            AREA   CHAR.L  WIDTH
HS30002500   209.   5.0     5.0
HS30002600   0
*
HS30003000   3       1
HS30003001   'WALL 300'
HS30003002   0.0     1.0                       * BOTTOM AT 0.0 M, VERTICAL
HS30003100   -1      1       0.0
HS30003101   0.3048     3
HS30003200   -1
HS30003201   'CONCRETE'     2
HS30003300   0
HS30003400   1      300   EXT   0.0   0.0
*            AREA   CHAR.L  WIDTH
HS30003500   229.5   3.0    3.0
HS30003600   1      150   EXT   0.0  0.0
*            AREA   CHAR.L  WIDTH
HS30003700   229.5   3.0    3.0
*
*
*
HS35001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS35001001   'FLOOR 350'                      * STRUCTURE NAME
HS35001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS35001100   -1      1       0.0              * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS35001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS35001200   -1                               * DEFINE MATERIAL
HS35001201   'CONCRETE'     2                 * 2 MESH POINTS
HS35001300   0                                * NO INTERNAL POWER SOURCE
HS35001400   0                                * ADIABATIC LOWER BC
HS35001600   1    350  EXT 0.0  0.0           * UPPER BC
*            AREA   CHAR.L  WIDTH             * EXTERNAL HEAT TRANSFER
HS35001700   325.2   20.0    20.0              * SUFRACE AREA M**2
*
HS35002000   3       1
HS35002001   'CEILING 350'
HS35002002   4.0    0.0                       * BOTTOM NB
HS35002100   -1      1       0.0
HS35002101   0.3048     3
HS35002200   -1
HS35002201   'CONCRETE'      2
HS35002300   0
HS35002400   1    350  EXT 0.0  0.0
*            AREA   CHAR.L  WIDTH
HS35002500   325.2   5.0     5.0
HS35002600   0
*
HS35003000   3       1
HS35003001   'WALL 350'
HS35003002   0.0     1.0                       * BOTTOM AT 0.0 M, VERTICAL
HS35003100   -1      1       0.0
HS35003101   0.3048     3
HS35003200   -1
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HS35003201   'CONCRETE'      2
HS35003300   0
HS35003400   1       350   EXT   0.0   0.0
*            AREA    CHAR.L  WIDTH
HS35003500   326.1    3.0     3.0
HS35003600   1       150   EXT   0.0  0.0
*            AREA    CHAR.L  WIDTH
HS35003700   326.1    3.0     3.0
*
*
*
HS40001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS40001001   'FLOOR 400'                      * STRUCTURE NAME
HS40001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS40001100   -1      1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS40001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS40001200   -1                              * DEFINE MATERIAL
HS40001201   'CONCRETE'      2                * 2 MESH POINTS
HS40001300   0                               * NO INTERNAL POWER SOURCE
HS40001400   0                               * ADIABATIC LOWER BC
HS40001600   1    400  EXT 0.0  0.0          * UPPER BC
*            AREA    CHAR.L  WIDTH           * EXTERNAL HEAT TRANSFER
HS40001700   292.6    20.0     20.0           * SUFRACE AREA M**2
*
HS40002000   3       1
HS40002001   'CEILING 400'
HS40002002   4.0     0.0                      * BOTTOM NB
HS40002100   -1      1        0.0
HS40002101   0.3048     3
HS40002200   -1
HS40002201   'CONCRETE'       2
HS40002300   0
HS40002400   1    400  EXT 0.0  0.0
*            AREA    CHAR.L  WIDTH
HS40002500   292.6    5.0      5.0
HS40002600   0
*
HS40003000   3       1
HS40003001   'WALL 400'
HS40003002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS40003100   -1      1        0.0
HS40003101   0.3048     3
HS40003200   -1
HS40003201   'CONCRETE'      2
HS40003300   0
HS40003400   1       400   EXT   0.0   0.0
*            AREA    CHAR.L  WIDTH
HS40003500   277.8    3.0     3.0
HS40003600   1       150   EXT   0.0  0.0
*            AREA    CHAR.L  WIDTH
HS40003700   277.8    3.0     3.0
*
*
*
HS45001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS45001001   'FLOOR 450'                      * STRUCTURE NAME
HS45001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS45001100   -1      1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS45001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS45001200   -1                              * DEFINE MATERIAL
HS45001201   'CONCRETE'      2                * 2 MESH POINTS
HS45001300   0                               * NO INTERNAL POWER SOURCE
HS45001400   0                               * ADIABATIC LOWER BC
HS45001600   1    450  EXT 0.0  0.0          * UPPER BC
*            AREA    CHAR.L  WIDTH           * EXTERNAL HEAT TRANSFER
HS45001700   92.9     20.0     20.0           * SUFRACE AREA M**2
*
HS45002000   3       1
HS45002001   'CEILING 450'
HS45002002   4.0     0.0                      * BOTTOM NB
HS45002100   -1      1        0.0
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HS45002101   0.3048      3
HS45002200   -1
HS45002201   'CONCRETE'       2
HS45002300   0
HS45002400   1     450  EXT 0.0  0.0
*            AREA    CHAR.L  WIDTH
HS45002500   92.9     5.0      5.0
HS45002600   0
*
HS45003000   3        1
HS45003001   'WALL 450'
HS45003002   0.0      1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS45003100   -1       1        0.0
HS45003101   0.3048      3
HS45003200   -1
HS45003201   'CONCRETE'      2
HS45003300   0
HS45003400   1       450    EXT    0.0    0.0
*            AREA    CHAR.L  WIDTH
HS45003500   265.7    3.0     3.0
HS45003600   1       150    EXT    0.0  0.0
*            AREA    CHAR.L  WIDTH
HS45003700   265.7    3.0     3.0
*
*
*
HS50001000   3        1
HS50001001   'FLOOR 500'
HS50001002   0.0    0.0
HS50001100   -1       1        0.0
HS50001101   0.3      3
HS50001200   -1
HS50001201   'CONCRETE'      2
HS50001300   0
HS50001400   0
HS50001600   1       500    EXT    0.0  0.0
HS50001700   0.0001  0.0001    0.0001           * AREA
*
*
*
HS60001000   3        1
HS60001001   'FLOOR 600'
HS60001002   0.0    0.0
HS60001100   -1       1        0.0
HS60001101   0.3      3
HS60001200   -1
HS60001201   'CONCRETE'      2
HS60001300   0
HS60001400   0
HS60001600   1       600    EXT    0.0  0.0
HS60001700   0.0001  0.0001    0.0001           * AREA
*
*
*
HS70001000   3        1
HS70001001   'FLOOR 700'
HS70001002   0.0    0.0
HS70001100   -1       1        0.0
HS70001101   0.3      3
HS70001200   -1
HS70001201   'CONCRETE'      2
HS70001300   0
HS70001400   0
HS70001600   1       700    EXT    0.0  0.0
HS70001700   0.0001  0.0001    0.0001           * AREA
*
*
*
HS80001000   3        1
HS80001001   'FLOOR 800'
HS80001002   0.0    0.0
```

```
HS80001100   -1       1        0.0
HS80001101   0.3      3
HS80001200   -1
HS80001201   'CONCRETE'      2
HS80001300   0
HS80001400   0
HS80001600   1       800    EXT    0.0  0.0
HS80001700   0.0001  0.0001     0.0001          * AREA
*
* AEROSOL SECTION
* SEE THE RNUSERGUIDE DOCUMENT FOR EXTENDED DETAILS
RN1000  0  *   ACTIVATE RADIO NUCLIDE PACKAGE (MODULE)
RNCA100 0  *   CHEMISORPTION NOT ACTIVE
*
* SEE PAGE 15 OF RNUSERGUIDE FOR NEXT CARD INPUT DETAILS (RN1001)
*
RN1001 20 2 17 0 0 1 0
* SEE PAGE 26 OF RNUSERGUIDE FOR NEXT CARD INPUT DETAILS (RN1100)
RN1100 1.0E-8 3.0E-6 11.46E+3 * MINIMUM AEROSOL PARTICLE DIAMETER,
* MAXIMUM AEROSOL PARTICLE DIAMETER, NOMINAL DENSITY OF AEROSOL

* SEE PAGE 26 OF RNUSERGUIDE FOR NEXT CARD INPUT DETAILS (RNACOEF)
RNACOEF   1
* SEE PAGE 31 OF RNUSERGUIDE FOR NEXT CARD INPUT DETAILS (RNASXXX)
RNAS000 350 2 1 1. 1.0 601 2 * 350 IS THE VOLUME NUMBER WHERE THE AEROSOL
* IS ORIGINALLY LOCATED
RNAS001 2.3E-6 2. * AEROSOL MASS MEDIAN DIAMETER, GEOMETRIC STANDARD
* DEVIATION
*
* DEFINE TABULAR FUNCTION AEROSOL RELEASE RATE
*
* TABULAR FUNCTION TO DEFINE THE AEROSOL TIME-RELEASE
TF60100   'AEROSOL'   5   1.0
TF60110   0.0      0.000    *  TIME  KG RELEASE
TF60111   10.0     0.000
TF60112   11.0     1.0
TF60113   12.0     0.0
TF60114   200000.  0.0
* END OF MELGEN INPUT DATA
.
* BEGIN MELCOR INPUT DATA
*EOR* MELCOR
*
**********************************
*          MELCOR INPUT          *
**********************************
*
TITLE     'TEST PROBLEM'
*
RESTART   0       * RESTART FROM CYCLE 0
*
TEND      72000.0  * END OF SIMULATION TIME
*
CPULIM    100000.0  * SET THIS NUMBER TO A HIGH VALUE
CPULEFT   20.0
*
CRTOUT            * 80-COLUMN OUTPUT FORMAT
*
*********
* FILES *
*********
*
RESTARTFILE  SAMPLE.RST
OUTPUTFILE   SAMPLE.OUT
PLOTFILE     SAMPLE.PTF
DIAGFILE     SAMPLE.DIA
MESSAGEFILE  SAMPLE.MES
*
******************************
* TIME STEP AND EDIT CONTROL *
******************************
```

```
* SEE THE EXECUSERGUIDE DOCUMENT FOR EXTENDED DETAILS
*          TIME      DTMAX      DTMIN        DTEDT      DTPLT      DTRST
TIME1      0.0       0.1        0.000000001   5.0       100.0      10.0
TIME2      1000.0     10.0      0.000000001   500.0     100.0      1000.0
TIME3      1100.0     30.0      0.000000001   500.0     100.0      1000.0
TIME4      1300.0     100.0     0.000000001   1000.0    200.0      5000.0
TIME5      2500.0     200.0     0.000000001   1000.0    200.0      5000.0
.
```

Appendix D. Seismic Problem (Ventilation Operating) Input File

```
*eor* melgen
*
**********************************
********** MELGEN INPUT **********
**********************************
*
TITLE     'TEST PROBLEM'
*
DTTIME    0.0001  * Initial time-step of 1 ms
*
CRTOUT            * 80-column output format
*
*********
* FILES *
*********
*  DEFINITION OF OUTPUT FILE NAMES
*
OUTPUTFILE   SAMPLEG.OUT
DIAGFILE     SAMPLEG.DIA
RESTARTFILE  SAMPLE.RST
*
*
* DEFINITION OF DEFAULT FLUID
* AIR DEFINITION
NCG001    N2  4          * N2 IS MATERIAL NO. 4
NCG002    O2  5          * O2 IS MATERIAL NO. 5
* END AIR DEFINITION
**************************
* PRIMARY SYSTEM VOLUMES *
**************************
*
CV10000   ROOM100     2  1  1    * ROOM-100
*  VOLUME ENV. CONDITIONS
CV100A1   PVOL 101352.9          * INITIAL PRESSURE
CV100A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV100B1     0.0       0.0              * BOTTOM 0.0
CV100B2     4.        1104.4           * TOTAL VOLUME
*
*
CV15000   ROOM150     2  1  1    * ROOM-150
*  VOLUME ENV. CONDITIONS
CV150A1   PVOL 101352.9          * INITIAL PRESSURE
CV150A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV150B1    0.0       0.0         * BOTTOM AT 0.0
CV150B2    4.        1689.7      * TOTAL VOLUME
*
*
CV20000   ROOM200     2  1  1    * ROOM-200
CV200A1   PVOL 101352.9          * INITIAL PRESSURE
CV200A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV200B1    0.0       0.0         * BOTTOM AT 0.0
CV200B2    4.0       1689.7      * TOTAL VOLUME
*
*
CV25000   ROOM250     2  1  1    * ROOM-250
CV250A1   PVOL 101352.9          * INITIAL PRESSURE
CV250A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV250B1    0.0       0.0         * BOTTOM AT 0.0
CV250B2    4.0       375.5       * TOTAL VOLUME
*
*
CV30000   ROOM300     2  1  1    * ROOM-300
CV300A1   PVOL 101352.9          * INITIAL PRESSURE
```

```
CV300A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV300B1    0.0       0.0        * BOTTOM AT 0.0
CV300B2    4.0       828.3      * TOTAL VOLUME
*
*
CV35000   ROOM350     2  1  1   * ROOM-350
CV350A1   PVOL 101352.9          * INITIAL PRESSURE
CV350A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV350B1   0.0        0.0          * BOTTOM AT 0.0
CV350B2   4.0        1288.4       * TOTAL VOLUME
*
*
CV40000   ROOM400     2  1  1   * ROOM-400
CV400A1   PVOL 101352.9          * INITIAL PRESSURE
CV400A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV400B1   0.0      0.0           * BOTTOM AT 0.0
CV400B2   4.0      1159.6        * TOTAL VOLUME
*
*
CV45000   ROOM450     2  1  1   * ROOM-400
CV450A1   PVOL 101352.9          * INITIAL PRESSURE
CV450A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV450B1   0.0      0.0           * BOTTOM AT 0.0
CV450B2   4.0      368.1         * TOTAL VOLUME
*
*
****************************************
* ENVIRONMENTAL VOLUME - OUTSIDE CELLS *
****************************************
*
CV50000   WEST-VOL500     2  1  1   * ENV-500 WEST
CV500A1   PVOL 101351.6992          * INITIAL PRESSURE
CV500A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV500B1   0.0      0.0           * BOTTOM AT 0.0
CV500B2   4.0      1.0E10        * TOTAL VOLUME
*
*
CV60000   NORTH-VOL600     2  1  1   * ENV-600 NORTH
CV600A1   PVOL 101351.8493          * INITIAL PRESSURE
CV600A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV600B1   0.0      0.0           * BOTTOM AT 0.0
CV600B2   4.0      1.0E10        * TOTAL VOLUME
*
*
*  WIND FROM EAST AT 5 MPH
CV70000   EAST-VOL700     2  1  1    * ENV-700 EAST
CV700A1   PVOL 101355.0013          * INITIAL PRESSURE
CV700A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV700B1   0.0      0.0           * BOTTOM AT 0.0
CV700B2   4.0      1.0E10        * TOTAL VOLUME
*
*
CV80000   SOUTH-VOL800     2  1  1   * ENV-800 SOUTH
CV800A1   PVOL 101351.8493          * INITIAL PRESSURE
CV800A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV800B1   0.0      0.0           * BOTTOM AT 0.0
CV800B2   4.0      1.0E10        * TOTAL VOLUME
*
*
* FILTER SYSTEM VOLUME
CV90000   FILTER-VOL900     2  1  1    * FILTER VOLUME
CV900A1   PVOL 101352.9                 * INITIAL PRESSURE
CV900A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0 * 80% N2, 20% O2
```

```
*       ALTITUDE OF CELL AND VOLUME
CV900B1   0.0      0.0          * BOTTOM AT 0.0
CV900B2   4.0      1.0E10       * TOTAL VOLUME
************************
* INTERNAL FLOW PATHS *
************************
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL11000   100-300       100   300     1.      1.
FL11001    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL11003    1.5    1.5                            * LOSS COEFFICIENT
FL110S0    0.0387       0.0508       0.0254      * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL11500   100-250       100   250     1.      1.
FL11501    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL11503    1.5    1.5                            * LOSS COEFFICIENT
FL115S0    0.0387       0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL12000   150-100       150   100     1.      1.
FL12001    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL12003    1.5    1.5                            * LOSS COEFFICIENT
FL120S0    0.0387       0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL12500   300-350       300   350     1.      1.
FL12501    0.0387        0.05    1.0               * A, L, FRACTION OPEN
FL12503    1.5    1.5                             * LOSS COEFFICIENT
FL125S0    0.0387        0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL13000   150-250       150   250     1.      1.
FL13001    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL13003    1.5    1.5                            * LOSS COEFFICIENT
FL130S0    0.0387       0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL13500   150-200       150   200     1.      1.
FL13501    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL13503    1.5    1.5                            * LOSS COEFFICIENT
FL135S0    0.0387       0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL14000   200-250       200   250     1.      1.
FL14001    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL14003    1.5    1.5                            * LOSS COEFFICIENT
FL140S0    0.0387       0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL14500   250-350       250   350     1.      1.
FL14501    0.0387       0.05    1.0              * A, L, FRACTION OPEN
FL14503    1.5    1.5                            * LOSS COEFFICIENT
FL145S0    0.0387       0.0508    0.0254        * A, L, HYD.DIAM.
*
*
*                        Volumes      Junct.Elev.
```

```
*                       From  To     From    To
FL15000   250-400       250   400    1.      1.
FL15001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL15003    1.5    1.5                          * LOSS COEFFICIENT
FL150S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL15500   350-400       350   400    1.      1.
FL15501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL15503    1.5    1.5                          * LOSS COEFFICIENT
FL155S0    0.0387       0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL16000   350-450       350   450    1.      1.
FL16001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL16003    1.5    1.5                          * LOSS COEFFICIENT
FL160S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL16500   450-400       450   400    1.      1.
FL16501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL16503    1.5    1.5                          * LOSS COEFFICIENT
FL165S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
**********************************
* FLOW PATHS FROM/TO EXTERNAL VOLUMES *
**********************************
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL17000    300-500      300   500    1.      1.
FL17001    0.0639       0.05    1.0            * A, L, FRACTION OPEN
FL17003    1.5    1.5                          * LOSS COEFFICIENT
FL170S0    0.0639       0.0508     0.0254      * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL17500   200-600       200   600    1.      1.
FL17501    0.0639       0.05    1.0            * A, L, FRACTION OPEN
FL17503    1.5    1.5                          * LOSS COEFFICIENT
FL175S0    0.0639       0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL18000   400-700       400   700    1.      1.
FL18001    0.0639       0.05    1.0            * A, L, FRACTION OPEN
FL18003    1.5    1.5                          * LOSS COEFFICIENT
FL180S0    0.0639       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL18500   450-800       450   800    1.      1.
FL18501    3.9     0.05    1.0             * A, L, FRACTION OPEN
FL18503    1.5     1.5                     * LOSS COEFFICIENT
FL185S0    3.9     0.0508  1.6             * A, L, HYD.DIAM.
FL185V0    -1   251  251
* USE A CONTROL FUNCTION
CF25100    'JUN CONROL' TAB-FUN 1  1.0  * TRIP ON TIME
CF25101    0.0
CF25103    233  * TAB FUNCTION NUMBER
CF25110   1.0  0.0  TIME
*  TAB FUNCTION NEXT
```

```
TF23300    'MOD DOOR'  6  1.0  0.
TF23310    0.0        0.0164
TF23311    120.       0.0164
TF23312    120.       1.0
TF23313    720.       1.0
TF23314    720.       0.0164
TF23315    200000.    0.0164
*
*  VENTILATION SUPPLY WALL OPENING
*                       Volumes     Junct.Elev.
*                     From  To      From    To
FL19000   700-200       700   200    1.      1.
FL19001    2.0      0.05    1.0                * A, L, FRACTION OPEN
FL19003    1.5    1.5                          * LOSS COEFFICIENT
FL190S0    2.0    0.3048    2.0                * A, L, HYD.DIAM.
*
********************
* TO FILTER SYSTEM *
********************
*
*  FIXED FLOW CONDITION TO FILTER SYSTEM
*                       Volumes     Junct.Elev.
*                     From  To      From    To
FL20100   100-900       100   900    1.      1.
FL20101    1.0      0.05    1.0             * A, L, FRACTION OPEN
FL201S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL201T0     1   201
TF20100     'FIXED FLOW' 3 1.0 0.0
TF20110     0.       1.226
TF20111     10.      1.226
TF20112     500000.  1.226
*
*
*                       Volumes     Junct.Elev.
*                     From  To      From    To
FL20200   150-900       150   900    1.      1.
FL20201    1.0      0.05    1.0             * A, L, FRACTION OPEN
FL202S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL202T0     1   202
TF20200     'FIXED FLOW' 3 1.0 0.0
TF20210     0.       1.876
TF20211     10.      1.876
TF20212     500000.  1.876
*
*
*                       Volumes     Junct.Elev.
*                     From  To      From    To
FL20300   200-900       200   900    1.      1.
FL20301    1.0      0.05    1.0             * A, L, FRACTION OPEN
FL203S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL203T0     1   203
TF20300     'FIXED FLOW' 3 1.0 0.0
TF20310     0.       1.876
TF20311     10.      1.876
TF20312     500000.  1.876
*
*
*                       Volumes     Junct.Elev.
*                     From  To      From    To
FL20400   250-900       250   900    1.      1.
FL20401    1.0      0.05    1.0             * A, L, FRACTION OPEN
FL204S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL204T0     1   204
TF20400     'FIXED FLOW' 3 1.0 0.0
TF20410     0.       0.417
TF20411     10.      0.417
TF20412     500000.  0.417
*
*
*                       Volumes     Junct.Elev.
*                     From  To      From    To
```

```
FL20500   300-900       300    900     1.       1.
FL20501    1.0       0.05     1.0             * A, L, FRACTION OPEN
FL20SS0    1.0       0.3048           1.0     * A, L, HYD.DIAM.
FL205T0     1   205
TF20500     'FIXED FLOW' 3 1.0 0.0
TF20510     0.       0.919
TF20511     10.      0.919
TF20512     500000. 0.919
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20600   350-900       350    900     1.       1.
FL20601    1.0       0.05     1.0             * A, L, FRACTION OPEN
FL206S0    1.0       0.3048           1.0     * A, L, HYD.DIAM.
FL206T0     1   206
TF20600     'FIXED FLOW' 3 1.0 0.0
TF20610     0.       1.430
TF20611     10.      1.430
TF20612     500000. 1.430
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20700   400-900       400    900     1.       1.
FL20701    1.0       0.05     1.0             * A, L, FRACTION OPEN
FL207S0    1.0       0.3048           1.0     * A, L, HYD.DIAM.
FL207T0     1   207
TF20700     'FIXED FLOW' 3 1.0 0.0
TF20710     0.       1.287
TF20711     10.      1.287
TF20712     500000. 1.287
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20800   450-900       450    900     1.       1.
FL20801    1.0       0.05     1.0             * A, L, FRACTION OPEN
FL208S0    1.0       0.3048           1.0     * A, L, HYD.DIAM.
FL208T0     1   208
TF20800     'FIXED FLOW' 3 1.0 0.0
TF20810     0.       0.409
TF20811     10.      0.409
TF20812     500000. 0.409
*
*
*************************
* HEAT STRUCTURES INPUT *
*************************
*
*
*
HS10001000   3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS10001001   'FLOOR 100'                     * STRUCTURE NAME
HS10001002   0.0   0.0                       * BOTTOM AT 0.0 M, HORIZONTAL
HS10001100   -1      1       0.0       * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS10001101   0.3048     3                   * THIRD NODE NODE AT 0.3048 M
HS10001200   -1                             * DEFINE MATERIAL
HS10001201   'CONCRETE'     2               * 2 MESH POINTS
HS10001300   0                              * NO INTERNAL POWER SOURCE
HS10001400   0                              * ADIABATIC LOWER BC
HS10001600   1    100  EXT 0.0  0.0         * UPPER BC
*            Area   Char.L  Width           * EXTernal heat transfer
HS10001700   278.7  20.0    20.0            * SUFRACE AREA M**2
*
HS10002000   3       1
HS10002001   'CEILING 100'
HS10002002   4.0     0.0                     * Bottom NB
HS10002100   -1      1       0.0
HS10002101   0.3048     3
HS10002200   -1
```

```
HS10002201   'CONCRETE'      2
HS10002300   0
HS10002400   1    100  EXT 0.0  0.0
*            Area   Char.L  Width
HS10002500   278.7  5.0     5.0
HS10002600   0
*
HS10003000   3       1
HS10003001   'WALL 100'
HS10003002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS10003100   -1      1       0.0
HS10003101   0.3048     3
HS10003200   -1
HS10003201   'CONCRETE'     2
HS10003300   0
HS10003400   1      100   EXT   0.0   0.0
*            Area   Char.L  Width
HS10003500   265.7   3.0    3.0
HS10003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS10003700   265.7   3.0    3.0
*
*
*
HS15001000   3       1                     * 3 NODES, RECTANGULAR GEOMETRY
HS15001001   'FLOOR 150'                   * STRUCTURE NAME
HS15001002   0.0   0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS15001100   -1      1       0.0           * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS15001101   0.3048     3                 * THIRD NODE NODE AT 0.3048 M
HS15001200   -1                           * DEFINE MATERIAL
HS15001201   'CONCRETE'     2             * 2 MESH POINTS
HS15001300   0                            * NO INTERNAL POWER SOURCE
HS15001400   0                            * ADIABATIC LOWER BC
HS15001600  1    150  EXT 0.0  0.0        * UPPER BC
*            Area   Char.L  Width          * EXTernal heat transfer
HS15001700   426.4  20.0    20.0          * SUFRACE AREA M**2
*
HS15002000   3       1
HS15002001   'CEILING 150'
HS15002002   4.0     0.0                   * Bottom NB
HS15002100   -1      1       0.0
HS15002101   0.3048     3
HS15002200   -1
HS15002201   'CONCRETE'      2
HS15002300   0
HS15002400   1    150  EXT 0.0  0.0
*            Area   Char.L  Width
HS15002500   426.4  5.0     5.0
HS15002600   0
*
HS15003000   3       1
HS15003001   'WALL 150'
HS15003002   0.0     1.0                   * BOTTOM AT 0.0 M, VERTICAL
HS15003100   -1      1       0.0
HS15003101   0.3048     3
HS15003200   -1
HS15003201   'CONCRETE'     2
HS15003300   0
HS15003400   1      150   EXT   0.0   0.0
*            Area   Char.L  Width
HS15003500   335.8   3.0    3.0
HS15003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS15003700   335.8   3.0    3.0
*
*
*
HS20001000   3       1                     * 3 NODES, RECTANGULAR GEOMETRY
HS20001001   'FLOOR 200'                   * STRUCTURE NAME
HS20001002   0.0   0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS20001100   -1      1       0.0           * DEFINE NODE POSITIONS, FIRST AT 0.0 M
```

```
HS20001101   0.3048      3                    * THIRD NODE NODE AT 0.3048 M
HS20001200   -1                               * DEFINE MATERIAL
HS20001201   'CONCRETE'      2                * 2 MESH POINTS
HS20001300   0                                * NO INTERNAL POWER SOURCE
HS20001400   0                                * ADIABATIC LOWER BC
HS20001600   1    200  EXT 0.0  0.0           * UPPER BC
*            Area   Char.L  Width             * EXTernal heat transfer
HS20001700   426.4  20.0    20.0             * SUFRACE AREA M**2
*
HS20002000   3       1
HS20002001   'CEILING 200'
HS20002002   4.0     0.0                      * Bottom NB
HS20002100   -1      1       0.0
HS20002101   0.3048     3
HS20002200   -1
HS20002201   'CONCRETE'      2
HS20002300   0
HS20002400   1    200  EXT 0.0  0.0
*            Area   Char.L  Width
HS20002500   426.4  5.0     5.0
HS20002600   0
*
HS20003000   3       1
HS20003001   'WALL 200'
HS20003002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS20003100   -1      1       0.0
HS20003101   0.3048     3
HS20003200   -1
HS20003201   'CONCRETE'     2
HS20003300   0
HS20003400   1      200   EXT   0.0   0.0
*            Area   Char.L  Width
HS20003500   335.8   3.0    3.0
HS20003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS20003700   335.8   3.0    3.0
*
*
*
HS25001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS25001001   'FLOOR 250'                      * STRUCTURE NAME
HS25001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS25001100   -1      1       0.0              * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS25001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS25001200   -1                               * DEFINE MATERIAL
HS25001201   'CONCRETE'     2                * 2 MESH POINTS
HS25001300   0                                * NO INTERNAL POWER SOURCE
HS25001400   0                                * ADIABATIC LOWER BC
HS25001600   1    250  EXT 0.0  0.0           * UPPER BC
*            Area   Char.L  Width             * EXTernal heat transfer
HS25001700   94.8   20.0    20.0             * SUFRACE AREA M**2
*
HS25002000   3       1
HS25002001   'CEILING 250'
HS25002002   4.0     0.0                      * Bottom NB
HS25002100   -1      1       0.0
HS25002101   0.3048     3
HS25002200   -1
HS25002201   'CONCRETE'      2
HS25002300   0
HS25002400   1    250  EXT 0.0  0.0
*            Area   Char.L  Width
HS25002500   94.8   5.0     5.0
HS25002600   0
*
HS25003000   3       1
HS25003001   'WALL 250'
HS25003002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS25003100   -1      1       0.0
HS25003101   0.3048     3
HS25003200   -1
```

```
HS25003201   'CONCRETE'     2
HS25003300   0
HS25003400   1      250   EXT   0.0   0.0
*            Area   Char.L  Width
HS25003500   425.1   3.0    3.0
HS25003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS25003700   425.1   3.0    3.0
*
*
*
HS30001000   3       1                      * 3 NODES, RECTANGULAR GEOMETRY
HS30001001   'FLOOR 300'                    * STRUCTURE NAME
HS30001002   0.0   0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS30001100   -1      1       0.0            * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS30001101   0.3048     3                  * THIRD NODE NODE AT 0.3048 M
HS30001200   -1                           * DEFINE MATERIAL
HS30001201   'CONCRETE'     2              * 2 MESH POINTS
HS30001300   0                            * NO INTERNAL POWER SOURCE
HS30001400   0                            * ADIABATIC LOWER BC
HS30001600   1    300  EXT 0.0  0.0        * UPPER BC
*            Area   Char.L  Width          * EXTernal heat transfer
HS30001700   209.   20.0    20.0           * SUFRACE AREA M**2
*
HS30002000   3       1
HS30002001   'CEILING 300'
HS30002002   4.0    0.0                    * Bottom NB
HS30002100   -1      1       0.0
HS30002101   0.3048     3
HS30002200   -1
HS30002201   'CONCRETE'      2
HS30002300   0
HS30002400   1    300  EXT 0.0  0.0
*            Area   Char.L  Width
HS30002500   209.   5.0     5.0
HS30002600   0
*
HS30003000   3       1
HS30003001   'WALL 300'
HS30003002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS30003100   -1      1       0.0
HS30003101   0.3048     3
HS30003200   -1
HS30003201   'CONCRETE'     2
HS30003300   0
HS30003400   1      300   EXT   0.0   0.0
*            Area   Char.L  Width
HS30003500   229.5   3.0    3.0
HS30003600   1      150   EXT   0.0  0.0
*            Area   Char.L  Width
HS30003700   229.5   3.0    3.0
*
*
*
HS35001000   3       1                      * 3 NODES, RECTANGULAR GEOMETRY
HS35001001   'FLOOR 350'                    * STRUCTURE NAME
HS35001002   0.0   0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS35001100   -1      1       0.0            * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS35001101   0.3048     3                  * THIRD NODE NODE AT 0.3048 M
HS35001200   -1                           * DEFINE MATERIAL
HS35001201   'CONCRETE'     2              * 2 MESH POINTS
HS35001300   0                            * NO INTERNAL POWER SOURCE
HS35001400   0                            * ADIABATIC LOWER BC
HS35001600   1    350  EXT 0.0  0.0        * UPPER BC
*            Area   Char.L  Width          * EXTernal heat transfer
HS35001700   325.2   20.0    20.0           * SUFRACE AREA M**2
*
HS35002000   3       1
HS35002001   'CEILING 350'
HS35002002   4.0    0.0                    * Bottom NB
HS35002100   -1      1       0.0
```

```
HS35002101   0.3048      3
HS35002200   -1
HS35002201   'CONCRETE'       2
HS35002300   0
HS35002400   1     350  EXT 0.0  0.0
*            Area    Char.L  Width
HS35002500   325.2    5.0      5.0
HS35002600   0
*
HS35003000   3        1
HS35003001   'WALL 350'
HS35003002   0.0      1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS35003100   -1       1        0.0
HS35003101   0.3048      3
HS35003200   -1
HS35003201   'CONCRETE'      2
HS35003300   0
HS35003400   1       350    EXT    0.0    0.0
*            Area    Char.L  Width
HS35003500   326.1    3.0     3.0
HS35003600   1       150    EXT    0.0  0.0
*            Area    Char.L  Width
HS35003700   326.1    3.0     3.0
*
*
*
HS40001000   3        1                        * 3 NODES, RECTANGULAR GEOMETRY
HS40001001   'FLOOR 400'                       * STRUCTURE NAME
HS40001002   0.0    0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS40001100   -1       1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS40001101   0.3048      3                     * THIRD NODE NODE AT 0.3048 M
HS40001200   -1                               * DEFINE MATERIAL
HS40001201   'CONCRETE'      2                 * 2 MESH POINTS
HS40001300   0                                * NO INTERNAL POWER SOURCE
HS40001400   0                                * ADIABATIC LOWER BC
HS40001600   1     400  EXT 0.0  0.0          * UPPER BC
*            Area    Char.L  Width             * EXTernal heat transfer
HS40001700   292.6    20.0     20.0            * SUFRACE AREA M**2
*
HS40002000   3        1
HS40002001   'CEILING 400'
HS40002002   4.0     0.0                       * Bottom NB
HS40002100   -1       1        0.0
HS40002101   0.3048      3
HS40002200   -1
HS40002201   'CONCRETE'       2
HS40002300   0
HS40002400   1     400  EXT 0.0  0.0
*            Area    Char.L  Width
HS40002500   292.6    5.0      5.0
HS40002600   0
*
HS40003000   3        1
HS40003001   'WALL 400'
HS40003002   0.0      1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS40003100   -1       1        0.0
HS40003101   0.3048      3
HS40003200   -1
HS40003201   'CONCRETE'      2
HS40003300   0
HS40003400   1       400    EXT    0.0    0.0
*            Area    Char.L  Width
HS40003500   277.8    3.0     3.0
HS40003600   1       150    EXT    0.0  0.0
*            Area    Char.L  Width
HS40003700   277.8    3.0     3.0
*
*
*
HS45001000   3        1                        * 3 NODES, RECTANGULAR GEOMETRY
HS45001001   'FLOOR 450'                       * STRUCTURE NAME
```

```
HS45001002   0.0    0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS45001100   -1       1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS45001101   0.3048      3                     * THIRD NODE NODE AT 0.3048 M
HS45001200   -1                                 * DEFINE MATERIAL
HS45001201   'CONCRETE'      2                 * 2 MESH POINTS
HS45001300   0                                  * NO INTERNAL POWER SOURCE
HS45001400   0                                  * ADIABATIC LOWER BC
HS45001600   1    450  EXT 0.0  0.0            * UPPER BC
*            Area    Char.L  Width              * EXTernal heat transfer
HS45001700   92.9     20.0     20.0             * SUFRACE AREA M**2
*
HS45002000   3       1
HS45002001   'CEILING 450'
HS45002002   4.0     0.0                        * Bottom NB
HS45002100   -1       1        0.0
HS45002101   0.3048      3
HS45002200   -1
HS45002201   'CONCRETE'       2
HS45002300   0
HS45002400   1    450  EXT 0.0  0.0
*            Area    Char.L  Width
HS45002500   92.9     5.0      5.0
HS45002600   0
*
HS45003000   3       1
HS45003001   'WALL 450'
HS45003002   0.0      1.0                       * BOTTOM AT 0.0 M, VERTICAL
HS45003100   -1       1        0.0
HS45003101   0.3048      3
HS45003200   -1
HS45003201   'CONCRETE'      2
HS45003300   0
HS45003400   1       450   EXT   0.0   0.0
*            Area    Char.L  Width
HS45003500   265.7    3.0     3.0
HS45003600   1       150   EXT   0.0  0.0
*            Area    Char.L  Width
HS45003700   265.7    3.0     3.0
*
*
*
HS50001000   3       1
HS50001001   'FLOOR 500'
HS50001002   0.0    0.0
HS50001100   -1       1        0.0
HS50001101   0.3      3
HS50001200   -1
HS50001201   'CONCRETE'      2
HS50001300   0
HS50001400   0
HS50001600   1       500   EXT   0.0  0.0
HS50001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS60001000   3       1
HS60001001   'FLOOR 600'
HS60001002   0.0    0.0
HS60001100   -1       1        0.0
HS60001101   0.3      3
HS60001200   -1
HS60001201   'CONCRETE'      2
HS60001300   0
HS60001400   0
HS60001600   1       600   EXT   0.0  0.0
HS60001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS70001000   3       1
HS70001001   'FLOOR 700'
```

```
HS70001002   0.0    0.0
HS70001100   -1       1        0.0
HS70001101   0.3      3
HS70001200   -1
HS70001201   'CONCRETE'      2
HS70001300   0
HS70001400   0
HS70001600   1       700    EXT    0.0  0.0
HS70001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS80001000   3        1
HS80001001   'FLOOR 800'
HS80001002   0.0    0.0
HS80001100   -1       1        0.0
HS80001101   0.3      3
HS80001200   -1
HS80001201   'CONCRETE'      2
HS80001300   0
HS80001400   0
HS80001600   1       800    EXT    0.0  0.0
HS80001700   0.0001  0.0001    0.0001          * AREA
*
HS90001000   3        1
HS90001001   'FLOOR 900'
HS90001002   0.0    0.0
HS90001100   -1       1        0.0
HS90001101   0.3      3
HS90001200   -1
HS90001201   'CONCRETE'      2
HS90001300   0
HS90001400   0
HS90001600   1       900    EXT    0.0  0.0
HS90001700   0.0001  0.0001    0.0001          * AREA
*
* AEROSOL SECTION
RN1000 0  *   ACTIVATE
RNCA100 0 *   NOT ACTIVE
*
RN1001 20 2 17 0 0 1 0
RN1100 1.0e-8 3.0e-6 11.46e+3
RNACOEF   1
*
RNAS000 350 2 1 1. 1.0 601 2
RNAS001 2.3e-6 2.

* DEFINE TABULAR FUNCTION AEROSOL RELEASE RATE
*
TF60100   'AEROSOL'   5   1.0
TF60110   0.0       0.000     *  TIME  1 KG RELEASE
TF60111   10.0      0.000
TF60112   11.0      1.0
TF60113   12.0      0.0
TF60114   200000.   0.0
.
*eor* melcor
*
**********************************
*          MELCOR INPUT          *
**********************************
*
TITLE     'TEST PROBLEM'
*
RESTART   0       * RESTART FROM CYCLE 0
*
TEND      72000.0  * END TIME S
*
CPULIM    100000.0
CPULEFT   20.0
*
```

```
CRTOUT            * 80-COLUMN OUTPUT FORMAT
*
*********
* FILES *
*********
*
RESTARTFILE  SAMPLE.RST
OUTPUTFILE   SAMPLE.OUT
PLOTFILE     SAMPLE.PTF
DIAGFILE     SAMPLE.DIA
MESSAGEFILE  SAMPLE.MES
*
******************************
* TIME STEP AND EDIT CONTROL *
******************************
*          TIME      DTMAX      DTMIN         DTEDT      DTPLT      DTRST
TIME1      0.0       0.1      0.000000001     5.0        100.0      10.0
TIME2      1000.0     10.0    0.000000001     500.0      100.0      1000.0
TIME3      1100.0     30.0    0.000000001     500.0      100.0      1000.0
TIME4      1300.0     100.0   0.000000001     1000.0     200.0      5000.0
TIME5      2500.0     200.0   0.000000001     1000.0     200.0      5000.0
.
```

Appendix E. Fire Problem Input File

```
*eor* melgen
*
**********************************
********** MELGEN INPUT **********
**********************************
*
TITLE     'TEST PROBLEM'
*
DTTIME    0.001  * Initial time-step of 1 ms
*
CRTOUT           * 80-column output format
*
*********
* FILES *
*********
*  DEFINITION OF OUTPUT FILE NAMES
*
OUTPUTFILE   SAMPLEG.OUT
DIAGFILE     SAMPLEG.DIA
RESTARTFILE  SAMPLE.RST
*
*
* DEFINITION OF DEFAULT FLUID
* AIR DEFINITION
NCG001    N2  4          * N2 IS MATERIAL NO. 4
NCG002    O2  5          * O2 IS MATERIAL NO. 5
* END AIR DEFINITION
**************************
* PRIMARY SYSTEM VOLUMES *
**************************
*
CV10000   ROOM100     2  1  1   * ROOM-100
*  VOLUME ENV. CONDITIONS
CV100A1   PVOL 101352.9          * INITIAL PRESSURE
CV100A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV100B1     0.0       0.0              * BOTTOM 0.0
CV100B2     4.        1104.4           * TOTAL VOLUME
*
*
CV15000   ROOM150     2  1  1   * ROOM-150
*  VOLUME ENV. CONDITIONS
CV150A1   PVOL 101352.9          * INITIAL PRESSURE
CV150A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV150B1    0.0       0.0         * BOTTOM AT 0.0
CV150B2    4.        1689.7      * TOTAL VOLUME
*
*
CV20000   ROOM200     2  1  1   * ROOM-200
CV200A1   PVOL 101352.9          * INITIAL PRESSURE
CV200A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV200B1    0.0       0.0         * BOTTOM AT 0.0
CV200B2    4.0       1689.7      * TOTAL VOLUME
*
*
CV25000   ROOM250     2  1  1   * ROOM-250
CV250A1   PVOL 101352.9          * INITIAL PRESSURE
CV250A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV250B1    0.0       0.0         * BOTTOM AT 0.0
CV250B2    4.0       375.5       * TOTAL VOLUME
*
*
CV30000   ROOM300     2  1  1   * ROOM-300
CV300A1   PVOL 101352.9          * INITIAL PRESSURE
```

```
CV300A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV300B1    0.0        0.0        * BOTTOM AT 0.0
CV300B2    4.0        828.3      * TOTAL VOLUME
*
*
CV35000   ROOM350     2  1  1    * ROOM-350
CV350A1   PVOL 101352.9          * INITIAL PRESSURE
CV350A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV350B1   0.0        0.0         * BOTTOM AT 0.0
CV350B2   4.0        1288.4      * TOTAL VOLUME

CV350C1   MASS.3   RATE  CF.998  * VAPOR MASS C-FUNCTION
CV350C2   ENERGY.A RATE  CF.999  * CORRESPONDING ENTALPY
CF99800   'VAPOR MASS'  TAB-FUN  1   1.0
CF99803   998                    * TF NUMBER
CF99810   1.0   0.0  TIME        * ARGUMENT IS TIME
TF99800   'VAPOR MASS'   5   1.0
TF99810   0.0    0.0
TF99811   300.   0.001
TF99812   900.   0.001
TF99813   1200.  0.0
TF99814   200000.  0.0
*
CF99900   'ENTHALPY'  MULTIPLY  2   1.0  * ENTHALPY RATE
CF99910   1.0   0.0     CFVALU.998
CF99911   0.0   1.0E+9  TIME
*
* END FIRE SOURCE
*
*
CV40000   ROOM400     2  1  1    * ROOM-400
CV400A1   PVOL 101352.9          * INITIAL PRESSURE
CV400A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV400B1   0.0      0.0          * BOTTOM AT 0.0
CV400B2   4.0      1159.6       * TOTAL VOLUME
*
*
CV45000   ROOM450     2  1  1    * ROOM-400
CV450A1   PVOL 101352.9          * INITIAL PRESSURE
CV450A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV450B1   0.0      0.0          * BOTTOM AT 0.0
CV450B2   4.0      368.1        * TOTAL VOLUME
*
*
****************************************
* ENVIRONMENTAL VOLUME - OUTSIDE CELLS *
****************************************
*
CV50000   WEST-VOL500     2  1  1    * ENV-500 WEST
CV500A1   PVOL 101351.6992           * INITIAL PRESSURE
CV500A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV500B1   0.0      0.0          * BOTTOM AT 0.0
CV500B2   4.0      1.0E10       * TOTAL VOLUME
*
*
CV60000   NORTH-VOL600     2  1  1    * ENV-600 NORTH
CV600A1   PVOL 101351.8493           * INITIAL PRESSURE
CV600A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV600B1   0.0      0.0          * BOTTOM AT 0.0
CV600B2   4.0      1.0E10       * TOTAL VOLUME
*
*
*  WIND FROM EAST AT 5 MPH
CV70000   EAST-VOL700     2  1  1     * ENV-700 EAST
CV700A1   PVOL 101355.0013           * INITIAL PRESSURE
```

```
CV700A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV700B1   0.0     0.0          * BOTTOM AT 0.0
CV700B2   4.0     1.0E10       * TOTAL VOLUME
*
*
CV80000   SOUTH-VOL800     2  1  1   * ENV-800 SOUTH
CV800A1   PVOL 101351.8493             * INITIAL PRESSURE
CV800A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV800B1   0.0     0.0          * BOTTOM AT 0.0
CV800B2   4.0     1.0E10       * TOTAL VOLUME
*
*
*
***********************
* INTERNAL FLOW PATHS *
***********************
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL11000   100-300       100   300    1.      1.
FL11001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL11003    1.5    1.5                          * LOSS COEFFICIENT
FL110S0    0.0387       0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL11500   100-250       100   250    1.      1.
FL11501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL11503    1.5    1.5                          * LOSS COEFFICIENT
FL115S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL12000   150-100       150   100    1.      1.
FL12001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL12003    1.5    1.5                          * LOSS COEFFICIENT
FL120S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL12500   300-350       300   350    1.      1.
FL12501    0.0387        0.05    1.0             * A, L, FRACTION OPEN
FL12503    1.5    1.5                           * LOSS COEFFICIENT
FL125S0    0.0387        0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL13000   150-250       150   250    1.      1.
FL13001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL13003    1.5    1.5                          * LOSS COEFFICIENT
FL130S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL13500   150-200       150   200    1.      1.
FL13501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL13503    1.5    1.5                          * LOSS COEFFICIENT
FL135S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL14000   200-250       200   250    1.      1.
FL14001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL14003    1.5    1.5                          * LOSS COEFFICIENT
```

```
FL140S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL14500   250-350      250   350    1.      1.
FL14501    0.0387      0.05    1.0            * A, L, FRACTION OPEN
FL14503    1.5    1.5                         * LOSS COEFFICIENT
FL145S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL15000   250-400      250   400    1.      1.
FL15001    0.0387      0.05    1.0            * A, L, FRACTION OPEN
FL15003    1.5    1.5                         * LOSS COEFFICIENT
FL150S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL15500   350-400      350   400    1.      1.
FL15501    0.0387      0.05    1.0            * A, L, FRACTION OPEN
FL15503    1.5    1.5                         * LOSS COEFFICIENT
FL155S0    0.0387      0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL16000   350-450      350   450    1.      1.
FL16001    0.0387      0.05    1.0            * A, L, FRACTION OPEN
FL16003    1.5    1.5                         * LOSS COEFFICIENT
FL160S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL16500   450-400      450   400    1.      1.
FL16501    0.0387      0.05    1.0            * A, L, FRACTION OPEN
FL16503    1.5    1.5                         * LOSS COEFFICIENT
FL165S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
**********************************
* FLOW PATHS FROM/TO EXTERNAL VOLUMES *
**********************************
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL17000    300-500     300   500    1.      1.
FL17001    0.0639      0.05    1.0            * A, L, FRACTION OPEN
FL17003    1.5    1.5                         * LOSS COEFFICIENT
FL170S0    0.0639      0.0508     0.0254      * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL17500   200-600      200   600    1.      1.
FL17501    0.0639      0.05    1.0            * A, L, FRACTION OPEN
FL17503    1.5    1.5                         * LOSS COEFFICIENT
FL175S0    0.0639      0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL18000   400-700      400   700    1.      1.
FL18001    0.0639      0.05    1.0            * A, L, FRACTION OPEN
FL18003    1.5    1.5                         * LOSS COEFFICIENT
FL180S0    0.0639      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
```

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*                       From  To     From    To
FL18500   450-800       450   800    1.      1.
FL18501    3.9     0.05    1.0             * A, L, FRACTION OPEN
FL18503    1.5     1.5                     * LOSS COEFFICIENT
FL185S0    3.9     0.0508  1.6             * A, L, HYD.DIAM.
FL185V0    -1   251  251
* USE A CONTROL FUNCTION
CF25100    'JUN CONROL' TAB-FUN 1  1.0  * TRIP ON TIME
CF25101    0.0
CF25103    233  * TAB FUNCTION NUMBER
CF25110   1.0  0.0  TIME
*  TAB FUNCTION NEXT
TF23300    'MOD DOOR'  6  1.0  0.
TF23310    0.0       0.0164
TF23311    120.      0.0164
TF23312    120.      1.0
TF23313    720.      1.0
TF23314    720.      0.0164
TF23315    200000.   0.0164
*
*  VENTILATION SUPPLY WALL OPENING
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL19000   700-200       700   200    1.      1.
FL19001    2.0      0.05    1.0               * A, L, FRACTION OPEN
FL19003    1.5    1.5                         * LOSS COEFFICIENT
FL190S0    2.0    0.3048    2.0               * A, L, HYD.DIAM.
*
*
*
*
*************************
* HEAT STRUCTURES INPUT *
*************************
*
*
*
HS10001000   3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS10001001   'FLOOR 100'                     * STRUCTURE NAME
HS10001002   0.0   0.0                       * BOTTOM AT 0.0 M, HORIZONTAL
HS10001100   -1      1       0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS10001101   0.3048     3                   * THIRD NODE NODE AT 0.3048 M
HS10001200   -1                              * DEFINE MATERIAL
HS10001201   'CONCRETE'     2               * 2 MESH POINTS
HS10001300   0                               * NO INTERNAL POWER SOURCE
HS10001400   0                               * ADIABATIC LOWER BC
HS10001600   1    100  EXT 0.0  0.0          * UPPER BC
*            Area   Char.L  Width            * EXTernal heat transfer
HS10001700   278.7  20.0    20.0             * SUFRACE AREA M**2
*
HS10002000   3       1
HS10002001   'CEILING 100'
HS10002002   4.0    0.0                      * Bottom NB
HS10002100   -1      1       0.0
HS10002101   0.3048     3
HS10002200   -1
HS10002201   'CONCRETE'      2
HS10002300   0
HS10002400   1    100  EXT 0.0  0.0
*            Area   Char.L  Width
HS10002500   278.7  5.0     5.0
HS10002600   0
*
HS10003000   3       1
HS10003001   'WALL 100'
HS10003002   0.0     1.0                     * BOTTOM AT 0.0 M, VERTICAL
HS10003100   -1      1       0.0
HS10003101   0.3048     3
HS10003200   -1
HS10003201   'CONCRETE'     2
HS10003300   0
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HS10003400   1       100   EXT   0.0   0.0
*            Area    Char.L  Width
HS10003500   265.7    3.0     3.0
HS10003600   1       300   EXT   0.0   0.0
*            Area    Char.L  Width
HS10003700   265.7    3.0     3.0
*
*
*
HS15001000   3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS15001001   'FLOOR 150'                     * STRUCTURE NAME
HS15001002   0.0    0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS15001100   -1      1       0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS15001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS15001200   -1                             * DEFINE MATERIAL
HS15001201   'CONCRETE'     2               * 2 MESH POINTS
HS15001300   0                              * NO INTERNAL POWER SOURCE
HS15001400   0                              * ADIABATIC LOWER BC
HS15001600  1    150  EXT 0.0  0.0          * UPPER BC
*            Area    Char.L  Width           * EXTernal heat transfer
HS15001700   426.4   20.0    20.0            * SUFRACE AREA M**2
*
HS15002000   3       1
HS15002001   'CEILING 150'
HS15002002   4.0     0.0                     * Bottom NB
HS15002100   -1      1       0.0
HS15002101   0.3048     3
HS15002200   -1
HS15002201   'CONCRETE'      2
HS15002300   0
HS15002400   1    150  EXT 0.0  0.0
*            Area    Char.L  Width
HS15002500   426.4   5.0     5.0
HS15002600   0
*
HS15003000   3       1
HS15003001   'WALL 150'
HS15003002   0.0     1.0                     * BOTTOM AT 0.0 M, VERTICAL
HS15003100   -1      1       0.0
HS15003101   0.3048     3
HS15003200   -1
HS15003201   'CONCRETE'     2
HS15003300   0
HS15003400   1       150   EXT   0.0   0.0
*            Area    Char.L  Width
HS15003500   335.8    3.0     3.0
HS15003600   1       300   EXT   0.0   0.0
*            Area    Char.L  Width
HS15003700   335.8    3.0     3.0
*
*
*
HS20001000   3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS20001001   'FLOOR 200'                     * STRUCTURE NAME
HS20001002   0.0    0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS20001100   -1      1       0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS20001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS20001200   -1                             * DEFINE MATERIAL
HS20001201   'CONCRETE'     2               * 2 MESH POINTS
HS20001300   0                              * NO INTERNAL POWER SOURCE
HS20001400   0                              * ADIABATIC LOWER BC
HS20001600   1    200  EXT 0.0  0.0          * UPPER BC
*            Area    Char.L  Width           * EXTernal heat transfer
HS20001700   426.4   20.0    20.0            * SUFRACE AREA M**2
*
HS20002000   3       1
HS20002001   'CEILING 200'
HS20002002   4.0     0.0                     * Bottom NB
HS20002100   -1      1       0.0
HS20002101   0.3048     3
HS20002200   -1
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HS20002201   'CONCRETE'      2
HS20002300   0
HS20002400   1    200  EXT 0.0  0.0
*            Area   Char.L  Width
HS20002500   426.4  5.0     5.0
HS20002600   0
*
HS20003000   3       1
HS20003001   'WALL 200'
HS20003002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS20003100   -1      1       0.0
HS20003101   0.3048    3
HS20003200   -1
HS20003201   'CONCRETE'     2
HS20003300   0
HS20003400   1      200   EXT   0.0   0.0
*            Area   Char.L  Width
HS20003500   335.8   3.0    3.0
HS20003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS20003700   335.8   3.0    3.0
*
*
*
HS25001000   3       1                     * 3 NODES, RECTANGULAR GEOMETRY
HS25001001   'FLOOR 250'                   * STRUCTURE NAME
HS25001002   0.0   0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS25001100   -1      1       0.0           * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS25001101   0.3048    3                   * THIRD NODE NODE AT 0.3048 M
HS25001200   -1                           * DEFINE MATERIAL
HS25001201   'CONCRETE'     2             * 2 MESH POINTS
HS25001300   0                            * NO INTERNAL POWER SOURCE
HS25001400   0                            * ADIABATIC LOWER BC
HS25001600   1    250  EXT 0.0  0.0       * UPPER BC
*            Area   Char.L  Width          * EXTernal heat transfer
HS25001700   94.8   20.0    20.0          * SUFRACE AREA M**2
*
HS25002000   3       1
HS25002001   'CEILING 250'
HS25002002   4.0     0.0                   * Bottom NB
HS25002100   -1      1       0.0
HS25002101   0.3048    3
HS25002200   -1
HS25002201   'CONCRETE'      2
HS25002300   0
HS25002400   1    250  EXT 0.0  0.0
*            Area   Char.L  Width
HS25002500   94.8   5.0     5.0
HS25002600   0
*
HS25003000   3       1
HS25003001   'WALL 250'
HS25003002   0.0     1.0                   * BOTTOM AT 0.0 M, VERTICAL
HS25003100   -1      1       0.0
HS25003101   0.3048    3
HS25003200   -1
HS25003201   'CONCRETE'     2
HS25003300   0
HS25003400   1      250   EXT   0.0   0.0
*            Area   Char.L  Width
HS25003500   425.1   3.0    3.0
HS25003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS25003700   425.1   3.0    3.0
*
*
*
HS30001000   3       1                     * 3 NODES, RECTANGULAR GEOMETRY
HS30001001   'FLOOR 300'                   * STRUCTURE NAME
HS30001002   0.0   0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS30001100   -1      1       0.0           * DEFINE NODE POSITIONS, FIRST AT 0.0 M
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HS30001101   0.3048      3                    * THIRD NODE NODE AT 0.3048 M
HS30001200   -1                               * DEFINE MATERIAL
HS30001201   'CONCRETE'      2                * 2 MESH POINTS
HS30001300   0                                * NO INTERNAL POWER SOURCE
HS30001400   0                                * ADIABATIC LOWER BC
HS30001600   1    300  EXT 0.0  0.0           * UPPER BC
*            Area    Char.L  Width            * EXTernal heat transfer
HS30001700   209.    20.0    20.0             * SUFRACE AREA M**2
*
HS30002000   3       1
HS30002001   'CEILING 300'
HS30002002   4.0     0.0                      * Bottom NB
HS30002100   -1      1       0.0
HS30002101   0.3048     3
HS30002200   -1
HS30002201   'CONCRETE'      2
HS30002300   0
HS30002400   1    300  EXT 0.0  0.0
*            Area    Char.L  Width
HS30002500   209.    5.0     5.0
HS30002600   0
*
HS30003000   3       1
HS30003001   'WALL 300'
HS30003002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS30003100   -1      1       0.0
HS30003101   0.3048     3
HS30003200   -1
HS30003201   'CONCRETE'      2
HS30003300   0
HS30003400   1      300   EXT   0.0   0.0
*            Area    Char.L  Width
HS30003500   229.5   3.0     3.0
HS30003600   1      150   EXT   0.0  0.0
*            Area    Char.L  Width
HS30003700   229.5   3.0     3.0
*
*
*
HS35001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS35001001   'FLOOR 350'                      * STRUCTURE NAME
HS35001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS35001100   -1      1       0.0              * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS35001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS35001200   -1                               * DEFINE MATERIAL
HS35001201   'CONCRETE'      2                * 2 MESH POINTS
HS35001300   0                                * NO INTERNAL POWER SOURCE
HS35001400   0                                * ADIABATIC LOWER BC
HS35001600   1    350  EXT 0.0  0.0           * UPPER BC
*            Area    Char.L  Width            * EXTernal heat transfer
HS35001700   325.2   20.0    20.0              * SUFRACE AREA M**2
*
HS35002000   3       1
HS35002001   'CEILING 350'
HS35002002   4.0     0.0                      * Bottom NB
HS35002100   -1      1       0.0
HS35002101   0.3048     3
HS35002200   -1
HS35002201   'CONCRETE'      2
HS35002300   0
HS35002400   1    350  EXT 0.0  0.0
*            Area    Char.L  Width
HS35002500   325.2   5.0     5.0
HS35002600   0
*
HS35003000   3       1
HS35003001   'EAST WALL'
HS35003002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS35003100   -1      1       0.0
HS35003101   0.3048     3
HS35003200   -1
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HS35003201   'CONCRETE'     2
HS35003300   0
HS35003400   1       350   EXT   0.0   0.0
*            Area    Char.L  Width
HS35003500   42.27    3.0     3.0
HS35003600   1       400   EXT   0.0  0.0
*            Area    Char.L  Width
HS35003700   42.27    3.0     3.0
*
*
HS35004000   3       1
HS35004001   'WEST WALL'
HS35004002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS35004100   -1      1       0.0
HS35004101   0.3048     3
HS35004200   -1
HS35004201   'CONCRETE'     2
HS35004300   0
HS35004400   1       350   EXT   0.0   0.0
*            Area    Char.L  Width
HS35004500   42.27    3.0     3.0
HS35004600   1       300   EXT   0.0  0.0
*            Area    Char.L  Width
HS35004700   42.27    3.0     3.0
*
HS35005000   3       1
HS35005001   'NORTH WALL'
HS35005002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS35005100   -1      1       0.0
HS35005101   0.3048     3
HS35005200   -1
HS35005201   'CONCRETE'     2
HS35005300   0
HS35005400   1       350   EXT   0.0   0.0
*            Area    Char.L  Width
HS35005500   120.77   3.0     3.0
HS35005600   1       250   EXT   0.0  0.0
*            Area    Char.L  Width
HS35005700   120.77   3.0     3.0
*
HS35006000   3       1
HS35006001   'SOUTH WALL'
HS35006002   0.0     1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS35006100   -1      1       0.0
HS35006101   0.3048     3
HS35006200   -1
HS35006201   'CONCRETE'     2
HS35006300   0
HS35006400   1       350   EXT   0.0   0.0
*            Area    Char.L  Width
HS35006500   120.77   3.0     3.0
HS35006600   1       450   EXT   0.0  0.0
*            Area    Char.L  Width
HS35006700   120.77   3.0     3.0
*
*
*
HS40001000   3       1                      * 3 NODES, RECTANGULAR GEOMETRY
HS40001001   'FLOOR 400'                    * STRUCTURE NAME
HS40001002   0.0   0.0                      * BOTTOM AT 0.0 M, HORIZONTAL
HS40001100   -1      1       0.0            * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS40001101   0.3048     3                   * THIRD NODE NODE AT 0.3048 M
HS40001200   -1                           * DEFINE MATERIAL
HS40001201   'CONCRETE'     2              * 2 MESH POINTS
HS40001300   0                            * NO INTERNAL POWER SOURCE
HS40001400   0                            * ADIABATIC LOWER BC
HS40001600   1    400  EXT 0.0  0.0        * UPPER BC
*            Area    Char.L  Width         * EXTernal heat transfer
HS40001700   292.6   20.0    20.0          * SUFRACE AREA M**2
*
HS40002000   3       1
```

```
HS40002001   'CEILING 400'
HS40002002   4.0     0.0                        * Bottom NB
HS40002100   -1       1        0.0
HS40002101   0.3048      3
HS40002200   -1
HS40002201   'CONCRETE'       2
HS40002300   0
HS40002400   1     400  EXT 0.0  0.0
*            Area    Char.L  Width
HS40002500   292.6    5.0      5.0
HS40002600   0
*
HS40003000   3        1
HS40003001   'WALL 400'
HS40003002   0.0      1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS40003100   -1       1        0.0
HS40003101   0.3048      3
HS40003200   -1
HS40003201   'CONCRETE'      2
HS40003300   0
HS40003400   1       400    EXT    0.0    0.0
*            Area    Char.L  Width
HS40003500   277.8    3.0     3.0
HS40003600   1       150    EXT    0.0  0.0
*            Area    Char.L  Width
HS40003700   277.8    3.0     3.0
*
*
*
HS45001000   3        1                         * 3 NODES, RECTANGULAR GEOMETRY
HS45001001   'FLOOR 450'                        * STRUCTURE NAME
HS45001002   0.0   0.0                          * BOTTOM AT 0.0 M, HORIZONTAL
HS45001100   -1       1        0.0              * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS45001101   0.3048      3                     * THIRD NODE NODE AT 0.3048 M
HS45001200   -1                                 * DEFINE MATERIAL
HS45001201   'CONCRETE'      2                  * 2 MESH POINTS
HS45001300   0                                  * NO INTERNAL POWER SOURCE
HS45001400   0                                  * ADIABATIC LOWER BC
HS45001600   1     450  EXT 0.0  0.0            * UPPER BC
*            Area    Char.L  Width              * EXTernal heat transfer
HS45001700   92.9     20.0     20.0              * SUFRACE AREA M**2
*
HS45002000   3        1
HS45002001   'CEILING 450'
HS45002002   4.0     0.0                        * Bottom NB
HS45002100   -1       1        0.0
HS45002101   0.3048      3
HS45002200   -1
HS45002201   'CONCRETE'       2
HS45002300   0
HS45002400   1     450  EXT 0.0  0.0
*            Area    Char.L  Width
HS45002500   92.9     5.0      5.0
HS45002600   0
*
HS45003000   3        1
HS45003001   'WALL 450'
HS45003002   0.0      1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS45003100   -1       1        0.0
HS45003101   0.3048      3
HS45003200   -1
HS45003201   'CONCRETE'      2
HS45003300   0
HS45003400   1       450    EXT    0.0    0.0
*            Area    Char.L  Width
HS45003500   265.7    3.0     3.0
HS45003600   1       150    EXT    0.0  0.0
*            Area    Char.L  Width
HS45003700   265.7    3.0     3.0
*
*
```

```
*
HS50001000   3        1
HS50001001   'FLOOR 500'
HS50001002   0.0    0.0
HS50001100   -1       1        0.0
HS50001101   0.3      3
HS50001200   -1
HS50001201   'CONCRETE'      2
HS50001300   0
HS50001400   0
HS50001600   1       500    EXT    0.0  0.0
HS50001700   0.0001  0.0001     0.0001          * AREA
*
*
*
HS60001000   3        1
HS60001001   'FLOOR 600'
HS60001002   0.0    0.0
HS60001100   -1       1        0.0
HS60001101   0.3      3
HS60001200   -1
HS60001201   'CONCRETE'      2
HS60001300   0
HS60001400   0
HS60001600   1       600    EXT    0.0  0.0
HS60001700   0.0001  0.0001     0.0001          * AREA
*
*
*
HS70001000   3        1
HS70001001   'FLOOR 700'
HS70001002   0.0    0.0
HS70001100   -1       1        0.0
HS70001101   0.3      3
HS70001200   -1
HS70001201   'CONCRETE'      2
HS70001300   0
HS70001400   0
HS70001600   1       700    EXT    0.0  0.0
HS70001700   0.0001  0.0001     0.0001          * AREA
*
*
*
HS80001000   3        1
HS80001001   'FLOOR 800'
HS80001002   0.0    0.0
HS80001100   -1       1        0.0
HS80001101   0.3      3
HS80001200   -1
HS80001201   'CONCRETE'      2
HS80001300   0
HS80001400   0
HS80001600   1       300    EXT    0.0  0.0
HS80001700   0.0001  0.0001     0.0001          * AREA
*
* AEROSOL SECTION
RN1000 0  *    ACTIVATE
RNCA100 0 *    NOT ACTIVE

RN1001 20 2 17 0 0 1 0
RN1100 1.0e-8 3.0e-6 11.46E+3
RNACOEF    1

RNAS000 350 2 1 1. 1.0 601 2
RNAS001 2.3e-6 2.

* DEFINE TABULAR FUNCTION AEROSOL RELEASE RATE
*
TF60100    'AEROSOL'    5    1.0
TF60110    0.0          0.000     *  TIME  KG RELEASE
TF60111    500.0        0.000
```

```
TF60112   501.0      1.0
TF60113   502.0      0.0
TF60114   200000.    0.0
.
*eor* melcor
*
**********************************
*          MELCOR INPUT          *
**********************************
*
TITLE     'TEST PROBLEM'
*
RESTART   0       * RESTART FROM CYCLE 0
*
TEND      36000.0  * END TIME S
*
CPULIM    36000.0
CPULEFT   20.0
*
CRTOUT            * 80-COLUMN OUTPUT FORMAT
*
*********
* FILES *
*********
*
RESTARTFILE  SAMPLE.RST
OUTPUTFILE   SAMPLE.OUT
PLOTFILE     SAMPLE.PTF
DIAGFILE     SAMPLE.DIA
MESSAGEFILE  SAMPLE.MES
*
*******************************
* TIME STEP AND EDIT CONTROL *
*******************************
*         TIME      DTMAX      DTMIN         DTEDT      DTPLT      DTRST
TIME1     0.0       0.1      0.000000001    5.0        100.0      10.0
TIME2     1200.0     10.0    0.000000001    500.0      100.0      1000.0
TIME3     1300.0     30.0    0.000000001    500.0      100.0      1000.0
TIME4     1400.0     100.0   0.000000001    1000.0     200.0      5000.0
TIME5     2500.0     200.0   0.000000001    1000.0     200.0      5000.0
.
```

Appendix F. Fire Plus Seismic (Ventilation Operating) Input File

```
*eor* melgen
*
**********************************
********** MELGEN INPUT **********
**********************************
*
TITLE     'TEST PROBLEM'
*
DTTIME    0.001  * Initial time-step of 1 ms
*
CRTOUT           * 80-column output format
*
*********
* FILES *
*********
*  DEFINITION OF OUTPUT FILE NAMES
*
OUTPUTFILE   SAMPLEG.OUT
DIAGFILE     SAMPLEG.DIA
RESTARTFILE  SAMPLE.RST
*
*
* DEFINITION OF DEFAULT FLUID
* AIR DEFINITION
NCG001    N2  4          * N2 IS MATERIAL NO. 4
NCG002    O2  5          * O2 IS MATERIAL NO. 5
* END AIR DEFINITION
**************************
* PRIMARY SYSTEM VOLUMES *
**************************
*
CV10000   ROOM100     2  1  1    * ROOM-100
*  VOLUME ENV. CONDITIONS
CV100A1   PVOL 101352.9          * INITIAL PRESSURE
CV100A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV100B1     0.0       0.0              * BOTTOM 0.0
CV100B2     4.        1104.4           * TOTAL VOLUME
*
*
CV15000   ROOM150     2  1  1    * ROOM-150
*  VOLUME ENV. CONDITIONS
CV150A1   PVOL 101352.9          * INITIAL PRESSURE
CV150A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV150B1    0.0       0.0         * BOTTOM AT 0.0
CV150B2    4.        1689.7      * TOTAL VOLUME
*
*
CV20000   ROOM200     2  1  1    * ROOM-200
CV200A1   PVOL 101352.9          * INITIAL PRESSURE
CV200A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV200B1    0.0       0.0         * BOTTOM AT 0.0
CV200B2    4.0       1689.7      * TOTAL VOLUME
*
*
CV25000   ROOM250     2  1  1    * ROOM-250
CV250A1   PVOL 101352.9          * INITIAL PRESSURE
CV250A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV250B1    0.0       0.0         * BOTTOM AT 0.0
CV250B2    4.0       375.5       * TOTAL VOLUME
*
*
CV30000   ROOM300     2  1  1    * ROOM-300
CV300A1   PVOL 101352.9          * INITIAL PRESSURE
```

```
CV300A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV300B1    0.0       0.0        * BOTTOM AT 0.0
CV300B2    4.0       828.3      * TOTAL VOLUME
*
*
CV35000   ROOM350     2  1  1   * ROOM-350
CV350A1   PVOL 101352.9          * INITIAL PRESSURE
CV350A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV350B1   0.0        0.0         * BOTTOM AT 0.0
CV350B2   4.0        1288.4      * TOTAL VOLUME

CV350C1   MASS.3   RATE  CF.998  * VAPOR MASS C-FUNCTION
CV350C2   ENERGY.A RATE  CF.999  * CORRESPONDING ENTALPY
CF99800   'VAPOR MASS'  TAB-FUN  1   1.0
CF99803   998                    * TF NUMBER
CF99810   1.0   0.0  TIME        * ARGUMENT IS TIME
TF99800   'VAPOR MASS'   5   1.0
TF99810   0.0    0.0
TF99811   300.   0.001
TF99812   900.   0.001
TF99813   1200.  0.0
TF99814   200000.  0.0
*
CF99900   'ENTHALPY'  MULTIPLY  2   1.0  * ENTHALPY RATE
CF99910   1.0   0.0     CFVALU.998
CF99911   0.0   1.0E+9  TIME
*
* END FIRE SOURCE
*
*
CV40000   ROOM400     2  1  1   * ROOM-400
CV400A1   PVOL 101352.9          * INITIAL PRESSURE
CV400A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV400B1   0.0      0.0          * BOTTOM AT 0.0
CV400B2   4.0      1159.6       * TOTAL VOLUME
*
*
CV45000   ROOM450     2  1  1   * ROOM-400
CV450A1   PVOL 101352.9          * INITIAL PRESSURE
CV450A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV450B1   0.0      0.0          * BOTTOM AT 0.0
CV450B2   4.0      368.1        * TOTAL VOLUME
*
*
****************************************
* ENVIRONMENTAL VOLUME - OUTSIDE CELLS *
****************************************
*
CV50000   WEST-VOL500     2  1  1   * ENV-500 WEST
CV500A1   PVOL 101351.6992          * INITIAL PRESSURE
CV500A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV500B1   0.0      0.0          * BOTTOM AT 0.0
CV500B2   4.0      1.0E10       * TOTAL VOLUME
*
*
CV60000   NORTH-VOL600     2  1  1   * ENV-600 NORTH
CV600A1   PVOL 101351.8493          * INITIAL PRESSURE
CV600A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV600B1   0.0      0.0          * BOTTOM AT 0.0
CV600B2   4.0      1.0E10       * TOTAL VOLUME
*
*
*  WIND FROM EAST AT 5 MPH
CV70000   EAST-VOL700     2  1  1    * ENV-700 EAST
CV700A1   PVOL 101355.0013          * INITIAL PRESSURE
```

```
CV700A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV700B1   0.0     0.0          * BOTTOM AT 0.0
CV700B2   4.0     1.0E10       * TOTAL VOLUME
*
*
CV80000   SOUTH-VOL800     2  1  1   * ENV-800 SOUTH
CV800A1   PVOL 101351.8493             * INITIAL PRESSURE
CV800A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV800B1   0.0     0.0          * BOTTOM AT 0.0
CV800B2   4.0     1.0E10       * TOTAL VOLUME
*
*
* FILTER SYSTEM VOLUME
CV90000   FILTER-VOL900     2  1  1    * FILTER VOLUME
CV900A1   PVOL 101352.9                * INITIAL PRESSURE
CV900A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0 * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV900B1   0.0     0.0          * BOTTOM AT 0.0
CV900B2   4.0     1.0E10       * TOTAL VOLUME
*
************************
* INTERNAL FLOW PATHS *
************************
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL11000   100-300       100   300    1.      1.
FL11001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL11003    1.5    1.5                          * LOSS COEFFICIENT
FL110S0    0.0387       0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL11500   100-250       100   250    1.      1.
FL11501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL11503    1.5    1.5                          * LOSS COEFFICIENT
FL115S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL12000   150-100       150   100    1.      1.
FL12001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL12003    1.5    1.5                          * LOSS COEFFICIENT
FL120S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL12500   300-350       300   350    1.      1.
FL12501    0.0387        0.05    1.0             * A, L, FRACTION OPEN
FL12503    1.5    1.5                           * LOSS COEFFICIENT
FL125S0    0.0387        0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL13000   150-250       150   250    1.      1.
FL13001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL13003    1.5    1.5                          * LOSS COEFFICIENT
FL130S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL13500   150-200       150   200    1.      1.
FL13501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL13503    1.5    1.5                          * LOSS COEFFICIENT
FL135S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
```

```
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL14000   200-250      200   250     1.      1.
FL14001    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL14003    1.5    1.5                           * LOSS COEFFICIENT
FL140S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL14500   250-350      250   350     1.      1.
FL14501    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL14503    1.5    1.5                           * LOSS COEFFICIENT
FL145S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL15000   250-400      250   400     1.      1.
FL15001    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL15003    1.5    1.5                           * LOSS COEFFICIENT
FL150S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL15500   350-400      350   400     1.      1.
FL15501    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL15503    1.5    1.5                           * LOSS COEFFICIENT
FL155S0    0.0387      0.0508      0.0254       * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL16000   350-450      350   450     1.      1.
FL16001    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL16003    1.5    1.5                           * LOSS COEFFICIENT
FL160S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL16500   450-400      450   400     1.      1.
FL16501    0.0387      0.05    1.0              * A, L, FRACTION OPEN
FL16503    1.5    1.5                           * LOSS COEFFICIENT
FL165S0    0.0387      0.0508    0.0254         * A, L, HYD.DIAM.
*
*
**********************************
* FLOW PATHS FROM/TO EXTERNAL VOLUMES *
**********************************
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL17000    300-500     300   500     1.      1.
FL17001    0.0639      0.05    1.0              * A, L, FRACTION OPEN
FL17003    1.5    1.5                           * LOSS COEFFICIENT
FL170S0    0.0639      0.0508     0.0254        * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
FL17500   200-600      200   600     1.      1.
FL17501    0.0639      0.05    1.0              * A, L, FRACTION OPEN
FL17503    1.5    1.5                           * LOSS COEFFICIENT
FL175S0    0.0639      0.0508      0.0254       * A, L, HYD.DIAM.
*
*
*                       Volumes      Junct.Elev.
*                      From  To      From    To
```

```
FL18000   400-700      400   700    1.      1.
FL18001    0.0639      0.05    1.0            * A, L, FRACTION OPEN
FL18003    1.5    1.5                         * LOSS COEFFICIENT
FL180S0    0.0639      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL18500   450-800      450   800    1.      1.
FL18501    3.9     0.05    1.0            * A, L, FRACTION OPEN
FL18503    1.5     1.5                    * LOSS COEFFICIENT
FL185S0    3.9     0.0508  1.6            * A, L, HYD.DIAM.
FL185V0    -1   251  251
* USE A CONTROL FUNCTION
CF25100    'JUN CONROL' TAB-FUN 1  1.0  * TRIP ON TIME
CF25101    0.0
CF25103    233  * TAB FUNCTION NUMBER
CF25110   1.0  0.0  TIME
*  TAB FUNCTION NEXT
TF23300    'MOD DOOR'  6  1.0  0.
TF23310    0.0       0.0164
TF23311    120.      0.0164
TF23312    120.      1.0
TF23313    720.      1.0
TF23314    720.      0.0164
TF23315    200000.   0.0164
*
*  VENTILATION SUPPLY WALL OPENING
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL19000   700-200      700   200    1.      1.
FL19001    2.0      0.05    1.0              * A, L, FRACTION OPEN
FL19003    1.5    1.5                        * LOSS COEFFICIENT
FL190S0    2.0    0.3048    2.0              * A, L, HYD.DIAM.
*
*
********************
* TO FILTER SYSTEM *
********************
*
*  FIXED FLOW CONDITION TO FILTER SYSTEM
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL20100   100-900      100   900    1.      1.
FL20101    1.0      0.05    1.0           * A, L, FRACTION OPEN
FL201S0    1.0      0.3048         1.0    * A, L, HYD.DIAM.
FL201T0     1   201
TF20100     'FIXED FLOW' 3 1.0 0.0
TF20110     0.       1.839
TF20111     10.      1.839
TF20112     500000. 1.839
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL20200   150-900      150   900    1.      1.
FL20201    1.0      0.05    1.0           * A, L, FRACTION OPEN
FL202S0    1.0      0.3048         1.0    * A, L, HYD.DIAM.
FL202T0     1   202
TF20200     'FIXED FLOW' 3 1.0 0.0
TF20210     0.       2.813
TF20211     10.      2.813
TF20212     500000. 2.813
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL20300   200-900      200   900    1.      1.
FL20301    1.0      0.05    1.0           * A, L, FRACTION OPEN
FL203S0    1.0      0.3048         1.0    * A, L, HYD.DIAM.
FL203T0     1   203
```

```
TF20300     'FIXED FLOW' 3 1.0 0.0
TF20310     0.      2.813
TF20311     10.     2.813
TF20312     500000. 2.813
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20400   250-900      250   900    1.      1.
FL20401    1.0      0.05    1.0            * A, L, FRACTION OPEN
FL204S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL204T0     1   204
TF20400     'FIXED FLOW' 3 1.0 0.0
TF20410     0.      0.625
TF20411     10.     0.625
TF20412     500000. 0.625
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20500   300-900      300   900    1.      1.
FL20501    1.0      0.05    1.0            * A, L, FRACTION OPEN
FL205S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL205T0     1   205
TF20500     'FIXED FLOW' 3 1.0 0.0
TF20510     0.      1.379
TF20511     10.     1.379
TF20512     500000. 1.379
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20600   350-900      350   900    1.      1.
FL20601    1.0      0.05    1.0            * A, L, FRACTION OPEN
FL206S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL206T0     1   206
TF20600     'FIXED FLOW' 3 1.0 0.0
TF20610     0.      2.145
TF20611     10.     2.145
TF20612     500000. 2.145
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20700   400-900      400   900    1.      1.
FL20701    1.0      0.05    1.0            * A, L, FRACTION OPEN
FL207S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL207T0     1   207
TF20700     'FIXED FLOW' 3 1.0 0.0
TF20710     0.      1.931
TF20711     10.     1.931
TF20712     500000. 1.931
*
*
*                       Volumes     Junct.Elev.
*                      From  To     From    To
FL20800   450-900      450   900    1.      1.
FL20801    1.0      0.05    1.0            * A, L, FRACTION OPEN
FL208S0    1.0      0.3048         1.0     * A, L, HYD.DIAM.
FL208T0     1   208
TF20800     'FIXED FLOW' 3 1.0 0.0
TF20810     0.      0.613
TF20811     10.     0.613
TF20812     500000. 0.613
*
*
************************
* HEAT STRUCTURES INPUT *
************************
*
*
```

```
*
HS10001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS10001001   'FLOOR 100'                      * STRUCTURE NAME
HS10001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS10001100   -1      1       0.0              * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS10001101   0.3048     3                     * THIRD NODE NODE AT 0.3048 M
HS10001200   -1                               * DEFINE MATERIAL
HS10001201   'CONCRETE'     2                 * 2 MESH POINTS
HS10001300   0                                * NO INTERNAL POWER SOURCE
HS10001400   0                                * ADIABATIC LOWER BC
HS10001600   1    100  EXT 0.0  0.0           * UPPER BC
*            Area   Char.L  Width              * EXTernal heat transfer
HS10001700   278.7  20.0    20.0              * SUFRACE AREA M**2
*
HS10002000   3       1
HS10002001   'CEILING 100'
HS10002002   4.0    0.0                       * Bottom NB
HS10002100   -1      1       0.0
HS10002101   0.3048     3
HS10002200   -1
HS10002201   'CONCRETE'      2
HS10002300   0
HS10002400   1    100  EXT 0.0  0.0
*            Area   Char.L  Width
HS10002500   278.7  5.0     5.0
HS10002600   0
*
HS10003000   3       1
HS10003001   'WALL 100'
HS10003002   0.0     1.0                       * BOTTOM AT 0.0 M, VERTICAL
HS10003100   -1      1       0.0
HS10003101   0.3048     3
HS10003200   -1
HS10003201   'CONCRETE'     2
HS10003300   0
HS10003400   1      100   EXT   0.0   0.0
*            Area   Char.L  Width
HS10003500   265.7   3.0    3.0
HS10003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS10003700   265.7   3.0    3.0
*
*
*
HS15001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS15001001   'FLOOR 150'                      * STRUCTURE NAME
HS15001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS15001100   -1      1       0.0              * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS15001101   0.3048     3                     * THIRD NODE NODE AT 0.3048 M
HS15001200   -1                               * DEFINE MATERIAL
HS15001201   'CONCRETE'     2                 * 2 MESH POINTS
HS15001300   0                                * NO INTERNAL POWER SOURCE
HS15001400   0                                * ADIABATIC LOWER BC
HS15001600   1    150  EXT 0.0  0.0           * UPPER BC
*            Area   Char.L  Width              * EXTernal heat transfer
HS15001700   426.4  20.0    20.0              * SUFRACE AREA M**2
*
HS15002000   3       1
HS15002001   'CEILING 150'
HS15002002   4.0    0.0                       * Bottom NB
HS15002100   -1      1       0.0
HS15002101   0.3048     3
HS15002200   -1
HS15002201   'CONCRETE'      2
HS15002300   0
HS15002400   1    150  EXT 0.0  0.0
*            Area   Char.L  Width
HS15002500   426.4  5.0     5.0
HS15002600   0
*
HS15003000   3       1
```

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HS15003001   'WALL 150'
HS15003002   0.0      1.0                    * BOTTOM AT 0.0 M, VERTICAL
HS15003100   -1       1        0.0
HS15003101   0.3048      3
HS15003200   -1
HS15003201   'CONCRETE'      2
HS15003300   0
HS15003400   1       150    EXT    0.0    0.0
*            Area    Char.L  Width
HS15003500   335.8    3.0     3.0
HS15003600   1       300    EXT    0.0   0.0
*            Area    Char.L  Width
HS15003700   335.8    3.0     3.0
*
*
*
HS20001000   3        1                     * 3 NODES, RECTANGULAR GEOMETRY
HS20001001   'FLOOR 200'                    * STRUCTURE NAME
HS20001002   0.0    0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS20001100   -1       1        0.0          * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS20001101   0.3048      3                  * THIRD NODE NODE AT 0.3048 M
HS20001200   -1                            * DEFINE MATERIAL
HS20001201   'CONCRETE'      2              * 2 MESH POINTS
HS20001300   0                             * NO INTERNAL POWER SOURCE
HS20001400   0                             * ADIABATIC LOWER BC
HS20001600   1    200  EXT 0.0  0.0        * UPPER BC
*            Area    Char.L  Width          * EXTernal heat transfer
HS20001700   426.4   20.0    20.0           * SUFRACE AREA M**2
*
HS20002000   3        1
HS20002001   'CEILING 200'
HS20002002   4.0      0.0                   * Bottom NB
HS20002100   -1       1        0.0
HS20002101   0.3048      3
HS20002200   -1
HS20002201   'CONCRETE'       2
HS20002300   0
HS20002400   1    200  EXT 0.0  0.0
*            Area    Char.L  Width
HS20002500   426.4   5.0     5.0
HS20002600   0
*
HS20003000   3        1
HS20003001   'WALL 200'
HS20003002   0.0      1.0                   * BOTTOM AT 0.0 M, VERTICAL
HS20003100   -1       1        0.0
HS20003101   0.3048      3
HS20003200   -1
HS20003201   'CONCRETE'      2
HS20003300   0
HS20003400   1       200    EXT    0.0    0.0
*            Area    Char.L  Width
HS20003500   335.8    3.0     3.0
HS20003600   1       300    EXT    0.0   0.0
*            Area    Char.L  Width
HS20003700   335.8    3.0     3.0
*
*
*
HS25001000   3        1                     * 3 NODES, RECTANGULAR GEOMETRY
HS25001001   'FLOOR 250'                    * STRUCTURE NAME
HS25001002   0.0    0.0                     * BOTTOM AT 0.0 M, HORIZONTAL
HS25001100   -1       1        0.0          * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS25001101   0.3048      3                  * THIRD NODE NODE AT 0.3048 M
HS25001200   -1                            * DEFINE MATERIAL
HS25001201   'CONCRETE'      2              * 2 MESH POINTS
HS25001300   0                             * NO INTERNAL POWER SOURCE
HS25001400   0                             * ADIABATIC LOWER BC
HS25001600   1    250  EXT 0.0  0.0        * UPPER BC
*            Area    Char.L  Width          * EXTernal heat transfer
HS25001700   94.8    20.0    20.0           * SUFRACE AREA M**2
```

```
*
HS25002000   3       1
HS25002001   'CEILING 250'
HS25002002   4.0     0.0                        * Bottom NB
HS25002100   -1      1        0.0
HS25002101   0.3048     3
HS25002200   -1
HS25002201   'CONCRETE'      2
HS25002300   0
HS25002400   1    250  EXT 0.0  0.0
*            Area    Char.L  Width
HS25002500   94.8    5.0     5.0
HS25002600   0
*
HS25003000   3       1
HS25003001   'WALL 250'
HS25003002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS25003100   -1      1        0.0
HS25003101   0.3048     3
HS25003200   -1
HS25003201   'CONCRETE'     2
HS25003300   0
HS25003400   1      250   EXT   0.0   0.0
*            Area    Char.L  Width
HS25003500   425.1    3.0     3.0
HS25003600   1      300   EXT   0.0  0.0
*            Area    Char.L  Width
HS25003700   425.1    3.0     3.0
*
*
*
HS30001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS30001001   'FLOOR 300'                        * STRUCTURE NAME
HS30001002   0.0   0.0                          * BOTTOM AT 0.0 M, HORIZONTAL
HS30001100   -1      1        0.0               * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS30001101   0.3048     3                      * THIRD NODE NODE AT 0.3048 M
HS30001200   -1                                 * DEFINE MATERIAL
HS30001201   'CONCRETE'     2                   * 2 MESH POINTS
HS30001300   0                                  * NO INTERNAL POWER SOURCE
HS30001400   0                                  * ADIABATIC LOWER BC
HS30001600   1    300  EXT 0.0  0.0             * UPPER BC
*            Area    Char.L  Width              * EXTernal heat transfer
HS30001700   209.    20.0    20.0               * SUFRACE AREA M**2
*
HS30002000   3       1
HS30002001   'CEILING 300'
HS30002002   4.0     0.0                        * Bottom NB
HS30002100   -1      1        0.0
HS30002101   0.3048     3
HS30002200   -1
HS30002201   'CONCRETE'      2
HS30002300   0
HS30002400   1    300  EXT 0.0  0.0
*            Area    Char.L  Width
HS30002500   209.    5.0     5.0
HS30002600   0
*
HS30003000   3       1
HS30003001   'WALL 300'
HS30003002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS30003100   -1      1        0.0
HS30003101   0.3048     3
HS30003200   -1
HS30003201   'CONCRETE'     2
HS30003300   0
HS30003400   1      300   EXT   0.0   0.0
*            Area    Char.L  Width
HS30003500   229.5    3.0     3.0
HS30003600   1      150   EXT   0.0  0.0
*            Area    Char.L  Width
HS30003700   229.5    3.0     3.0
```

```
*
*
*
HS35001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS35001001   'FLOOR 350'                        * STRUCTURE NAME
HS35001002   0.0   0.0                          * BOTTOM AT 0.0 M, HORIZONTAL
HS35001100   -1      1       0.0                * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS35001101   0.3048     3                      * THIRD NODE NODE AT 0.3048 M
HS35001200   -1                                 * DEFINE MATERIAL
HS35001201   'CONCRETE'     2                   * 2 MESH POINTS
HS35001300   0                                  * NO INTERNAL POWER SOURCE
HS35001400   0                                  * ADIABATIC LOWER BC
HS35001600   1    350  EXT 0.0  0.0             * UPPER BC
*            Area   Char.L  Width               * EXTernal heat transfer
HS35001700   325.2   20.0    20.0               * SUFRACE AREA M**2
*
HS35002000   3       1
HS35002001   'CEILING 350'
HS35002002   4.0     0.0                        * Bottom NB
HS35002100   -1      1       0.0
HS35002101   0.3048     3
HS35002200   -1
HS35002201   'CONCRETE'      2
HS35002300   0
HS35002400   1    350  EXT 0.0  0.0
*            Area   Char.L  Width
HS35002500   325.2   5.0     5.0
HS35002600   0
*
HS35003000   3       1
HS35003001   'EAST WALL'
HS35003002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS35003100   -1      1       0.0
HS35003101   0.3048     3
HS35003200   -1
HS35003201   'CONCRETE'     2
HS35003300   0
HS35003400   1      350   EXT   0.0   0.0
*            Area   Char.L  Width
HS35003500   42.27   3.0     3.0
HS35003600   1      400   EXT   0.0  0.0
*            Area   Char.L  Width
HS35003700   42.27   3.0     3.0
*
*
HS35004000   3       1
HS35004001   'WEST WALL'
HS35004002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS35004100   -1      1       0.0
HS35004101   0.3048     3
HS35004200   -1
HS35004201   'CONCRETE'     2
HS35004300   0
HS35004400   1      350   EXT   0.0   0.0
*            Area   Char.L  Width
HS35004500   42.27   3.0     3.0
HS35004600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS35004700   42.27   3.0     3.0
*
HS35005000   3       1
HS35005001   'NORTH WALL'
HS35005002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS35005100   -1      1       0.0
HS35005101   0.3048     3
HS35005200   -1
HS35005201   'CONCRETE'     2
HS35005300   0
HS35005400   1      350   EXT   0.0   0.0
*            Area   Char.L  Width
HS35005500   120.77   3.0     3.0
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HS35005600   1       250   EXT   0.0   0.0
*            Area    Char.L  Width
HS35005700   120.77   3.0     3.0
*
HS35006000   3       1
HS35006001   'SOUTH WALL'
HS35006002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS35006100   -1      1        0.0
HS35006101   0.3048     3
HS35006200   -1
HS35006201   'CONCRETE'     2
HS35006300   0
HS35006400   1       350   EXT   0.0    0.0
*            Area    Char.L  Width
HS35006500   120.77   3.0     3.0
HS35006600   1       450   EXT   0.0   0.0
*            Area    Char.L  Width
HS35006700   120.77   3.0     3.0
*
*
*
HS40001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS40001001   'FLOOR 400'                      * STRUCTURE NAME
HS40001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS40001100   -1      1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS40001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS40001200   -1                              * DEFINE MATERIAL
HS40001201   'CONCRETE'     2                 * 2 MESH POINTS
HS40001300   0                               * NO INTERNAL POWER SOURCE
HS40001400   0                               * ADIABATIC LOWER BC
HS40001600   1    400  EXT 0.0  0.0          * UPPER BC
*            Area    Char.L  Width           * EXTernal heat transfer
HS40001700   292.6   20.0    20.0            * SUFRACE AREA M**2
*
HS40002000   3       1
HS40002001   'CEILING 400'
HS40002002   4.0     0.0                      * Bottom NB
HS40002100   -1      1        0.0
HS40002101   0.3048     3
HS40002200   -1
HS40002201   'CONCRETE'      2
HS40002300   0
HS40002400   1    400  EXT 0.0  0.0
*            Area    Char.L  Width
HS40002500   292.6   5.0     5.0
HS40002600   0
*
HS40003000   3       1
HS40003001   'WALL 400'
HS40003002   0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS40003100   -1      1        0.0
HS40003101   0.3048     3
HS40003200   -1
HS40003201   'CONCRETE'     2
HS40003300   0
HS40003400   1       400   EXT   0.0    0.0
*            Area    Char.L  Width
HS40003500   277.8   3.0     3.0
HS40003600   1       150   EXT   0.0   0.0
*            Area    Char.L  Width
HS40003700   277.8   3.0     3.0
*
*
*
HS45001000   3       1                        * 3 NODES, RECTANGULAR GEOMETRY
HS45001001   'FLOOR 450'                      * STRUCTURE NAME
HS45001002   0.0   0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS45001100   -1      1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS45001101   0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS45001200   -1                              * DEFINE MATERIAL
HS45001201   'CONCRETE'     2                 * 2 MESH POINTS
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HS45001300   0                                  * NO INTERNAL POWER SOURCE
HS45001400   0                                  * ADIABATIC LOWER BC
HS45001600   1    450  EXT 0.0  0.0             * UPPER BC
*            Area   Char.L  Width               * EXTernal heat transfer
HS45001700   92.9    20.0    20.0                * SUFRACE AREA M**2
*
HS45002000   3       1
HS45002001   'CEILING 450'
HS45002002   4.0    0.0                         * Bottom NB
HS45002100   -1      1       0.0
HS45002101   0.3048     3
HS45002200   -1
HS45002201   'CONCRETE'      2
HS45002300   0
HS45002400   1    450  EXT 0.0  0.0
*            Area   Char.L  Width
HS45002500   92.9    5.0     5.0
HS45002600   0
*
HS45003000   3       1
HS45003001   'WALL 450'
HS45003002   0.0     1.0                         * BOTTOM AT 0.0 M, VERTICAL
HS45003100   -1      1       0.0
HS45003101   0.3048     3
HS45003200   -1
HS45003201   'CONCRETE'     2
HS45003300   0
HS45003400   1      450   EXT   0.0   0.0
*            Area   Char.L  Width
HS45003500   265.7   3.0    3.0
HS45003600   1      150   EXT   0.0  0.0
*            Area   Char.L  Width
HS45003700   265.7   3.0    3.0
*
*
*
HS50001000   3       1
HS50001001   'FLOOR 500'
HS50001002   0.0   0.0
HS50001100   -1      1       0.0
HS50001101   0.3     3
HS50001200   -1
HS50001201   'CONCRETE'     2
HS50001300   0
HS50001400   0
HS50001600   1      500   EXT   0.0  0.0
HS50001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS60001000   3       1
HS60001001   'FLOOR 600'
HS60001002   0.0   0.0
HS60001100   -1      1       0.0
HS60001101   0.3     3
HS60001200   -1
HS60001201   'CONCRETE'     2
HS60001300   0
HS60001400   0
HS60001600   1      600   EXT   0.0  0.0
HS60001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS70001000   3       1
HS70001001   'FLOOR 700'
HS70001002   0.0   0.0
HS70001100   -1      1       0.0
HS70001101   0.3     3
HS70001200   -1
HS70001201   'CONCRETE'     2
```

```
HS70001300   0
HS70001400   0
HS70001600   1       700   EXT   0.0  0.0
HS70001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS80001000   3       1
HS80001001   'FLOOR 800'
HS80001002   0.0   0.0
HS80001100   -1      1       0.0
HS80001101   0.3     3
HS80001200   -1
HS80001201   'CONCRETE'     2
HS80001300   0
HS80001400   0
HS80001600   1       800   EXT   0.0  0.0
HS80001700   0.0001  0.0001    0.0001          * AREA
*
*
HS90001000   3       1
HS90001001   'FLOOR 900'
HS90001002   0.0   0.0
HS90001100   -1      1       0.0
HS90001101   0.3     3
HS90001200   -1
HS90001201   'CONCRETE'     2
HS90001300   0
HS90001400   0
HS90001600   1       900   EXT   0.0  0.0
HS90001700   0.0001  0.0001    0.0001          * AREA
*
* AEROSOL SECTION
RN1000 0  *   ACTIVATE
RNCA100 0 *   NOT ACTIVE

RN1001 20 2 17 0 0 1 0
RN1100 1.0e-8 3.0e-6 11.46E+3
RNACOEF   1

RNAS000 350 2 1 1. 1.0 601 2
RNAS001 2.3e-6 2.

* DEFINE TABULAR FUNCTION AEROSOL RELEASE RATE
*
TF60100   'AEROSOL'   5   1.0
TF60110   0.0       0.000    *  TIME  KG RELEASE
TF60111   500.0     0.000
TF60112   501.0     1.0
TF60113   502.0     0.0
TF60114   200000.   0.0
.
*eor* melcor
*
**********************************
*          MELCOR INPUT          *
**********************************
*
TITLE     'TEST PROBLEM'
*
RESTART   0      * RESTART FROM CYCLE 0
*
TEND      36000.0  * END TIME S
*
CPULIM    36000.0
CPULEFT   20.0
*
CRTOUT           * 80-COLUMN OUTPUT FORMAT
*
*********
* FILES *
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*********
*
RESTARTFILE   SAMPLE.RST
OUTPUTFILE    SAMPLE.OUT
PLOTFILE      SAMPLE.PTF
DIAGFILE      SAMPLE.DIA
MESSAGEFILE   SAMPLE.MES
*
******************************
* TIME STEP AND EDIT CONTROL *
******************************
*          TIME      DTMAX      DTMIN         DTEDT      DTPLT      DTRST
TIME1      0.0       0.1      0.000000001     5.0       100.0      10.0
TIME2      1200.0     10.0    0.000000001     500.0     100.0      1000.0
TIME3      1300.0     30.0    0.000000001     500.0     100.0      1000.0
TIME4      1400.0     100.0   0.000000001     1000.0    200.0      5000.0
TIME5      2500.0     200.0   0.000000001     1000.0    200.0      5000.0
.
```

Appendix G. Seismic Problem with Multiple Spills (Ventilation Operating) Input File

```
*eor* melgen
*
**********************************
********** MELGEN INPUT **********
**********************************
*
TITLE     'TEST PROBLEM'
*
DTTIME    0.0001  * Initial time-step of 1 ms
*
CRTOUT           * 80-column output format
*
*********
* FILES *
*********
*  DEFINITION OF OUTPUT FILE NAMES
*
OUTPUTFILE   SAMPLEG.OUT
DIAGFILE     SAMPLEG.DIA
RESTARTFILE  SAMPLE.RST
*
*
* DEFINITION OF DEFAULT FLUID
* AIR DEFINITION
NCG001    N2  4          * N2 IS MATERIAL NO. 4
NCG002    O2  5          * O2 IS MATERIAL NO. 5
* END AIR DEFINITION
**************************
* PRIMARY SYSTEM VOLUMES *
**************************
*
CV10000   ROOM100     2  1  1   * ROOM-100
*  VOLUME ENV. CONDITIONS
CV100A1   PVOL 101352.9         * INITIAL PRESSURE
CV100A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV100B1     0.0       0.0             * BOTTOM 0.0
CV100B2     4.        1104.4          * TOTAL VOLUME
*
*
CV15000   ROOM150     2  1  1   * ROOM-150
*  VOLUME ENV. CONDITIONS
CV150A1   PVOL 101352.9         * INITIAL PRESSURE
CV150A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV150B1    0.0       0.0        * BOTTOM AT 0.0
CV150B2    4.        1689.7     * TOTAL VOLUME
*
*
CV20000   ROOM200     2  1  1   * ROOM-200
CV200A1   PVOL 101352.9         * INITIAL PRESSURE
CV200A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV200B1    0.0       0.0        * BOTTOM AT 0.0
CV200B2    4.0       1689.7     * TOTAL VOLUME
*
*
CV25000   ROOM250     2  1  1   * ROOM-250
CV250A1   PVOL 101352.9         * INITIAL PRESSURE
CV250A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV250B1    0.0       0.0        * BOTTOM AT 0.0
CV250B2    4.0       375.5      * TOTAL VOLUME
*
*
CV30000   ROOM300     2  1  1   * ROOM-300
CV300A1   PVOL 101352.9         * INITIAL PRESSURE
```

```
CV300A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV300B1    0.0       0.0        * BOTTOM AT 0.0
CV300B2    4.0       828.3      * TOTAL VOLUME
*
*
CV35000   ROOM350     2  1  1   * ROOM-350
CV350A1   PVOL 101352.9          * INITIAL PRESSURE
CV350A4   MLFR.4 .8  MLFR.5 .2  TATM 294.3 RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV350B1   0.0         0.0         * BOTTOM AT 0.0
CV350B2   4.0         1288.4      * TOTAL VOLUME
*
*
CV40000   ROOM400     2  1  1   * ROOM-400
CV400A1   PVOL 101352.9          * INITIAL PRESSURE
CV400A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV400B1   0.0     0.0          * BOTTOM AT 0.0
CV400B2   4.0     1159.6       * TOTAL VOLUME
*
*
CV45000   ROOM450     2  1  1   * ROOM-400
CV450A1   PVOL 101352.9          * INITIAL PRESSURE
CV450A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV450B1   0.0     0.0          * BOTTOM AT 0.0
CV450B2   4.0     368.1        * TOTAL VOLUME
*
*
****************************************
* ENVIRONMENTAL VOLUME - OUTSIDE CELLS *
****************************************
*
CV50000   WEST-VOL500     2  1  1   * ENV-500 WEST
CV500A1   PVOL 101351.6992          * INITIAL PRESSURE
CV500A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV500B1   0.0     0.0          * BOTTOM AT 0.0
CV500B2   4.0     1.0E10       * TOTAL VOLUME
*
*
CV60000   NORTH-VOL600     2  1  1   * ENV-600 NORTH
CV600A1   PVOL 101351.8493          * INITIAL PRESSURE
CV600A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV600B1   0.0     0.0          * BOTTOM AT 0.0
CV600B2   4.0     1.0E10       * TOTAL VOLUME
*
*
*  WIND FROM EAST AT 5 MPH
CV70000   EAST-VOL700     2  1  1    * ENV-700 EAST
CV700A1   PVOL 101355.0013          * INITIAL PRESSURE
CV700A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV700B1   0.0     0.0          * BOTTOM AT 0.0
CV700B2   4.0     1.0E10       * TOTAL VOLUME
*
*
CV80000   SOUTH-VOL800     2  1  1   * ENV-800 SOUTH
CV800A1   PVOL 101351.8493          * INITIAL PRESSURE
CV800A4   MLFR.4 .8  MLFR.5 .2 TATM 294.3  RHUM 0.0  * 80% N2, 20% O2
*       ALTITUDE OF CELL AND VOLUME
CV800B1   0.0     0.0          * BOTTOM AT 0.0
CV800B2   4.0     1.0E10       * TOTAL VOLUME
*
*
*
************************
* INTERNAL FLOW PATHS *
************************
```

```
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL11000   100-300       100   300    1.      1.
FL11001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL11003    1.5    1.5                          * LOSS COEFFICIENT
FL110S0    0.0387      0.0508      0.0254      * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL11500   100-250       100   250    1.      1.
FL11501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL11503    1.5    1.5                          * LOSS COEFFICIENT
FL115S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL12000   150-100       150   100    1.      1.
FL12001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL12003    1.5    1.5                          * LOSS COEFFICIENT
FL120S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL12500   300-350       300   350    1.      1.
FL12501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL12503    1.5    1.5                          * LOSS COEFFICIENT
FL125S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL13000   150-250       150   250    1.      1.
FL13001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL13003    1.5    1.5                          * LOSS COEFFICIENT
FL130S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL13500   150-200       150   200    1.      1.
FL13501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL13503    1.5    1.5                          * LOSS COEFFICIENT
FL135S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL14000   200-250       200   250    1.      1.
FL14001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL14003    1.5    1.5                          * LOSS COEFFICIENT
FL140S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL14500   250-350       250   350    1.      1.
FL14501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL14503    1.5    1.5                          * LOSS COEFFICIENT
FL145S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                      Volumes     Junct.Elev.
*                     From  To     From    To
FL15000   250-400       250   400    1.      1.
FL15001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL15003    1.5    1.5                          * LOSS COEFFICIENT
FL150S0    0.0387      0.0508    0.0254       * A, L, HYD.DIAM.
*
```

```
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL15500   350-400       350   400    1.      1.
FL15501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL15503    1.5    1.5                          * LOSS COEFFICIENT
FL155S0    0.0387       0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL16000   350-450       350   450    1.      1.
FL16001    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL16003    1.5    1.5                          * LOSS COEFFICIENT
FL160S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL16500   450-400       450   400    1.      1.
FL16501    0.0387       0.05    1.0            * A, L, FRACTION OPEN
FL16503    1.5    1.5                          * LOSS COEFFICIENT
FL165S0    0.0387       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
**********************************
* FLOW PATHS FROM/TO EXTERNAL VOLUMES *
**********************************
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL17000    300-500      300   500    1.      1.
FL17001    0.0639       0.05    1.0            * A, L, FRACTION OPEN
FL17003    1.5    1.5                          * LOSS COEFFICIENT
FL170S0    0.0639       0.0508     0.0254      * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL17500   200-600       200   600    1.      1.
FL17501    0.0639       0.05    1.0            * A, L, FRACTION OPEN
FL17503    1.5    1.5                          * LOSS COEFFICIENT
FL175S0    0.0639       0.0508      0.0254     * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL18000   400-700       400   700    1.      1.
FL18001    0.0639       0.05    1.0            * A, L, FRACTION OPEN
FL18003    1.5    1.5                          * LOSS COEFFICIENT
FL180S0    0.0639       0.0508    0.0254       * A, L, HYD.DIAM.
*
*
*                        Volumes     Junct.Elev.
*                       From  To     From    To
FL18500   450-800       450   800    1.      1.
FL18501    3.9     0.05    1.0            * A, L, FRACTION OPEN
FL18503    1.5     1.5                    * LOSS COEFFICIENT
FL185S0    3.9     0.0508  1.6            * A, L, HYD.DIAM.
FL185V0    -1   251  251
* USE A CONTROL FUNCTION
CF25100    'JUN CONROL' TAB-FUN 1  1.0  * TRIP ON TIME
CF25101    0.0
CF25103    233  * TAB FUNCTION NUMBER
CF25110   1.0  0.0  TIME
*  TAB FUNCTION NEXT
TF23300    'MOD DOOR'  6  1.0  0.
TF23310    0.0       0.0164
TF23311    120.      0.0164
TF23312    120.      1.0
TF23313    720.      1.0
TF23314    720.      0.0164
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TF23315    200000.    0.0164
*
*  VENTILATION SUPPLY WALL OPENING
*                        Volumes      Junct.Elev.
*                       From  To      From    To
FL19000   700-200        700   200     1.      1.
FL19001    2.0       0.05     1.0                * A, L, FRACTION OPEN
FL19003    1.5     1.5                          * LOSS COEFFICIENT
FL190S0    2.0     0.3048     2.0                * A, L, HYD.DIAM.
*
*
*
*
*************************
* HEAT STRUCTURES INPUT *
*************************
*
*
*
HS10001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS10001001   'FLOOR 100'                        * STRUCTURE NAME
HS10001002   0.0   0.0                          * BOTTOM AT 0.0 M, HORIZONTAL
HS10001100   -1      1       0.0                * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS10001101   0.3048     3                      * THIRD NODE NODE AT 0.3048 M
HS10001200   -1                                 * DEFINE MATERIAL
HS10001201   'CONCRETE'     2                   * 2 MESH POINTS
HS10001300   0                                  * NO INTERNAL POWER SOURCE
HS10001400   0                                  * ADIABATIC LOWER BC
HS10001600   1    100  EXT 0.0  0.0             * UPPER BC
*            Area   Char.L  Width               * EXTernal heat transfer
HS10001700   278.7  20.0    20.0               * SUFRACE AREA M**2
*
HS10002000   3       1
HS10002001   'CEILING 100'
HS10002002   4.0    0.0                         * Bottom NB
HS10002100   -1      1       0.0
HS10002101   0.3048     3
HS10002200   -1
HS10002201   'CONCRETE'      2
HS10002300   0
HS10002400   1    100  EXT 0.0  0.0
*            Area   Char.L  Width
HS10002500   278.7  5.0     5.0
HS10002600   0
*
HS10003000   3       1
HS10003001   'WALL 100'
HS10003002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS10003100   -1      1       0.0
HS10003101   0.3048     3
HS10003200   -1
HS10003201   'CONCRETE'     2
HS10003300   0
HS10003400   1      100   EXT   0.0   0.0
*            Area   Char.L  Width
HS10003500   265.7   3.0    3.0
HS10003600   1      300   EXT   0.0  0.0
*            Area   Char.L  Width
HS10003700   265.7   3.0    3.0
*
*
*
HS15001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS15001001   'FLOOR 150'                        * STRUCTURE NAME
HS15001002   0.0   0.0                          * BOTTOM AT 0.0 M, HORIZONTAL
HS15001100   -1      1       0.0                * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS15001101   0.3048     3                      * THIRD NODE NODE AT 0.3048 M
HS15001200   -1                                 * DEFINE MATERIAL
HS15001201   'CONCRETE'     2                   * 2 MESH POINTS
HS15001300   0                                  * NO INTERNAL POWER SOURCE
HS15001400   0                                  * ADIABATIC LOWER BC
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HS15001600  1    150  EXT 0.0  0.0          * UPPER BC
*           Area   Char.L  Width             * EXTernal heat transfer
HS15001700  426.4  20.0    20.0              * SUFRACE AREA M**2
*
HS15002000  3       1
HS15002001  'CEILING 150'
HS15002002  4.0    0.0                      * Bottom NB
HS15002100  -1      1       0.0
HS15002101  0.3048     3
HS15002200  -1
HS15002201  'CONCRETE'      2
HS15002300  0
HS15002400  1    150  EXT 0.0  0.0
*           Area   Char.L  Width
HS15002500  426.4  5.0     5.0
HS15002600  0
*
HS15003000  3       1
HS15003001  'WALL 150'
HS15003002  0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS15003100  -1      1       0.0
HS15003101  0.3048     3
HS15003200  -1
HS15003201  'CONCRETE'     2
HS15003300  0
HS15003400  1      150   EXT   0.0   0.0
*           Area   Char.L  Width
HS15003500  335.8   3.0    3.0
HS15003600  1      300   EXT   0.0  0.0
*           Area   Char.L  Width
HS15003700  335.8   3.0    3.0
*
*
*
HS20001000  3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS20001001  'FLOOR 200'                     * STRUCTURE NAME
HS20001002  0.0   0.0                       * BOTTOM AT 0.0 M, HORIZONTAL
HS20001100  -1      1       0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS20001101  0.3048     3                    * THIRD NODE NODE AT 0.3048 M
HS20001200  -1                              * DEFINE MATERIAL
HS20001201  'CONCRETE'     2                * 2 MESH POINTS
HS20001300  0                               * NO INTERNAL POWER SOURCE
HS20001400  0                               * ADIABATIC LOWER BC
HS20001600  1    200  EXT 0.0  0.0          * UPPER BC
*           Area   Char.L  Width             * EXTernal heat transfer
HS20001700  426.4  20.0    20.0              * SUFRACE AREA M**2
*
HS20002000  3       1
HS20002001  'CEILING 200'
HS20002002  4.0    0.0                      * Bottom NB
HS20002100  -1      1       0.0
HS20002101  0.3048     3
HS20002200  -1
HS20002201  'CONCRETE'      2
HS20002300  0
HS20002400  1    200  EXT 0.0  0.0
*           Area   Char.L  Width
HS20002500  426.4  5.0     5.0
HS20002600  0
*
HS20003000  3       1
HS20003001  'WALL 200'
HS20003002  0.0     1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS20003100  -1      1       0.0
HS20003101  0.3048     3
HS20003200  -1
HS20003201  'CONCRETE'     2
HS20003300  0
HS20003400  1      200   EXT   0.0   0.0
*           Area   Char.L  Width
HS20003500  335.8   3.0    3.0
```

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HS20003600   1       300    EXT    0.0   0.0
*            Area    Char.L  Width
HS20003700   335.8    3.0     3.0
*
*
*
HS25001000   3        1                        * 3 NODES, RECTANGULAR GEOMETRY
HS25001001   'FLOOR 250'                       * STRUCTURE NAME
HS25001002   0.0    0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS25001100   -1       1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS25001101   0.3048      3                    * THIRD NODE NODE AT 0.3048 M
HS25001200   -1                               * DEFINE MATERIAL
HS25001201   'CONCRETE'      2                 * 2 MESH POINTS
HS25001300   0                                * NO INTERNAL POWER SOURCE
HS25001400   0                                * ADIABATIC LOWER BC
HS25001600   1    250  EXT 0.0  0.0           * UPPER BC
*            Area    Char.L  Width            * EXTernal heat transfer
HS25001700   94.8    20.0    20.0             * SUFRACE AREA M**2
*
HS25002000   3        1
HS25002001   'CEILING 250'
HS25002002   4.0     0.0                       * Bottom NB
HS25002100   -1       1        0.0
HS25002101   0.3048      3
HS25002200   -1
HS25002201   'CONCRETE'       2
HS25002300   0
HS25002400   1    250  EXT 0.0  0.0
*            Area    Char.L  Width
HS25002500   94.8    5.0     5.0
HS25002600   0
*
HS25003000   3        1
HS25003001   'WALL 250'
HS25003002   0.0      1.0                      * BOTTOM AT 0.0 M, VERTICAL
HS25003100   -1       1        0.0
HS25003101   0.3048      3
HS25003200   -1
HS25003201   'CONCRETE'      2
HS25003300   0
HS25003400   1       250    EXT    0.0    0.0
*            Area    Char.L  Width
HS25003500   425.1    3.0     3.0
HS25003600   1       300    EXT    0.0   0.0
*            Area    Char.L  Width
HS25003700   425.1    3.0     3.0
*
*
*
HS30001000   3        1                        * 3 NODES, RECTANGULAR GEOMETRY
HS30001001   'FLOOR 300'                       * STRUCTURE NAME
HS30001002   0.0    0.0                        * BOTTOM AT 0.0 M, HORIZONTAL
HS30001100   -1       1        0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS30001101   0.3048      3                    * THIRD NODE NODE AT 0.3048 M
HS30001200   -1                               * DEFINE MATERIAL
HS30001201   'CONCRETE'      2                 * 2 MESH POINTS
HS30001300   0                                * NO INTERNAL POWER SOURCE
HS30001400   0                                * ADIABATIC LOWER BC
HS30001600   1    300  EXT 0.0  0.0           * UPPER BC
*            Area    Char.L  Width            * EXTernal heat transfer
HS30001700   209.    20.0    20.0             * SUFRACE AREA M**2
*
HS30002000   3        1
HS30002001   'CEILING 300'
HS30002002   4.0     0.0                       * Bottom NB
HS30002100   -1       1        0.0
HS30002101   0.3048      3
HS30002200   -1
HS30002201   'CONCRETE'       2
HS30002300   0
HS30002400   1    300  EXT 0.0  0.0
```

```
*           Area    Char.L  Width
HS30002500  209.    5.0     5.0
HS30002600  0
*
HS30003000  3       1
HS30003001  'WALL 300'
HS30003002  0.0     1.0                     * BOTTOM AT 0.0 M, VERTICAL
HS30003100  -1      1       0.0
HS30003101  0.3048      3
HS30003200  -1
HS30003201  'CONCRETE'      2
HS30003300  0
HS30003400  1       300   EXT   0.0   0.0
*           Area    Char.L  Width
HS30003500  229.5   3.0     3.0
HS30003600  1       150   EXT   0.0  0.0
*           Area    Char.L  Width
HS30003700  229.5   3.0     3.0
*
*
*
HS35001000  3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS35001001  'FLOOR 350'                     * STRUCTURE NAME
HS35001002  0.0   0.0                       * BOTTOM AT 0.0 M, HORIZONTAL
HS35001100  -1      1       0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS35001101  0.3048      3                   * THIRD NODE NODE AT 0.3048 M
HS35001200  -1                              * DEFINE MATERIAL
HS35001201  'CONCRETE'      2               * 2 MESH POINTS
HS35001300  0                               * NO INTERNAL POWER SOURCE
HS35001400  0                               * ADIABATIC LOWER BC
HS35001600  1    350  EXT 0.0  0.0          * UPPER BC
*           Area    Char.L  Width           * EXTernal heat transfer
HS35001700  325.2   20.0    20.0             * SUFRACE AREA M**2
*
HS35002000  3       1
HS35002001  'CEILING 350'
HS35002002  4.0     0.0                     * Bottom NB
HS35002100  -1      1       0.0
HS35002101  0.3048      3
HS35002200  -1
HS35002201  'CONCRETE'      2
HS35002300  0
HS35002400  1    350  EXT 0.0  0.0
*           Area    Char.L  Width
HS35002500  325.2   5.0     5.0
HS35002600  0
*
HS35003000  3       1
HS35003001  'WALL 350'
HS35003002  0.0     1.0                     * BOTTOM AT 0.0 M, VERTICAL
HS35003100  -1      1       0.0
HS35003101  0.3048      3
HS35003200  -1
HS35003201  'CONCRETE'      2
HS35003300  0
HS35003400  1       350   EXT   0.0   0.0
*           Area    Char.L  Width
HS35003500  326.1   3.0     3.0
HS35003600  1       150   EXT   0.0  0.0
*           Area    Char.L  Width
HS35003700  326.1   3.0     3.0
*
*
*
HS40001000  3       1                       * 3 NODES, RECTANGULAR GEOMETRY
HS40001001  'FLOOR 400'                     * STRUCTURE NAME
HS40001002  0.0   0.0                       * BOTTOM AT 0.0 M, HORIZONTAL
HS40001100  -1      1       0.0             * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS40001101  0.3048      3                   * THIRD NODE NODE AT 0.3048 M
HS40001200  -1                              * DEFINE MATERIAL
HS40001201  'CONCRETE'      2               * 2 MESH POINTS
```

```
HS40001300   0                                  * NO INTERNAL POWER SOURCE
HS40001400   0                                  * ADIABATIC LOWER BC
HS40001600   1    400  EXT 0.0  0.0             * UPPER BC
*            Area   Char.L  Width               * EXTernal heat transfer
HS40001700   292.6   20.0    20.0                * SUFRACE AREA M**2
*
HS40002000   3       1
HS40002001   'CEILING 400'
HS40002002   4.0     0.0                        * Bottom NB
HS40002100   -1      1       0.0
HS40002101   0.3048     3
HS40002200   -1
HS40002201   'CONCRETE'      2
HS40002300   0
HS40002400   1    400  EXT 0.0  0.0
*            Area   Char.L  Width
HS40002500   292.6   5.0     5.0
HS40002600   0
*
HS40003000   3       1
HS40003001   'WALL 400'
HS40003002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS40003100   -1      1       0.0
HS40003101   0.3048     3
HS40003200   -1
HS40003201   'CONCRETE'     2
HS40003300   0
HS40003400   1      400   EXT   0.0   0.0
*            Area   Char.L  Width
HS40003500   277.8   3.0     3.0
HS40003600   1      150   EXT   0.0  0.0
*            Area   Char.L  Width
HS40003700   277.8   3.0     3.0
*
*
*
HS45001000   3       1                          * 3 NODES, RECTANGULAR GEOMETRY
HS45001001   'FLOOR 450'                        * STRUCTURE NAME
HS45001002   0.0   0.0                          * BOTTOM AT 0.0 M, HORIZONTAL
HS45001100   -1      1       0.0                * DEFINE NODE POSITIONS, FIRST AT 0.0 M
HS45001101   0.3048     3                      * THIRD NODE NODE AT 0.3048 M
HS45001200   -1                                 * DEFINE MATERIAL
HS45001201   'CONCRETE'     2                   * 2 MESH POINTS
HS45001300   0                                  * NO INTERNAL POWER SOURCE
HS45001400   0                                  * ADIABATIC LOWER BC
HS45001600   1    450  EXT 0.0  0.0             * UPPER BC
*            Area   Char.L  Width               * EXTernal heat transfer
HS45001700   92.9    20.0    20.0                * SUFRACE AREA M**2
*
HS45002000   3       1
HS45002001   'CEILING 450'
HS45002002   4.0     0.0                        * Bottom NB
HS45002100   -1      1       0.0
HS45002101   0.3048     3
HS45002200   -1
HS45002201   'CONCRETE'      2
HS45002300   0
HS45002400   1    450  EXT 0.0  0.0
*            Area   Char.L  Width
HS45002500   92.9    5.0     5.0
HS45002600   0
*
HS45003000   3       1
HS45003001   'WALL 450'
HS45003002   0.0     1.0                        * BOTTOM AT 0.0 M, VERTICAL
HS45003100   -1      1       0.0
HS45003101   0.3048     3
HS45003200   -1
HS45003201   'CONCRETE'     2
HS45003300   0
HS45003400   1      450   EXT   0.0   0.0
```

```
*            Area    Char.L  Width
HS45003500   265.7    3.0     3.0
HS45003600   1       150    EXT    0.0  0.0
*            Area    Char.L  Width
HS45003700   265.7    3.0     3.0
*
*
*
HS50001000   3        1
HS50001001   'FLOOR 500'
HS50001002   0.0    0.0
HS50001100   -1       1         0.0
HS50001101   0.3      3
HS50001200   -1
HS50001201   'CONCRETE'      2
HS50001300   0
HS50001400   0
HS50001600   1       500    EXT    0.0  0.0
HS50001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS60001000   3        1
HS60001001   'FLOOR 600'
HS60001002   0.0    0.0
HS60001100   -1       1         0.0
HS60001101   0.3      3
HS60001200   -1
HS60001201   'CONCRETE'      2
HS60001300   0
HS60001400   0
HS60001600   1       600    EXT    0.0  0.0
HS60001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS70001000   3        1
HS70001001   'FLOOR 700'
HS70001002   0.0    0.0
HS70001100   -1       1         0.0
HS70001101   0.3      3
HS70001200   -1
HS70001201   'CONCRETE'      2
HS70001300   0
HS70001400   0
HS70001600   1       700    EXT    0.0  0.0
HS70001700   0.0001  0.0001    0.0001          * AREA
*
*
*
HS80001000   3        1
HS80001001   'FLOOR 800'
HS80001002   0.0    0.0
HS80001100   -1       1         0.0
HS80001101   0.3      3
HS80001200   -1
HS80001201   'CONCRETE'      2
HS80001300   0
HS80001400   0
HS80001600   1       800    EXT    0.0  0.0
HS80001700   0.0001  0.0001    0.0001          * AREA
*
* AEROSOL SECTION
RN1000 0  *   ACTIVATE
RNCA100 0 *   NOT ACTIVE

RN1001 20 2 17 0 0 3 0
RN1100 1.0e-8 3.0e-6 11.46E+3
RNACOEF   1

RNAS000 350 2 1 1. 1.0 601 2
```

```
RNAS001 2.3e-6 2.
RNAS002 200 2 1 1. 1.0 602 2
RNAS003 2.3e-6 2.
RNAS004 250 2 1 1. 1.0 603 2
RNAS005 2.3e-6 2.

* DEFINE TABULAR FUNCTION AEROSOL RELEASE RATE
*
TF60100   'AEROSOL1'   5   1.0
TF60110   0.0      0.000    *  TIME  KG RELEASE
TF60111   10.0     0.000
TF60112   11.0     0.3
TF60113   12.0     0.0
TF60114   200000.  0.0

TF60200   'AEROSOL2'   5   1.0
TF60210   0.0      0.000    *  TIME  KG RELEASE
TF60211   10.0     0.000
TF60212   11.0     0.3
TF60213   12.0     0.0
TF60214   200000.  0.0

TF60300   'AEROSOL3'   5   1.0
TF60310   0.0      0.000    *  TIME  KG RELEASE
TF60311   10.0     0.000
TF60312   11.0     0.4
TF60313   12.0     0.0
TF60314   200000.  0.0
.
*eor* melcor
*
**********************************
*          MELCOR INPUT          *
**********************************
*
TITLE     'TEST PROBLEM'
*
RESTART   0      * RESTART FROM CYCLE 0
*
TEND      72000.0  * END TIME S
*
CPULIM    100000.0
CPULEFT   20.0
*
CRTOUT           * 80-COLUMN OUTPUT FORMAT
*
*********
* FILES *
*********
*
RESTARTFILE  SAMPLE.RST
OUTPUTFILE   SAMPLE.OUT
PLOTFILE     SAMPLE.PTF
DIAGFILE     SAMPLE.DIA
MESSAGEFILE  SAMPLE.MES
*
******************************
* TIME STEP AND EDIT CONTROL *
******************************
*         TIME     DTMAX     DTMIN        DTEDT     DTPLT     DTRST
TIME1     0.0      0.1      0.000000001   5.0       100.0     10.0
TIME2     1000.0    10.0    0.000000001   500.0     100.0     1000.0
TIME3     1100.0    30.0    0.000000001   500.0     100.0     1000.0
TIME4     1300.0    100.0   0.000000001   1000.0    200.0     5000.0
TIME5     2500.0    200.0   0.000000001   1000.0    200.0     5000.0
.
```

SEPARATION

PAGE

GENII Computer Code
Application Guidance for
Documented Safety Analysis

Final Report

U.S. Department of Energy
Office of Environment, Safety, and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

June 2004

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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the GENII computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the GENII documentation provided by the code developer. GENII is one of six computer codes designated by the DOE Office of Environmental, Safety and Health as a toolbox code for safety analysis.

Suggestions for corrections or improvements to this document should be addressed to –

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REVISION STATUS

Page/Section	Revision	Change
1. Entire Document	1. Final Draft for Review	1. Original Issue
2. Entire Document	2. Final Report	2. Updated all sections per review comments.

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GENII

Computer Code Application Guidance for Support of Documented Safety Analysis

EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in the *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications (DOE, 2002b). The Generalized Environmental Radiation Dosimetry Software System – Hanford Dosimetry System (GENII) code is one of the designated toolbox codes.

The GENII code has two versions available, and both GENII versions may require some degree of quality assurance improvement before meeting current SQA standards. The first, version 1.485, was subjected to strict SQA standards as it was developed. The second, version 2.0, is still undergoing final testing. It will require completion of quality assurance improvement measures before meeting current SQA standards. In addition, version 2.0 has not been developed for Documented Safety Analysis work and therefore cannot be recommended until several recommendations are implemented. In the interim period before these changes are completed, GENII is considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available code documentation information.

The GENII guidance report includes the following:

(i) Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis

(ii) Code development information and SQA background

(iii) Appropriate regimes and code limitations

(iv) Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and

(v) Default input value recommendations for site-independent parameters.

Use of the information contained here, although not ensuring correct use of GENII in each analytical context, will minimize potential user errors and the likelihood of GENII use outside its regime of applicability.

This guidance report is supplemental in nature to documentation from the code developer such as the user's guide and model description. The DOE safety analyst should obtain a complete and up to date set of documentation from the GENII code maintainer.

1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25 (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and in the variability of guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its Recommendation to DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the DNFSB concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include

(i) Identification of a set of accident analysis software that is widely used in the DOE Complex, and

(ii) Issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regimes in accident analysis, default inputs, and special conditions for use.

Safety analysis software for the DOE "toolbox" status was designated by the DOE Office of Environment, Safety, and Health (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications* (see http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf). It includes the Generalized Environmental Radiation Dosimetry Software System – Hanford Dosimetry System (GENII) code.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in its guidance report. The code-specific document will be maintained and updated until a minimum qualification software package is completed, or until such time that it is determined to no longer be necessary to update.

The contents of this report are applicable in the interim period until measures are completed to bring GENII into compliance with defined SQA standards. The primary objective of this guidance report is to provide information on the use of GENII for supporting DOE safety-basis accident analysis. Specifically, the report contains:

(iii) Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis

(iv) Appropriate regimes, recommended configurations

(v) Overcoming known vulnerabilities and avoiding code errors

(vi) Valid ranges of input parameters consistent with code capability and DOE safety basis applications

(vii) Default input value recommendations for site-independent parameters, and

(viii) Citations of currently available SQA documentation.

Thus, this report is intended to complement existing GENII user's documentation. The latter tends to be much broader in coverage of the full range of capabilities of GENII and the spectrum of inputs that might be needed depending upon the application, but lack cohesive and targeted guidance for particular applications such as DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The GENII guidance document is written using the following outline. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830 (CFR, 2001). More information follows on the scope and purpose of this document. The next major section is a summary description of GENII. A third section discusses applicable regimes for using GENII in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, is next. Following this discussion are sections on special conditions for use of the software and software limitations. A sample case is then provided, followed by acronyms and definitions, references, and appendices. Appendix A is an overview of atmospheric dispersion consequence analysis provided for safety analysts new to this field. Appendix B provides important GENII software defect notices as taken from the Radiation Safety Information Computational Center (RSICC) website. Appendix C provides joint frequency distribution input file prepared to run the sample case.

1.1 Background: Overview of Toolbox Software in Context of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software will be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements, and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA

pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes, out of more than one hundred software packages applied in the DOE Complex for accident analysis purposes, have been designated as "toolbox" codes (DOE, 2002b). Other non-toolbox dispersion and consequence software can still be applied in the context of support safety-basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

This GENII guidance report includes the following:

(ix) Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis

(x) Code development information and SQA background

(xi) Appropriate regimes and code limitations

(xii) Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and

(xiii) Default input value recommendations for site-independent parameters.

1.3 Purpose

The GENII code, while part of the toolbox collection of software, still may require Software Quality Assurance (SQA) upgrades prior to meeting current established standards for software. However, until these GENII upgrades are completed, GENII can be applied safely under the condition that the guidance contained in this and related reports is followed. Once upgrades are finalized with GENII, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of GENII in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

It is recognized that other computer codes besides GENII exist that perform similar type of atmospheric dispersion and radiological consequence calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for some accident analysis applications that involve releases of radiological material. The relative merits of using a different computer program or using a hand calculation for a given application are a judgment that must be made by the analyst on a case-by-case basis.

The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology

Evaluation Program. As part of this program, the radiological dispersion and consequence assessment (RDCA) Working Group (WG) was established to address issues and evaluate methodologies in the RDCA domain. The RDCA WG (also referred to as WG 5) issued a report that identifies and evaluates methodologies and computer codes to support RDCA applications (O'Kula, 1998).

The RDCA WG 5 report identified the GENII computer code as a recommended code with generally broad suitability to safety-basis documentation applications. In addition to code recommendations, the report also provides a broad set of recommended "best practices" for modeling radiological releases to the atmosphere.

This report builds upon the WG 5 work to provide guidance and recommendations that are targeted to the use of the GENII code for atmospheric dispersion and radiological consequence calculations in the context of DSA-type applications. Specifically, the guidance is best suited for

(xiv) Accident analysis calculations,

(xv) Bounding analysis for final hazard categorization analysis, and

(xvi) Confirmatory calculations for evaluating mitigative and preventive safety controls.

2.0 SUMMARY DESCRIPTION OF THE GENII CODE

This section provides a summary form description of the GENII code followed by an overview of the use of GENII for regulatory applications, in particular, for supporting accident analysis in DSA documents. Users requiring additional background information on dispersion and consequence analysis are referred to Chapter 5 (*Atmospheric Dispersion and Consequence Modeling*) of the Nuclear Fuel Cycle Facility Accident Analysis Handbook (NRC, 1998) and to Appendix A of this guidance document.

2.1 GENII Summary Description

The GENII computer code was developed at Pacific Northwest National Laboratory (PNNL) to provide a state-of-the art, technically peer-reviewed, documented set of programs for calculating radiation dose and risk from radionuclides released to the environment[1]. Although the code was initially developed at Hanford, it was designed with the flexibility to accommodate input parameters for a wide variety of generic sites.

The latest version of GENII, Version 2.0, incorporates the internal dosimetry models recommended by the International Commission on Radiological Protection (ICRP) and the radiological risk estimating procedures of Federal Guidance Report (FGR) 13 into updated versions of existing environmental pathway analysis models. The resulting environmental dosimetry computer codes are compiled in the GENII Environmental Dosimetry System. The earlier version, GENII 1.485, on the other hand, incorporated internal dosimetry models from earlier ICRP recommendations, namely, ICRP publications 26, 30, and 48, which are incorporated into FGR 11.

The development history of the GENII code is outlined below (Napier, 1999d):

(xvii) 1988 - Version 1, released (ICRP-26/30/48 dosimetry)

(xviii) 1990 - Version 1.485 finalized

(xix) 1992 - GENII-S stochastic version

(xx) 1998 - GENII Version 2.0 (ICRP-72 age-dependent dosimetry).

Table 2-1 lists summary information for GENII versions 1.485 and 2.0. A stochastic edition of GENII Version 1, named GENII-S, was developed for the Waste Isolation Pilot Plant assessments by Sandia National Laboratory (Leigh et al. 1992). GENII Version 2 is completely stochastic, using the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) Sensitivity/Uncertainty Multimedia Modeling Module (SUM) driver.

[1] Much of the information presented here can be found on the EPA website on air quality computer models, http://www.epa.gov/radiation/neshaps/models.htm.

Table 2-1. Summary Description of GENII Software – Versions 1.485 and 2.0

Type	Specific Information GENII Version 1.485	Specific Information GENII Version 2.0
Code Name	GENII - Generalized Environmental Radiation Dosimetry Software System - Hanford Dosimetry System (Generation II)	
Developing Organization and Sponsor	Pacific Northwest National Laboratories (PNNL) for the U.S. Department of Energy	Pacific Northwest National Laboratories (PNNL) for the U.S. Environmental Protection Agency (current)
Version of the Code	Version 1.485	Version 2.0
Auxiliary Codes	APPRENTICE: Interactive input processor. ENVIN: controls input for ENV ENV: calculates transfer and uptake DOSE: calculates dose from all exposures EXTDF: calculates external dose rate factors INTDF: calculates internal dose rate factors DITTY: calculates population exposure MASS: Enables the mass production of GENII output using a file containing one or more nuclide groups and several input files.	Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) and Sensitivity/Uncertainty Multimedia Modeling Module (SUM). GENII 2.0 has four atmospheric codes, one surface water code, three environmental accumulation models, one exposure model, and one dose/risk model, each with its specific user-interface code.
Software Platform/Portability	Software on four DS/HD 3.5-in. (1.44 MB) diskettes in self-extracting compressed DOS files. Documentation separate (PNL-6584).	Software and documentation on CD or downloadable from website.
Code Procurement	Radiation Safety Information Computational Center (RSICC) Oak Ridge National Laboratory Post Office Box 2008 Bethel Valley Road Oak Ridge, Tennessee 37831-6171 Phone: 865-574-6176; Fax: 865-241-4046 Email: pdc@ornl.gov	See EPA NESHAPs Website for the NESHAPS version of GENII 2, which limits the user to change certain variables: http://www.epa.gov/radiation/neshaps/models.htm
Coding and Computer	FORTRAN 77 and Quick Basic. IBM PC or compatible. Operates in a DOS environment. RSICC claims that it also functions properly in a DOS window in Windows 95. It also runs in a DOS window of Windows-98 but it may not always run properly under Windows-XP.	FORTRAN 99. Requires Windows operating system (95 or later), a Pentium-class CPU, and 60 MB of disk storage (formerly 20 MB). Runs fastest with ≥ 256 MB of memory.
Technical Support	Bruce Napier Pacific Northwest National Laboratories P.O. Box 999 Richland, Washington 99352 509-375-3896/Phone 509-375-3896/Facsimile Bruce.Napier@pnl.gov	Bruce Napier Pacific Northwest National Laboratories P.O. Box 999 Richland, Washington 99352 509-375-3896/Phone 509-375-3896/Facsimile Bruce.Napier@pnl.gov
Code Package	RSICC Code Package CCC-601 MICRO	Available from author
Contributors	Pacific Northwest National Laboratory, Richland, Washington through the Energy Science & Technology Software Center, Oak Ridge, Tennessee. Hanford Engineering Development Laboratory, Richland, Washington.	

Table 2-1. Summary Description of GENII Software (Continued)

Type	Specific Information GENII Version 1.485	Specific Information GENII Version 2.0
Documentation Supplied with Code Transmittal (Not all documents are routinely transmitted with code)	B. A. Napier, R.A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII - The Hanford Environmental Radiation Dosimetry Software System, Volume 1: Conceptual Representation*, PNL-6584 Vol. 1 (December 1988). B. A. Napier, R. A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII - The Hanford Environmental Radiation Dosimetry Software System, Volume 2: Users' Manual*, PNL-6584 Vol. 2 (November 1988). P. D. Rittmann, *Verification Tests for the July 1993 Revision to the GENII Radionuclide and Dose Increment Libraries*, WHC-SD-WM-TI-596, Rev. 0 (October 1993).	Leigh, C. D., B. M. Thompson, J. E. Campbell, D. E. Longsine, R. A. Kennedy, and B. A. Napier. 1992. *User's Guide for GENII-S: A Code for Statistical and Deterministic Simulations of Radiation Doses to Humans from Radionuclides in the Environment*, SAND91-0561A, Sandia National Laboratories, Albuquerque, New Mexico. Napier, B. A., D. L. Strenge, J. V. Ramsdell, Jr., P.W. Eslinger, and C. F. Fosmire, 1999. *GENII Version 2 Software Design Document*, Pacific Northwest National Laboratory, Richland, Washington. Napier, B.A. 1999, *GENII Version 2 Example Calculation Descriptions*. Pacific Northwest National Laboratory, Richland Washington. Gelston, G.M., M.A. Pelton, K.J. Castleton, B.L. Hoopes, R.Y Taira, P.W. Eslinger, G. Whelan, P.D. Meyer, and B.A. Napier, 1998, *GENII Version 2 Sensitivity/Uncertainty Multimedia Modeling Module Users' Guidance*, Pacific Northwest National Laboratory, Richland, Washington.

Table 2-1. Summary Description of GENII Software (Continued)

Nature of Problem	GENII was developed to incorporate the internal dosimetry models recommended by the International Commission on Radiological Protection (ICRP) into the environmental pathway analysis models used at Hanford. GENII is a coupled system of programs and the associated data libraries that comprise the Hanford Dosimetry System (Generation II) to estimate potential radiation doses to individuals or populations from both routine and accidental releases of radionuclides to air or water and residual contamination from spills or decontamination operations. The GENII system includes interactive menu-driven programs to assist the user with scenario generation and data input, internal and external dose factor generators, and environmental dosimetry programs. The programs analyze environmental contamination resulting from both far-field and near-field scenarios. A far-field scenario focuses outward from a source, while a near-field scenario focuses in toward a receptor. GENII can calculate annual dose, committed dose, and accumulated dose from acute and chronic releases from ground or elevated sources to air or water and from initial contamination of soil or surfaces and can evaluate exposure pathways including direct exposure via water (swimming, boating, and fishing), soil (surface and buried sources), air (semi-infinite and finite cloud geometries), inhalation pathways, and ingestion pathways. In addition, GENII can perform 10,000-years migration analyses and can be used for retrospective calculations of potential radiation doses resulting from routine emissions and for prospective dose calculations for purposes such as siting facilities, environmental impact statements, and safety analysis reports. The alternate data added in March 1995 were contributed by HEDL, and are intended to improve the treatment of decay chains for calculations of doses from contaminated soil allowed to decay for hundreds of years. Air transport calculations are largely unaffected by these changes due to the short decay times involved.
Method of Solution	GENII 1.485: APPRENTICE interactively prepares a text input file for the near-term (Approximately 1 to 100 years) environmental dosimetry programs and a batch processing file to manage the file handling needed to control the operations of the five subsequent codes and prepare an output report. ENVIN controls the reading and organization of the input files for ENV, which then calculates the environmental transfer, uptake, and human exposure to radionuclides that result from the chosen scenario for the defined source term. ENV writes the annual media concentrations and intake rates to intermediate data transfer files for use by DOSE. DOSE converts these data to radiation dose, calculating the external dose using factors generated by EXTDF and the internal dose using factors generated in INTDF. DOSE calculates the one-year dose, committed dose, cumulative dose, and maximum annual dose and prepares the normal output report of doses and optional doses by pathway and by radionuclide. EXTDF calculates the external dose-rate factors for submersion in an infinite cloud of radioactive materials, immersion in contaminated water, and direct exposure to plane or slab sources of contamination. EXTDF used the ISOSHLD point-kernel integration technique whereby numerical integration is carried out over the source volume to obtain the total dose. INTDF estimates the dose equivalents in a number of target organs from the activity in a given source organ based on ICRP-30 models and biokinetic values for radionuclide residency and transport in the body. The dose equivalent in a target organ is the product of the total number of nuclear transformations of the radionuclide and the energy absorbed per gram in the target organ. This initial value problem is solved using a coupled set of differential equations. DITTY calculates long-term total population exposure based on air and water source terms, atmospheric dispersion patterns, and exposed population. A straight-line cross-wind-averaged Gaussian plume model is used for the dispersion calculation, and the regional population is defined as a function of time for airborne and waterborne pathways. The time frame may be any 10,000-year period, broken into 143 periods of 70 years each. GENII 2.0: The FRAMES user interface is used in place of APPRENTICE and its supporting programs. The capabilities of GENII 2.0 are similar to GENII 1.485 but with enhancements, such as SUM for stochastic evaluations, and an improved user interface.

Table 2-1. Summary Description of GENII Software (Continued)

Restrictions or Limitations	The atmospheric model included in the code does not model the impact of terrain effects on atmospheric dispersion. The code also does not model dispersion close to the source (less than 100 meters from the source) or long-range dispersion. Maximum of 100 radionuclides, 5 shields. For GENII 1.485, there are 16 sectors and 10 distance intervals in a radial grid but only one distance and one sector can be run at a time.	The atmospheric model included in the code does not model the impact of terrain effects on atmospheric dispersion. The code also does not model dispersion close to the source (less than 100 meters from the source) or long-range dispersion. GENII 2.0 includes a 36 sector radial grid and a square grid (for puffs). The user can specify up to 10 receptor locations in the grid and GENII 2.0 will assign those locations to the nearest grid points.
Run Time	The sample problems took a total of 30 minutes on an IBM PC-AT under DOS 3.3. Under Windows, the sample problems take less than one minute for most runs (~ 5 s)	GENII 2.0 is machine-dependent and requires a few seconds for most problems.
Computer Hardware Requirements	GENII requires an IBM PC/AT or compatible computer, an 80287 math coprocessor, 640 Kbytes of random access memory, and a minimum of 5 MB on-line disk storage.	GENII Version 2 requires Windows 95, 98, NT, 2000, or XP using Pentium processors (or equivalent), and disk storage in excess of 60 Mbytes. As FRAMES and GENII make use of the memory swapping capabilities of Windows, the programs should run on any Windows compatible machine. Best performance is with machines with 256 Mbytes or more.
Computer Software Requirements	Lahey F77L (92%) and Microsoft QuickBASIC 3.0 (8%) were used to create the executables, which runs under DOS 3.1 or later. RSICC claims that it also runs from a DOS window of Windows 95. Experience shows that this also runs under Windows 98 but problems may be encountered for some scenarios when run under Windows XP. The GENII and APPRENTICE source files were added to the package in the March 1995 update. APPRENTICE, which is written in Microsoft QuickBASIC 3.0, uses modules and subroutines from the Komputerwerk Modules libraries.	Pentium-class processor, Windows 95 or later, 60 MB disk space, preferably ≥ 256 MB memory. Does not run under DOS.
Other Versions Available	GENII-S (Stochastic); GENII Version 2.0	GENII-S (Stochastic); GENII Version 1.485

Capabilities and Exposure Pathways

The GENII system includes the capabilities for calculating radiation doses following chronic and acute atmospheric releases. Radionuclide transport via air, water, or biological activity may be considered. Air transport options include both puff and plume models, each allow use of an effective stack height or calculation of plume rise from buoyant and momentum effects. Building wake effects can be included in acute atmospheric release scenarios. The code provides risk estimates for health effects to individuals or populations; these can be obtained using the

code by applying appropriate risk factors to the effective dose equivalent or organ dose. Data entry is accomplished via interactive, menu-driven user interfaces.

Default exposure and consumption parameters are provided for both the average (population) and maximum individual; however these may be modified by the user. Source term information may be entered as radionuclide release quantities for transport scenarios, or as basic radionuclide concentrations in environmental media (air, water, soil). For input of basic or derived concentrations, decay of parent radionuclides and ingrowth of radioactive decay products prior to the start of the exposure scenario may be considered. A single code run can accommodate unlimited numbers of radionuclides including the source term and any radionuclides that accumulate from decay of the parent, because the system works sequentially on individual decay chains.

Interface System

The Version 1.485 user interface is APPRENTICE. It interfaces with other codes for input of data, computations, and output of results. The code package for Version 2.0 also provides interfaces, through the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES). Both versions provide external calculations of atmospheric dispersion, geohydrology, biotic transport, and surface water transport. Target populations are identified by direction and distance (radial or square grids for Version 2.0) for individuals, populations, and for intruders into contained sources.

Dosimetry Models

GENII Version 1.485 implemented dosimetry models recommended by the ICRP in Publications 26, 30, and 48, and approved for use by DOE Order 5400.5. GENII Version 2.0 implements these models plus those of ICRP Publications 56 through 72, and the related risk factors published in Federal Guidance Report 13. Risk factors in the form of EPA developed "slope factors" are also included. The dosimetry and risk models are considered to be 'state of the art' by the international radiation protection community and have been adopted by most national and international organizations as their standard dosimetry methodology.

Component Programs

GENII Version 1.485 consists of seven coupled programs (listed above) for input, processing, and output. Version 2.0 consists of four independent atmospheric models, one surface water model, three independent environmental accumulation models, one exposure module, and one dose/risk module, each with a specific user interface code. The computer programs are of several types: user interfaces (i.e., interactive, menu-driven programs to assist the user with scenario generation and data input), internal and external dose factor libraries, the environmental dosimetry programs, and FRAMES-supplied file-viewing routines. For maximum flexibility, the code has been divided into several interrelated, but separate, exposure and dose calculations.

Documented Safety Analysis Calculations

The GENII code executes consequence calculations that can be used to support applications such as site evaluations, DSAs, and environmental impact statements. Source term information may

be entered as radionuclide release quantities for transport scenarios or as radionuclide concentrations in air, water, or soil media. Algorithms model transport of radioactive material through the atmosphere, surface water, and biotic activity. Atmospheric releases are modeled as plumes or as a series of puffs. The GENII code includes models for stack releases, plume rise from momentum and buoyancy effects, and building-wake influences on trajectory and dispersion. Radionuclide decay and ingrowth during plume transport are computed.

Exposure pathways include direct external exposure via air, water, or soil and internal exposure through inhalation and ingestion. The tritium model also considers exposures via skin absorption. Dose conversion factors (DCFs) relate environmental concentrations and intakes to resultant human doses for specific exposure pathways, organs, and radionuclides.

2.2 Overview of GENII for Regulatory Applications

For documented safety analysis purposes, the consequences of interest are the centerline Total Effective Dose Equivalent (TEDE) incurred by the Maximally Exposed Offsite Individual (MOI) evaluated at the 95th percentile dose level. The statistical evaluation of consequences from meteorological variability is handled in one of two ways. In GENII 2.0, hourly meteorological data of wind direction, wind speed, and atmospheric stability class over a one-year period is randomly sampled. In GENII 1.485, a joint frequency distribution of wind direction, wind speed, and atmospheric stability class is first determined from the hourly meteorological data and then used in the calculations. GENII 1.485 can calculate the 95th percentile dose for a given distance and direction. It has to be run 16 times, once for each sector and for the distance to the site boundary for that sector. The largest of these 95th percentile values is reported, rather than the overall sector-independent 95th percentile dose discussed in DOE-STD-3009-94, CN#2 (DOE 2002a). The present GENII 2.0 version, however, cannot be used to generate 95th percentile values without considerable effort.

The MOI TEDE will most easily be evaluated with GENII at the closest site boundary without regard to sector (i.e., sector independent). Although this method is not identical with NRC Regulatory Guide 1.145, the calculated dose at the closest offsite boundary without regard to sector can be shown to be conservative relative to that calculated with regard to sector.

Accident duration is defined in terms of plume passage at the location of the dose calculation, for a period not to exceed 2 hours normally, or 8 hours for slow-developing release scenarios (DOE, 2002a). Prolonged effects, such as resuspension, need not be modeled. The acute puff and plume models in GENII are applicable to releases or exposures that occur over a relatively short period, such as a few hours. Thus, these models are appropriate for modeling accidental releases for DSA applications.

2.3 GENII Applications

GENII 1.485 has been applied in many safety analysis applications for determination of MOI doses. Studies using GENII include, but are not limited to those performed for:

(xxi) Safety analysis reports - Hanford site nuclear facilities, the Waste Isolation Pilot Plant

(xxii) One-year worker dose from postulated accidents - Solid Waste Material Facilities (Savannah River Site), and

(xxiii) Environmental Impact Statement chronic and accident release analysis, the Mixed Oxide Fuel Fabrication Facility.

As indicated in Table 2-1, GENII Version 2.0 is EPA-sponsored, and has been applied mostly for Environmental Impact Statement (EIS) and National Emissions Standards for Hazardous Air Pollutants (NESHAPS) compliance analyses for routine release calculations.

3.0 APPLICABLE REGIMES

The objective of this section is to present a discussion of GENII applicability from two perspectives: (1) in terms of its overall function as a key step in accident analysis; and (2) noting the phenomenological regimes in which it provides an approximate model of dispersion in the environment and the resulting radiological exposure to downwind individuals (receptors).

3.1 Overall Application in Safety Analysis

The Department of Energy (DOE) evaluates and approves the operation of its nuclear facilities via the safety analysis process outlined in 10CFR830 – Subpart B (CFR, 2001) and DOE-STD-3009-94 (DOE, 2002a). This safety analysis process requires the development of a Documented Safety Analysis (DSA) per the Rule language and includes two key types of analyses: (1) hazard analysis and (2) accident analysis.

Hazard analysis is the cornerstone of the DOE safety analysis process and is largely a qualitative process by which

(xxiv) the hazards in the facility are identified,

(xxv) a spectrum of accidents are postulated for each hazard,

(xxvi) a qualitative evaluation of accident likelihood and consequence is made, and

(xxvii) all preventive and mitigative systems or controls are identified along with a qualitative measure of their importance.

The final product of the hazard analysis gives rise to a list of which systems or controls are important to safety and therefore are designated as safety-significant. This designation will lead to a formal commitment on the part of the facility contractor to maintain the safety function of these systems through technical safety requirements (TSRs).

Accident analysis is a follow-on activity to the hazard analysis. The focus of the Design Basis Accidents (DBAs) is public exposure, and therefore, a quantitative calculation of dose to the maximally exposed offsite individual (MOI) is made for each DBA. The purpose of the dose calculations is to determine if some of the safety-significant systems identified in the hazard analysis should have their safety designation raised to safety-class. The standard approach for the accident analysis is outlined below in terms of the source term and the radiological dispersion and consequence analysis phases.

3.1.1 Source Term Analysis

The radiological consequences are typically established using the methods discussed in the DOE-HDBK-3010-94 (DOE, 1994a). Since the dose from the inhalation pathway will usually dominate the overall dose from most non-reactor facilities, the source term may be quantified using the five-factor formula:

$$ST = MAR \cdot DR \cdot ARF \cdot RF \cdot LPF \qquad (3\text{-}1)$$

where:

(xxviii)Source term (ST) is the total quantity of respirable material released to the atmosphere during the postulated accident condition.

(xxix) Material-at-Risk (MAR) is the total quantity of radionuclides (in grams or curies of activity for each radionuclide) available to be acted on by a given physical stress.

(xxx) Damage Ratio (DR) is the fraction of the MAR actually impacted by the accident-generated conditions.

(xxxi) Airborne Release Fraction (ARF) is the fraction of a radioactive material suspended in air as an aerosol and thus available for transport due to a physical stress from a specific accident condition.

(xxxii) Respirable Fraction (RF) is the fraction of airborne radionuclides as particles that can be transported through air and inhaled into the human respiratory system and is commonly assumed to include particles 10-μm Aerodynamic Equivalent Diameter (AED) and less.

(xxxiii)Leakpath Factor (LPF) is the fraction of the radionuclides in the aerosol transported through some confinement deposition system (e.g., facility rooms, ductwork) or filtration mechanism (e.g., HEPA or sand filters).

For most accident analyses, the MAR is best defined as the maximum inventory that is permitted within the room, area, or facility. While it is permissible to exclude material forms that are considered to be unaffected by an accident condition from the MAR, experience suggests that for these forms the DR is usually best set to zero for the release mechanism. The overall result using either approach is the same. However, by assigning DR values to each combination of inventory form and release mechanism, there is the expectation that each credited form (e.g., a shipping package certified to withstand the postulated fire severity) is also reviewed against secondary events (e.g., building collapse initiated by a fire) and therefore, less likely to be overlooked.

The ARF and RF values presented in DOE-HDBK-3010-94 (DOE 1994a) are derived from discrete experiments that typically evaluated a single release mechanism. For example, in a severe fire there may be many mechanisms occurring simultaneously. Powdered metals might be subject to entrainment by fire-induced air currents, falling because of equipment (glove box) collapse, and impact because of objects falling into the exposed fire. In addition, multiple occurrences could be possible for specific mechanisms (e.g., impact of falling object on a stable powder). Aqueous solutions could be subject to boiling within the storage tank, spillage because of a tank collapse, and rapid evaporation plus splashing as the liquid sits in a diked area during the same postulated fire. Solid metals can melt, drip, and burn during the same event. To accommodate multiple-mechanism events, it is common to consider the ARF and RF values for each mechanism in the source term estimate.

Just as with the ARF·× RF term, there can be multiple LPF terms applied to a single material form (e.g., room leakage, ventilation system deposition, filtration system effectiveness). Thus, their cumulative effect must be accounted for. There can be interdependence between the LPF and DR in some applications. If a shipping package is considered to leak during a fire, the leakpath effect as the material exits the packaging can be accounted for as an LPF or a DR.

Based on experience, it is recommended that source term reductions related to localized conditions such as at shipping packages, and glove boxes be accounted for in the DR term. This approach allows the source term contribution from individual rooms to be readily compared. It also simplifies comparisons between the room source term and the building source term.

Based on the above discussion, Equation (1) can be generally reformatted as:

$$ST_{jk} = \sum_{i=1}^{n_i} \left\{ MAR_{ij} \cdot DR_{ijk} \cdot \left[(ARF \cdot RF)_{ijk} \cdot \left(\prod_{m=1}^{n_m} LPF_m \right)_{ijk} \right] \right\} \quad (3\text{-}2)$$

where:

- i is the index for the MAR component in a specific form (e.g., powder, liquid)
- j is the index for the MAR component by type (e.g., ^{238}Pu, ^{239}Pu)
- k is the index for the release mechanism (e.g., fire, spill)
- m is the index for the filtration or deposition stage (successive stages)
- n is the index for the number of parameters for the form, type, mechanism or stage based on the subscript.

Thus, the source term is usually expressed in terms of an isotopic activity distribution for each release mechanism. Source term components that are associated with the same release duration can be combined, but source term components that have different release mechanisms should be kept separate to account for time-dependent variance in atmospheric dispersion for consequence assessment. Note that the LPF term is the product of the successive factors, not their sum.

Note that the DR, but not the MAR, is shown in Equation (2) as a function of the release mechanism (k subscript), based upon the recommendation above on how to best handle the interplay between the MAR and the DR. Frequently, the DR, ARF, RF, and LPF terms are specified independently of the type, and the j subscript can be dropped from these terms as applicable.

3.1.2 Dispersion and Consequence Analysis

Once the source term is established, the consequences to the receptors can be estimated. For fire scenarios at facilities relatively close to the site boundary, the receptor at the site boundary may be exposed to lower concentrations if plume buoyancy lofts the plume above the receptor. Under these circumstances, higher receptor exposures can be expected downwind of the site boundary as the effects of increasing downwind plume growth progressively makes plume rise effect less significant. The 'touchdown' point refers to the location of maximum receptor concentration. Thus, the maximally exposed individual for a lofted plume is not at the site boundary, but rather at the touchdown point. Rather than evaluating for this point, it can be more cost effective to estimate the fire consequences as a ground level release with the maximally exposed individual at the site boundary. While the results will be higher than the plume-buoyancy credited analysis,

the increase may not be significant when compared to the uncertainties in the analysis and the analysis complexity.

Typically, the off-site radiological consequences are expressed as the total effective dose equivalent (TEDE) to the receptor at the highest exposure conditions. For most accident types, this is at or near the site boundary. The TEDE includes the 50-year committed effective dose equivalent (CEDE) from inhalation both during plume passage and later from resuspension, the cloudshine effective dose equivalent (EDE), the groundshine EDE, and the skin absorption EDE. This TEDE calculation generally does not include the ingestion CEDE from consumption of contaminated water and foodstuffs, although in principle it could. The inhalation CEDE is usually the dominant contributor and its relationship to the source term is highlighted below.

The basic equation for the radiological consequences to an individual receptor (i.e., stationary at a specific downwind location) from the inhalation pathway during plume passage is:

$$\text{Receptor Inhalation CEDE} = BR \cdot \sum_{k=1}^{n_k} \left\{ \left(\frac{\chi}{Q} \right)_k \sum_{j=1}^{n_j} \left[ST_{jk} \cdot C_j \cdot IDCF_j \right] \right\} \qquad (3\text{-}3)$$

where: j, k, n are as defined in Equation 3-2 above

BR is the breathing rate of the individual exposed to the plume of released radiological material, with typical units of m^3/s.

C_j is the specific activity of isotope j, with typical units of Ci/kg if ST is in mass units (kg) and unity if ST is in activity units (Ci).

$IDCF_j$ is the inhalation dose conversion factor for unit activity uptake of isotope j, with typical units of [rem/Ci] or [Sv/Bq].

$(\chi/Q)_k$ is the downwind dilution factor from atmospheric dispersion, which represents the time-integrated concentration at a specific downwind location that is normalized by the quantity released to the atmosphere, with typical units of s/m^3.

When the ST value is input into the GENII code, the GENII output provides the TEDE value at the requested receptor location that will include the contribution from the plume-passage inhalation CEDE as well as the contributions from resuspension inhalation CEDE, cloudshine EDE, groundshine EDE, and skin absorption EDE.

3.1.3 Computer Codes for Accident Analysis

The safety analyst may use hand calculations or computer codes to calculate source term and dispersion values. The computer codes chosen by the safety analyst fall into several categories. The categories of codes are

(xxxiv) Radiological atmospheric dispersion codes,

(xxxv) Chemical atmospheric dispersion codes,

(xxxvi) Fire modeling codes, and

(xxxvii) Leakpath analysis codes.

The analyst typically applies one or more of these types of codes to calculate parameters such as DR, LPF, and χ/Q, or to integrate over groups of these parameters. The effect of the quality of these codes on the overall safety analysis process can be evaluated qualitatively by examining the role that these parameters play in the overall safety process.

3.1.4 Qualitative Effect of the Codes on Safety Analysis

The gross effect of the use of computer codes can be evaluated by examining their effect on the final MOI dose values calculated as part of the accident analysis. The values chosen or calculated for each parameter in the dose equation are near the conservative tail of any distribution that would be assigned to the individual parameter. Therefore, when each parameter is multiplied using Equations 3-2 and 3-3 to obtain the dose, the conservatism in the calculation grows. If applied consistently in each phase of the process and in a reasonably bounding manner, this large conservatism in the calculation has always provided the DOE safety analysis process with sufficient margin when the doses are used to make decisions regarding safety. Even if a single value in the dose calculation were off by an order of magnitude, the resulting value would still not approach the mean value of dose if a cumulative distribution of dose also were calculated.

GENII is used to calculate the appropriate dilution factor and ultimately quantify the radiological dose. The net effect on safety then is related to GENII's use in selecting safety-class systems, structures, and components (SSCs).

GENII, and other atmospheric dispersion and radiological consequence codes, are used in analyzing atmospheric dispersion and the subsequent radiological consequence of accidental releases of radioactivity from postulated accident conditions. Codes of this type are used primarily to calculate the appropriate dilution factor for atmospheric transport of puffs or plumes and ultimately quantify the radiological dose that is received by the maximally exposed offsite individual (MOI). The 95th percentile of the distribution of doses to the MOI is the comparison point for assessment against the evaluation guideline (EG). Consequently, the importance of these classes of accident analysis codes on safety is related to their contribution in selecting safety-class (SC) systems, structures, and components (SSCs).[2]

Appendix A to DOE-STD-3009-94 prescribes the statistical method to be used to calculate the MOI dose, which is based on the method described in Position 3 of the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (NRC 1983). Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based doses calculated for a postulated release to downwind receptors at the site boundary that would result in a dose that is exceeded 5% of the time. Appendix A to DOE-STD-3009-94 allows for variations in distance to the site boundary as a function of distance to be taken into consideration. Assuming the

[2] The selection of safety-class SSCs is an important decision, but the decision to make an SSC safety-significant is made initially in the hazard analysis. Thus, the quality of the dose value will not affect the SSC being made a safety-significant SSC and having TSR coverage, only the designation of safety-class, and therefore, possibly the pedigree of the SSC.

minimum distance to the site boundary applies in all directions is a conservative implementation that is easily supported by GENII and that essentially makes the calculations sector independent.

3.2 Phenomenological Regimes of Applicability

The GENII class of atmospheric dispersion codes is based on the Gaussian model of dispersion. As such, these types of computer model are best suited for specific types of conditions. The chief phenomenological regimes for applying GENII include:

(xxxviii) Temporal regime – The use of these codes is best suited for "short" duration plumes, on the order of a few hours or less.

(xxxix) Spatial regime – The class of code also does not model dispersion close to the source (less than 100 meters from the source), especially where the influence of structures or other obstacles is still significant. Dispersion influenced by several, collocated facilities, within several hundred meters of each other should be modeled with care. Similarly, the GENII class of codes should be applied with caution at distances greater than ten to fifteen miles, especially if meteorological conditions are likely to be different from those at the source of the release. Long-range projections of dose conditions are better calculated with mesoscale, regional models that are able to account for multiple weather observations. Nevertheless, some applications may require fifty-mile or greater radius analysis to meet requirements, e.g., Environmental Impact Statements (EISs).

(xl) Terrain variability – Gaussian models are inherently flat-earth models, and perform best over regions of transport where there is minimal variation in terrain.

(xli) Energetic releases – GENII does not account for releases originating from detonation type events without appreciable post-processing of boundary and initial conditions. Using the latter approach, Steele (Steele, 1998) has demonstrated a segmented methodology for a detonation source term that was found to compare well with observations. (The Steele report used the MACCS2 code, not GENII, but in principle GENII 2.0 could be used in this way as it uses hourly meteorological data, as does MACCS2.)

(xlii) Thermal buoyancy – In plumes arising from fire-related source terms, the user should exercise caution with the models that use the Briggs algorithm. The Briggs approach for accounting for sensible energy in a plume is valid for "open-field" releases (not impacted by buildings and other obstacles), or if used in combination with building wake effects. In GENII, plume lofting is calculated only as a combination of buoyancy and momentum rise effects. GENII uses plume temperature rather than sensible heat in calculating thermal buoyancy. However, as a result of the work documented in Section 7.0 of this report, it has been determined that GENII cannot be used to model fires.

(xliii) Dose conversion factor applicability – The user should ensure that the dose conversion factors used in GENII are applicable to the radionuclides in the source term and the physicochemical characteristics. For example, plutonium nitrates and oxides have different time scales for dosimetric effects in the body with different resulting dose conversion factors. Thus, the appropriate lung absorption type should be used in the dose

conversion factor file used in the GENII run. GENII 1.485 does not allow user-prescribed DCFs.

4.0 INPUTS AND RECOMMENDATIONS

Safety analysts with experience with both versions of GENII prefer GENII 1.485 to GENII 2.0 for DSA purposes. Among other things, GENII 2.0 cannot be used to determine 95th percentile values of χ/Q without considerable effort. The potential method to do this with GENII 2.0 has not been tried. Furthermore, the full suite of subroutines for GENII 2.0 has not yet been completely tested. Therefore, because GENII 2.0 cannot yet be recommended for DSA analyses, the inputs and recommendations cited below are for GENII 1.485.

The GENII 1.485 computer code consists of models for atmospheric transport, surface water transport, terrestrial (i.e., plant and animal) transport, and human exposure and dosimetry. Since surface water transport and terrestrial transport are not of interest for support of a DSA, inputs associated with these models are not discussed here. The water transport and terrestrial transport models, for example, support the calculation of drinking water and food ingestion doses that are not required for DSA dose determinations.

4.1 General Code Input and Output Assumptions

A number of input parameters are unique when using GENII for a specific DSA application. Some of these parameters will be related to the source term being released or more specifically the radionuclide inventory being released. When defining the radionuclide inventory for GENII input, one must consider the activity of the inventory, under what conditions the material is being released (i.e. filtered or unfiltered conditions), and the material type being released. The material type influences the selection of CEDE inhalation dose conversion factors (IDCFs).

For DSA purposes, the consequences of interest are the centerline Total Effective Dose Equivalent (TEDE) incurred by the Maximally Exposed Offsite Individual (MOI) evaluated at the 95th percentile dose level (DOE, 2002a). In GENII 1.485, each sector is evaluated independently through executing the code for each of the 16 sectors individually. The maximum value at the site boundary among the 95th percentile dose-level results for the 16 sectors is chosen to represent the MOI dose. Although this sector approach is not identical with the guidance of Appendix A of DOE-STD-3000-94 (CN#2) (DOE, 2002a), it is considered conservative with respect to the guidance. It may also be noted that the joint frequency distribution (JFD) data that has been used with GENII 1.485 for safety analysis work at Hanford may not be compliant with the sampling algorithm that is prescribed by Appendix A of DOE-STD-3000-94 (CN#2) or with its basis, NRC Regulatory Guide 1.145 (NRC, 1983). This older JFD was prepared before the prescription of DOE-STD-3009-94, Appendix A (CN#2) was promulgated. However, it is possible for a user to create a new JFD as input to the code.

4.2 Recommended Inputs for Specific Scenario Parameters

The user is prompted for a set of input data for a scenario when using the APPRENTICE interactive input processor. Guidance is given below for those parameters that are common to DSA applications. Other parameters are set with default values and should remain unchanged unless the user has good reason to change them. These are covered in Section 4.3.

4.2.1 Scenario Type

The user is given the choice of specifying either near-field or far-field for the scenario type. According to the user documentation, a far-field scenario is generally applicable to safety analysis applications. A typical far-field type of a scenario involves a release of radioactive material, its downwind transport, and dose impact on an individual or distributed populations. Conversely, the focus of the near-field scenario type is the dose that an individual receives at a particular location that has an external source or initial contamination.

Recommendation: The far-field scenario type is specified for most DSA applications.

4.2.2 Receptor Dose

For a far-field scenario, GENII will calculate either the dose that is received by an individual or by a distributed population.

Recommendation: The individual receptor is specified for DSA applications.

4.2.3 Release Type

GENII models both acute and chronic releases. An acute release scenario defines an accidental, one-time release of radioactive material over a short period of time such as a few hours or less. Chronic releases occur over a longer period.

Recommendation: An acute release should be specified for DSA applications.

4.2.4 Individual Type

The individual-type input establishes a set of individual exposure parameters that are used to model inhalation, ingestion, and external exposure effects. The user specifies either average individual or maximum individual for this input. The parameter specifications for the average individual type are recommended by the user documentation for most population dose calculations, but for DSA applications, the maximum individual should be selected.

Recommendation: The maximum individual type should be specified for DSA applications.

4.2.5 Transport Pathway

The GENII Version 1.485 computer code consists of models for atmospheric air transport and surface water transport.

Recommendation: Airborne transport is specified for DSA applications.

4.2.6 Exposure Pathways

The GENII Version 1.485 computer code consists of models for various exposure pathways related to inhalation, ingestion, and external exposure.

Recommendation: Ingestion exposure effects are not considered in DSA applications. Receptor doses in DSA are based on inhalation, direct shine from the plume, and ground shine from deposited material.

4.2.7 Inventory Radionuclides and Source Term Release Quantity

The number of inventory radionuclides cannot exceed 100. The user specifies the activity, in curies, of each radionuclide released over a specified release period, up to one year. For acute airborne releases, the radioactive material is effectively released over the period that is specified for the plume duration.

Recommendation: If the number of radionuclides is greater than 100, either the inventory must be divided into groups with a maximum of 100 radionuclides each, or only those radionuclides that contribute to the overall TEDE should be retained. A useful cut-off for considering a group of radionuclides is the dose consequence contributed by one or more radionuclides is $\leq 0.1\%$. Below this value, the radionuclides in question can be ignored because they contribute insignificantly to the dose.

The curies released for each radionuclide of the inventory should have an appropriate amount of conservatism to account for any variability or uncertainty.

4.2.8 Atmospheric Transport and Dispersion Characterization

A cloud of released material undergoes dilution during atmospheric transport and diffusion that is characterized by the χ/Q value, which represents the time-integrated concentration at a specific downwind location, normalized by the quantity released to the atmosphere, with typical units of s/m^3. The user may specify the χ/Q value or provide a JFD of meteorological data consisting of wind speed, wind direction, and atmospheric stability.

Recommendation: If the user specifies the χ/Q value, it should represent the 95^{th} percentile χ/Q value as prescribed by Appendix A of DOE-STD-3000-94 (CN#2) (DOE, 2002a) with the statistical basis consistent with regulatory position 3 of NRC Regulatory Guide 1.145 (NRC, 1983). If a JFD file of meteorological data is used, it should be developed in accordance with guidance given in the user documentation. Note that wind speeds in the JFD file should correspond to the release height of the plume. If the release takes place at or near ground level, it is common practice to base the wind speed at 10 m above ground.

When a JFD file is used, the user is prompted to specify the wind direction (i.e., one of the 16 sectors) and the site boundary distance or equivalently the distance from the source to the receptor of interest if the receptor is not at the site boundary. Regulatory position 3 of NRC Regulatory Guide 1.145 provides instructions on how to take into consideration variations in distance to the site boundary as a function of angular direction. Each sector is evaluated independently in GENII 1.485, which requires 16 separate executions of the code for a given scenario. The maximum value among the 95^{th} percentile dose results for the 16 sectors is chosen to represent the MOI dose, but is different from the methodology described in Regulatory Guide 1.145.

4.2.9 Source Height

With elevated plumes from a stack, the separation of the plume centerline from the ground lowers the plume concentration at ground level. The effective source height can exceed the stack height through plume rise from buoyancy or momentum effects. The user has the option of either specifying the effective source height or specifying separately the source height and plume-rise parameters that GENII will use to calculate the effective source height. Elevated releases, however, can be negated by nearby structures as the released cloud can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs. The input for the height of adjacent structures is addressed in the next section and following sections address plume-rise input parameters.

Recommendation: It is generally conservative to specify a ground-level release (source height of zero) in an open field (adjacent structure height of zero) while taking no credit for plume rise effects from either momentum or buoyancy. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. In addition, the local terrain may have hills that reduce the effective stack height with respect to the ground. The source height should be conservatively estimated on the low side when there is some uncertainty or variability in its value.

4.2.10 Building Height

As mentioned above, plumes from elevated discharges can be drawn downward and entrained into the wake in the wind field caused by the building. NRC Regulatory Guides 1.111 and 1.145 define a stack release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977, 1983). Releases are generally considered to be at ground level if the point of release is below the height of the facility in question and its collocated buildings. The intermediate case of releases that occur in the range between 2.5 times the height of adjacent buildings and the building height, escape the building wake under certain conditions, become completely entrained into the building wake under other conditions, or behave as a "mixture" of these types for still other conditions (NRC, 1998). Technical details of the algorithms that are used by GENII are given in (Napier, 1988b).

The identification of adjacent structures must take into account the extent of influence that the building has on the flow field in its vicinity. The wind flow that is directly over the top of the building is entrained downward into the wake cavity. The extent of the wake cavity downwind, as measured from the lee face of the building, can range from 2.5 times the building height (H_b) to approximately 10 H_b for buildings that have large width-to-height ratios (Hanna, 1982). The wake cavity is marked by increased turbulence levels that decay progressively as a function of distance from the building. For releases from stacks not meeting the criterion of 2.5 times the height of adjacent solid structures, the combination of downward-directed entrainment into the wake cavity and increased dispersion due to high turbulence levels serve to increase ground-level concentrations above what would be observed in the absence of the building. The term downwash is frequently used to collectively describe these effects. An accepted practice by the

EPA is to assume that downwash effects can influence plumes that are released from stacks that are located in the range of 2 L upwind to 5 L downwind of building, where L is the lesser of the building height or projected width (EPA, 1995).

Recommendation: It is generally conservative to specify a ground-level release (source height of zero) in an open field (adjacent structure height of zero) while taking no credit for plume rise effects from either momentum or buoyancy. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs. Moreover, increased dispersion due to high turbulence levels serve to stretch the plume vertically (as well as horizontally), which may lead to higher ground-level concentrations especially close to the source (e.g., instead of the elevated plume simply passing over the close-in receptor, part of the plume may extend to ground-level when this increased dispersion is taken into account).

Adjacent buildings should be identified using the EPA method or an equivalent method with technical justification. Additionally, the building-height input should be conservatively estimated on the high side when used with elevated releases if there is some uncertainty or variability with its value. Conversely, the building-height input should be conservatively estimated on the low side when used with ground-level releases with no initial momentum or buoyancy.

4.2.11 Plume Rise Parameters

Just as with elevated releases, plume rise from momentum and buoyancy effects can result in the separation of the plume centerline from the ground that lowers the plume concentration that is observed at ground level. The specific input parameters that are used for the plume rise calculations are the source volume flow rate, source exit temperature, and stack radius. Fires in open areas cannot be modeled with GENII. Technical details of the algorithms that are used by GENII are given in (Napier, 1988b).

Recommendation: The recommendation here closely parallels the one above for source height. With elevated plumes either from a stack or because of plume-rise mechanisms, the separation of the plume centerline from the ground lowers the plume concentration at ground level. Thus, the most conservative approach is generally to assume a ground-level, open-field release with no initial momentum or buoyancy. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with plume lofting. Site observation is necessary since plume lofting can be negated by nearby structures as has been discussed above.

Specific input recommendations are given in multiple parts in order to account for the various component inputs that are needed to characterize the plume rise from buoyancy or momentum effects.

Source volume flow rate – The best basis for the input would be from measurement, but for most DSA applications, the input will likely be from an external calculation. The latter can be the result of either a manual calculation or the output from another code. Plume rise from momentum effects increase with increasing stack volume flow rate. The stack exit volume flow rate should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

Stack radius – The best basis for the input would be from measurement. For generic applications, in which the stack radius is unknown, it is conservative to estimate a large radius in order to minimize the exit velocity.

Source exit temperature – The basis for the input can be measurement or external calculation. Plume rise from buoyancy effects increase with increasing effluent temperature. The effluent temperature should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

4.2.12 End of Intake Period

The time step for the GENII 1.485 simulations is integer years. The intake period for an acute release will be much less than one year, but one year is the minimum specification for such a release. Note that the exposure times (in hours) for external exposure from ground contamination and inhalation will be specified later, in Sections 4.2.15 and 4.2.16, respectively.

Recommendation: A specification of one year for this input parameter is appropriate for DSA applications that involve accidental releases that occur over a short period.

4.2.13 Dose Commitment Period

The evaluation guideline for radiological releases is based on total dose effective dose equivalent (TEDE). The TEDE is the sum of the external (short-term) and the internal (committed, long-term) effective doses. When a radioactive particle is inhaled, it will cause long-term damage to the body as it remains in the body and continues to disintegrate and irradiate organs and tissues. The committed effective dose equivalent (CEDE) is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults.

Recommendation: The dose commitment period should be specified to be 50 years for DSA applications.

4.2.14 Fraction of Time Submersed in Acute Cloud

This input is used by GENII 1.485 to model acute plume exposure. A value of one means the receptor is present during the entire time of plume passage. For chronic releases, this parameter input is typically set to zero.

Recommendation: A specification of one for this input parameter is appropriate for DSA applications that involve acute, accidental releases that occur over a short period.

4.2.15 Period of Time for Soil Contamination Exposure

This input is used by GENII 1.485 to model external exposure from ground contamination, that is, groundshine.

Recommendation: For DSA applications, accident duration is not to exceed 8 hours (DOE, 2002a). Prolonged effects, such as resuspension, need not be modeled.

4.2.16 Period of Time for Inhalation Exposure

This input is used by GENII 1.485 to specify the plume release duration. For acute airborne releases, the radioactive material is effectively released over the period specified by this input value.

Recommendation: Accident duration in DSA applications is defined in terms of plume passage at the location of the dose calculation, for a period not to exceed 2 hours normally, or 8 hours for slow-developing release scenarios (DOE, 2002a). If the scenario involves release duration that is shorter than 2 hours, the scenario-specific release duration should be specified.

4.3 Recommended Inputs for Default Parameters

The following guidance is for those parameters having default values that should be not be changed except for compelling reasons.

4.3.1 Deposition Velocity

The deposition velocity represents the ratio of the ground surface contamination rate from deposition to the contaminant concentration in the plume above. Larger solid particles released in a plume will fall to the ground due to gravitational settling. Smaller particles and even some gases will deposit on ground surface elements (e.g., ground vegetation) through a variety of processes that can include chemical, biological, and physical interactions between the contaminant (particle or gas) in the plume and the ground surface elements. The GENII 1.485 code treats deposition of particles from the plume to ground surface elements in a way that mass is not conserved. Specifically, deposition velocities are applied in a standard way to deposit contaminants on the ground over the region of travel; however, this deposited material is not subtracted from the contaminants in the plume. As a result, air concentrations of contaminants and calculated CEDEs from inhalation are conservatively over-estimated.

Recommendation: In GENII 1.485, the default deposition velocity for particles is 0.001 m/s. However, GENII does not conserve mass with respect to the particles in the plume and that which is deposited out. While a reasonable assumption for routine releases, under postulated accident conditions, this will tend to artificially maintain concentrations in the plume and consequently increase doses in the far-field. In the context of consequence analysis, the focus is particles in the respirable size range.[3] For iodine, the deposition velocity is 0.01 m/s. A value of

[3] The DOE handbook for release fractions and respirable fractions uses a broad definition of respirable range to include particles of size 10-μm aerodynamic equivalent diameter (AED) and less (DOE, 1994a). Narrower respirable ranges have been used by the U.S. Atomic Energy Commission (up to 3.5-μm AED) and the American

zero is used for noble gases. These are reasonable values and should generally be used. Data in the literature support higher deposition velocities for respirable-sized particles. In computer codes that support plume depletion from deposition (i.e., mass is conserved), the use of a higher deposition velocity generally will result in a lower receptor TEDE since the inhalation CEDE is usually the dominant contributor to the TEDE. In GENII 1.485, the use of a higher deposition velocity only creates more ground contamination and increases ground shine exposure, which generally is a small contributor to the TEDE.

4.3.2 Breathing Rate

The inhalation CEDE that is calculated for a receptor is proportional to the assumed breathing rate.

Recommendation: The breathing rate should be set equal to the GENII 1.485 default value for acute releases of 3.3×10^{-4} m^3/s, which represents the DOE occupational breathing rate (DOE, 1998). Note that the chronic release model in GENII 1.485, which is not recommended for DSA analysis, has a smaller default value for the breathing rate of 2.7×10^{-4} m^3/s.

4.3.3 Inhalation Dose Conversion Factors

Dose conversion factors (DCFs) relate environmental concentrations and intakes to resultant human doses for specific exposure pathways, organs, and radionuclides. Doses arise from both internal and external exposures. The internal exposures consist of inhalation (from the plume and from resuspension) and ingestion. The external exposures are from cloudshine, groundshine, and skin deposition.

For DSA purposes, the consequences of interest are the centerline TEDE incurred by the MOI evaluated at the 95th percentile dose level.

Dose coefficients for external radiation should be based on FGR-12, which is available in both GENII 1.485 and GENII 2.0. For internal radiation, GENII 1.485 uses dose coefficients based on FGR 11[4]. GENII 2.0 offers these as well as the newer ICRP 72 recommendations[5], but these are not available in GENII 1.485.

Conference of Governmental Industrial Hygienists (up to 2-μm AED) (DOE, 1994a).

[4] FGR 11 contains IDCFs based on weighting factors from ICRP 26 (ICRP, 1977) and organ/tissue models documented in ICRP 30 and 48 (ICRP, 1979-82, and ICRP, 1986). The IDCF values in FGR 11 are based on exposure to an adult worker and a particle size of 1.0 μm Activity Median Aerodynamic Diameter (AMAD). The AMAD signifies that fifty percent of the activity in the aerosol is associated with particles of aerodynamic diameter greater than the AMAD. The values are applied uniformly for all ages in the general public population and all release conditions.

[5] ICRP Publication 72 provides updated dosimetry for the public, whereas ICRP 68 covers radiation workers (ICRP, 1995, 1996a, 1996b). Both include age specific models and parameters (ICRP, 2001). The IDCFs contained in these reports are based on ICRP 1990 Recommendation on radiation protection standards in Publication 60 (ICRP, 1991) and as well as the revised kinetic and dosimetric model of the respiratory tract in Publication 66 (ICRP, 1994). The inhalation DCFs in ICRP 72 are only for the CEDE and a 1.0 μm AMAD particle (ICRP, 1996a). Since the issuance of ICRP Publications 68 and 72, the ICRP has issued a compact disc with a dose coefficient database (ICRP, 2001) using the same models. However, the database gives both organ and effective dose coefficients. Additionally, the database gives the user greater flexibility by including dose coefficients for ten particle sizes and

Recommendation: The FGR-11 and -12 dose conversion coefficients must be used in GENII 1.485 because the user cannot choose the newer dose conversion factors.

Note that if the source term includes tritium oxide, its 50-year committed inhalation dose conversion factor should be increased by 50% to include the effects of skin absorption as directed by International Commission on Radiological Protection (ICRP) in their publication 30 (ICRP, 1978).

4.4 Radiological Dispersion and Consequence Analysis Recommendation

Recommendations on inputs for GENII modeling radiological dispersion and consequences and their bases are summarized in Table 4-1. In most cases, the standard practices and recommendations are site-insensitive.

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ten periods as well as six ages at exposure (ICRP2, 2001).

Table 4-1. Standard Practices and Assumptions Recommended for Consequence Analysis

Model/Attribute	Recommendation/Basis
Model Basis	Gaussian plume or puff model; DOE-STD-3009-94, CN#2, Appendix A.
Receptor Distances & Meteorology	• MOI: Evaluate using a conservative 95th percentile methodology per DOE-STD-3009-94, CN#2, Appendix A and NRC Regulatory Guide 1.145. • Evaluate at touchdown point for elevated releases or releases involving plume lofting.
Dispersion Parameters (see Appendix A for a discussion of these options)	▪ Urban terrain: (Briggs, 1973) urban conditions. ▪ Other terrain and >100 meters from source: (Briggs, 1973) open country; (Eimutis and Konicek, 1972); or (EPA, 1995) [based on (Turner, 1970)]. • Other terrain and < 100 meters from source: (Eimutis and Konicek, 1972).
Mixing Layer Height	Apply local site/laboratory recommendations for seasonal and time-of-day estimates for the mixing layer height.
Release Duration and Exposure	Should be consistent with accident analysis, not to not to exceed 2 hours normally, or 8 hours for slow-developing release scenarios. Two hours: DOE-STD-3009-94, CN#2, App. A; RG 1.145 (to MOI). Eight hours: DOE-STD-3009-94, CN#2, App. A.
Particle Size (dry deposition)	Particle: based on respirable-sized particles (e.g., 1 μm AED to 4 μm AED) and properties of the dispersed material if known. If the airborne particles pass through a filtration system (e.g., HEPA filters), the particles that are released to the environment and are transported to the receptor can typically be expected to be less than 1 μm AED.
Dose Conversion Factors (DCFs)	ICRP-26 for metabolic model; ICRP 30/48-based: Federal Guidance Report (FGR) 11for inhalation and ingestion DCFs and FGR 12 for external dose coefficients. (The newer DCFs are not available in GENII 1.485.)
Pathways	Primary: Inhalation; DOE-STD-3009-94, CN#2, Appendix A Secondary: Cloudshine, Groundshine (Important only for criticality source terms in non-reactor applications).
Dose Commitment	50-year, per definition of TEDE in DOE-STD-3009-94, CN#2, Appendix A.
Evaluation Criterion	Offsite/MOI Evaluation Guideline – 25 rem; DOE-STD-3009-94, CN#2, Appendix A.
Terrain	Flat earth acceptable for most near-field and MOI estimates.
Sensible heat in plume	1. The conservative assumption generally is to not credit plume rise, apply a short duration, and assume ground-level release in an open field. 2. More realistic results are obtained using judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures.
Protective Actions	None. Conservatively assume no shielding by any structure or cut-off of ventilation (sheltering), or movement to avoid plume (evacuation).
Meteorological Sampling	Sampling of hourly meteorological data or use of joint frequency of occurrence data. For GENII 1.485, sampling of hourly meteorological data is not an option.
Meteorological Data	At least one year of representative, qualified, hourly data. Two to five years is recommended (Regulatory Guide 1.23 (NRC, 1972)).

5.0 SPECIAL CONDITIONS FOR USE

The GENII code has additional capabilities that generally are not used in standard DSA applications. For example, food ingestion doses can be calculated, but these results are not part of the DOE 3009 Appendix A requirement for safety basis dose calculations. In addition, GENII can be used to calculate population doses, but neither are these used for DSA applications.

GENII can evaluated chronic releases to air and water, and initial contamination of soil or surfaces near the point of release.

Results of these types are not needed for safety-basis dose calculations.

6.0 SOFTWARE LIMITATIONS

This section summarizes GENII software limitations in terms of past occurrences of errors and defects in various versions of the code.

6.1 Software Quality Assurance (SQA)

The GENII code developer has indicated that both GENII versions were developed under SQA plans based on the American National Standards Institute (ANSI) standard NQA-1 as implemented in the PNNL Quality Assurance Manual. The documentation accompanying the releases of both GENII 1.485 and 2.0, as well as the current air quality website for the EPA, state that all steps of code development for both versions have been documented and tested, and hand calculations have verified the code's implementation of major transport and exposure pathways for a subset of the radionuclide library. In addition, a collection of hand calculations and other verification activities is available. Additional testing is currently underway for Version 2.0.

The earlier version of GENII has been included in the International Atomic Energy Agency's VAMP project (Validation of Model Predictions - an acronym for the Coordinated Research Program on Validation of Models for the Transfer of Radionuclides in Terrestrial, Urban and Aquatic Environments), an international effort to compare environmental radionuclide transport models with measured environmental data. Results for test scenario CB (based on environmental measurements following the Chernobyl accident) indicated that dose estimates from GENII were comparable to, although slightly higher than, those of other participating models. The models included in the code have been validated to various degrees by additional studies, however these have not been compared directly to output from the code.

6.1.1 GENII 1.485 Issues

Several user experiences with GENII 1.485 should be discussed in light of potential upgrades. Most significant are:

(xliv) GENII 1.485 was developed for Disk Operating System (DOS)-based computers. It can be operated in a DOS window on a Windows-95 or –98 based computer but caution must be exercised when operating under Windows-XP, as problems may be encountered for some scenarios when used in this way. This arises from the different memory management techniques used in DOS-based and Windows-based computers. The safest approach is to use GENII 1.485 on a DOS-based computer. This is addressed further in Section 7.

(xlv) Joint Frequency Distribution – The JFD file used originally at the Hanford Site, and similar ones developed for other sites, were developed before the sampling algorithm in Appendix A of DOE-STD-3000-94 (CN#2) was promulgated and it is not clear if these JFD file are compliant. Users should assure that the JFD file used is compliant.

(xlvi) Non-conservative plume deposition – The GENII 1.485 code allows standard deposition velocities to be used to account for dry deposition over the region of travel. However, the plume concentration is not reduced by deposition and is therefore overly conservative.

(xlvii) Hydrogen equilibrium model – The tritium model in GENII assumes equilibrium is reached between tritium concentrations in air and vegetation. This is a good assumption for long-term, chronic release conditions, but may over-predict short-duration, time-dependent, release consequences.

(xlviii) Food pathway modeling – In some EIS sensitivity studies, the potential population dose incurred from consumption of contaminated food is evaluated. In these cases, GENII can be used to quantify this component of dose. However, using the food ingestion dose capability, the code may over-predict the dose if one of the radionuclides is tritium (^{3}H) or Carbon-14 (^{14}C). The potential exists for a limited combination of options: specifically, only for cases of acute, atmospheric release when the "food production grid" input option is used, if "food export" is chosen, and one of the input radionuclides is ^{3}H or ^{14}C. Because ^{3}H and ^{14}C are handled with special specific-activity models, calculations for these two radionuclides do not have the same path through the code logic. If the above combination of options is used, the food production grid is inappropriately applied to ^{3}H and ^{14}C. The total amount of food input of the full 80-km (50 mile) circle is assumed contaminated with these two radionuclides, rather than just that from the selected downwind sector. The estimated dose provided by the GENII 1.485 code is too large by factors of about 10 to 20.

The developers of GENII 1.485 have no intention at this time of making changes to the code. The code update, GENII 2.0, is scheduled to undergo formal peer review in the near future, and is intended to replace GENII 1.485 after comment resolution is completed. However, unless the shortcomings of GENII 2.0 for DSA applications are addressed, the safety analyst is advised to use GENII 1.485 on a DOS-based or Windows-95 or –98 computers instead of GENII 2.0.

6.1.2 GENII 2.0 Issues

Current support of GENII 2.0 is from the Environmental Protection Agency's NESHAPs office. Since its release, GENII 2.0 has not been applied in safety analysis studies for assessment of consequences due to postulated accident releases. Most work that has been documented is for routine release assessment, or dose reconstruction studies from DOE sites. The principal shortcoming of GENII 2.0 for DSA work is that it cannot be used to calculate 95th percentile dose according to DOE-STD-3009-94, Appendix A (CN#2).

6.2 Outcome of Gap Analysis

A gap analysis for Version 1.485 and 2.0 of the GENII software has been completed (DOE, 2004a). The gap analysis reviewed the program, practices, and procedures associated with development of GENII compared with NQA-1 based requirements as contained in U.S. Department of Energy, Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes (DOE, 2003a). It was determined that GENII 1.485 code does meet its intended function for use in supporting documented safety analysis, providing it is not used on a Windows-XP based computer. It was determined that GENII 2.0 will not meet its intended function. Therefore, only GENII 1.485 can be recommended for DSA use at this time. As with all safety-related software, users should be aware of current limitations and capabilities of GENII for supporting safety analysis. Informed use of the software can be assisted by the current set of GENII reports, and this code guidance report for DOE safety analysts. Furthermore, while SQA

improvement actions are recommended for GENII, no evidence has been found of programming, logic, or other types of software errors in GENII that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

Of the ten primary SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), nine requirements are met at an acceptable level for GENII 1.485, (items 1-9). Improvement actions are recommended for GENII 1.485 to fully meet the requirement for *Error Impact* (item 10). For GENII 2.0, of the ten primary SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), two requirements are met at an acceptable level, i.e., *Software Classification* (1) and *Configuration Control* (9). Improvement actions are recommended for GENII 2.0 to fully meet the requirement for five that are partially met, i.e., *SQA Procedures and Plans* (2), *Requirements Phase* (3), *Design Phase* (4), *Implementation Phase* (5), and *User Instructions* (7) and for the remaining three, *Testing Phase* (6), *Acceptance Test* (8), and *Error Impact* (10). This evaluation outcome is deemed acceptable because: (1) GENII is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of GENII is limited to those analytic applications for which the software is intended.

Table 6-1 below is a copy of Table 2-1 of (DOE, 2004a) giving a summary of important exceptions, reasoning, and suggested remediation for GENII 2.0.

Table 6-1 Summary of Important Exceptions, Reasoning, and Suggested Remediation for GENII 2.0

No.	Criterion	Reason Not Met	Remedial Action(s)
1.	Testing Phase	Testing not yet complete	Document all testing of GENII 2.0
2.	Acceptance Test	Testing not yet complete	Develop and document acceptance criteria for GENII 2.0 and document acceptance testing.
3.	Error Impact	A formal error reporting and corrective action procedure is not followed.	Create and follow a formal error reporting and corrective action process (applies to GENII 1.485 as well)

By order of priority, it is recommended that GENII software improvement actions be taken, especially:

1. correct known defects
2. upgrade user technical support activities
3. provide training on a regular basis, and
4. revise software documentation.

Performing these four primary actions should satisfactorily improve the SQA compliance status of GENII relative to the primary evaluation criteria cited in this report.

A new software baseline set of documents is recommended for GENII 2.0 to demonstrate completion of item 4 (above), revise software documentation. The list of baseline documents for revision includes:

1. Software Quality Assurance Plan
2. Software Model Description, including, but not limited to,
    a. Software Requirements
    b. Software Design
3. User's Manual, including, but not limited to,
    a. User Instructions
    b. Test Case Description and Report
    c. Software Configuration and Control
4. Error Notification and Corrective Action Procedure.

It is estimated that nearly ten full-time equivalent (FTE) months would be required to perform all SQA upgrade tasks covered in Section 4.0 (DOE, 2004a) for GENII 2.0. Because GENII 1.485 has been in use for many years and the code author does not intend to make any further modifications, no similar estimates need be made. The error-reporting estimate for GENII 2.0 may be applied to GENII 1.485. In order to use GENII 1.485 in all Windows environments, it will be necessary to recompile the code using a Windows-XP compatible compiler. A side-by-side testing on DOS-based and Windows-based computers would then follow this. The GENII 1.485 documentation would not need to be changed if the results were the same but documentation of the results should be included with the RSICC distribution package for GENII 1.485. The recompiled version would have to be given a new number, such as 1.486.

Training opportunities exist for both versions of GENII, but these are not routinely offered. It is recommended that user training for safety analysis applications be conducted formally on at a minimum, an annual basis. Prerequisites for, and core knowledge needed by, the user prior to initiating GENII applications should be documented by the code developer.

While completion of the GENII 2.0 development is encouraged, current DOE DSA support should be through the earlier code version, GENII 1.485. Use of Windows-XP based computers should be avoided for GENII 1.485 until such time that a Windows-XP based version is available.

7.0 SAMPLE CALCULATIONS

This section discusses installation and execution of GENII 1.485 as obtained from the Radiation Safety Information Computational Center (RSICC) at Oak Ridge. A final part of the discussion then illustrates use of GENII for analyzing a ^{239}Pu release, and compares the results to the results from another designated toolbox code.

7.1 Installation of GENII 1.485

Version 1.485 of GENII comes in four folders, labeled DISK01 through DISK04 (as they were originally provided on four floppy disks). This version of the code is best run in the DOS mode, not in Windows proper[6]. The only way to run GENII 1.485 on Windows-based computers is to operate it in a DOS window. In the earlier versions of Windows (such as Windows 95 or 98), one can enter the DOS mode by clicking on "Start", then "Programs", then "MS-DOS Prompt". In the later version (such as Windows XP), one can enter the DOS window by clicking on "Start", then "run" and type "command" in the "open" line and press "enter". If the DOS window that opens is not at the root directory (the prompt should be C:\>, assuming that "C" is the hard disk drive), type "cd C:\", which should switch to the root directory. It must be emphasized that the analyst must be wary of the results when operating in a DOS window (as opposed to DOS mode), as will be evident below.

There are several ways one can install GENII 1.485. Here is one simple way:

1. Copy the contents of the file "DISK01" onto a blank floppy disk in drive A.

2. Open a DOS Window on drive C as described above.

3. At the C:\> prompt type "A:\genii –d", or "A:\DISK01\genii –d" if the files on the floppy disk are in a folder called "DISK01".

The latter command will install the software in the folder c:\genii.

7.2 Execution of GENII 1.485

GENII is menu driven and executed as follows:

1. Make a folder where you want to place your input and output files. This can be done using Windows or in DOS mode. If in DOS mode, use the "md" command. For example, if the folder name is to be SAMPLE, at the C:\> prompt type "md SAMPLE". The Joint Frequency Distribution file (typically named "jointfre.in") does not have to be

[6] Documentation issued by RSICC with the GENII 1.485 distribution disks states that it can be run in a DOS window in Windows 95. Experience shows it can also be run under Windows 98. However, when GENII 1.485 was developed, computers were limited to 640 KB of memory and this limitation had to be addressed during code development. Windows, however, manages memory differently than does DOS and unexpected problems may arise when GENII 1.485 is run in a DOS window within the Windows-XP environment.

copied to this folder although it is useful to do so. If population doses are to be calculated, a population file (typically named "pop.in") also needs to be available. The population file does not have to be in the input/output folder but it is useful if it is.

2. Navigate to this folder in DOS mode by typing "cd SAMPLE". The prompt should be C:\SAMPLE>.

3. At the prompt type "\genii\apprenti" (e.g., the command line would appears as "C:\SAMPLE>\genii\apprenti").

Follow the instructions given in the menu-driven prompts to input the various data. The help file can be accessed by pressing the F1 key.

The following figures are screenshots from the GENII front-end processor (Apprentice). These figures show some of the steps the user must take to generate the input file to run GENII, including the execution script (batch file). Not all of the screens are shown, as there are too many possibilities to show them all here. The method is intuitive and straightforward. It is noted that Apprentice functions properly in Windows XP, generating proper input and batch files. However, execution of these files in Windows XP may lead to errors and is not recommended.

Figure 7-1 is a sample of the DOS window where the front-end processor is called (step 3 above). The main screen for GENII is then displayed, as in Figure 7-2.

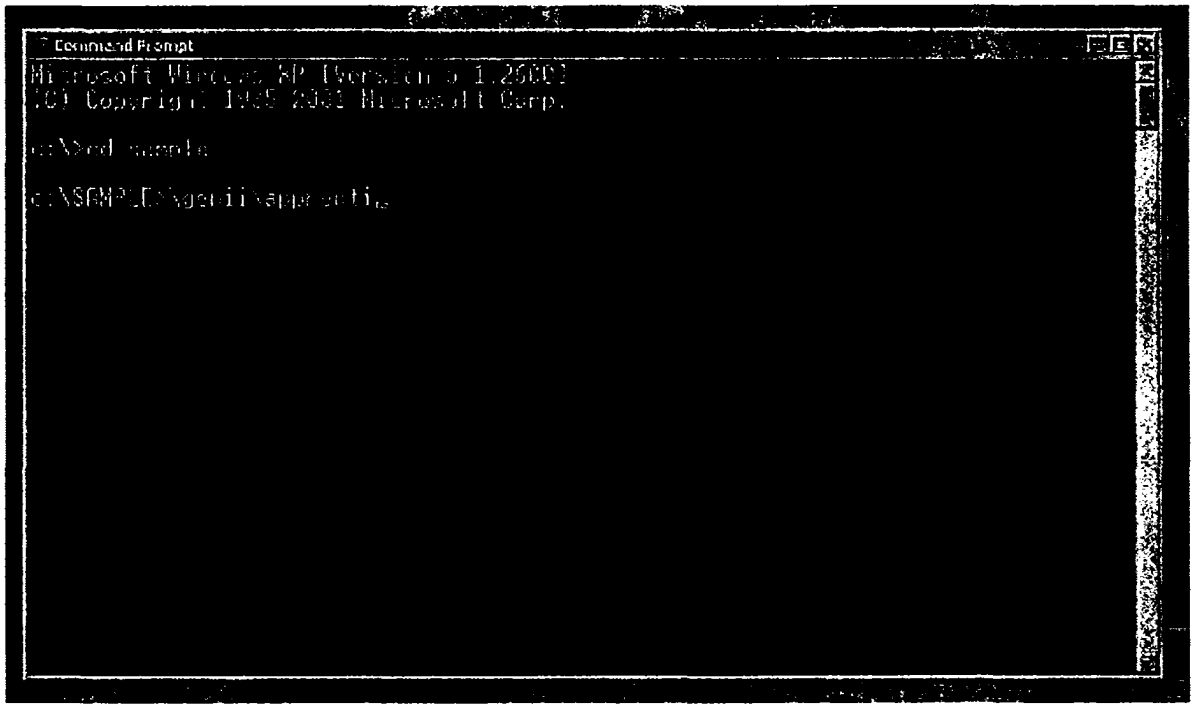

Figure 7-1. DOS Window where GENII 1.485 front-end processor (Apprentice) is called.

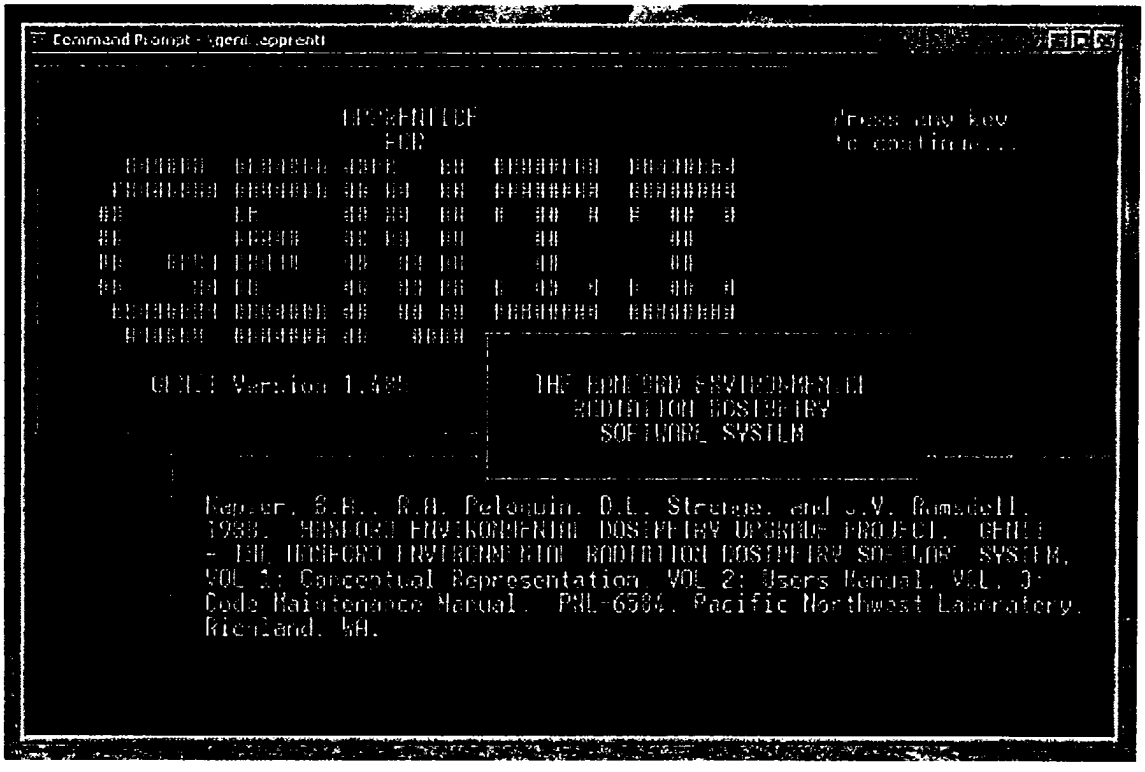

Figure 7-2. GENII 1.485 introduction screen.

Pressing any key then takes you to a page giving an overview to GENII. To get help on using Apprentice, press "H", which leads you into a set of help screens. Otherwise, pressing any other key leads to the first input screen, as shown in Figure 7-3. This screen allows you to input selections for individual type (average or maximum individual), scenario (far or near field), dose to population or individual, and whether the release is chronic or acute. The selections are chosen using the up- and down-arrow keys to move within a group and the left- and right-arrow keys to move between pages[7]. Use the "enter" key to select an option. For the screen shown in Figure 7-3, the pages would be "Scenario", "Dose to", "Release", "Individual Type", and "Next", as shown along the top of the screen. The first four are for making selections on this page, whereas "Next" navigates to the next set of selections.

[7] Note that the arrow keys on the numeric keypad must be used for some screens (such as radionuclide selection), as the arrow keypad keys will not work there. On other screens, the arrow keys from either the numeric keypad or arrow keypad work equally well. For a laptop computer, which doesn't have a normal numeric keypad, the 8, 9, 0, u, i, o, j ,k, and l keys can be converted into a numeric keypad with the use of a function key. The right-arrow key, for example, would be "o" and the down-arrow key would be "k". (The key selections may vary with computer manufacturer. See user guide for the laptop computer to learn how to activate this capability.)

Figure 7-3. First input selection screen.

Figure 7-4 shows the types of output reports requested (annual EDE only, by radionuclide, by pathway, and screen debug), the selected transport medium (air or surface water), the selected exposure (various choices for external and internal), and inventory location for air or surface water.

Figure 7-5 is a screen view of the panel to select the radionuclides. For the screen shown, ^{137}Cs and ^{239}Pu have been chosen. The activity unit is chosen on the previous screen, the edge of which is barely visible in the figure. In this case, Curies (Ci) had been chosen.

Figure 7-6 shows the panel where the radionuclide inventory is input. These are for the radionuclides chosen in the previous screen(s).

Figure 7-7 shows the panel where various release parameters are chosen: wind sector, location of receptor, option for release elevation, and option for building wake model. Note that only one direction and one distance can be selected for each run and that wind direction is the direction *toward* which the wind is blowing, not *from* which it is blowing (the meteorological convention).

Figures 7-8 through 7-12 show the various panels for setting exposure parameters. The figures are self-explanatory.

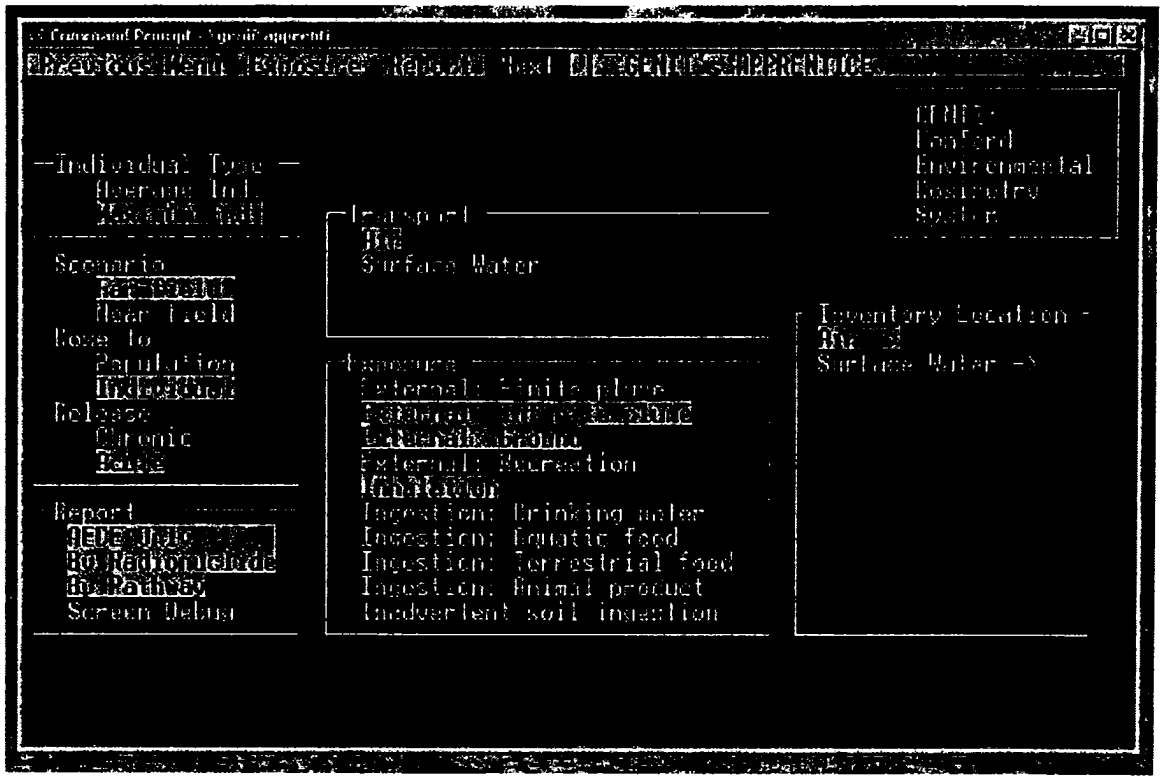

Figure 7-4. Selections of report type, transport medium, and exposure types.

Figure 7-5. Radionuclide selection screen.

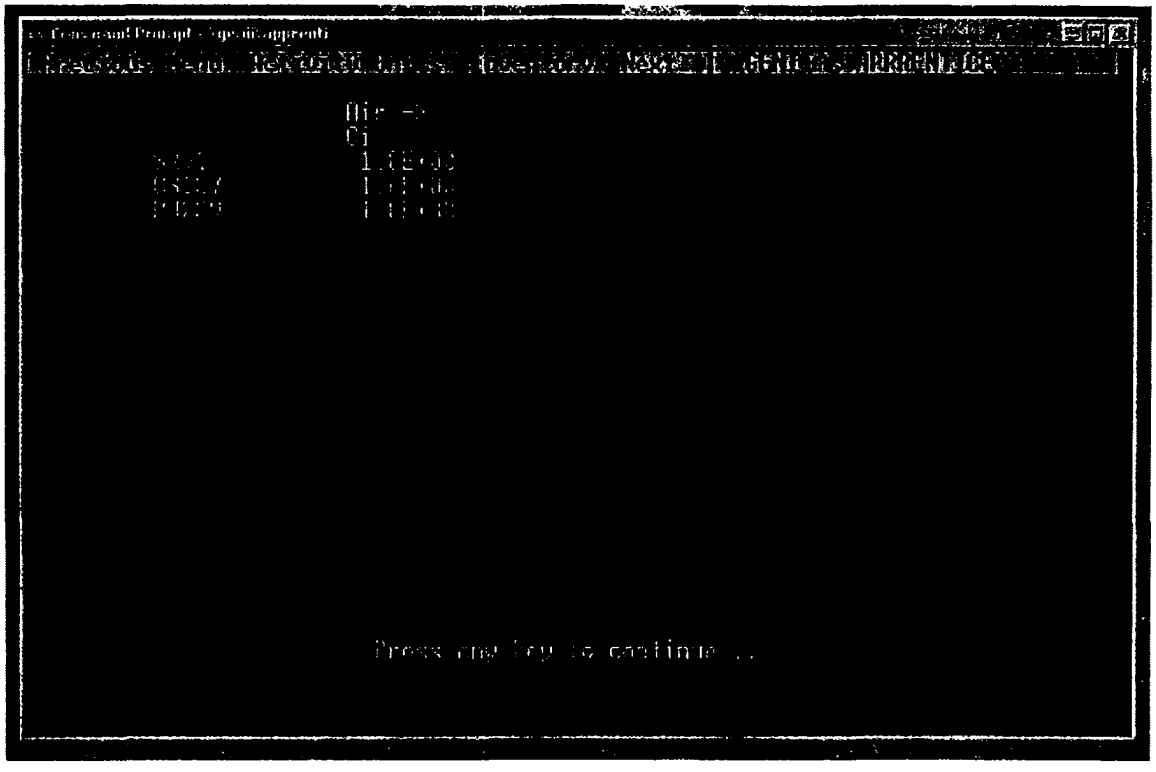

Figure 7-6. Activity specification screen for each selected radionuclide.

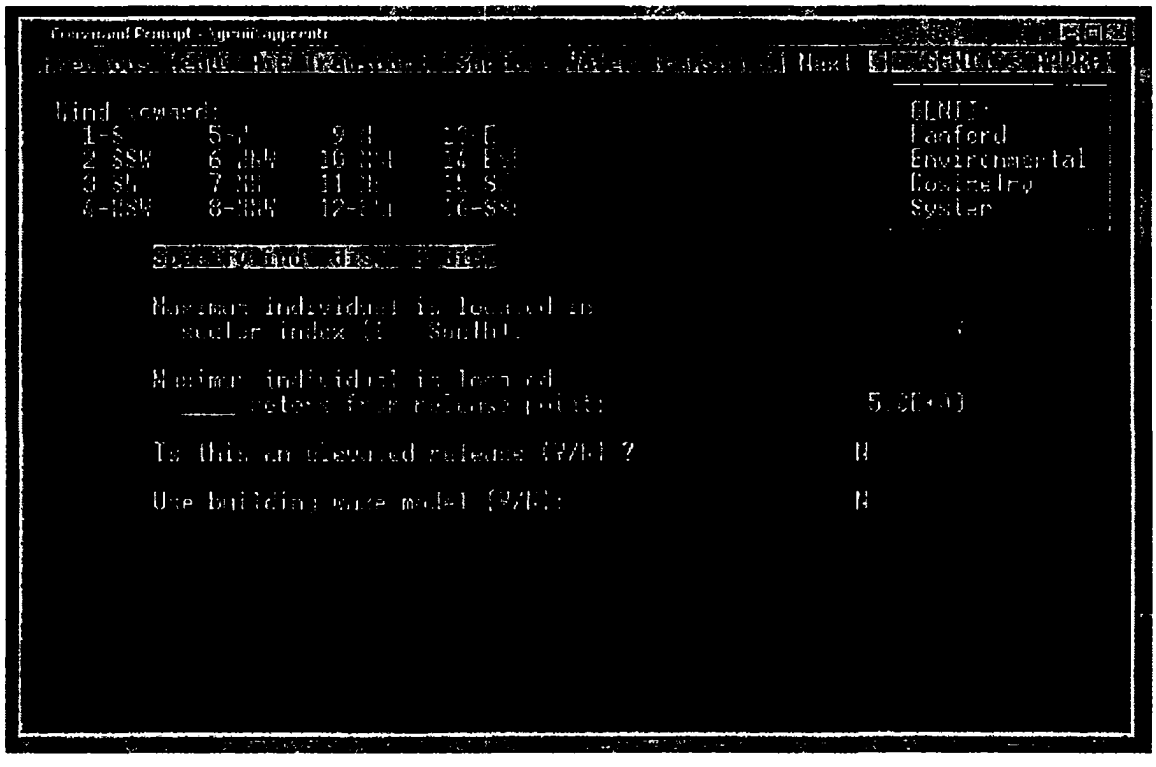

Figure 7-7. Release parameters are selected at this screen.

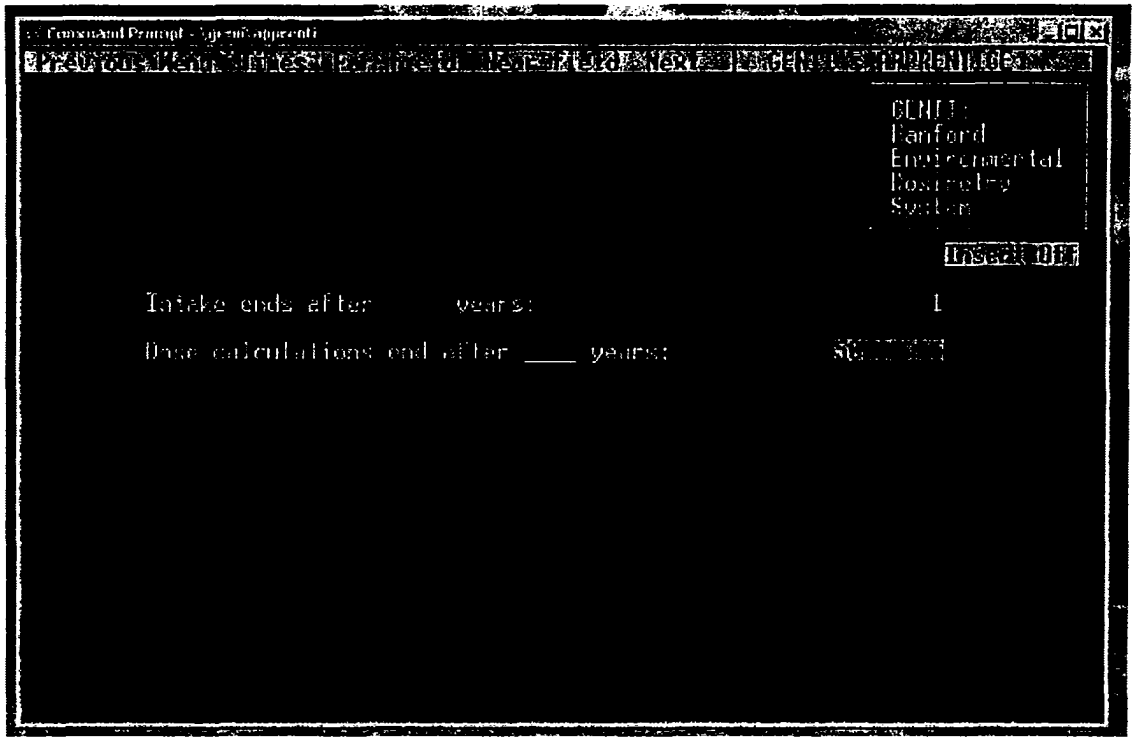

Figure 7-8. Screen for specifying durations for intake and dose calculations.

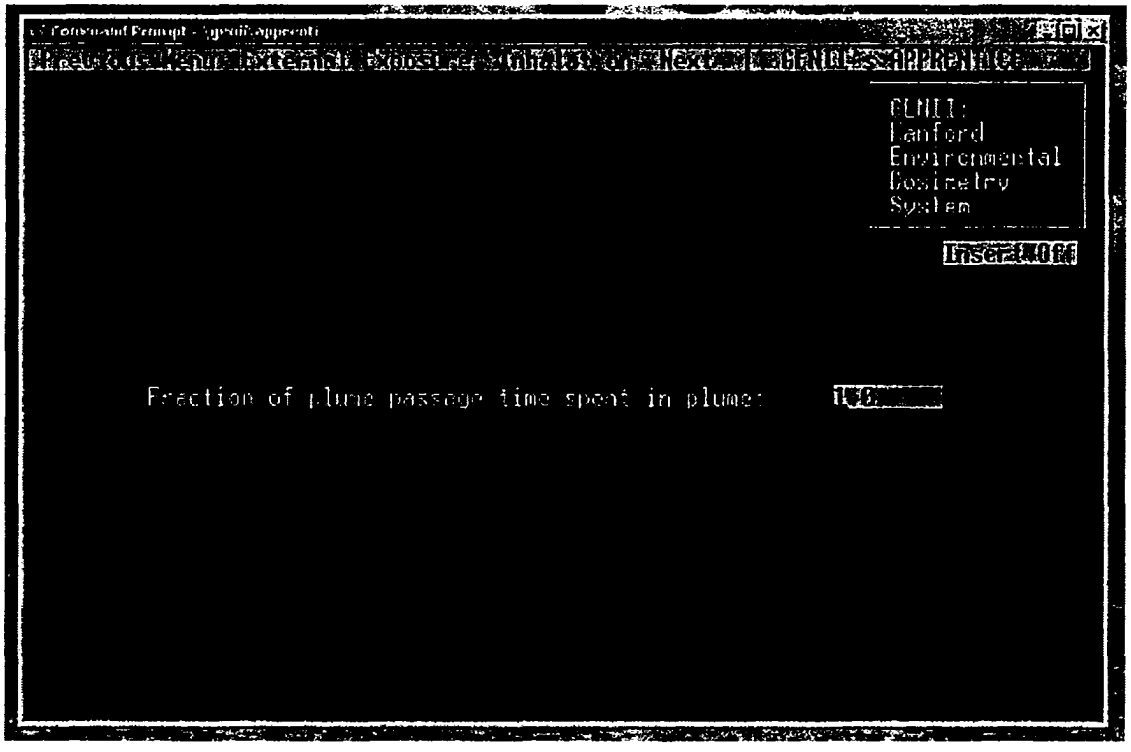

Figure 7-9. Screen for specifying fraction of plume passage time that receptor is exposed.

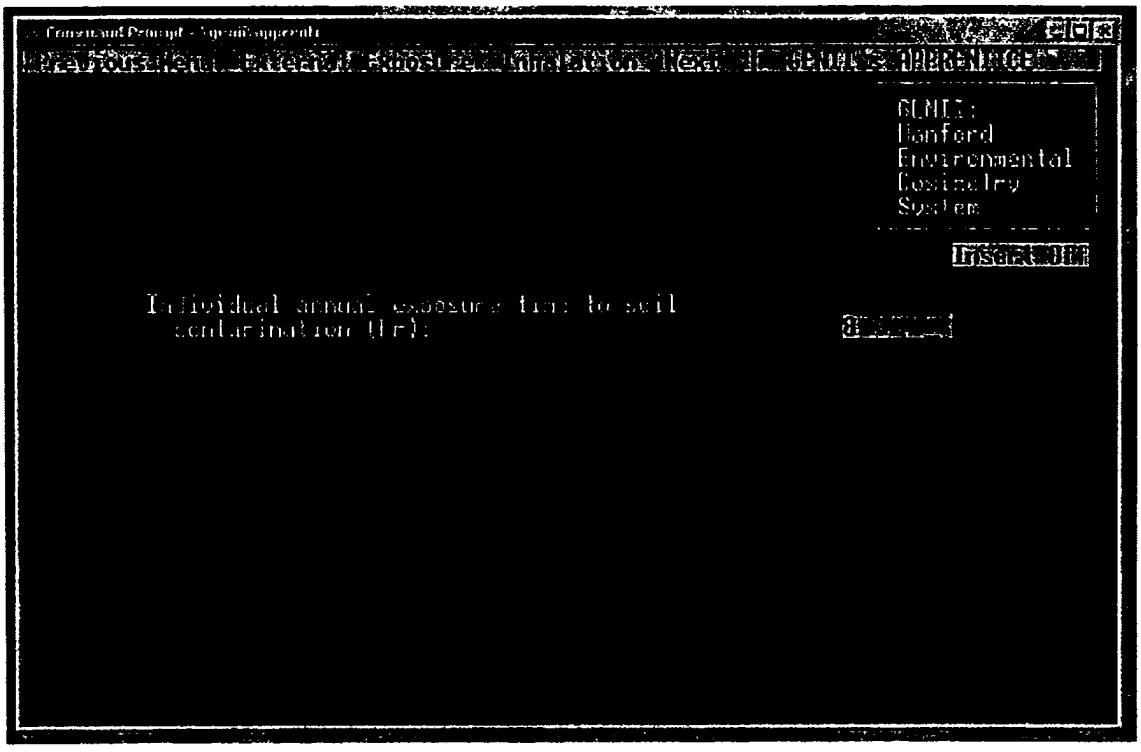

Figure 7-10. Receptor exposure time to groundshine is specified here.

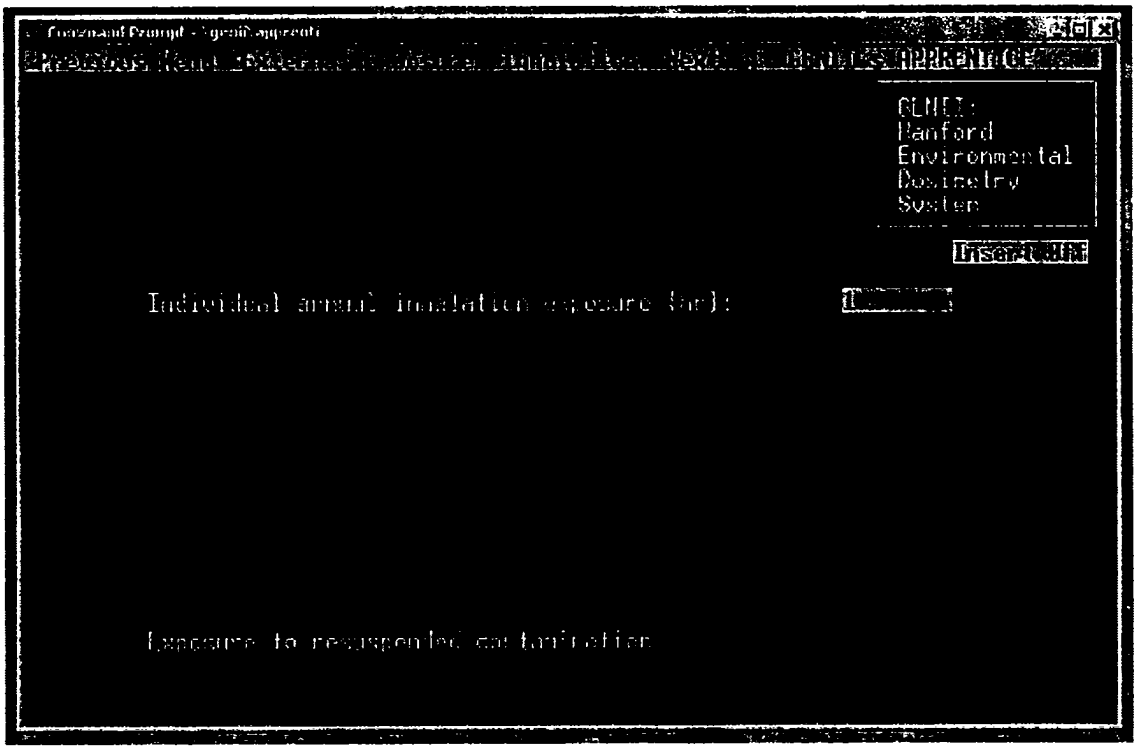

Figure 7-11. Receptor inhalation duration is specified here.

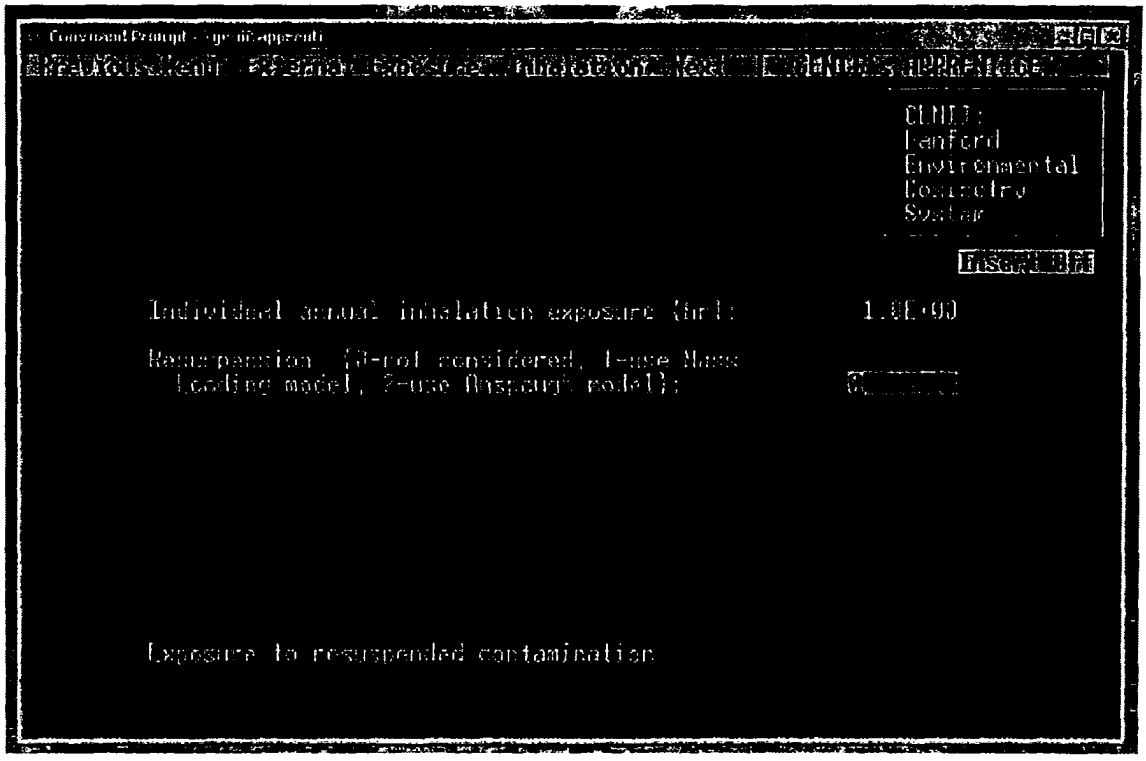

Figure 7-12. Resuspension specification (not chosen in this case)

7.3 Sample Problem

The sample problem chosen for GENII 1.485 is the same as the one chosen for the MACCS2 guidance document (DOE 2004b). For MACCS2, four scenarios were addressed. However, two of them involved fires, which cannot be modeled with GENII 1.485 and therefore are not included here. The two scenarios analyzed are 1) no buoyancy and without building wake, and 2) no buoyancy and with building wake for a building 13 m high and 90 m wide.

The main objective of this section is to provide sample files that illustrate the guidance discussed in this report. A secondary objective is to provide a comparison with MACCS2 for the same scenarios shown in the MACCS2 guidance document (DOE 2004b).

The following are the major assumptions associated with this analysis:

(xlix) The radial distances to the receptor are 150, 250, 350, 450, 750, 1250, 1750, 2250, 2750, 3250, 3750, 4250, 4750, 5250, 5750, 6250, 6750, 7250, 7750, and 9000 m. This corresponds to the radial ring endpoints of 0.1, 0.2, 0.3, 0.4, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0, 7.5, 8.0, and 10.0 km used in the MACCS2 sample problem. (In MACCS2, the representative receptors are at the midpoints between the radial ring endpoints.) Note that in GENII 1.485, receptor distances less than 100 m are not allowed.

(l) The base case is assumed an open-area release (no buildings in the vicinity) with a non-buoyant plume. The horizontal dispersion half-widths (the σ_ys) in GENII 1.485 are calculated in a manner identical to that of MACCS2. However, the vertical dispersion

half-widths (the σ_zs) are calculated with distance-dependent coefficients (different sets of coefficients for < 100m, 100 m to 1000 m, and > 1000 m).

(li) In the building wake cases, the building is assumed to have a height of 42.5 ft (13 m) and width of 296 ft (90 m).

(lii) One curie of ^{239}Pu is released over a ten-minute period. The default dose conversion factor (DCF) used in GENII 1.485 for ^{239}Pu is taken from ICRP-30 for lung clearance class Y, for which the inhalation DCF is 8.33×10^{-5} Sv/Bq. This default cannot be overridden by the user. In contrast, the MACCS2 analysis used class W for the ^{239}Pu, for which the DCF is 1.16×10^{-4} Sv/Bq. Thus, MACCS2 uses a DCF that is 1.4 times larger than used in GENII 1.485.

(liii) No wet deposition is assumed.

(liv) The default dry deposition velocity used in GENII 1.485 is 0.001 m/s. This is less than the value used in the MACCS2 sample problem (0.01 m/s). Although GENII 1.485 allows for dry deposition, it does not deplete the plume and therefore is overly conservative. Therefore, dry deposition was turned off in the GENII 1.485 runs.

(lv) The surface roughness length is not specified in GENII 1.485.

(lvi) The assumed breathing rate is 3.3×10^{-4} m^3/s, which is the DOE occupational breathing rate (DOE, 1998). It is also the default GENII 1.485 value.

(lvii) The doses to the maximum individuals at the specified distances are calculated. The population distribution is not needed.

(lviii) No shielding is assumed.

(lix) No evacuation or sheltering is assumed nor does GENII 1.485 allow for it.

(lx) Results reported are the plume centerline TEDE value for 95th percentile meteorological conditions for all distances.

The site meteorological data file used was a joint-distribution file based on the same hourly data used in the MACCS2 sample problem. It was for a specific calendar year of qualified data, measured at wind speed height of 10 meters. Appendix C provides this data file.

The 95th percentile TEDEs for all the selected distances and directions can be generated in two ways. Each generates one or more input files (extension of .IN), which are then executed with a batch file (extension of .BAT).

The first technique, and the most straightforward, is to produce a separate input file for each distance-direction combination, using APPRENTICE. For this sample problem, the following selections were made:

(lxi) After the introductory pages of APPRENTICE, these options were chosen: scenario was "far field", dose was to "individual", release was "acute", and individual was "maximum individual".

(lxii) On the subsequent page: transport was "air", inventory location was skipped (it was automatically selected once "air" was chosen), exposures were "infinite plume" and

"inhalation", and report was "AEDE only" (the default selection). Note that ground exposure was not chosen in order to suppress the calculation of groundshine. Cloudshine, however, was included.

(lxiii) Activity unit was "Ci", inventory selection was "Pu239" (using the keypad keys, not arrows, F3 to move to second screen where Pu239 is located, F2 to select it, F10 exit this screen), and input of inventory quantity was "1".

(lxiv) For air transport the χ/Q choice was "specify ind. dist & dir.", the input direction desired was a number ("1" is south, "2" is SSW, etc.), input distance was 150, 250, etc.

(lxv) This is followed by "Y" or "N" choices for elevated release and building wake model. If either of these is chosen ("Y"), additional information must be input. If the building wake model is to be run, the stack flow rate must be input (use zero for no fire). This is followed by the specification of "Building cross-sectional (vertical) area", which is "1170"in this example.

(lxvi) Subsequent pages provide for input of "Intake ends after ___ years" (enter "1"), "Dose calculations end after ___ years" (enter "50"), "Fraction of plume passage time spent in plume:" (enter 1.0), "Individual annual inhalation exposure (hr):" (enter "0.1667", which is ten minutes), and resuspension option (enter "0" for no resuspension).

(lxvii) Enter a name for this input file, specify name and location of the joint frequency distribution file (and confirm choice), choose "N" for printing output file, and give a title to be included in the output file. Then specify "write file". At this point, the user can exit or choose "Next Scenario", which proceeds again through the above choices. If only the single scenario is to be run, choose Quit and confirm it. The name of the batch file will be the same as the name chosen for the input file if only one case is run. If more than one scenario is to be run, the name of the batch file must be specified, which can be the same as one of the input files but need not be.

Several scenarios can be combined into a single batch file run by using the "Next Scenario" option in APPRENTICE. For example, the runs for all 16 directions and a selected distance can be run together. An example of this is shown below.

A second, faster, technique is to use the "population" option in place of "individual" on the first selection page of APPRENTICE (see first bullet above). The other selections are the same, except that the name of the population distribution file must also be given. (For DSAs, populations doses are not calculated so the standard population file ("pop.in") can be used as only the χ/Q' values are of interest. The χ/Q' values are then converted to TEDE using a conversion factor of 1.02×10^{5} rem-m^3/s, which is the product of the DCF (8.33×10^{-5} Sv/Bq), breathing rate (3.3×10^{-4} m^3/s), and conversion factors of 3.7×10^{10} Bq/Ci and 100 rem/Sv.) In this technique, values of χ/Q' for one direction and ten distances are calculated at a time. As before, the various directions can be combined into a single batch file run by using the "Next Scenario" option. This technique gives the χ/Q' values for the various distances but does not give TEDEs (except for the population dose). However, once the ratio of TEDE to χ/Q' has been established (1.02×10^{5} rem-m^3/s in this case), the χ/Q' values can be converted to TEDEs as discussed above. This second technique, however, requires modifying the DEFAULT.IN file. The original default distances in this file are based on the population distances in the population distribution file, but these won't be used for DSA analyses. Up to ten distances can be specified.

If more than ten distances are needed (as in this sample problem), then two or more DEFAULT.IN files will be needed. Each should be given a unique name. Before running the batch file, change the original DEFAULT.IN name to something like DEFAULT.org, change the unique name to DEFAULT.IN, run the batch file, and change the name back to the unique name afterwards.

A very large number of runs of GENII 1.485 were required to analyze these scenarios. One example of the input data file generated by the GENII front-end (Apprentice) is given in Exhibit A (see following pages), the corresponding output hard copy from GENII is given in Exhibit B, and the batch file generated by Apprentice that included this input/output is given in Exhibit C. In Exhibit B, the redundant page headers have been removed to save space. In Exhibit C, batch commands for directions other WSW have been removed for brevity.

GENII 1.485 was run repeatedly for all 16-wind sectors and receptor distances. Sectors are numbered clockwise from the south. Thus, S = 1, SSW = 2, etc. The sample problem shown in the following Exhibits are for no fire, no building wake, a distance of 150 m, and sector 4, that is, to the WSW, which typically had the largest doses for the weather data used. The 95th percentile χ/Q' (labeled E/Q in the output) for this sector at 150 m was 4.2×10^{-3} s/m^3 and the corresponding dose (TEDE) was 430 rem. (Only two significant figures are used in data transfers between subroutines in GENII 1.485, so some round-off error is expected. Thus, the expected result of 420 rem (i.e., 4.2×10^{-3} s/m^3)(1.02×10^5 rem-m^3/s) differed slightly from the output value of 430 rem.)

The results for the base case (no lofting, no wake) and case of building wake without lofting are given in Figure 7-13 as the solid curves. The results from MACCS2 for these same scenarios are included in the figure as dashed curves. For the base case, the MACCS2 results are somewhat larger at close-in distances but decrease much more rapidly with distance compared to GENII, the cross-over occurring at about 1,500 m. For the wake-effects case without lofting, the GENII results are smaller at all distances compared to its base case. For MACCS2 the doses are very similar to its base case, being somewhat smaller than the base case for close-in distances but beyond about 400 m, they are larger. The MACCS2 doses are larger than those from GENII at distances closer than about 3,500 m but are smaller at greater distances.

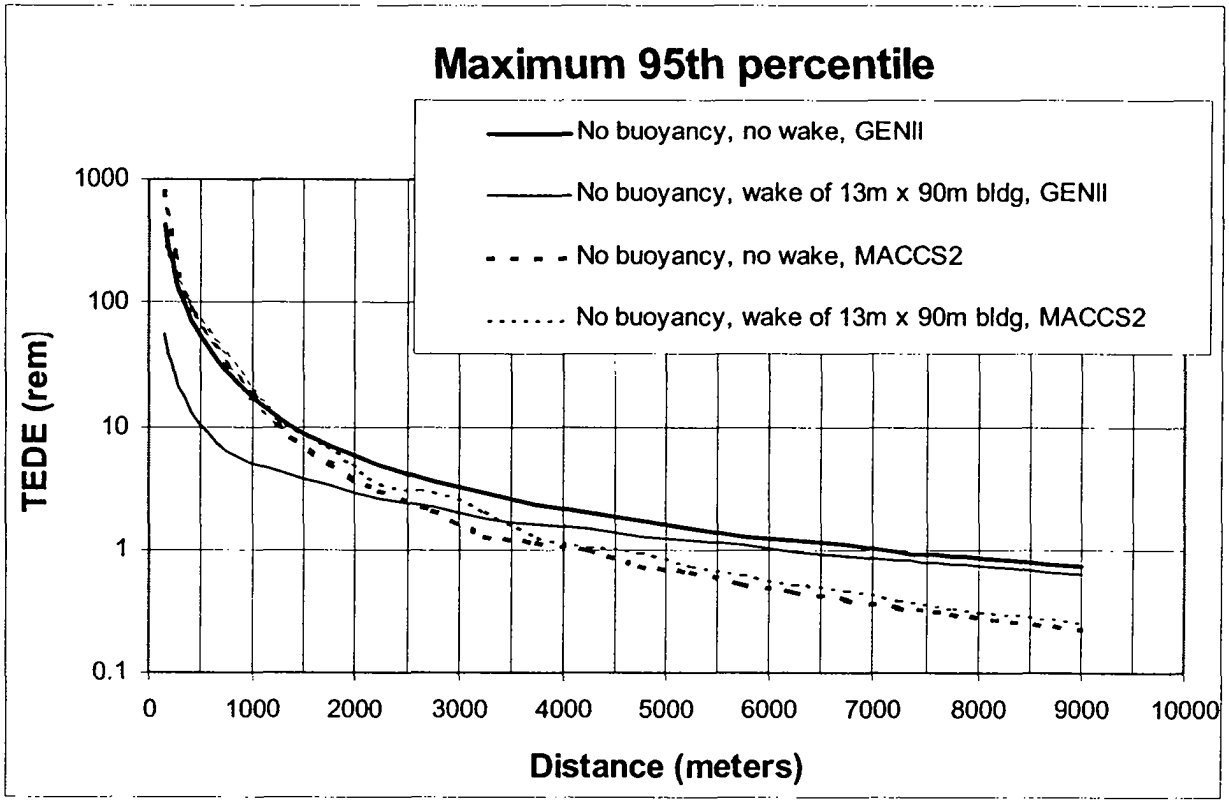

Figure 7-13. 95th percentile TEDE vs. distance for the maximum sector. Base case (no lofting, no wake) and building wake without lofting.

EXHIBIT A: Input file created by Apprentice for base case.

```
Title: no buoyancy no wake 150 m WSW
       \WSMSCALC\nn150wsw.in                    Created on 02-26-2004 at 20:34
OPTIONS======================== Default ====================================
F    Near-field scenario?      (Far-field)    NEAR-FIELD: narrowly-focused
F    Population dose?         (Individual)                release, single site
T    Acute release?             (Chronic)    FAR-FIELD:  wide-scale release,
     Maximum Individual data set used                     multiple sites
                              Complete                                  Complete
TRANSPORT OPTIONS============ Section   EXPOSURE PATHWAY OPTIONS===== Section
T  Air Transport                   1     F  Finite plume, external       5
F  Surface Water Transport         2     T  Infinite plume, external     5
F  Biotic Transport (near-field)  3,4    F  Ground, external             5
F  Waste Form Degradation (near)  3,4    F  Recreation, external         5
                                         T  Inhalation uptake            5,6
REPORT OPTIONS=======================    F  Drinking water ingestion     7,8
T  Report AEDE only                      F  Aquatic foods ingestion      7,8
F  Report by radionuclide                F  Terrestrial foods ingestion  7,9
F  Report by exposure pathway            F  Animal product ingestion     7,10
F  Debug report on screen                F  Inadvertent soil ingestion

INVENTORY ##############################################################################

 4   Inventory input activity units: (1-pCi  2-uCi  3-mCi  4-Ci  5-Bq)
 0   Surface soil source units (1- m2  2- m3  3- kg)
     Equilibrium question goes here

     --------|----Release Terms------|----------Basic Concentrations---------|
     Use when|  transport selected   |  near-field scenario, optionally      |
     --------|-----------------------|---------------------------------------|
     Release |        Surface Buried |        Surface Deep    Ground  Surface|
     Radio-  |Air     Water   Waste  |Air     Soil    Soil    Water   Water  |
     nuclide |/yr     /yr     /m3    |/m3     /unit   /m3     /L      /L     |
     --------|------- ------- -------|------- ------- ------- ------- -------|
     PU239    1.0E+00

     --------|----Derived Concentrations-----|
     Use when|   measured values are known   |
     --------|-------------------------------|
     Release |Terres. Animal  Drink   Aquatic|
     Radio-  |Plant   Product Water   Food   |
     nuclide |/kg     /kg     /L      /kg    |
     --------|------- ------- ------- -------|

TIME ###################################################################################

1    Intake ends after (yr)
50   Dose calc. ends after (yr)
0    Release ends after (yr)
0    No. of years of air deposition prior to the intake period
0    No. of years of irrigation water deposition prior to the intake period

FAR-FIELD SCENARIOS (IF POPULATION DOSE) ###############################################

0          Definition option: 1-Use population grid in file POP.IN
0                             2-Use total entered on this line

NEAR-FIELD SCENARIOS ###################################################################

           Prior to the beginning of the intake period: (yr)
0            When was the inventory disposed?  (Package degradation starts)
```

```
0           When was LOIC?  (Biotic transport starts)
0         Fraction of roots in upper soil (top 15 cm)
0         Fraction of roots in deep soil
0         Manual redistribution: deep soil/surface soil dilution factor
0         Source area for external dose modification factor (m2)
TRANSPORT ##########################################################################
          ====AIR TRANSPORT=====================================SECTION 1=====
                  0-Calculate PM             |0        Release type (0-3)
3         Option: 1-Use chi/Q or PM value    |F        Stack release (T/F)
                  2-Select MI dist & dir     |0        Stack height (m)
                  3-Specify MI dist & dir    |0        Stack flow (m3/sec)
0         Chi/Q or PM value                  |0        Stack radius (m)
4         MI sector index (1=S)              |0        Effluent temp. (C)
150.0     MI distance from release point (m)|0        Building x-section (m2)
T         Use jf data, (T/F) else chi/Q grid|0        Building height (m)

          ====SURFACE WATER TRANSPORT=========================SECTION 2=====
0         Mixing ratio model: 0-use value, 1-river, 2-lake
0         Mixing ratio, dimensionless
0         Average river flow rate for: MIXFLG=0 (m3/s), MIXFLG=1,2 (m/s),
0         Transit time to irrigation withdrawl location (hr)
          If mixing ratio model > 0:
0           Rate of effluent discharge to receiving water body (m3/s)
0           Longshore distance from release point to usage location (m)
0           Offshore distance to the water intake (m)
0           Average water depth in surface water body (m)
0           Average river width (m), MIXFLG=1 only
0           Depth of effluent discharge point to surface water (m), lake only

          ====WASTE FORM AVAILABILITY=========================SECTION 3=====
0         Waste form/package half life, (yr)
0         Waste thickness, (m)
0         Depth of soil overburden, m

          ====BIOTIC TRANSPORT OF BURIED SOURCE===============SECTION 4=====
T         Consider during inventory decay/buildup period (T/F)?
T         Consider during intake period (T/F)?   | 1-Arid non agricultural
0         Pre-Intake site condition.............| 2-Humid non agricultural
                                                 | 3-Agricultural

EXPOSURE ###########################################################################

          ====EXTERNAL EXPOSURE================================SECTION 5=====
          Exposure time:                |   Residential irrigation:
0           Plume (hr)                  | T       Consider: (T/F)
0           Soil contamination (hr)     | 0       Source: 1-ground water
0           Swimming (hr)               |                 2-surface water
0           Boating (hr)                | 0       Application rate (in/yr)
0           Shoreline activities (hr)   | 0       Duration (mo/yr)
0         Shoreline type: (1-river, 2-lake, 3-ocean, 4-tidal basin)
0         Transit time for release to reach aquatic recreation (hr)
1.0       Average fraction of time submersed in acute cloud (hr/person hr)

          ====INHALATION=======================================SECTION 6=====
0.1667    Hours of exposure to contamination per year
0         0-No resus-  1-Use Mass Loading          2-Use Anspaugh model
0           pension      Mass loading factor (g/m3)   Top soil available (cm)

          ====INGESTION POPULATION=============================SECTION 7=====
0         Atmospheric production definition (select option):
0           0-Use food-weighted chi/Q, (food-sec/m3), enter value on this line
            1-Use population-weighted chi/Q
            2-Use uniform production
```

```
            3-Use chi/Q and production grids (PRODUCTION will be overridden)
0           Population ingesting aquatic foods, 0 defaults to total (person)
0           Population ingesting drinking water, 0 defaults to total (person)
F           Consider dose from food exported out of region (default=F)

            Note below: S* or Source: 0-none, 1-ground water, 2-surface water
                                      3-Derived concentration entered above
            ==== AQUATIC FOODS / DRINKING WATER INGESTION=========SECTION 8====

F           Salt water? (default is fresh)

            USE        TRAN-  PROD-     -CONSUMPTION- |
            ?   FOOD   SIT    UCTION    HOLDUP   RATE |
            T/F TYPE   hr     kg/yr     da       kg/yr |      DRINKING WATER
            --- ------ -----  -------   ------   ----- |-------------------------
            F   FISH    0.00  0.0E+00    0.00     0.0  | 0      Source (see above)
            F   MOLLUS  0.00  0.0E+00    0.00     0.0  | T      Treatment? T/F
            F   CRUSTA  0.00  0.0E+00    0.00     0.0  | 0      Holdup/transit(da)
            F   PLANTS  0.00  0.0E+00    0.00     0.0  | 0      Consumption (L/yr)

            ====TERRESTRIAL FOOD INGESTION=======================SECTION 9=====

            USE        GROW   --IRRIGATION--          PROD-    --CONSUMPTION--
            ?   FOOD   TIME   S RATE   TIME    YIELD  UCTION   HOLDUP   RATE
            T/F TYPE   da     * in/yr  mo/yr   kg/m2  kg/yr    da       kg/yr
            --- ------ -----  - -----  -----   -----  -------  ------   ------
            F   LEAF V  0.00  0   0.0    0.0     0.0  0.0E+00    0.0      0.0
            F   ROOT V  0.00  0   0.0    0.0     0.0  0.0E+00    0.0      0.0
            F   FRUIT   0.00  0   0.0    0.0     0.0  0.0E+00    0.0      0.0
            F   GRAIN   0.00  0   0.0    0.0     0.0  0.0E+00    0.0      0.0

            ====ANIMAL PRODUCTION CONSUMPTION====================SECTION 10====

            ---HUMAN----  TOTAL   DRINK    -------------STORED FEED--------------
USE         CONSUMPTION   PROD-   WATER    DIET  GROW  -IRRIGATION--          STOR-
?   FOOD    RATE  HOLDUP  UCTION  CONTAM   FRAC- TIME  S RATE  TIME    YIELD  AGE
T/F TYPE    kg/yr   da    kg/yr   FRACT.   TION  da    * in/yr mo/yr   kg/m3  da
--- ------  ------ -----  ------  -------  ----  ----  - -----  -----   -----  -----
F   BEEF      0.0   0.0    0.00     0.00  0.00   0.0  0   0.0   0.00    0.00    0.0
F   POULTR    0.0   0.0    0.00     0.00  0.00   0.0  0   0.0   0.00    0.00    0.0
F   MILK      0.0   0.0    0.00     0.00  0.00   0.0  0   0.0   0.00    0.00    0.0
F   EGG       0.0   0.0    0.00     0.00  0.00   0.0  0   0.0   0.00    0.00    0.0
                                          -------------FRESH FORAGE------------
    BEEF                                  0.00   0.0  0   0.0   0.00    0.00    0.0
    MILK                                  0.00   0.0  0   0.0   0.00    0.00    0.0
```

EXHIBIT B: Output file created by GENII 1.485 for base case.

```
                        GENII  Dose Calculation Program
                           (Version 1.485 3-Dec-90)

 Case title:   no buoyancy no wake 150 m WSW

 Executed on:  02/26/:4 at 20:51:14                                    Page A.  1
 ------------------------------------------------------------------------------

           This is a far-field (wide-scale release, multiple site) scenario.
           Release is acute
           Individual dose

           THE FOLLOWING TRANSPORT MODES ARE CONSIDERED
                Air

           THE FOLLOWING EXPOSURE PATHS ARE CONSIDERED:
                Infinite plume, external
                Inhalation uptake

           THE FOLLOWING TIMES ARE USED:
                Intake ends after (yr):                1.0
                Dose calculations ends after (yr):    50.0

========== FILENAMES AND TITLES OF FILES/LIBRARIES USED ======================

 Input file name: \WSMSCALC\nn150wsw.in
 GENII Default Parameter Values (28-Mar-90 RAP)
 Radionuclide Master Library   (11/28/90 RAP)
 External Dose Factors for GENII in person Sv/yr per Bq/n (8-May-90 R
 Internal Dose Increments, PNL Solubility Choices Rerun 12/3/90 PDR
 MACCS2 CONVERSION MET DATA

==============================================================================

           -------- ----Release Terms------
           Release           Surface Buried
           Radio-   Air      Water   Source
           nuclide   Ci/yr    Ci/yr   Ci/m3
           -------- ------- ------- -------
           PU239    1.0E+00 0.0E+00 0.0E+00

========== AIR TRANSPORT ======================================================
           Joint frequency data input.
1.5E+02    Maximum individual distance from release point (m)
4.0E+00    Maximum individual sector index (Wind Toward WSW)
           Ground level release.

========== EXTERNAL EXPOSURE ==================================================
 1.0E+00   Fraction of time spent in cloud

========== INHALATION =========================================================
           Resuspension not considered

==============================================================================


Input prepared by: _____________________________  Date: _____________

Input checked by: _____________________________  Date: _____________
```

	Probability	E/Q (sec/m3)	DOQ (m2)	Travel Time (sec)	Population-Weighted E/Q (person-sec/m3)
Sector index: 4					
Distance: 150.0					
	0.0050	7.6E-03	7.6E-05	48.	
	0.0500	4.2E-03	4.2E-05	48.	
	0.1000	2.6E-03	2.6E-05	27.	
	0.2500	1.2E-03	1.2E-05	27.	
	0.5000	4.1E-04	4.1E-06	22.	
4.2E-03 Individual E/Q					

Acute release
Uptake/exposure period: 1.0
Dose commitment period: 50.0
Dose units: Rem

Organ	Committed Dose Equivalent	Weighting Factors	Weighted Dose Equivalent
Gonads	5.9E+01	2.5E-01	1.5E+01
Breast	4.2E-04	1.5E-01	6.4E-05
R Marrow	3.4E+02	1.2E-01	4.0E+01
Lung	1.6E+03	1.2E-01	1.9E+02
Thyroid	4.1E-04	3.0E-02	1.2E-05
Bone Sur	4.4E+03	3.0E-02	1.3E+02
Liver	7.8E+02	6.0E-02	4.7E+01
LL Int.	1.4E-01	6.0E-02	8.4E-03
UL Int.	4.7E-02	6.0E-02	2.8E-03
S Int.	8.3E-03	6.0E-02	5.0E-04
Stomach	3.6E-03	6.0E-02	2.2E-04
Internal Effective Dose Equivalent			4.3E+02
External Dose			8.8E-08
Annual Effective Dose Equivalent			4.3E+02

Controlling Organ:	Bone Sur
Controlling Pathway:	Inh
Controlling Radionuclide:	PU239
Total Inhalation EDE:	4.3E+02
Total Ingestion EDE:	0.0E+00

Acute release
Uptake/exposure period: 1.0
Dose commitment period: 50.0
Dose units: Rem

	Dose Commitment Year 1	2	3	...		
Internal Intake : Year: 3			0.0E+00	...		
			+			
2		0.0E+00	0.0E+00	...		Internal Effective Dose Equivalent
		+	+			
1	4.1E+01	+ 2.9E+01	+ 2.2E+01	+ ...	= 4.3E+02	
	||	||	||			
Internal Annual Dose	4.1E+01	+ 2.9E+01	+ 2.2E+01	+ ...	= 4.3E+02	Cumulative Internal Dose
	+	+	+		+	
External Annual Dose	8.8E-08	0.0E+00	0.0E+00	...	8.8E-08	
	||	||	||		||	
Annual Dose	4.1E+01	+ 2.9E+01	+ 2.2E+01	+ ...	= 4.3E+02	Cumulative Dose
					4.1E+01	Maximum Annual Dose Occurred In Year 1

EXHIBIT C: Batch file created by Apprentice for base case.

```
CLS
rem
rem
rem
rem
rem                GENII
rem                Hanford Environmental Dosimetry Software System
rem
rem                Pacific Northwest Laboratory
rem                Richland WA
rem
rem                Contact:  Bruce Napier (509) 375-3896
rem
 echo off
 erase  \genii\genii.in
 erase  \genii\pop.in
 erase  \genii\jointfre.in
 erase  \genii\chiq.in
 erase  \genii\foodprod.in
 erase  \genii\env.in
 erase  \genii\genii.out
 erase  \genii\env.out
 erase  \genii\genii2.out
 erase  \genii\dose.out
 copy C:\WSMSCALC\jointfre.in \genii\jointfre.in
echo on

<snip:  batch commands for other directions have been removed for brevity.>

 copy \WSMSCALC\nn150wsw.in \genii\genii.in
 \genii\envin
 if errorlevel 1 goto stop4
 \genii\env
 if errorlevel 1 goto stop4
 \genii\dose
 if errorlevel 1 goto stop4
rem
 copy \genii\genii.out+ \genii\genii2.out+ \genii\dose.out \WSMSCALC\nn150wsw.out
rem
:stop4

<snip:  batch commands for other directions have been removed for brevity.>
```

Only the batch commands for a distance of 150 m and direction of WSW are shown above.

8.0 ACRONYMS & DEFINITIONS

ACRONYMS:

ALARA	As Low As Reasonably Achievable
ALI	Annual Limit on Intake
ALOHA	Areal Locations of Hazardous Atmospheres (designated toolbox software)
ANSI	American National Standards Institute
ARF	Airborne Release Fraction
ARR	Airborne Release Rate
BR	Breathing Rate
CDE	Committed Dose Equivalent (see definition below)
CEDE	Committed Effective Dose Equivalent (see definition below)
CFAST	Consolidated Fire and Smoke Transport Model (designated toolbox software)
CFR	Code of Federal Regulations
DAC	Derived Air Concentration
DBA	Design Basis Accident
DCF	Dose Conversion Factor
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DR	Damage Ratio
DSA	Documented Safety Analysis
EFCOG	Energy Facility Contractors Group
EH	DOE Office of Environment, Safety and Health
EIS	Environmental Impact Statement
EM	DOE Office of Environmental Management
EPIcode	Emergency Prediction Information code (designated toolbox software)
FRAMES	Framework for Risk Analysis in Multimedia Environmental Systems
GENII	Generalized Environmental Radiation Dosimetry Software System - Hanford Dosimetry System (Generation II) (designated toolbox software)
GEP	Good Engineering Practice
HT	Tritiated Hydrogen Gas
HTO	Tritium Oxide
ICRP	International Commission for Radiological Protection
IDCF	Inhalation Dose Conversion Factor
IEEE	Institute of Electrical and Electronics Engineers
IP	Implementation Plan
ISO	International Organization for Standardization
JFD	Joint Frequency Distribution
LANL	Los Alamos National Laboratory
LET	Linear Energy Transfer
LHS	Latin Hyper-cubed Square
LPF	Leak Path Factor
MACCS2	MELCOR Accident Consequence Code System 2 (designated toolbox software)
MAR	Material at Risk
MELCOR	Methods for Estimation of Leakages and Consequences of Releases (designated toolbox software)
MOI	Maximally Exposed Offsite Individual (see definition below)

NESHAPS	National Emissions Standards for Hazardous Air Pollutants
NNSA	National Nuclear Security Administration
NRC	Nuclear Regulatory Commission
OEP	Onsite Evaluation Point/Person (see definition below)
PNNL	Pacific Northwest National Laboratory
PSA	Probabilistic Safety Analysis (or Assessment)
RF	Respirable Fraction
RSICC	Radiation Safety Information Computational Center
SASG	Safety Analysis Software Group (see definition below)
SC	Safety Class
SC SSC	Safety Class Structures Systems or Components (see definition below)
SNL	Sandia National Laboratories
SQA	Software Quality Assurance
SS	Safety Significant
SSC	Systems Structures or Components
SSCs	Safety Structures Systems and Components (see definition below)
SS SSC	Safety Significant Structures Systems or Components (see definition below)
ST	Source Term
SUM	Sensitivity/Uncertainty Multimedia Modeling Module
TEDE	Total Effective Dose Equivalent (see definition below)
TSR	Technical Safety Requirement
V&V	Verification and Validation
WSMS	Washington Safety Management Solutions
WSRC	Westinghouse Savannah River Company

Selected Terms and Definitions Used in Accident and Consequence Analysis & Software Quality Assurance

Absorbed Dose (D) – The energy absorbed by matter from ionizing radiation per unit mass of irradiated material at the place of interest in that material. The absorbed dose is expressed in units of rad (or gray) (1 rad = 0.01 gray).

Committed Dose Equivalent ($H_{T,50}$) – The dose equivalent calculated to be received by a tissue or organ over a 50-year period after the intake of a radionuclide into the body. It does not include contributions from radiation sources external to the body. Committed dose equivalent is expressed in units of rem (or sievert) (1 rem = 0.01 sievert).

Committed Effective Dose Equivalent (CEDE) – The sum of the committed dose equivalents ($H_{T,50}$) over a fifty-year period to various organs or tissues in the body, each multiplied by the appropriate weighting factor (w_T) -- that is $H_{E,50} = \Sigma\, w_T\, H_{T,50}$. CEDE is applicable to exposure from internally deposited radionuclides.

Gap Analysis – Evaluation of the Software Quality Assurance attributes of specific computer software against identified criteria.

Gray (Gy) – Systeme' International (SI) unit of absorbed dose. One gray is equal to an absorbed dose of 1 joule per kilogram. One Gy equals 100 rad.

Maximally Exposed Offsite Individual (MOI) – A theoretical offsite receptor defined to allow dose comparison with numerical offsite evaluation guides. The MOI is located at the maximum air concentration point (ground-level) at or beyond the DOE site boundary. The latter may occur with elevated or buoyant releases that do not land within the site boundary, but reach ground level beyond the boundary (touchdown point).

Nuclear Facility – A reactor or a nonreactor nuclear facility where an activity is conducted for or on behalf of DOE and includes any related area, structure, facility, or activity to the extent necessary to ensure proper implementation of the requirements established by 10 CFR 830. [10 CFR 830]

Onsite Evaluation Point/Person (OEP) – A theoretical onsite receptor defined to allow dose comparison with numerical onsite evaluation guides. This point may be at a fixed distance (e.g. 100 m, 600 m, or 640 m), or located at the closest point on the facility or facility area exclusion zone. For elevated or buoyant releases that do not land within the exclusion zone, the OEP is the point beyond the exclusion zone where the maximum air concentration is located (touchdown point).

Rad – The unit of absorbed dose, equal to 0.01 Gy.

Rem – A measure of biological damage from radiation. It is the unit of dose equivalent, effective dose equivalent, or committed effective dose equivalent. The rem is numerically equal to the absorbed dose in rad multiplied by a quality factor,

distribution factor, and any other necessary modifying factor (1 rem = 0.01 sievert).

Safety Analysis and Design Software – Computer software that is not part of a structure, system, or component (SSC) but is used in the safety classification, design, and analysis of nuclear facilities to ensure

- proper accident analysis of nuclear facilities;
- proper analysis and design of safety SSCs; and
- proper identification, maintenance, and operation of safety SSCs.

Safety Analysis Software Group (SASG) – A group of technical experts formed by the DOE Deputy Secretary in October 2000 in response to Technical Report 25 issued by the Defense Nuclear Facilities Safety Board (DNFSB). This group was responsible for determining the safety analysis and instrument and control (I&C) software needs to be fixed or replaced, establishing plans and cost estimates for remedial work, providing recommendations for permanent storage of the software and coordinating with the Nuclear Regulatory Commission on code assessment as appropriate.

Safety-Class Structures, Systems, and Components (SC SSCs) – SSCs, including portions of process systems, whose preventive and mitigative function is necessary to limit radioactive hazardous material exposure to the public, as determined from the safety analyses. [10 CFR 830]

Safety-Significant Structures, Systems, and Components (SS SSCs) – SSCs which are not designated as safety-class SSCs, but whose preventive or mitigative function is a major contributor to defense in depth and/or worker safety as determined from safety analyses [10 CFR 830]. As a general rule of thumb, SS SSC designations based on worker safety are limited to those systems, structures, or components whose failure is estimated to result in prompt worker fatalities, serious injuries, or significant radiological or chemical exposure to workers. The term 'serious injuries', as used in this definition, refers to medical treatment for immediately life-threatening or permanently disabling injuries (e.g., loss of eye, loss of limb). The general rule of thumb cited above is neither an evaluation guideline nor a quantitative criterion. It represents a lower threshold of concern for which an SS SSC designation may be warranted. Estimates of worker consequences for the purpose of SS SSC designation are not intended to require detailed analytical modeling. Consideration should be based on engineering judgment of possible effects and the potential added value of SS SSC designation [DOE G 420.1-1].

Safety Software – Includes both safety system software and safety analysis and design software.

Safety Structures, Systems, and Components (SSCs) – The set of safety-class SSCs and safety-significant SSCs for a given facility. [10 CFR 830]

Safety System Software – Computer software and firmware that performs a safety system function as part of a structure, system, or component (SSC) that has been

functionally classified as Safety Class (SC) or Safety Significant (SS). This also includes computer software such as human-machine interface software, network interface software, programmable logic controller (PLC) programming language software, and safety management databases that are not part of an SSC but whose operation or malfunction can directly affect SS and SC SSC function.

Sievert (Sv) – The Systeme' Internationale (SI) unit of any of the quantities expressed as dose equivalent. The dose equivalent in sievert is equal to the absorbed dose in gray multiplied by the quality factor (1 Sv = 100 rem).

Software – Computer programs, operating systems, procedures, and possibly associated documentation and data pertaining to the operation of a computer system. [IEEE Standard 610.12-1990, *IEEE Standard Glossary of Software Engineering Terminology*].

Toolbox Codes – A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and of appropriate qualification that are maintained, managed, and distributed by a central source. Toolbox codes meet minimum quality assurance criteria. They may be applied to support 10 CFR 830 DSAs provided the application domain and input parameters are valid. In addition to public domain software, commercial or proprietary software may also be considered. In addition to safety analysis software, design codes may also be included if there is a benefit to maintain centralized control of the codes [modified from DOE N 411.1].

Total Effective Dose Equivalent (TEDE) – The sum of the deep dose equivalent (from external exposure) and the committed effective dose equivalent (from internal exposure). Note that the TEDE is equivalent to the EDE. For purposes of compliance, deep dose equivalent to the whole body may be used as effective dose equivalent for external exposures.

Whole Body – For the purposes of external exposure, head, trunk (including male gonads), arm above and including the elbow, and the legs above and including the knee.

95th Percentile Consequence – A method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to define the meteorological conditions assumed to be present for consequence analysis. Given site-specific data, the 95th percentile meteorology is the set of meteorological conditions assumed during a postulated release to a downwind receptor location that would result in a dose that is exceeded 5% of the time (based on a yearly average). This consequence level is direction-independent, i.e. averaged over all 360° at the distance of interest.

99.5th Percentile, Worst-Sector Consequence – A method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to define the meteorological conditions assumed to be present for consequence analysis. Given site-specific data, the sector 99.5th percentile meteorology is the set of meteorological conditions assumed during a postulated release to a downwind

receptor location that would result in a dose that is exceeded 0.5% of the time (based on a yearly average) in one of sixteen 22.5 ° sectors. The highest of the sixteen 22.5 ° sectors is then defined as the 99.5 Percentile, Worst-Sector Meteorology/Consequence condition. The MOI dose consideration takes distance to the site boundary in each direction into account.

9.0 REFERENCES

AIChE, 1996. Guidelines for Use of Vapor Cloud Dispersion Models, 2nd Edition. Publication 1439, American Institute of Chemical Engineers (AIChE) Center for Chemical Process Safety, New York, NY, 1996.

AMS, 1978. American Meteorological Society, Accuracy of Dispersion Models – A Position Paper of the AMS 1977 Committee on Atmospheric Turbulence and Diffusion, *Bulletin of the American Meteorological Society*, 9 (8), (August 1978).

Briggs, 1971, G. A. Briggs, *Some Recent Analyses of Plume Rise Observations,* Proceedings of the Second International Clean Air Congress, H. M. England and W. T. Berry. Eds., Academic Press.

Briggs, 1973, G. A. Briggs, *Lift Off of Buoyant Gas Initially on the Ground,*" ADTL Contribution File No. 87, November 1973. Air Resources Atmospheric Turbulence and Diffusion Laboratory NOAA, Oak Ridge, TN.

Carpenter, S.B., T.L. Montgomery, J.M. Leavitt, W.C. Colbaugh, and F.W. Thomas. 1971. "Principal plume dispersion model: TVA power plants." *Journal of the Air Pollution Control Association* 23:491-495.

CFR, 1991, 10 CFR 20, 1991. *Standards for Protection Against Radiation*, Title 10 Code of Federal Regulations Part 20, Office of the Federal Register, Washington, DC, May 21, 1991.

CFR, 1992, 29 CFR Part 1910, *Process Safety Management of Highly Hazardous Chemicals; Explosives and Blasting Agents*; Final Rule, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

CFR, 2001, 10 CFR Part 830, *Nuclear Safety Management Rule*, Code of Federal Regulations, Office of the Federal Register, Washington, DC.

Chamberlain, 1953, A. C. Chamberlain. *Aspects of Travel and Deposition Aerosol and Vapour Clouds,* Atomic Energy Research Establishment, Harwell, United Kingdom, British Report AERE-HP/R 1261.

DNFSB, 2000, Defense Nuclear Facilities Safety Board, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, Technical Report DNFSB/TECH-25, (January 2000).

DNFSB, 2002, Defense Nuclear Facilities Safety Board, *Recommendation 2002-1, Quality Assurance for Safety-Related Software*, (September 2002).

DOE, 1994a, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities*, DOE-HDBK-3010-94, U.S. Department of Energy, Washington, DC, Change Notice 1 (January, 1999).

DOE, 1998, Implementation Guide for use with DOE Order 440.1 Occupational Exposure Assessment, U.S. Department of Energy, Washington, D.C. DOE G 440.1-3.

DOE, 2002a, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports*, DOE-STD-3009-94, U.S. Department of Energy, Washington, DC, Change Notice 2 (April 2002).

DOE (2002b). *Selection of Computer Codes for DOE Safety Analysis Applications, Department of Energy*, National Nuclear Security Agency - Defense Programs Technical Report, (May 2002).

DOE, 2003a, *Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes*, (draft), U.S. Department of Energy, Washington, DC (September 2003).

DOE, 2004a. *Software Quality Assurance Improvement Plan: GENII Gap Analysis*, U.S. Department of Energy, Washington DC (May 2004).

DOE, 2004b, *MACCS2 Computer Code Application Guidance for Documented Safety Analysis*, U.S. Department of Energy, Washington, DC (May 2004).

DOE/EH, 2003, U.S. Department of Energy (2003), *Designation of Initial Safety Analysis Toolbox Codes*, Letter, (March 28, 2003).

Eckerman 1988, K.F. Eckerman, A.B. Wolbarst, A.C.B. Richardson. *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion.* Federal Guidance Report No. 11, U.S. Environmental Protection Agency, Washington, DC, DE89-011065.

Eckerman 1993, K.F. Eckerman and J.C. Ryman. *External Exposure to Radionuclides in Air, Water, and Soil. Federal Guidance Report 12*, U.S. Environmental Protection Agency, Washington, DC, PB94-114451.

Eimutis, 1972. E.C. Eimutis and M.G. Konicek, Derivations of Continuous Functions for the Lateral and Vertical Atmospheric Dispersion Coefficients, Atm. Env.,6, pp. 859-863.

EPA, 1995. *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volume II – Description of Model Algorithms*, EPA-454/B-95-003b, U.S. Environmental Protection Agency, Research Triangle Park, NC, September 1995.

EPA, 1988. K.F. Eckerman, A.B. Wolbarst, and A.C.B. Richardson, *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion*, Federal Guidance Report No. 11, U.S. Environmental Protection Agency, Washington, DC, 1988.

Fallon, 1982, R.D. Fallon, "Molecular Tritium Uptake in Southeastern U.S. Soils" *Soil Biol. Biochem,* Vol. 14, pp. 553 to 556.

Gelston, 1998, G. M. Gelston, M.A. Pelton, K.J. Castleton, B.L. Hoopes, R.Y. Taira, P.W. Eslinger, G. Whelan, P.D. Meyer and B.A. Napier, GENII Version 2 Sensitivity/Uncertainty Multimedia Modeling *Module Users' Guidance*, Pacific Northwest National Laboratory, Richland, Washington (1998).

Gifford, 1975. "Atmospheric Dispersion Models for Environmental Pollution Applications," in *Lectures on Air Pollution and Environmental Impact Analysis,* D. A. Haugen, ed., American Meteorological Society.

Gifford, 1976, F.A. Gifford, "Turbulent Diffusion Typing Schemes - a Review." *Nuclear Safety* 17:68-86.

Hanna, 1982. S.R. Hanna, G.A. Briggs, and R.P. Hosker, Handbook on Atmospheric Diffusion. DOE/TIC-11223, U.S. Department of Energy, Washington, DC, 1982.

Haugen, 1959, D.A. Haugen, editor, *Project Prairie Grass: A Field Program in Diffusion,* Geophysical Research Papers, #59, Vol. III, Report AFCRC-TR-58-235, Air Force Cambridge Research Center, *Hanscom Field, MA, 1959.*

Healy, 1984, J.W. Healy, *Radioactive Cloud Dose Calculation,* in Atmospheric Sciences and Power Production, DOE/TIC-27601, D. Randerson, Editor, U.S. Department of Energy, Washington, DC, 1984.

Holzworth, 1972, G.C. Holzworth, *Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution Throughout the Contiguous United States,* EPA Report AP-101, Environmental Protection Agency, Research Triangle Park, NC, p. 109, January 1972.

Hunter, 1993, C. H. Hunter, *Revised Onsite Meteorological data for Emergency Planning Hazards Assessments,* Savannah River Technology Center, Westinghouse Savannah River Company, SRT-ETS-931167 (1993).

ICRP, 1977. *Recommendations of the ICRP,* Annals of the ICRP 1 (#3), ICRP Publication 26, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1977.

ICRP, 1978, Radiation Protection: ICRP Publication 30 Part 1 Limits for Intakes of Radionuclides by Workers, Pergamon Press, New York, NY.

ICRP, 1979-82. *Limits for Intakes of Radionuclides by Workers,* Annals of the ICRP 2 (#3-4), 4 (#3-4), 6 (#2-3), 7, 8 (#1-4), and 19 (#4), ICRP Publication 30, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1979 - 1982.

ICRP, 1986. "The Metabolism of Plutonium and Related Elements," ICRP Publication 48 *Annals of the ICRP* Volume 16, Numbers 2-3, Pergamon Press, New York, NY.

ICRP, 1991. *1990 Recommendations of the International Commission of Radiological Protection,* Annals of the ICRP 21 (#1-3), ICRP Publication 60, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1991.

ICRP, 1994. *Human Respiratory Tract Model for Radiological Protection,* Annals of the ICRP 24 (#1-3), ICRP Publication 66, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 1994.

ICRP, 1995. "Dose Coefficients for Intakes of Radionuclides by Workers: A Report of a Task Group of Committee 2 of the International Commission on Radiological Protection Replacement of ICRP Publication 61," ICRP Publication 68 *Annals of the ICRP* Volume 24, Number 2, Pergamon Press, New York, NY.

ICRP, 1996a. "Age-dependent Doses to the Members of the Public from Intake of Radionuclides: Part 5," ICRP Publication 72 *Annals of the ICRP* Volume 26, Number 1, Pergamon Press, New York, NY.

ICRP, 1996b. "Age-dependent Doses to Members of the Public from Intake of Radionuclides: Part 4, Inhalation Dose Coefficients," ICRP Publication 71 *Annals of the ICRP* Volume 25, Number 3, Pergamon Press, New York, NY.

ICRP, 2001. *The ICRP Database of Dose Coefficients: Workers and Members of the Public*, Version 2.0, CD-ROM of ICRP Publication 68 and 72, published for the International Commission for Radiological Protection by Pergamon Press, Oxford, England, 2000.

Jow, 1990. H-N Jow, J. L. Sprung, J. A. Rollstin, L. T. Ritchie, and D. I. Chanin, *MELCOR Accident Consequence Code System (MACCS), Volume 2, Model Description*, NUREG/CR-4691, SAND86-1562, Sandia National Laboratories, Albuquerque, NM (February 1990).

LANL, 1995. J.F. McInroy, *A True Measure of Exposure*, Los Alamos Science 23, p 235, Los Alamos National Laboratory, Los Alamos, NM, 1995.

Lazaro, 1997, M. A. Lazaro, K. Woodward, S. R. Hanna, D.J. Hesse, J. C. Huang, J. Lewis, and C. A. Mazzola. *Model Review and Evaluation for Application in DOE Safety Basis Documentation of Chemical Accidents – Modeling Guidance for Atmospheric Dispersion and Consequence Assessment*, ANL/EAD/TM-75, Environmental Assessment Division (EAD), Argonne National Laboratory (ANL), Argonne, IL.

Leigh, 1992, C. D. Leigh, B. M. Thompson, J. E. Campbell, D. E. Longsine, R. A. Kennedy, and B. A. Napier, *User's Guide for GENII-S: A Code for Statistical and Deterministic Simulations of Radiation Doses to Humans from Radionuclides in the Environment*, SAND91-0561A, Sandia National Laboratories, Albuquerque, New Mexico (1992).

McElroy, 1968, J.L. McElroy and F. Pooler. *The St. Louis Dispersion Study*. U.S. Public Heath Service, National Air Pollution Control Administration, Report AP-53.

Mills, 1987, M. T. Mills, *Modeling the Release and Dispersion of Toxic Combustion Products from Chemical Fires*, Presented at International Conference on Vapor Cloud Modeling, November 2–4, Cambridge, MA, (1987).

Napier, 1988a, B. A. Napier, R.A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII - The Hanford Environmental Radiation Dosimetry Software System*, Volume 1: Conceptual Representation, PNL-6584 Vol. 1 (December 1988).

Napier, 1988b, B. A. Napier, R. A. Peloquin, D. L. Strenge, and J. V. Ramsdell, *GENII - The Hanford Environmental Radiation Dosimetry Software System*, Volume 2: Users' Manual, PNL-6584 Vol. 2 (November 1988).

Napier, 1999a, B. A. Napier, *GENII Version 2 User's Guide*, Prepared for U.S. Environmental Protection Agency, (January, 1999).

Napier, 1999b, B. A. Napier, *GENII Version 2 Example Calculation Descriptions*, Prepared for U.S. Environmental Protection Agency, (January , 1999).

Napier, 1999c, B. A. Napier, D.L. Strenge, J. V. Ramsdell, Jr., P. W. Eslinger, and C. Fosmire, *GENII Version 2 Software Design Document*, Prepared for U.S. Environmental Protection Agency, (January , 1999).

Napier, 1999d, B. A. Napier and L. Staven, *GENII Version 2 Training Power Point Slides*, Presented at the Safety Analysis Workshop of the annual meeting of the Energy Facility Contractors Group (EFCOG), (June, 1999).

NCRP, 1996. National Council on Radiation Protection and Measurements, *Screening Models for Releases of Radionuclides to Atmosphere, Surface Water, and Ground*, NCRP No. 123.

NRC, 1972. *Onsite Meteorological Programs*, U.S. Nuclear Regulatory Commission Regulatory Guide 1.23 (February 1972).

NRC, 1977. *Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water-Cooled Reactors*, Regulatory Guide 1.111, U.S. Nuclear Regulatory Commission, Washington, DC, (1977).

NRC, 1980. D. L. Strenge, *Models Selected for Calculation of Doses, Health Effects, and Economic Costs Due to Accidental Radionuclide Releases from Nuclear Power Plants.*

NRC, 1983. *Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants*, Regulatory Guide 1.145, U.S. Nuclear Regulatory Commission, Washington, DC, February 1983.

NRC, 1998. U.S. Nuclear Regulatory Commission, Nuclear Fuel Cycle Facility Accident Analysis Handbook, NUREG/CR-6410, Prepared by SAIC for the USNRC (1998).

NRC, 2003. *Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants*, U.S. Nuclear Regulatory Commission, Regulatory Guide 1.194, Washington, DC., (June 2003).

O'Kula, 1998, K.R. O'Kula, J.M. East, A.H. Weber, A.V. Savino, and C.A. Mazzola, *Evaluation of Current Computer Models in the DOE Complex for SAR Analysis of Radiological Dispersion & Consequences*, WSRC-TR-96-0126, Savannah River Site, Aiken, SC.

O'Kula 2000, K.R. O'Kula and J.M. East, *Evaluating Compliance with DOE-STD-3009-94, Appendix A Requirements (U)*, 2000 American Nuclear Society/European Nuclear Society International Meeting, Washington, D.C. (November 2000).

O'Kula, 2001, K.R. O'Kula, *Crediting Tritium Deposition Velocity in Accident Analysis*, Eleventh EFCOG Safety Analysis Workshop, Milwaukee, WI (June 2001)

Peterson, 1993, V.L. Peterson, *Reference Computations of Public Dose and Cancer Risk from Airborne Releases of Plutonium*, RFP-4910 (formerly NSTR-015-93), Safety Analysis Engineering/Nuclear Safety, EG&G Rocky Flats, Inc., December 23, 1993.

Peterson, 1995, V.L. Peterson, *Reference Computations of Public Dose and Cancer Risk from Airborne Releases of Uranium and Class W Plutonium*, RFP-4965 (formerly NSTR-026-94), Nuclear Safety/Safety Analysis, EG&G Rocky Flats Inc., Golden, Colorado, June 6, 1995.

Randerson, 1984, D. Randerson, Ed., Atmospheric Science and Power Production, Department of Energy, DOE/TIC-27601 (1984).

Rittman, 1978, P. D. Rittmann, *Verification Tests for the July 1993 Revision to the GENII Radionuclide and Dose Increment Libraries*, WHC-SD-WM-TI-596, Rev. 0 (October 1993).

Sehemel, 1978, G.A. Sehemel and W.H. Hodgson, A Model for Predicting Dry Deposition of Particles and Gases to Environmental Surfaces, Battelle Pacific Northwest Laboratories, Richland, WA, PNL-SA-6721.

Slade, 1968, D.H. Slade (editor), *Meteorology and Atomic Energy*, U.S. Atomic Energy Commission, Office of Information Services, Washington, D.C., 1968.

Smith, F.B. 1961. "An Analysis of Vertical Wind-fluctuation at Heights between 500 and 5,000 Feet." *Quarterly Journal of the Royal Meteorological Society* 87(372):180-193.

Steele, 1998, C.M. Steel, T.L. Wald, and D.I. Chanin, Plutonium Explosive Dispersal Modeling Using the MACCS2 Computer Code, Los Alamos National Laboratory, LA-UR-98-1901 (June 1998).

Sweet, 1984, C.W. Sweet, "The Relationship Between Tritiated Water Activities in Air, Vegetation and Soil Under Steady-state Conditions," *Health Physics*, Vol. 47, No. 4, pp. 635-639.

Tadmor, 1969, J. Tadmor and Y. Gur, *Analytical Expressions for the Vertical and Lateral Dispersion Coefficients in Atmospheric Diffusion*, Atmospheric Environment **3**, Pergamon Press, Great Britain, pp 688, 1969.

Turner, 1970. D.B. Turner. Workbook of Atmospheric Dispersion Estimates, Education, and Welfare report PB-191482, U.S. Department of Health, Washington, DC (1970).

Turner, 1986, J.E. Turner, *Atoms, Radiation, and Radiation Protection*, Pergamon Press, New York, 1986.

Turner ,1994, D. B. Turner, *Workbook of Atmospheric Dispersion Estimates, An Introduction to Dispersion Modeling*, Lewis Publishers, Ann Arbor, MI. (1994).

Weber, 1996. A. H. Weber and C.H. Hunter, *Estimating Dispersion from a Tornado Vortex and Mesocyclone (U)*, Savannah River Site, Aiken, SC, WSRC-TR-94-0386, Rev 2.

Yuan, 1993, Y.C. Yuan, S.Y. Chen, D. J. LePoire, and R. Rothman, RISKIND – A Computer Program for Calculating Radiological Consequences and Health Risks from Transportation of Spent Nuclear Fuel, ANL/EAIS-6, Rev. 0, Argonne National Laboratory, (February 1993).

Appendices

Appendix	Subject
A	Overview of Atmospheric Dispersion and Consequence Analysis
B	Software Defect Notifications
C	Sample Problem – Joint Frequency Distribution File

Appendix A. Overview of Atmospheric Dispersion and Consequence Analysis

Once the source term to the environment from a postulated accident condition has been calculated or estimated, the safety analyst must determine the concentration downwind to hypothetical receptors. A robust safety analysis will apply a sound technical basis for predicting the transport and diffusion of the airborne plume. Often this is based on a dispersion model that applies environmental data specific to the facility and site under consideration.[8]

This appendix provides an overview of atmospheric dispersion methods, focusing on Gaussian methodology, and discusses radiological consequence analysis "back end". Recommendations are provided where appropriate for specific data or assumptions.

A-1 Dispersion Methodology & Summary of DOE-STD-3009-94, App A

Appendix A to DOE-STD-3009-94, Change Notice 2 (CN#2) (DOE 2002a), specifies an Evaluation Guideline (EG) for radiological exposure to the offsite receptor, which is to be applied in specifying SSCs. The numerical value of the EG is 25 rem, Total Effective Dose Equivalent (TEDE). Dose estimates to be compared to the Evaluation Guideline (EG) are those received by a hypothetical maximally exposed offsite individual (MOI) at the site boundary for an exposure period of two hours. The nominal exposure period of two hours may be extended to eight hours for release scenarios that occur over a prolonged period.

Appendix A to DOE-STD-3009-94 notes that the airborne pathway is of primary interest for nonreactor nuclear facilities. NUREG-1140, *A Regulatory Analysis on Emergency Preparedness for Fuel Cycle and Other Radioactive Material Licenses*, previously noted that, "for all materials of greatest interest for fuel cycle and other radioactive material licenses, the dose from the inhalation pathway will dominate the (overall) dose." For some types of facilities such as waste storage, the surface and groundwater pathways may be more important, but accident releases usually would be expected to develop more slowly than airborne releases.

The dose calculation references Regulatory Guide 1.145 of the Nuclear Regulatory Commission (NRC) for determination of the five percent overall site relative concentration (χ/Q, often referred to as the dilution or dispersion factor) value at the exclusion area boundary (EAB). A straight-line Gaussian model is to be applied with one-hour averaged χ/Q values for the entire course of plume duration for a period not to exceed eight hours. Text from Section A.3.3 of Appendix A on Dose Estimation (p. A-8 to A-9) states

> The relevant factors for dose estimation are receptor location, meteorological dispersion, and dose conversion values ...

The first two of these three factors are addressed below.

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[8] The term dispersion is applied using the definition appearing as Footnote 2 in NRC Regulatory Guide 1.145 to encompass both transport (due to organized or mean airflow within the atmosphere) and diffusion (due to disorganized or random air motions) of the plume.

Dose Calculation Location. For the purposes of comparison to the EG, the comparison point is taken to be the location of a theoretical MOI standing at the site boundary. This location can also be beyond the DOE site boundary if a buoyant or elevated plume is not at ground level at the DOE site boundary. In such cases, the calculation location is taken at the point of maximum exposure, typically where the plume reaches ground level. It is DOE practice and expectation that onsite individuals, both workers and public, are protected under the Emergency Response plans and capabilities of its sites. This protection, along with implementation of defense-in-depth and worker safety philosophy, Safety Significant (SS) (and indirectly, through SC) SSC designation, and DOE's safety management programs, address onsite safety. However, an annual assessment of any changes in the site boundary and potential effects on safety SSC classification should be performed in association with the required annual update of the SAR for a facility. Privatization and site turnover initiatives may affect these determinations.

Atmospheric Dispersion. The 95th percentile of the distribution of doses to the MOI, accounting for variations in distance to the site boundary as a function of direction, is the comparison point for assessment against the EG. The method used should be consistent with the statistical treatment of calculated χ/Q values described in regulatory position 3 of NRC Regulatory Guide 1.145 for the evaluation of consequences along the exclusion area boundary. The determination of distance to the site boundary should be made in accordance with the procedure outlined in position 1.2 of Regulatory Guide 1.145. NRC Regulatory Guide 1.23 describes acceptable means of generating the meteorological data upon which dispersion is based. Accident phenomenology may be modeled assuming straight-line Gaussian dispersion characteristics, applying meteorological data representing a 1-hour average for the duration of the accident. Accident duration is defined in terms of plume passage at the location of dose calculation, for a period not to exceed 8 hours. Prolonged effects, such as resuspension, need not be modeled. The accident progression should not be defined so that the MOI is not substantially exposed (i.e., using a release rate that is specifically intended to expose the MOI to only a small fraction of the total material released). The exposure period begins from the time the plume reaches the MOI.

For ground level releases, the calculated dose equates to the centerline dose at the site boundary. For elevated, thermally buoyant, or jet releases, plume touchdown may occur beyond the site boundary. As noted in the discussion of receptor location, these cases should locate the dose calculation at the point of maximum dose beyond the site boundary, which is typically at the point of plume touchdown.

Accidents with unique dispersion characteristics, such as explosions, may be modeled using phenomenon-specific codes more accurately representing the release conditions. Discussion should be provided justifying the appropriateness of the model to the specific situation. For accident phenomena defined by weather extremes, actual meteorological condition associated with the phenomena may be used for comparison to the EG.

The guidance provided herein uses the prescriptive requirements of Appendix A as a basis, and is applicable for performing DSAs compliant with Subpart B of 10 CFR 83.

Before discussing choice of a model, the key important environmental transport values are summarized.

A-1.1 Atmospheric Dispersion Parameters and Statistical Bases

Most radiological source terms may be treated as neutrally buoyant. By neutrally buoyant, it is assumed that the cloud[9] of released material has approximately the same density as air. This is normally a valid assumption for radioactive releases that are gaseous in nature that contain trace amounts of very fine particulates, aerosols, and gases. As the cloud is carried downwind, it is common practice based on experimental data, to assume a Gaussian distribution in both the crosswind (lateral) and vertical directions. For continuous releases, the mean wind speed dilutes the pollutant but the downwind dispersion is negligible. As the cloud moves downwind it gets progressively larger due to lateral and vertical diffusion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the downwind direction becomes more important. Accordingly, a puff is described by a three-dimension Gaussian equation.

Several meteorological parameters affect the shape and size of a neutrally buoyant cloud. These are discussed in the following sections.

A-1.2 Meteorological Parameters

Earlier it was noted that downwind dispersion of a radioactive plume might be thought of as simultaneous transport and diffusion. In simplest terms, the transport term is mostly a function of wind and direction. The diffusion of the plume is due in large part to the atmospheric turbulence in the region of transport. The following sections discuss wind speed and direction, temperature profiles, and their impact on conditions in the atmosphere.

A-1.2.1 Wind Speed and Direction

Prevailing wind is a key determinant of the transport of the radioactive cloud. In terms of importance to accident analysis calculations, wind velocity is a vector quantity having both magnitude and direction. The wind speed at the height of the release determines both the initial diffusion of the pollutant and the travel time to reach a given downwind receptor. The initial diffusion and the plume travel are both directly proportional to the wind speed. It is also a factor in determining the magnitude of atmospheric stability. Atmospheric turbulence (i.e., mechanical turbulence) is generated when adjacent parcels of air move at different speeds or move in different directions. Thus, a change in wind speed with height above the ground, or a variation in wind direction at a given height, causes mechanical turbulence. Mechanical turbulence is also generated when air interacts with some fixed object, such as the ground, described as roughness length, or with a building, described by aerodynamic effects such as building wake and cavity.

[9] Cloud shall mean either a continuous (plume) or short-term release (puff).

The horizontal wind direction at the height of the release determines the direction of transport. It does not affect the magnitude of the concentration of the pollutant within the plume. The horizontal wind direction, or more commonly, wind direction, is the first moment, or average, of a series of "instantaneous" wind direction measurements. By convention, the wind direction is 180 degrees out of phase with the downwind or transport direction.

Atmospheric turbulence is directly related to the variability of wind direction. The variability of wind direction is normally expressed in terms of the standard deviation of a series of "instantaneous" wind direction measurements over a selected observation period, normally fifteen minutes. The standard deviation, or second moment of the horizontal wind direction, σ_θ, is commonly used to characterize atmospheric turbulence by stability classes. Alternatively, the standard deviation of the vertical wind component, σ_ϕ, is sometimes used as a basis to describe the category of atmospheric turbulence.

A-1.2.2 Vertical Temperature Profiles

In addition to wind direction variation, another technique that is used to type atmospheric turbulence is to use vertical temperature gradient measurements ($\Delta T/\Delta Z$). When a parcel of air is displaced in the vertical plane, it will expand (if rising) or contract (if sinking) to adjust its pressure to that of its surroundings. The expansion or contraction is accompanied by an adiabatic temperature change. As a parcel rises, it cools. If the surrounding air is warmer, the parcel will be heavier than its surroundings and sink back toward its original position, and its motion ceases. On the other hand, if the surrounding air is cooler, the parcel will be lighter and continue to move upward. Similarly, if the air parcel sinks, it warms up as it contracts. If the surrounding air is cooler, the parcel will be lighter and rise back toward its original position, and its motion ceases. If the surrounding air is warmer, the parcel will be heavier and continue to sink.

Thus, turbulence is suppressed if the temperature profile of the air (the so-called lapse rate) is less than adiabatic (subadiabatic), and enhanced if greater than adiabatic (superadiabatic). The adiabatic lapse rate near ground is about -9.8 °C/km (-5.4 °F/1,000 feet). Superadiabatic lapse rates are associated with unstable atmospheric conditions and labeled A, B, or C stability classes, with Class A representing the most unstable set of conditions. Subadiabatic lapse rates are associated with stable atmospheric conditions, inclusive of inversions (i.e., temperature increase with height) and labeled E, F, and G stability classes, with Class G representing the most stable conditions. Adiabatic lapse rates are associated with neutral atmospheric conditions and labeled as Class D. In practice, some sites limit the extent of classes to six, with G stability class being combined with F stability.

Thus, the vertical temperature profile affects atmospheric turbulence. The atmospheric layer near the ground is called the mixing, or the mixed layer. During daylight, the ground heats up, warming the air near the surface. The lapse rate near the surface thus becomes superadiabatic and buoyancy-driven vertical turbulence enhances in the existing mechanical turbulence due to ground roughness and wind shear. At night, the ground cools, causing the air near the surface to cool, and the lapse rate becomes subadiabatic and frequently inverted. Buoyancy-driven vertical turbulence thus suppresses the existing mechanical turbulence due to ground roughness and wind

shear. At greater heights, a few hundred to a few thousand meters in altitude, the lapse rate may change. It is common for the turbulent lower atmosphere to be capped by lapse rate that is subadiabatic so that turbulent eddies rising from below are suppressed. This layer near ground is thus called the mixed layer, for this is where turbulence in the strongest due primarily to the frictional effects of the earth's surface and the convective heat transfer from the earth's surface.

A-1.2.3 Atmospheric Stability Classes

A comprehensive treatment of atmospheric dispersion is so complex that many approximations are needed to make it tractable. Since turbulence is random and chaotic, it cannot be parameterized and one must resort to empirical formulations. One early attempt to simplify the treatment of turbulence was to define atmospheric stability classes and associate a rate of lateral and vertical diffusion with each class as a function of downwind distance only. Although computations based on these stability classes provide only a rough approximation to reality, they have proved extremely useful. They are still in use, although treatments that are more accurate are available. Wind direction variability and vertical temperature difference are the most common techniques that are employed to compute stability class. Wind direction variability provides the best approximation of mechanical turbulence, while vertical temperature difference approximates the buoyancy component.

Seven stability classes (i.e., Pasquill-Gifford-Turner classes) have been defined. These classes, with the original descriptions and conditions of occurrence given by Pasquill (Turner, 1994), are:

(lxviii) A: Extremely Unstable (Strong superadiabatic). Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).

(lxix) B: Moderately Unstable (Moderate superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 3 to 5 m/s range to dim sunshine with wind speeds < 2 m/s.

(lxx) C: Slightly Unstable (Slight superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 5 to 6 m/s range to dim sunshine with wind speed in the 2 to 3 m/s range.

(lxxi) D: Neutral (Adiabatic). Normally occurs with moderate to dim sunshine, cloudy conditions, and at night, with wind speeds > 3 m/s. It also occurs with very strong wind speeds on either sunny or cloudy days.

(lxxii) E: Slightly Stable (Slight subadiabatic with or without inversion). Normally occurs at night or early morning with some cloud cover and with wind speeds in 2 to 5 m/s range.

(lxxiii) F: Moderately Stable (Moderate subadiabatic with inversion). Normally occurs at night or early morning with little cloud cover and with relatively low wind speeds (< 3 m/s).

(lxxiv) G: Extremely Stable (Strong subadiabatic with inversion). Normally occurs at night or early morning with very light to nearly zero wind speed.

Unstable conditions result in rapid lateral and vertical diffusion of pollutants (i.e., wide plumes), whereas stable conditions result in slow lateral and vertical diffusion (i.e., narrow plumes). The latter will lead to higher air concentrations from ground-level releases.

Although Class A is not rare, it is not as common as Classes B through F. Class D is the most common stability class for many DOE sites. This is due to the large number of combinations that can result in Class D stability. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally Class D. Classes E and F are the most common stability classes at night.

Note that the meteorological conditions used as a basis for DOE-STD-1027-92 Hazard Characterization, Attachment 1 are D stability and 4.5 m/s wind speed. This set of conditions is also used as a basis by chemical process industry for determining limits on chemical inventories, and is representative of most U.S. regions (29 CFR 1910.119) (CFR, 1992). These are median dispersion conditions for most sites.

A-1.3 Dispersion Conditions for Accident Analysis

In calculating plume concentrations, and subsequently consequences to the receptor, both "unfavorable" and "typical" dispersion conditions are of special interest in accident analyses. For accident analysis consideration of the offsite MOI receptor, unfavorable meteorology should be based on site data. In practice, this is the dilution factor (χ/Q) that coupled with the source term would lead to doses that are exceeded less than five percent of the time. The method should be conservative or consistent to the discussion in the NRC Regulatory Guide 1.145 (Position 3) as summarized in Appendix A to DOE-STD-3009-94, CN#2. The 95th percentile of the distribution of doses to the MOI, accounting for variation in distance to the site boundary as a function of direction, is the comparison basis for assessment against the EG.

The size of the data set used in the meteorological assessments should be sufficiently large that it is representative of long-term meteorological trends at most sites. Meteorological data used in accident analysis should be qualified to meet the requirements of Regulatory Guide 1.23 (NRC, 1972) and representative of long-term trends. A five-year dataset is desirable, but a one-year data set can be applied under the right circumstances.[10] In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations, such as Class F stability and 1.0 m/s to 1.5 m/s wind speed, as an interim measure.

It should be noted that in the long run, site data is normally preferable over the default conditions for accident analysis.

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[10] In Draft Regulatory Guide DG-111, this subject is discussed as follows: "The NRC staff considers five years of hourly observations to be representative of long-term trends at most sites. With sufficient justification of its representativeness, the minimum meteorological data set is one complete year (including all four seasons) of hourly observations." (NRC, 2003)

For example, (Hunter, 1993) evaluated Savannah River Site data and found the 95th percentile conditions varied with release height and receptor distance. For most facility MOI distances, it was determined that 95th percentile conditions were E stability and

(lxxv) 1.7 m/s wind speed for a release height between 0 m and 10 m

(lxxvi) 2.1 m/s wind speed for a release height of 20 m, and

(lxxvii)3.0 m/s wind speed for a release height of 60-m.

(lxxviii) For mitigated hazard analysis, DOE has not established guidance for evaluating the mitigated benefit of SSCs. Both median statistical basis (i.e., 50th percentile) and 95th percentile bases have been applied to determine onsite receptor doses. While other measures of "typical" could be applied, each is problematic. The mean (i.e., average) and the mode (i.e., peak) of a distribution, unlike the median, are not heavily influenced by outliers (abnormally small or large values). For a bimodal distribution, which often occurs, the mean may fall between the peaks (i.e., modes) of the distribution and thus be comparatively infrequent, which could not be considered "typical". (The median could also be atypical in this sense but it has a relevant meaning.) In addition, if mode were chosen as "typical", a bimodal distribution could give two valid choices if the peaks are nearly as large.

(lxxix) Evaluation of site data for determining 95th and 50th percentile conditions has historically been of two types. A Joint Frequency Distribution (JFD) sampling of site hourly data sorts *all* data from high relative concentration to low relative concentration and identifies various percentile conditions by ranking the full data set. Another basis is use of a random sampling technique in which a sample of the full data is randomly selected and then typically sorted into pre-assigned consequence bins (normally chosen to find high-consequence conditions). An example of this approach is Latin Hypercube Sampling (LHS).

(lxxx) JFD sampling is usually done for a standard set of release conditions (e.g., one hour duration, ground-level release). The random sampling basis is normally determined on an accident case-by-case basis. The JFD profile tends to be composed of more data points and is generally "smoother".

A-1.4 Gaussian Model for Neutrally Buoyant Plumes

The choice of a dispersion model depends on factors such as the phase of safety analysis, complexity of facility, complexity of the accident sequence, and site topography and its affect on environmental transport conditions. Simply put, the most comprehensive, realistic computer model is not the best choice for all safety analysis situations. In most situations, peer-reviewed engineering calculations and spreadsheet analyses employing a Gaussian atmospheric dispersion model are sufficient. Data requirements for such calculations are typically less demanding than for models that are more complex. Ultimately, this type of accident analysis calculation is more scrutable and technically defensible during independent review if based on the Gaussian model.

The simple, straight-line Gaussian dispersion equation is used as the basis for a majority of the models used in DOE safety analysis of accidental releases. It is the basis for radionuclide inventories defining Hazard Category 2 and 3 facilities in DOE-STD-1027-92, CN 2. As noted

earlier, for compliance with Appendix A of DOE-STD-3009 and comparison with the EG, the Gaussian model can readily estimate time-integrated air concentrations (typical units of Ci-s/m^3 for radiological releases) at downwind locations and is recommended for most accident conditions (Figure A-1). While more sophisticated models are becoming more commonplace, especially in situations where complexities in physical or chemical properties, terrain, or nearby buildings influence the dispersion of radiological material, the data demands for these approaches may be prohibitive. However, for these situations, the basic Gaussian dispersion model can be bootstrapped to accommodate release and dispersion effects that are influenced by surface features or source term characteristics.

The user should exercise care over the distance for which the Gaussian model is applied. The American Meteorological Society (AMS) published a position paper indicating that the Gaussian model is estimated to be accurate within a factor of two for distances of 0.1 to 10 – 20 km when onsite meteorological tower data are available, and conditions are reasonably steady and horizontally homogeneous (AMS, 1978). For distances beyond 20 km and closer than 100 m, the Gaussian model should be considered to be order-of-magnitude estimates at best. Aerodynamic wakes, rough or urban terrain, dense gas effects, and dispersion under very stable conditions often render Gaussian model predictions inaccurate.

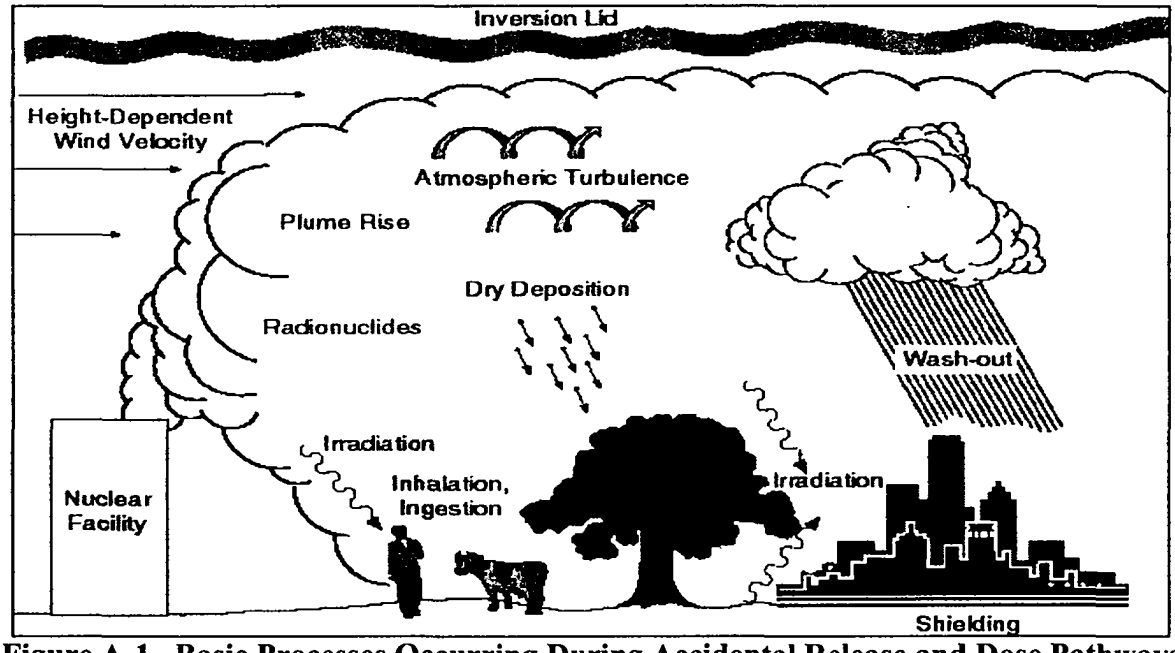

Figure A-1. Basic Processes Occurring During Accidental Release and Dose Pathways

For energetic releases, other models may be employed, as allowed under Appendix A of DOE-STD-3009-94, CN#2. However, data requirements for alternative model types may preclude use to support most DSA applications. Alternative techniques have been applied to "bootstrap" a Gaussian model and thereby apply it to cases normally outside the regime of Gaussian applicability (Steele, 1998).

It is the responsibility of the analyst to make the final determination of a dispersion basis. The determination must be weighed against the value of a complex, more realistic computer model

with its associated data demands; the requirements of the specific application; and the phase of the safety analysis.

Recommendation:

Apply the Gaussian model as a first choice. Accident phenomenology may be modeled assuming straight-line Gaussian dispersion characteristics, applying meteorological data representing a 1-hour average for the duration of the accident.

Use other special-purpose approaches as warranted for unique release situations, e.g. detonation or blast accident scenarios. Consider appropriate modifications for addressing weather extremes, such as tornado or high-wind conditions.

Basic Gaussian Equations

Intrinsic to the assumptions underlying the Gaussian approximation of atmospheric dispersion, as a plume is transported downwind, its horizontal expansion is essentially unlimited[11]. Vertical expansion is limited below by the earth's surface and above by inversion conditions. The downward expansion of the plume must obviously stop at the ground, while upward expansion may be stopped if there is a stable layer (i.e., a "cap") at the top of the mixing layer. This cap acts as a lid to rising "thermals" of air, thus restricting the range and magnitude of vertical turbulence. The plume is often considered to "reflect" off both the ground and the top of the mixing layer, causing the *vertical* profile to become increasingly uniform as the plume proceeds downwind.

The amount of atmospheric dilution and dispersion is usually expressed in terms of χ/Q, where χ is the concentration of the pollutant in air at some downwind location. For these formulations, χ represents either the instantaneous concentration (e.g., Ci/m^3 or Bq/m^3) or the time-integrated concentration (e.g., $Ci\text{-}s/m^3$ or $Bq\text{-}s/m^3$), and Q is the rate of release (e.g., Ci/s or Bq/s) of the pollutant, or total source strength (e.g., Ci or Bq) of the pollutant. The units of χ/Q are s/m^3 whether the instantaneous or time-integrated releases are considered. Thus, χ/Q is the concentration of the pollutant in air at the receptor per unit source rate, or time-integrated concentration per unit source. The actual concentration of the pollutant in air at the receptor is thus the product of χ/Q and the rate of release of the pollutant.

The Gaussian plume model (Slade, 1968), when not constrained in the vertical by the ground or the top of the mixed layer, is expressed as:

$$\frac{\chi(x,y,z,h)}{Q} = \frac{1}{2\pi u \sigma_y \sigma_z} e^{-y^2/2\sigma_y^2} \left[e^{-(z-h)^2/2\sigma_z^2} \right] \qquad \text{(A-1)}$$

Where x is the distance of the receptor downwind from the release point, y is the horizontal cross-wind distance of the receptor from the centerline of the plume, z is the distance of the

[11] Horizontal, or lateral, plume expansion may be somewhat limited by physical barriers, such as buildings and topographic obstacles, but these are normally treated as special cases.

receptor above the ground, h is the height of the plume centerline above the ground, σ_y is the standard deviation of the horizontal Gaussian distribution (i.e., the "half width"), σ_z is the standard deviation of the vertical Gaussian distribution (i.e., the "half thickness"), and u is the wind speed at 10 m height, the standard measurement height. The constant, 2π, is implicit in a Gaussian distribution, and is the product of lateral and vertical components each contributing $(2\pi)^{1/2}$. Note that the downwind distance x does not appear explicitly in this equation since downwind distance is an independent variable. The x dependence is implicit, as the σ_y and σ_z are functions of x only, for a given stability class. The wind speed (u) represents the direct dilution of the pollutant as soon as it is released into the atmosphere. The lateral and vertical Gaussian coefficients (σ_y, σ_z) approximate the diffusion or dispersion in the atmosphere as the plume is transported downwind.

The bracketed term in equation (A-1) defines the vertical distribution. If hazardous material released in the plume is reflected from the ground and from the top of the mixed layer, this term must be modified. This is done mathematically by adding multiple mirror source terms. The bracketed term in equation (A-1) thus is replaced with:

$$\left[e^{-(z-h)^2/2\sigma_z^2} + e^{-(z+h)^2/2\sigma_z^2} + \sum_{n=1}^{N} \left(e^{-(z-h-2nL)^2/2\sigma_z^2} + e^{-(z+h-2nL)^2/2\sigma_z^2} + e^{-(z-h+2nL)^2/2\sigma_z^2} + e^{-(z+h+2nL)^2/2\sigma_z^2} \right) \right] \quad \text{(A-1a)}$$

The term before the summation in expression (A-1a) is the ground reflection component since perfect reflection is assumed. The series of terms after the summation represent the perfect reflection of first the top of the plume and later the bottom of the plume on the top of the mixed layer. L represents the height of the top of the mixed layer and the summation is over the number (N) of reflections to be considered. The contribution of the summation term is minor, especially for distances close to the source and for larger values of L. The higher order terms contribute progressively less and the series is normally terminated after only a few terms. For a ground-level release (i.e., $h = 0$), the first two exponential terms become equivalent. Each of these terms subsequently becomes a value of one when the receptor is at ground level ($z = 0$). In these cases, the "2" in the denominator of equation (1) cancels out with the "2" in the numerator, if the summation term is ignored, as is often done. The maximum concentration occurs at plume centerline (i.e., $y = 0$). Thus, if the summation term is ignored, the Gaussian equation simplifies to a centerline condition:

$$\frac{\chi(x, y = 0, z = 0, h = 0)}{Q} = \frac{1}{\pi u \sigma_y \sigma_z} \quad \text{(A-2)}$$

Strictly speaking, the numerator in the above expression is slightly greater than one because of the contribution of the summation term. Equation (A-2), which is now only a function of downwind distance of the receptor, is often used for the MOI, as the plume centerline concentration represents a conservative value.

Similarly, a puff model using a Gaussian formulation may be used for instantaneous or near-instantaneous releases of hazardous material

$$\chi(x,y,z;H)=\frac{Q_T}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \quad \text{(A-3)}$$

Where:

Q_T = total source term (Ci)

σ_x = longitudinal dispersion coefficient, representing the standard deviation of the concentration distribution in the downwind axis direction (m) (AIChE, 1996).

The horizontal and vertical dispersion coefficients, σ_y and σ_z, required in the Gaussian dispersion equation are obtained either from site-specific meteorological measurements (standard deviations of wind angles) or indirectly through estimating an atmospheric stability class for which standard dispersion coefficients have been established. If the necessary meteorological measurements are not available, several methods for determining stability class may be used. The differences between puff and plume dispersion handled with the Gaussian dispersion equation should be taken into account when applying the model. Methods for calculating puff dispersion coefficients have been addressed by (Turner, 1970), (Gifford, 1977), and (Hanna, 1982). The puff dispersion equation is rarely used for radiological consequence calculations.

A-1.5 Special Gaussian Modeling Considerations

A-1.5.1 Plume Meander

The above expressions are for short-duration clouds released over relatively smooth terrain. However, as time passes after the initial release, larger sized eddies, mostly in the horizontal direction, may affect the cloud. Shifts in wind direction become likely with time increases since the start of release, and the cloud will tend to change direction, or meander. The meander factor is especially important for the longer duration releases. For a receptor that remains immersed in the plume for some time, meandering effectively widens the plume (i.e., increases horizontal dispersion) and thus decreases χ/Q. One formulation of the plume meander factor[12], the one attributed to Gifford (Gifford, 1975), is

$$\textit{meander factor} = (\textit{plume duration} / \textit{time base})^n \quad \text{(A-7)}$$

Where the time base is typically 10 minutes and the exponent n is 0.2 for plume duration of one hour or less and 0.25 for greater duration. The σ_y is increased by this meander factor and accordingly, the plume-centerline χ/Q would accordingly be reduced by this factor. The plume meander factor is never allowed to be less than one, and the experimental basis is limited to periods no longer than 100 hours.

Example: For a two-hour release and a time base of ten minutes, the plume meander factor is $[(2\text{ hr})(60\text{ min/hr})/10\text{ min}]^{0.25} = 1.86$.

[12] The meander factor is also called the plume expansion factor.

An alternative formulation (NRC, 1980) is

$$meander\,factor = (2 \times plume\,duration)^{1/3} \quad \text{(A-8)}$$

Where the plume duration is in hours (minimum of 0.5 hours). This gives results similar, but not identical, to those shown in equation (A-7).

A different type, and larger meander factor occurs under conditions that are very close to adverse meteorology for ground-level releases (i.e., very stable conditions with light wind speeds). Under such conditions, large eddies are present in the stably stratified atmosphere which augment the magnitude of the lateral turbulence. This theoretical effect was first empirically determined from tracer studies performed in the mid-1970s. After careful review of the results of the tracer study, the Nuclear Regulatory Commission incorporated this meander factor in Regulatory Guide 1.145 (NRC, 1983), and acknowledged it in several of their atmospheric dispersion models. The Regulatory Guide does not advise using this factor for relatively higher stability classes (A, B, and C).

The embedded equations in these models can simply be described by an augmentation of the lateral turbulence:

$$\Sigma_y = M\,\sigma_y \quad \text{(A-9)}$$

Where Σ_y is the augmented lateral turbulence and M is the meander factor.

The value of M increases for more stable conditions (i.e., from E to G stability class) and as wind speeds approach calm. This is exactly opposite to the aerodynamic building wake factor that is very small under these meteorological conditions, but increases significantly as the wind speeds increase and the stability class becomes neutral or slightly unstable.

Recommendation: Apply the Gifford model for recalibrating the time basis of the set of dispersion parameters to the release duration of interest.

A-1.5.2 Surface Roughness

Surface roughness mostly affects the magnitude of vertical turbulence, and hence, vertical atmospheric dispersion. The rougher the surface, the larger the turbulent eddies that are formed when the plume encounters the earth's surface. If the terrain is not smooth, which is frequently the case, a linear scaling factor needs to be introduced to increase the effective value of σ_z. A common approach to quantifying the "roughness" factor, is based on (AMS, 1977) and is usually expressed as:

$$roughness\,factor = (z_1/z_0)^{0.2} \quad (z_1 \geq z_0) \quad \text{(A-10)}$$

Where z_1 is the roughness length of the terrain over which the plume is passing and z_0 is the comparison standard length, normally taken as 3 cm, which represents the roughness factor associated with flat terrain. The roughness factor cannot be less than unity. Because σ_z is increased by the roughness factor, the plume-centerline χ/Q is proportionally reduced by this

amount. For grasslands, the roughness length is estimated to be 10 cm. In this case, the roughness factor is $(10/3)^{0.2} = 1.27$. For terrain that includes grasslands, trees, mountains, and cities, the average roughness length commonly applied ranges from 30 cm to 100 cm. For example, if it were about 24 cm, the roughness factor would be 1.52. (Note that in the Briggs formulation of σ_y and σ_z, this roughness factor is already taken into account in that different coefficients are used for open-country and urban terrain.). McElroy and Pooler first developed "urban" dispersion coefficients in the 1960's (McElroy, 1968). As a rough rule of thumb, the vertical dispersion increases by one stability class for urban areas (i.e., an atmospheric condition resulting in F stability in rural environments becomes E stability in urban environments).

Recommendation: Apply a roughness correction to adjust the vertical dispersion parameterization for the region of transport that is based on recommendations from the American Meteorological Society (AMS, 1977).

A-1.5.3 Depletion Processes

While atmospheric dispersion processes play the major role in determining cloud concentration, others processes exist that can remove both gases and particulates from the cloud and reinsert other radioactive species back into the atmosphere. The removal processes are dry deposition, which results from interaction of the lower portion of the plume with the ground and gravitational settling (fallout) of material from the plume, and wet deposition, or precipitation scavenging. Reinsertion of material back into the atmosphere is termed resuspension and will be discussed in more detail in the next section. These mass transfer processes are very important in determining the ultimate fate of small respirable particulates.

A-1.5.3.1 Dry Deposition

The physical characteristics of particulate and aerosol radionuclide species will tend to remove this component from a released cloud. Two common models for removal are the source model and the surface model. The source model is computationally simple, in which the rate at which materials in the cloud are deposited to the ground is the product of the ground level air concentration of the materials, and the dry deposition velocity of the material (Chamberlain, 1953). This approach uniformly depletes the cloud, that is, it does not perturb the normal distribution of the concentration in the vertical direction. This assumption is valid during neutral or unstable atmospheric conditions because the constant turn-over of material in the cloud maintains uniformity, but is not as valid for stable conditions, for which the turn-over is less vigorous.

Another approach is the surface depletion method. It is computationally more complex, and depletes the source primarily at the cloud/earth interface. This model changes the material distribution in the cloud.

The parameterization of dry deposition processes is usually accomplished by the use of a deposition velocity. Deposition velocity (v_d) is a mass-transfer boundary condition at the atmosphere-ground surface interface in atmospheric dispersion and transport models. The

deposition velocity is defined as a deposition flux (F_d) divided by the airborne concentration of radioactive material (χ):

$$v_d = F_d/\chi \quad \text{(A-11)}$$

In reality, the deposition velocity is a function of the particle size. The larger the particle, the larger its deposition velocity, up to the Stokes velocity limit. From various field experiments conducted over the years, dry deposition velocities range from 0.001 – 180 cm/s for particulates, while for gases it ranges from 0.002 – 26 cm/s.

Dispersion models such as GENII permit the treatment of particle sizes and assign different deposition velocities to each of user-prescribed particle size bins. The challenge facing the analyst is to assign radioactive material into these bins that has been generated under accident conditions. More than fifty variables exist that can influence the magnitude of the rate of dry deposition removal. These are categorized into micrometeorological, depositing material, and surface variable categories.

Typically, simplifying assumptions are made, based on radionuclide species, chemical form, and whether the emitted radioactive material is filtered or non-filtered. For noble gases and tritiated hydrogen gas (HT), no deposition should be modeled. For filtered particulate releases, the deposition velocity is assumed to 0.001 m/s. This dry deposition velocity corresponds to a particle with an approximate aerodynamic equivalent diameter (AED) of 0.2 μm to 0.4 μm (Sehemel, 1978). For unfiltered particulate releases, such as through cracks and open breaches assumed in the accident conditions, the deposition velocity is assumed to 0.01 m/s. This dry deposition velocity corresponds to a particle with an approximate aerodynamic equivalent diameter (AED) of 2 μm to 4 μm. Tritium oxide is normally taken to have a deposition velocity of 0.005 m/s (Fallon, 1982) and (Sweet, 1984).

A-1.5.3.2 Wet Deposition

Wet deposition through precipitation, depletes the plume to some degree. This phenomenon is difficult to parameterize due to its dependency on cloud physics variables which themselves vary over time and space. All types of precipitation (i.e., rain, snow, hail), passing through the plume will collect particulates and scavenge soluble gases. Wet deposition can be approximated by the following correction factor to a dispersion model:

$$D_w = exp\ (-vx/u) \quad \text{(A-12)}$$

where D_w represents the wet deposition and v represents a washout coefficient (s^{-1}), which itself is a complex function of precipitation particle-size spectrum, precipitation rate, radioactive or hazardous chemical particle-size distribution, and the solubility of the effluent. As previously, x is the downwind distance of the plume centerline from its release point, and u is the wind speed. Families of empirical curves have been developed for various rainfall rates (mm/hr) to estimate the washout coefficient. This procedure is made more complex by the spatial variability of the rainfall. Frequently, rainfall rates vary significantly within a rainfall event, and different

washout coefficients may need to be applied to various segments of the plume as it travels to the receptor.

Wet deposition is not modeled in consequence calculations for either the MOI receptor, or the onsite receptors supporting Mitigated Hazard Analysis. While not applicable to deterministic safety analysis, it is usually credited as part of a site's historical data patterns in probabilistic safety assessments (PSAs).

In addition to these mass-transfer processes, in-growth and decay of radioactive releases constantly occur during the transport and dispersion process. The process of in-growth and decay of radioactive isotopes in the plume is a function of the travel time and the half-life of each specific radionuclide present in the plume. In practice, this effect is appreciable for radioisotopes of half-life on the same order or shorter than the time to reach the receptor under consideration. For non-reactor facilities, an inadvertent criticality would be the primary accident type for which this factor is important.

Decay changes to the population of parent nuclide can be represented by the following factor:

$$A_i(t)/A_0 = exp(-\lambda_i t) = exp(-\lambda_i x/u) \qquad \text{(A-13)}$$

where λ_i is the decay constant of the i^{th} radionuclide species, $A_i(t)$ is its activity at time t, and A_0 its initial activity. Travel time, t, is the ratio of travel distance x, and the mean wind speed, u. Time zero ($t = 0$) is the moment of release into the environment.

Recommendation: Either the source model or surface model for depletion may be used in accident analysis. Do not model dry deposition for noble gases or tritium gas (HT or T_2). For filtered particulate releases, the deposition velocity can be taken as 0.001 m/s. For unfiltered releases, the deposition velocity is 0.01 cm/s. Tritium oxide (HTO or T_2O) has been characterized with a deposition characteristic of 0.005 m/s. Do not credit wet deposition for DSA accident conditions. Account for decay and in-growth if the initial radionuclides involved at the start of the accident condition have half-lives shorter than the travel time to the receptor.

A-1.5.4 Resuspension

Whereas deposition addresses mass-transfer from the plume to the ground surface, resuspension addresses the opposite processes. In resuspension, material that has already been deposited from the plume, or which has been on the ground for some time, is re-entrained by the wind. The particulates are reintroduced into the atmosphere and transported to a new location. While this effect can be non-negligible for DOE facilities in high-wind and environments without significant intervening vegetation, Appendix A to DOE-STD-3009-94, CN#2 indicates that resuspension "need not be modeled".

Recommendation: The analyst need not explicitly account for resuspension in the dose calculation of an accident condition for a DSA.

A-1.5.5 Deposition and Reemission of Tritium

While dry deposition is observed for most non-noble gas radioactive species and results in diminished plume concentrations as a function of downwind transport, tritium in particular, deposits and re-emits through mechanisms that are distinct from other radionuclides. The major biophysical processes are

(lxxxi) Initial settling to ground

(lxxxii)HT conversion to HTO by soil

(lxxxiii) HTO uptake by plants (and partial conversion to organically-bound tritium)

(lxxxiv) HTO re-emission from soil and plant

(lxxxv)Uptake by vegetation root systems

(lxxxvi) Transport into deeper soil regions.

In evaluating tritium-containing plumes in accident analysis, it is important to recognize that tritium will tend to move in the hydrogen pool throughout the environment. For tritiated water vapor, this will mean rapid uptake depending on difference in concentration. Furthermore, re-emission of tritium from soil and vegetation will take place after plume passage. The latter phenomenon usually takes place on a time scale much longer than the initial removal from the plume (O'Kula, 2001).

A-1.5.6 Plume Rise Mechanisms

Two physical processes can vertically propel a neutrally buoyant plume to a higher level above the ground from its initial point of release. Both of these mechanisms are collectively called plume rise. The first mechanism is termed momentum plume rise, in which the velocity of the release (i.e., efflux velocity) vertically propels the plume due to the excess momentum of the release itself. Accordingly, this is termed momentum plume rise.

The other plume rise mechanism is through buoyancy. Buoyancy plume rise occurs if the temperature of the release is warmer than the ambient air. It is also important to account for stack tip downwash of the plume under high wind speed conditions and plume downwash into the wake and cavity behind the building if the release is from a vent or small stack. A brief discussion follows on both of these plume rise components, and how they interact with forces that tend to downwash. Lastly a series of equations are identified that can be integrated into an atmospheric transport and dispersion model to account for the magnitude of these effects.

A-1.5.7 Momentum Rise

The estimation of the momentum rise component requires knowledge of the efflux velocity at the point of release, the wind speed at the point of release, and the diameter of the stack from which the effluent is released. The smaller the stack diameter, the faster the efflux velocity for a given efflux. The efflux velocity is directed vertically, normally, while the wind speed is directed horizontally. Therefore, the ratio of efflux velocity to wind speed determines the initial plume

rise. As the plume is transported downwind, the momentum from the efflux velocity vanishes and the wind speed bends the plume over into the horizontal plane. Any additional plume rise beyond the point of release only occurs due to plume buoyancy.

A-1.5.8 Plume Rise and Entrainment Methods

NRC Regulatory Guides 1.111 and 1.145 define a "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977, 1983). Open-field, "parking lot" dispersion calculations assume non-stack releases, but with no influence of neighboring structures. Releases can be considered to be at ground level if the point of release is below the height of the facility in question and collocated buildings. The intermediate case of releases that occur in the range between 2.5 times the height of adjacent buildings and the building height is difficult to parameterize. Under some circumstances, the plume escapes the building wake; under other conditions, it becomes completely entrained into the building wake; and under still other conditions, it behaves as a "mixture" of these types (NRC, 1998). Several rules of thumb are presented in this section to guide analysis under these conditions.

The NRC guidance differs moderately from the EPA Good Engineering Practice (GEP) stack height criteria. Applying the EPA criterion, the entire effluent escapes the influence of the facility structures if the stack height is 1.5 times the height of the nearest facility structure plus either the height or width of that structure, whichever is larger. For releases from structures that meet GEP stack height criteria, and under neutral or unstable stability conditions, the amount of plume rise, h_{pr}(m), is:

$$h_{pr} = 1.44d\,(v_e/u)^{0.667}(x/d)^{0.333} - C \qquad \text{(A-14)}$$

where v_e is the efflux velocity (m/s), u is the wind speed (m/s), x is the downwind distance (m), and d is the diameter of the stack (m). This equation shows the relationship between the two opposing parameters, v_e and u. C is the downwash correction factor (m), given by:

$$C = 3[1.5 - v_e/u]d \qquad \text{(A-15)}$$

Under stable (e.g., E-G stability classes) atmospheric conditions, two empirical equations are evaluated:

$$h_{pr} = 4\,(F_m/S)^{0.25} \qquad \text{(A-16a)}$$

and

$$h_{pr} = 1.5(S)^{-0.1666}\,(F_m/u)^{0.333} \qquad \text{(A-16b)}$$

The smaller value is chosen. In these two equations, the momentum flux is $F_m = v_e^2(0.5d)^2$, and the stability parameter is $S = g/[T(-d\theta/dz)]$. For these equations, g represents gravitational acceleration (m/s^2), T is the ambient temperature (K), and $d\theta/dz$ is the potential temperature lapse rate (K/m), which is related to the actual lapse rate.

For plume rise from non-GEP stacks or building vents, empirical relationships from field studies have been developed, where the v_e/u ratio is the driving parameter. When $v_e/u > 5$, the vertically-directed momentum flux (i.e., escape building effects) dominates the horizontally-directed wind speed (i.e., capture building effects), and the release is treated as elevated. This means that although the release emanated from a vent, it still will fully escape the aerodynamic effects of nearby buildings due to the high momentum flux coupled with low wind speed, and the GEP stack height equations apply. On the other end of the spectrum, when the $v_e/u < 1$, the release is ground level and no plume rise occurs. Two intermediate cases were also developed from field studies. These are the partially entrained and the partially elevated cases and are expressed in terms of an entrainment coefficient, E_t. The entrainment coefficient is defined as the fraction of the plume entrained in the wake and cavity of the building.

Partially Entrained: For cases where the $1.5 \leq v_e/u < 5$, a portion of the plume is entrained and the remainder of the plume remains elevated. The entrainment coefficient for this case is:

$$E_t = 0.30 - 0.06 v_e/u \qquad \text{(A-17)}$$

Partially Elevated: For cases where the $1 \leq v_e/u < 1.5$, the entrainment coefficient is:

$$E_t = 2.58 - 1.58 v_e/u \qquad \text{(A-18)}$$

In both of these cases, the elevated portion of the plume is subject to plume rise, while the entrained portion of the plume is downwashed to ground level. Building wake effects are discussed in more detail in a later section.

A-1.5.9 Buoyancy Rise

Buoyancy effects usually arise if significant sensible heat is contained in the cloud being released. For nonreactor DOE facilities, the primary sources of these cloud types are through postulated explosion or fire events. The estimation of the buoyancy component requires knowledge of the effluent and ambient temperatures at the point of release. If the effluent temperature is higher, positive (i.e., upward) buoyancy occurs, while for a cold or dense cloud, negative buoyancy will occur. The latter condition is normally associated with certain types of chemical releases, more so than for radiological releases. The stability class of the atmosphere is also very important, as it affects the magnitude of the buoyancy plume rise.

Buoyancy rise is usually calculated in two steps. The first is the initial rise and is dependent on the stability class. The second is the gradual rise and is independent of stability class. The larger of the two is then selected as representative.

Initial Plume Rise: For stability classes A – D, and buoyancy fluxes less than 55 m^4/s^3, the plume rise is given by (Briggs, 1971)

$$\Delta h = 21.425 \, F_b^{3/4} \, u^{-1} \qquad \text{(A-19a)}$$

where F_b is the buoyancy flux

$$F_b = g\, Q_h/(\pi\, C_p\, \rho_a\, T_a) \qquad \text{(A-19b)}$$

with units of [m^4/s^3]. In this equation, g is the gravitational acceleration, C_p is the specific heat of the effluent gases, ρ_a is the density of air, and T_a is the ambient air temperature.

For fluxes greater than 55 m^4/s^3, the plume rise is given by

$$\Delta h = 38.71\, F_b^{3/5}\, u^{-1} \qquad \text{(A-20)}$$

For stability classes E - G, the plume rise is given by (Randerson, 1984)

$$\Delta h = 2.6\ [F_b/(u\, S)]^{1/3} \qquad \text{(A-21)}$$

In calm conditions, a better approximation is provided by

$$\Delta h = 4\ F_b^{1/4}\, S^{3/8} \qquad \text{(A-22)}$$

In these last two equations, S is a stability parameter with units of inverse time squared (t^{-2}).

Gradual Plume Rise: The second portion of plume rise, gradual plume rise, is applicable to unstable to neutral conditions and can be calculated from

$$\Delta h = 1.6\, F_b^{1/3}\, x^{2/3}\, u^{-1} \qquad \text{(A-23)}$$

The buoyancy flux from a fire is $F_b = 8.79\times10^{-6}\ \Omega$, where Ω is the rate of release of sensible energy in watts (W).

Another model is that from Mills (1987). It is based on an area (pool) fire and is more correct for facility accident analysis where the assumed fire has compromised or breached an area in the facility. The Mills method adjusts the Briggs effective release height to a lower value using

$$H_{Mills} = \{\, (H_{Briggs})^3 + (R/\gamma)^3 \,\}^{1/3} - R/\gamma \qquad \text{(A-24)}$$

where

H_{Briggs} = effective release height estimated with the Briggs approach (equation A-19)

R = radius of burning pool

G = entrainment coefficient for buoyant plume rise.

An area or full facility fire event would fall in this category.

Several significant issues exist in modeling a fire event in accident analysis and the ensuing release into the environment. These include

- Sensible heat released
- Fire plume history

- Radiological material involvement in the fire.

Sensible heat – The fraction of the heat of combustion that is not radiated is available to cause a temperature increase in the air and other gases emitted in the plume. This energy is the sensible heat that acts to effectively increase the height of release. The radiated fraction can vary with the nature of the fire, but a typical value is 0.3 – 0.4, implying a sensible heat release of 0.6 - 0.7 of the total heat released. However, for indoor fires in complex facilities, the fraction can vary with the heat being radiated to structures (walls and ceilings) becoming available for heating of air. On the other hand, plumes released into a facility tend to be cooled before escaping the structure and therefore not be as buoyant as if released outdoors.

Fire plume history – Another uncertainty that exists is the temporal nature of the fire. For the same amount of radiological material released, short duration fires will lead to larger dose than longer fires due to less crosswind meander.

Radiological material involvement – Depending on facility type and location of radiological hazards with respect to the combustible loading, the fire may have a radiological component that is evenly distributed in time, localized to certain intervals, or some combination. The radioactive release history may not match up in time with the sensible heat release.

Thus, fires represent complex phenomenology that can demand an inordinate level of precision relative to the purpose of accident analysis. While MACCS and other codes allow use of an effective height model based on sensible heat released, the uncertainties in fire duration, sensible heat, and radiological material involvement introduce a significant burden to the analyst to defend.

Recommendation(s):

External (outdoor) fires: Determine the sensible heat fraction for well-defined fires. Credit only sensible heat fraction for the thermal buoyancy effect. Assume shortest duration consistent with fire sequence definition.

Internal (indoor fires): Assume no sensible heat release for release to environment. Assume shortest duration consistent with fire sequence definition.

If the source term analysis can defend the amount of sensible energy, the temporal history, and the spatial distribution, then this phenomenon may be modeled in the consequence analysis. If this cannot be defended adequately, then the source term from fire should be estimated using recommended five-factor methodology, and the consequent environmental model should assume a short duration fire, occurring as a ground-level release.

A-1.5.10 Building Wake Effects

As shown in an earlier section, releases from vents and small stacks can be entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs. Figure A-3 depicts the wake and cavity zones downwind of a nuclear facility. The downwind direction is x, the facility height is H_B, and A_B is the projected cross-sectional area

of the building most influencing the flow of the plume. For most bounding, screening purposes, A_B may be assumed the surface area of the largest wall of the building nearest the receptor. To a first approximation, the extent of the cavity zone may be taken to be approximately a downwind distance of 2.5 $A_B^{0.5}$. Similarly, the wake zone may extend to roughly ten times $A_B^{0.5}$.

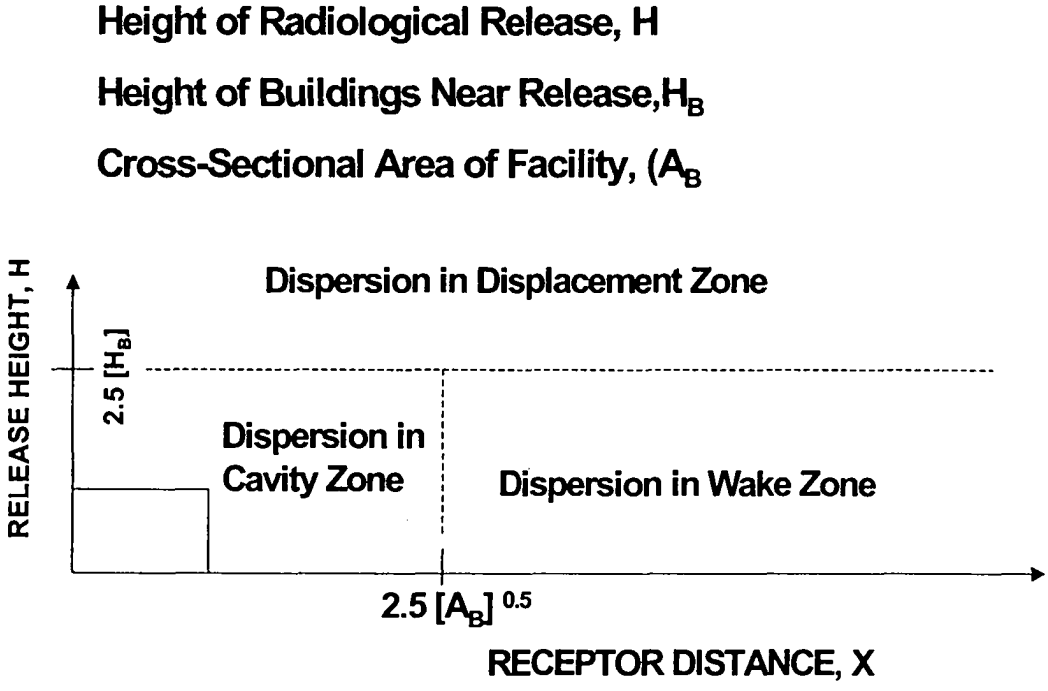

Figure A-2. Cavity and Wake Zones downwind of a Building Structure (Constant Wind Direction from Left to Right).

In order to account for aerodynamic effects of the building, the ground level dilution factor equation is modified as

$$\chi/Q = (u\,[\pi\,\sigma_y\,\sigma_z + c\,A])^{-1} \qquad \text{(A-25)}$$

where c is the building shape factor, usually taken to be 0.5, A is the smallest cross-sectional area of the building, u is the wind speed at 10-meter height, and the σ_z is corrected for the wake effect.

This formulation is to be applied in the context of NRC Regulatory Guide 1.145 for non-stack releases, e.g., vent and other building penetrations (NRC, 1983). Building wake effects tend to be appreciable under windy conditions, while the plume meander effects (discussed earlier) are more likely under light wind conditions.

An approximate form for the wake zone concentration of airborne release from a "squat" (length and width are > height) facility, up to a receptor distance of 10 building heights (10 H_B) is given by (Turner, 1970),

$$\chi/Q \approx 1/(u\ \pi\ \sigma'_y\ \sigma'_z) \qquad \text{(A-26)}$$

where

$$\sigma'_y = 0.35\ h_w + 0.067(x - 3\ H_B),$$
$$\sigma'_z = 0.70\ h_w + 0.067(x - 3\ H_B),$$
$$h_w = 0.866\ [(\text{Facility Length})^2 + (\text{Facility Width})^2]^{1/2}.$$

The dispersion parameters for this condition are those found in (EPA, 1995). The distance, x, is measured from the facility center.

For screening purposes, several empirical formulas are available for the cavity and wake zone concentrations. A suggested set is found in (NCRP, 1996).

A-1.5.11 Extreme Weather Conditions

Section A.3 of Appendix A to DOE-STD-3009-94, CN#2, indicates, "For accident phenomena defined by weather extremes, actual meteorological conditions associated with the phenomena may be used for comparison to the EG". A common weather extreme that is frequently addressed in many DSAs is that due to tornadoes.

The accident analysis should at minimum consider two periods for subsequent exposure evaluation: (1) that due to meteorological conditions from the tornado impact or strike itself; and (2) a second, more prolonged period after the tornado. The latter period would account for aerodynamic re-entrainment and resuspension acting to transport radiological material from the facility into the environment. The first period would be modeled with a design basis accident dilution factor (Ψ/Q, similar to χ/Q) designated for a specific class tornado and applied for the distance from the facility to the receptor. The second period is modeled using a standard consequence model for an exposure period of no longer than eight hours, to be consistent with the time period specification discussed in Appendix A to DOE-STD-3009-94, CN#2.

For the initial strike period, the appropriate Fujita scale should be applied. For most safety analyses, this is either Fujita-2 (F2) or F3. Figure A-2 shows the maximum time-integrated ground-level centerline air concentration (s/m^3) vs. downwind distance (km) for different mean translational speeds of the F2 tornado (Weber, 1996). The consequence analysis should pick a maximum Ψ/Q for the assumed translational speed. For example, the translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers downwind. This exposure should be added to that obtained for that distance using the standard 95th percentile methodology to estimate the full exposure due to the event. It is possible that the standard 95th percentile methodology at the site boundary may yield a larger dose than the total dose at the maximum Ψ/Q, in which case the MOI would be considered to be at the site boundary.

Another extreme weather condition is high straight-line winds, which are not rare at some sites. High winds correspond to a stability class of D, which is the same class that occurs for median (or "typical") conditions. In this case, the χ/Q value can be scaled from the median conditions by taking ratios of wind speeds for the two conditions, as χ/Q is inversely proportional to wind speed. For example, if median conditions correspond to a wind speed of 4.5 m/s (which is

common) and the high straight-line wind speed is 45 m/s (about 100 mph), the resultant χ/Q would be 10% of the median value.

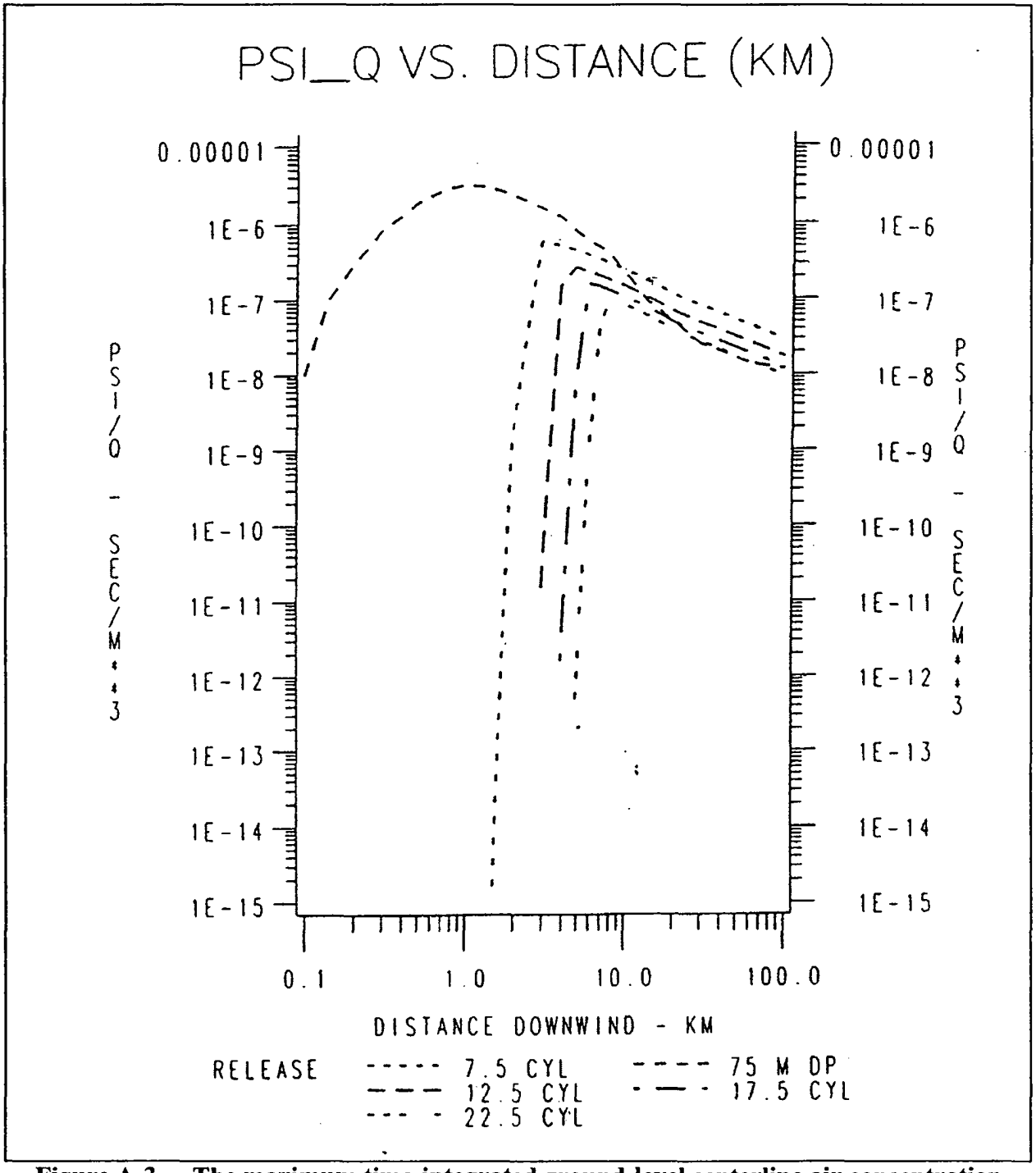

Figure A-3. The maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km) for tornado mean translational speeds from 7.5m/s to 22.5 m/s. The downdraft speed is 10 m/s and the height of the cylindrical mesocyclone is 3,500 m (from Weber and Hunter, 1996).

A-1.4.3 Mixing Layer Height

For an evaluation of χ/Q that includes reflections from the ground and the top of the mixing layer, an estimate of the depth of the mixing layer is required. This height varies throughout the day and throughout the seasons. During clear nights, when inversions are present, the mixed layer is relatively shallow, while during sunny days the mixing layer is much deeper. The magnitude of the depth of the mixing layer can be obtained from balloon soundings or from remote sensing techniques, such as acoustic or radar soundings. In the absence of such data, regional tables can be consulted, such as those of (Holzworth, 1972).

Recommendation: Calculate mixing layer depth from seasonal averages and time of day (viz., day vs. night), applying archived site meteorological data. If this is not applicable, use regional data as default input values, such as from (Holzworth, 1972).

A-1.4.4 Dispersion Parameters

Many schemes have been proposed for establishing the magnitudes of σ_y and σ_z. Most of these are based on empirical curve fitting of data taken during experiments over flat grassland (Haugen, 1959). One commonly used curve-fitting method is that of Tadmor and Gur Tadmor, 1969), in which each σ is expressed as a power law:

$$\sigma = a\,x^{b} + c \tag{A-4}$$

where a, b, and c are empirical constants, given in Table A-1.

Table A-1. Fitting Constants for σ_y and σ_z - Tadmor and Gur

Curve Fitting Constant	ATMOSPHERIC STABILITY CLASS					
	A	B	C	D	E	F
a_y	0.3658	0.2751	0.2089	0.1474	0.1046	0.0722
a_z	0.00025	0.0019	0.2	0.3	0.4	0.2
b_y	0.9031	0.9031	0.9031	0.9031	0.9031	0.9031
b_z	2.094	1.098	0.911	0.516	0.305	0.18
c_y	0.0	0.0	0.0	0.0	0.0	0.0
c_z	9.6	2.0	0.0	-13.0	-34.0	-48.6

Another commonly used curve-fitting method is that of Briggs (Briggs, 1973), for which each σ is expressed as

$$\sigma = a\,x(1 + bx)^{-\frac{1}{2}} \tag{A-5}$$

where a and b are constants, given in Table A-2.

Table A-2. Fitting Constants for σ_y and σ_z from Briggs

Curve Fitting Constant	ATMOSPHERIC STABILITY CLASS					
	A	B	C	D	E	F
	Open-Country Conditions					
a_y	0.22	0.16	0.11	0.08	0.06	0.04
a_z	0.20	0.12	0.08	0.06	0.03	0.016
b_y	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001
b_z	0	0	0.0002	0.0015	0.0003	0.0003
	Urban Conditions					
a_y	0.32	0.32	0.22	0.16	0.11	0.11
a_z	0.24	0.24	0.20	0.14	0.08	0.08
b_y	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004
b_z	0.001	0.001	0	0.0003	0.00015	0.00015

The most commonly used curves are the Pasquill-Gifford curves based on measurements at Project Prairie Grass in the mid-1950s. They are found in (Slade, 1968), and are based on three-minute averaging times. An empirical formula derived the Pasquill-Gifford parameters has the following form for σ_y and σ_z, and is based on work published by (Yuan, 1993), where

$$\sigma_y(x) = (0.000246\ \sigma_\theta^2 + 0.00576\ \sigma_\theta + 0.066)\ x^{0.9031} \quad \text{(A-6)}$$

and

$$\sigma_z(x) = a\ x^b + c \quad \text{(A-4)}$$

Coefficients and constants for various downwind distances and stability classes are given in Table A-3. The Tadmor-Gur and Briggs formulations, as well as others, give results that are nearly the same for some ranges and stability classes. However, they may differ by a factor of two or more for other ranges/classes. The coefficients given in these tables, and in other Gaussian models, are based on fitting curves to observational data of plumes released over flat grassland. In the case of the Briggs model, an adjustment for urban conditions has also been made. The Pasquill-Gifford formulations also specify different coefficients for different ranges of distance. It should be noted that the database underlying the empirical curve fits is valid for distances between 100 m and 1,000 m.

For distances less than about 100 m, these coefficients generally do not provide a good fit to the observations and the models are generally considered approximate. This is because the Gaussian models, with the underlying assumption of steady state, do not perform well in the near field.

In practice, the concentration at close-in receptor distances is frequently influenced by the physical presence of the facility from which the plume is released, as well as neighboring structures. Often, building wake effects are important for these smaller distances but the above coefficients ignore the enhancement of vertical turbulence from wake effects, downwashing into

the wake cavity behind the building, as well as recirculation. These effects can influence concentrations and building-geometry correction factors are often applied.

Recommendation: Consult with the laboratory or site meteorology organization responsible for recording and maintaining site data, and request a best-fit set of dispersion parameters for the region of transport applicable to the analysis. As a default, apply Tadmor-Gur, Briggs, or Pasquill-Gifford dispersion parameter sets, based on site-specific and surface roughness characteristics.

Table A-3. Pasquill-Gifford Dispersion Coefficients (Eimutis, 1972)

	Coefficients				
Applicable Distance, m	**Stability Class**	σ_θ	**a**	**b**	**c**
x > 1,000	A	25	0.00024	2.094	-9.6
	B	20	0.055	1.098	2.0
	C	15	0.113	0.911	0.0
	D	10	1.26	0.516	-13.0
	E	5	6.73	0.305	-34.0
	F	1.5	18.05	0.18	-48.6
100< x <1,000	A	25	0.00066	1.941	9.27
	B	20	0.0382	1.149	3.3
	C	15	0.113	0.911	0.0
	D	10	0.222	0.725	-1.7
	E	5	0.211	0.678	-1.3
	F	1.5	0.086	0.74	-0.35
x<100	A	25	0.192	0.936	0.0
	B	20	0.156	0.922	0.0
	C	15	0.116	0.905	0.0
	D	10	0.079	0.881	0.0
	E	5	0.063	0.871	0.0
	F	1.5	0.053	0.814	0.0

A-2 Radiological Consequences

This section provides guidance to the safety analyst regarding evaluation of radiological doses and health risks. It discusses the different types of radiation and the effect radiation can have on the human body, its organs, and its tissues. The factors that must be considered in estimating the dose a receptor may receive following the atmospheric release of radioactive material are covered in detail. Finally, the health risks associated with radiological doses and the standards for radiation protection, in terms of allowed dose or air concentration, are discussed.

A-2.1 Types of Radiological Exposures

Radiological doses can arise from exposure to clouds of radioactive material and fallout from the cloud, and from exposure to prompt (direct) radiation from a criticality. The modes of exposure include:

(lxxxvii) inhalation of radioactive material (particulates and gases) in a cloud,

(lxxxviii) inhalation of particulates from fallout that have been resuspended by traffic or by wind,

(lxxxix) ingestion of food products and water contaminated by fallout from the cloud,

(xc) gamma radiation from the plume (cloudshine)[13],

(xci) gamma radiation from particulates deposited on the ground from fallout (groundshine),

(xcii) skin contamination from fallout, and

(xciii) prompt (direct) radiation from a criticality.

Of especial concern to many DOE non-reactor facilities are inadvertent criticality events and exposure to actinide particulates. In the case of a criticality, doses arise from both the plume of fission products that may be released and from the prompt radiation. The primary contributor to dose from a criticality plume is cloudshine, although actinide particulates can also be important for an unfiltered release. Prompt radiation from a criticality is of concern only for workers located near the accident site. The distance of concern for prompt radiation depends upon the size of the criticality (number of fissions) and the amount of shielding (as from concrete walls) between the worker and the site of the criticality. On the other hand, for actinide exposure, inhalation of plutonium particulates is the primary radiological concern; cloudshine, groundshine, skin contamination, and ingestion doses are insignificant in comparison (Peterson, 1993). Inhalation of enriched uranium particulates is of lesser concern and inhalation of depleted uranium particulates are trivial by comparison (Peterson, 1995). For uranium, chemical toxicity is normally of greater concern than is the radioactivity.

A-2.2 Types of Radiation

Four types of radiation are important in accident analysis for DOE nuclear facilities: alpha (α), beta (β), gamma (γ), and neutron. The α, β, and γ radiations are emitted from atomic nuclei during radioactive disintegration (or decay) of the nucleus. The neutron radiation is emitted when a nucleus fissions (breaks into fragments), such as during an inadvertent criticality[14]. Alpha particles are energetic (fast-moving) helium nuclei – consisting of two protons, with a

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[13] Cloudshine also may contain a contribution from beta radiation and its attendant *bremsstrahlung* (discussed below), but this is normally minor compared to the gamma radiation.

[14] Neutrons can also be produced through (α,n) reactions, in which an alpha particle strikes the nucleus of an atom, causing the emission of a neutron. This is generally not important for dose calculations as the additional dose from the neutron radiation is balanced by the decreased dose from the lost alpha particle.

charge of +2[15], and two neutrons (no charge). Beta particles are energetic electrons, of charge -1, or positrons, of charge +1. They have a mass about 0.01% that of the alpha particle. Gamma radiation consists electromagnetic waves, or photons. Gamma rays have energy similar to that of X-rays, and, being photons, have neither charge nor mass. Gamma radiation typically accompanies alpha and beta radiation. Neutron radiation consists of energetic neutrons. Neutrons are particles with zero charge and mass similar to that of protons, that is, about 25% of the mass of alpha particles. When radiation strikes an organ or tissue of the body, it can deposit some or all of its energy, causing damage. The manner of energy deposition varies with the type of radiation. Some types of radiation, principally alpha and beta, deposit energy primarily by ionization. Upon striking an atom, an electron is stripped off, and the atom is said to be ionized. The two charged particles thus formed – the electron and the ion – are referred to as an ion-pair. The electron that is stripped off the atom may be sufficiently energetic that it can cause further ionization. The amount of ionization created depends upon the mass, charge, and energy of the particle. Particulate radiation (α, β, and neutron) can also deposit their energy through the dissociation of molecules and through elastic scattering, which causes heating.

Alpha-decay energy is typically on the order of several MeV (mega-electron volts)[16]. For example, plutonium, uranium, and americium all emit alpha particles with energies on the order of 5 MeV. Because an alpha particle is doubly charged and massive, it can ionize many atoms that it may encounter. For example, an alpha particle traveling through air will create on the order of 50,000 ion pairs for each centimeter it travels. Because it creates so much ionization, it deposits its energy quickly, and penetrates only a short distance into a tissue.

Beta-decay energy is typically on the order of tens of keV to a few MeV. For example, the beta-decay energy of ^{241}Pu is 21 keV. During beta decay, the emitted electron (or positron) is accompanied by a neutrino (or anti-neutrino), with which it shares the energy. The beta-decay energy is the sum of the energies of the electron and neutrino. Thus, for ^{241}Pu, the maximum energy the electron can have is 21 keV; normally, it will have only ~ 1/3 of this. Because the beta particle is singly charged and not very massive, it cannot create nearly the amount of ionization as can an alpha particle. For example, a beta particle traveling through air will create on the order of 100 ion pairs for each centimeter it travels. In addition to causing ionization, beta particles also can be scattered elastically by atomic electrons. Because a beta particle doesn't lose its energy as rapidly as does an alpha particle, and because of elastic scattering, it can penetrate more deeply into tissue. However, it travels an irregular path in tissue because of elastic scattering. This gives rise to the emission of electromagnetic radiation called *bremsstrahlung* (German for "braking radiation"), which in turn can deposit its energy in the surrounding tissue.

The energy of a gamma ray is typically on the order of tens of keV to a few MeV. For example, the energy of one of the (several possible) gamma rays that accompanies the alpha decay of ^{239}Pu is 52 keV. A gamma photon will typically create only about one ion-pair per centimeter in air.

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[15] The basic unit of charge is that of the electron, but with a reversal of sign. The charge of an electron is -1.60×10^{-19} coulomb.

[16] An electron volt is the kinetic energy of an electron after being accelerated through an electric potential difference of one volt. It is equal to 1.60×10^{-19} joule.

A gamma photon can also lose its energy through Compton scattering from electrons and even from interactions with the nucleus of an atom, although the latter are minor in comparison with photo ionization and Compton scattering. Gamma radiation is capable of penetrating deeply into the human body.

The energy of a fission neutron is typically on the order of a few keV to about 10 MeV. Because the neutron has no charge, it will not create many ion-pairs. It loses it energy primarily through elastic scattering. However, it can also cause nuclear transformations, especially when it has slowed (through elastic scattering) and become a "thermal" neutron. These nuclear transformations can lead to the emission of other radiation, such as α and γ. Neutron absorption through nuclear transformation is primarily by hydrogen and nitrogen in the body. Elastic scattering of neutrons is primarily by the hydrogen in the body. Like gamma radiation, neutron radiation is very penetrating.

A-2.3 Radioactivity

The *Système International d'Unités* (SI) unit of radioactivity, or simply *activity*, is the *becquerel* (*Bq*). It is equal to one disintegration per second (dps). The more commonly used, or traditional, unit of activity is the *curie* (*Ci*), and is equal to

$$1\ Ci = 3.7 \times 10^{10}\ Bq \qquad \text{(A-27a)}$$

This unit was derived from the activity of radium. The activity of one gram of ^{226}Ra was originally defined as one *Ci*. (Modern measurements, however, show that the activity of one gram of ^{226}Ra is slightly less than one *Ci*.) Conversely,

$$1\ Bq = 2.7 \times 10^{-11}\ Ci \qquad \text{(A-27b)}$$

The activity per unit mass is called *specific activity* and is measured in units such as *Bq/kg* or *Ci/g*. Thus, the specific activity of ^{226}Ra was originally defined as one *Ci/g*. The specific activity of a mixture of radionuclides is the sum, over all the radionuclides in the mixture, of the products of specific activities and mass fractions.

The activity of a sample of any given radionuclide decreases exponentially with time, providing it is not being created by the decay of another radionuclide. If N is the number of atoms of a specific type of radionuclide in a sample of material, the change in this number, dN, in a small interval of time, dt, is proportional to N and to dt. This is written

$$dN = -\lambda N\, dt \qquad \text{(A-28)}$$

where the negative sign is needed to show that N decreases with increasing time. The constant of proportionality, λ, is called the decay (or transformation) constant and is measured in inverse time units, such as s^{-1}. The disintegration rate, or activity (A), is given by

$$A = -dN/dt = \lambda N \qquad \text{(A-29)}$$

The solution to equation (A-28) is

$$N = N_0 e^{-\lambda t} \quad \text{(A-30)}$$

where N_0 is the number of atoms at time $t = 0$. Thus, equation (30) can be written

$$A = A_0 e^{-\lambda t} \quad \text{(A-31)}$$

where $A_0 = \lambda N_0$ is the activity at time $t=0$.

Because the decay is exponential, the time interval to decrease the number of atoms in a sample by a given factor is a constant. For example, the time to decrease by a factor of two, called the half-life ($t_{½}$), is obtained by inverting equation (A-30):

$$t_{½} = -(1/\lambda) \ln(½ N_0 / N_0) = (1/\lambda) \ln(2) = 0.693 / \lambda \quad \text{(A-32)}$$

The half-life of ^{239}Pu, for example, is 2.44×10^4 years and that of ^{235}U is 7.1×10^8 years. The specific activity of ^{235}U is therefore about 3×10^4 times smaller than that of ^{239}Pu, which is the reason it doesn't present as great a radiological hazard as ^{239}Pu for a given amount of material.

A-2.4 Effects of Radiation on the Body

Radiation damages the body as it deposits its energy (primarily through ionization) in organs and tissues. Because alpha radiation can be stopped by the body's epithelium (outer layer of dead skin cells), it poses no external hazard to the body; rather, its hazard is through inhalation and ingestion. Beta radiation can penetrate the skin (barely) to cause some damage; beta radiation can also damage the eye. Like alpha radiation, its damage comes principally from inhalation and ingestion, although less so than from alpha radiation. Gamma radiation and neutrons, on the other hand, cause damage as they penetrate the body directly from external sources. Material that emits gamma radiation and neutrons can, of course, be inhaled or ingested, but this is not the normal mode of exposure. Skin contamination from fallout causes tissue damage principally from β radiation.

Both short-term and long-term exposures are important. External radiation (from cloudshine, groundshine, skin contamination, or prompt radiation) typically gives a short-term, or even instantaneous dose, whereas internal radiation (from inhalation and ingestion) gives a long-term (committed) dose. A long-term dose can also arise from continual exposure to external radiation, as in a work place. If a radioactive particle is inhaled or ingested, it will cause damage as long as it remains in the body, because it contains many radioactive atoms that continue to disintegrate. If an organ or tissue is irradiated for an extended time, it can develop cancer or suffer other deleterious effects.

A-2.5 Dose Evaluation

The effects of exposure to ionizing radiation were originally defined in terms of the amount of ionization in air produced by gamma radiation and X-rays. The unit used was the *Roentgen* (R), now defined as the ratio $\Delta Q/\Delta m$, where ΔQ is the sum of all charges of one sign produced in air when all the electrons liberated by photons in a mass Δm of air are completely stopped in air. It

is equal to 2.58×10^{-4} coulombs produced in one kg of air. This is equivalent to 1.61×10^{15} ion-pairs produced per kg of air or an energy deposited of 87.3 erg per gram of air (Turner, 1986). Absorption of 1 *R* of radiation in tissue corresponds to about 95 ergs per gram of tissue.

Today, dose is expressed as an absorbed dose, i.e., the amount of energy deposited in matter, or as an equivalent dose, a measure of damage done in tissue. The traditional unit of absorbed dose is the *rad* and is defined as 100 ergs absorbed in one gram of material, slightly greater than the *Roentgen*. The newer (*SI*) unit is the *gray* (*Gy*) and is defined as one joule absorbed in one kilogram of material. Thus,

$$1 \text{ Gy} = 100 \text{ rad}$$

This definition applies to any type of radiation absorbed in any type of material.

The dose of most interest in accident analysis is the equivalent dose, as this is a measure of the biological damage. The amount of damage depends upon the type of radiation as well as the amount of energy absorbed. The equivalent dose, H_T, to a particular tissue *(T)* is equal to the absorbed dose, D_T, in that tissue times a radiation-weighting factor, w_R

$$H_T = w_R D_T \tag{A-33}$$

where w_R is a measure of the amount of damage done by the radiation.[17] If more than one type of radiation impacts the tissue, H_T is calculated by summing over all radiation types. Table A-4 gives the ICRP 60 radiation weight factors (ICRP, 1991) for the four radiation types considered here.

[17] The definitions given here are taken from the *1990 Recommendations of the International Commission on Radiological Protection,* ICRP-60 (ICRP, 1991). In earlier recommendations of the ICRP, the terminology was a little different. The following table gives the old and new terminology. The old terminology is still in use.

Old Terminology	New Terminology
Quality Factor	Radiation Weighting Factor
Dose Equivalent	Equivalent Dose
Committed Dose Equivalent	Committed Equivalent Dose
Effective Dose Equivalent	Effective Dose
Committed Effective Dose Equivalent	Committed Effective Dose

The effective dose is not identical to the effective dose equivalent in that the organ weighting factors are slightly different (Table A-5) and the organs included in "remainder" are different. A similar statement can be made for the differences between committed effective dose and committed effective dose equivalent.

Table A-4. Radiation Weighting Factors

Type, Energy Range		Radiation Weighting Factor, w_R
Alpha	any energy	20
Beta	any energy	1
Gamma	any energy	1
Neutrons	< 10 keV	5
	10 keV to 100 keV	10
	>100 keV to 2 MeV	20
	>2 MeV to 20 MeV	10
	> 20 MeV	5

The traditional unit for equivalent dose is the *rem* (roentgen-equivalent, man). The newer (*SI*) unit is the sievert (*Sv*). The relation between them is the same as between *gray* and *rad:*

$$1 \text{ Sv} = 100 \text{ rem}.$$

The radiation-weighting factor is related to the stopping power of the material, expressed as *Linear Energy Transfer* (*LET*)

$$LET = dE/dx \qquad \text{(A-34)}$$

where dE is the average energy locally imparted to the medium by a charged particle traversing the distance dx. Alpha and beta particles have high and low LET, respectively. Gamma radiation, although not a charged particle, is considered equivalent to low LET radiation. Neutrons have a moderate to high LET, depending upon their kinetic energy.

The definition of equivalent dose does not differentiate between short-term and long-term dose, or between external and internal exposure. A related term is committed equivalent dose, which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults (such as workers) or 70 years for children (as in the general population); it does not include external exposures. The committed equivalent dose is thus a subset of the equivalent dose. This has led to some confusion as it has led some workers to use (incorrectly) equivalent dose exclusively for external radiation, apparently as a counterpoint to committed equivalent dose, which is used exclusively for internal radiation. A new term, total organ dose equivalent (TODE), is now used to indicate the sum of the external (short-term) and internal (committed, long-term) doses to *an organ or tissue* (CFR, 1991).

Doses are also calculated for the body as a whole. This is done by summing over all organs the product of an organ weighting factor and the equivalent dose for that organ. This sum is called the effective dose (formerly, the effective dose equivalent (EDE) – a term still used). The organ weighting factors represent the fraction of the total health risk resulting from uniform whole-

body irradiation that could be attributed to that particular tissue or organ. These factors are between zero and one; their sum over all organs and tissues is one. The weighting factors for the various organs are shown in Table A-5, as taken from ICRP-60 (ICRP, 1991). For comparison, the ICRP-26 (ICRP, 1977) values are also shown, as they are still in use at many sites and laboratories.

Table A-5. Organ Weighting Factors

Organ	Organ Weighting Factor	
	ICRP-26	ICRP-60
Bladder	-	0.05
Bone Marrow (red)	0.12	0.12
Bone Surface (skeleton)	0.03	0.01
Breast	0.15	0.05
Colon	-	0.12
Esophagus	-	0.05
Gonads	0.25	0.20
Liver	-	0.05
Lung	0.12	0.12
Skin	-	0.01
Stomach	-	0.12
Thyroid	0.03	0.05
Remainder	0.30	0.05

A term similar to effective dose is committed effective dose (formerly, the committed effective dose equivalent – CEDE, a term still used), which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults, or 70 years for children. It does not include external exposures. Committed effective dose is thus a subset of effective dose. However, as with equivalent dose *cf.* committed equivalent dose, confusion has arisen in that some workers use (incorrectly) effective dose to refer to only external radiation, because committed effective dose refers only to internal radiation. A new term, total effective dose equivalent (TEDE), is now used to indicate the sum of the external (short-term) and the internal (committed, long-term) effective doses (CFR, 1991).

A-2.5.1 Types of Dose

Doses arise from both internal and external exposures, as noted above. The internal exposures consist of inhalation (from the plume and from resuspension) and ingestion. The external exposures are from cloudshine, groundshine, skin deposition, and direct (prompt) radiation from a criticality. These are discussed individually below. See the discussion earlier in this appendix for the calculation of the amount of material that falls out from a plume; this is important for the discussions of resuspension, ingestion, groundshine, and skin deposition.

A-2.5.2 Uptake through Inhalation

Inhalation dose from a cloud to a given organ or tissue from a given isotope (i) is the product of the amount of respirable radioactive material released (M_i), atmospheric dispersion factor (χ/Q), breathing rate (BR), and dose conversion factor (DCF_i)

$$Dose_i = M_i \times \chi/Q \times BR \times DCF_i \quad \text{(A-35)}$$

assuming the receptor remains exposed for the duration of the plume. The total dose to the organ or tissue is the sum over all isotopes inhaled. The amount of respirable material released (M_i), called the source term, is the product of the material at risk (MAR), damage ratio (DR), leakpath factor (LPF), airborne release fraction (ARF), and respirable fraction (RF). The breathing rate and dose conversion factors are discussed below and χ/Q was discussed earlier.

A-2.5.3 Breathing Rate

The breathing rates for the various activities, as have been used in accident analyses for the past several years at many DOE sites, are given in Table A-6 ICRP-2 (ICRP, 1977) and ICRP-30 (ICRP, 1979-82). The value used in the development of DOE-STD-1027-92 (Change Notice 1) tables is 3.5×10^{-4} m^3/s. ICRP-66 (ICRP, 1994) gives revised breathing for the "reference human"[18]. These are also listed in Table A-6. Still other breathing rates are appropriate for other individuals, such as infants, the elderly, and the infirm, and for other levels of activity perICRP-66, (ICRP, 1994). The analyst needs to choose which breathing rate is appropriate for the scenario being evaluated, taking into account the possible need to be consistent with earlier analyses.

Recommendation: Based on the DOE (DOE, 1998) directive, it is advised to apply the breathing rate of 3.33×10^{-4} m^3/s in dose calculations for DSAs.

[18] The reference human is male, 30 years old, height 176 cm (5 feet, 9 inches), and weight 73 kg (161 lb).

Table A-6. "Reference Human" Breathing Rates for Various Levels of Activity

Activity Level	Breathing Rate (m^3/s)
ICRP-2, ICPR-30, DOE 1998	
Chronic	2.66×10^{-4}
Light	3.33×10^{-4}
Heavy	3.47×10^{-4}
ICRP-66	
Sleep	1.25×10^{-4}
Rest, sitting	1.50×10^{-4}
Light exercise	4.17×10^{-4}
Heavy exercise	8.33×10^{-4}

A-2.5.4 Biokinetic Model and Dose Conversion Factors

Once radioactive material enters the lungs, it begins to migrate to other parts of the body. A portion is transferred directly to the blood and another portion to the stomach. Transfer of the material directly from the lungs into the blood depends upon where in the lungs it is deposited and how soluble it is. Material is also cleared from the lungs by means of the body's mucociliary mechanism and then swallowed, thus entering the gastro-intestinal (GI) tract. The fraction (f_1) of the material that passes from the GI tract into the blood (primarily from the small intestine) depends the solubility of the material. For some radionuclides, such as iodine, the transfer to the blood is nearly complete ($f_1 = 1.0$). For others, such as plutonium, the portion transferred to the blood is much less than 1%; the remainder is excreted. Once the material enters the blood, it can be carried to any part of the body. From there, it may preferentially target a given organ or tissue, as determined by the chemical properties of the radioactive material and the nature of the organ or tissue. For example, plutonium and americium become preferentially attached to bone surface (LANL, 1995), and tritium ultimately mixes uniformly with all tissues and organs.

The residence time of a radioactive particle in the lungs depends in part upon the solubility of the material. Three broad categories have been defined, and specify a characteristic half-time for inhaled material to clear from the pulmonary region of the lung to the blood and the gastrointestinal tract (Eckerman, 1988):

(xciv) Y: Radionuclides in insoluble compounds typically remain in the lungs for a long time; these are of Solubility Class Y (for years), also called Lung Clearance Class Y.

(xcv) W: Radionuclides in moderately soluble compounds remain in the lungs for weeks; these are of Solubility Class W (for weeks), also called Lung Clearance Class W.

(xcvi) D: Radionuclides in soluble compounds remain in the lungs for only a short time; these are of Solubility Class D (for days), also called Lung Clearance Class D.

According to Federal Guidance Report #11 (EPA, 1988), plutonium compounds can be Class Y (the oxides[19]) or Class W (all other Pu compounds). There are no Class D Pu compounds. Americium compounds are only Class W. Uranium compounds can be Class Y (UO_2 and U_3O_8), Class W (UO_3, UF_4, and UCl_4), or Class D (UF_6, UO_2F_2, and $UO_2(NO_3)_2$). Fission products are of all three classes. Should these compounds be involved in a fire, their chemical nature may change. For example, a plutonium salt (as in certain residues), which is class W, may change to an oxide (class Y) in a fire. However, such conversion will probably not be complete. To be conservative, it is best to assume that the resultant chemical form is the one that gives the largest dose; in the case of plutonium salts, for example, it is conservative to assume they remain class W.

In ICRP Publication 60, the lung clearance class term was dropped in favor of the term lung absorption type. Absorption types fast (F), medium (M), and slow (S) broadly correspond to older lung clearance classes of D, W, and Y (ICRP, 1991).

A-2.5.5 Dose Conversion Factors

The amount of biological damage that radioactive material may inflict on an organ or tissue is given by the Dose Conversion Factor (DCF) mentioned above. The DCFs take into account the migration of the radioisotope within the body, the decay of the radioisotope, and the formation of daughter isotopes that may be radioactive. For inhalation, this is typically expressed in units of Sv/Bq (or rem/Ci). This can be converted to Sv/g (or rem/g) by multiplying by the specific activity.

The older system of DCFs for a large number of radionuclides is given in Federal Guidance Report #11 (EPA, 1988). FGR 11 contains DCFs based on weighting factors from ICRP 26 (ICRP, 1977) and organ/tissue models documented in ICRP 30 and 48 (ICRP, 1979-82), and (ICRP, 1986). The DCF values in FGR 11 are based on exposure to an adult worker and a particle size of 1.0 μm Activity Median Aerodynamic Diameter (AMAD).[20] The values are applied uniformly for all ages in the general public population and all release conditions.

ICRP Publication 68 provides updated dosimetry for radiation workers, while ICRP 72 covers the general public. Both include age specific models and parameters (ICRP, 1995). The DCFs contained in these reports are based on ICRP 1990 Recommendation on radiation protection standards in Publication 60 (ICRP, 1991) and as well as the revised kinetic and dosimetric model of the respiratory tract in Publication 66 (ICRP, 1994). The inhalation DCFs in ICRP Publication 68 are for the CEDE and assume either 1.0 μm or 5.0 μm AMAD particle sizes. The inhalation DCFs in ICRP 72 are only for the CEDE and a 1.0 μm AMAD particle.

A combined data set is now available from the ICRP (ICRP, 2001) that not only provides dosimetric information for both worker and general public populations, but also extends the

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[19] Plutonium hydroxides have subsequently been added to Class Y.

[20] The AMAD signifies that fifty percent of the activity in the aerosol is associated with particles of aerodynamic diameter greater than the AMAD.

parameter space of the ICRP Publications 68 and 72. The combined data gives inhalation dose coefficients for ten aerosol sizes (0.001 μm to 10 μm AMAD) as well as ingestion coefficients. Effective doses and equivalent doses for all important tissues for a range of integration times (1, 7 and 30 days, 1, 5, 10, 20, 30, and 45 years) are given, together with the dose coefficients to age 70 years.

The Nuclear Regulatory Commission and at least one NRC Agreement State have granted license amendments to allow use of the newer ICRP 68/72 dosimetry. The newer data have been approved for use at least at one DOE site.

A-2.5.6 Inhalation (Resuspension)

Dose from resuspension inhalation is primarily of concern after plume passage. The ground concentration (GC_i) of a given isotope (i) under a plume can be calculated by the method discussed earlier, which also discusses resuspension factor (F_r) of this material. The resuspension inhalation dose to a given organ or tissue from this isotope is the product of the ground concentration, resuspension factor, breathing rate, and DCF_i for that organ and radionuclide.

$$Dose_i = GC_i \times F_r \times BR \times DCF_i \qquad \text{(A-36)}$$

The total dose to the organ or tissue is the sum of the doses from all isotopes resuspended. Correction factors can also be applied, as appropriate, to account for the receptor being off-centerline (if the GC_i was calculated for plume centerline) and for shielding, such as for the receptor being indoors. Off-centerline considerations and shielding are normally of greater importance for resuspension inhalation than for plume inhalation because resuspension takes place over an extended period and the routine activities of the receptors should be taken into account. This is especially important for inhalation doses to the public. The comparative magnitude of the resuspension dose depends on the amount material deposited on the ground from the plume. If the amount is large, the resuspension inhalation dose over a period of days, weeks, or months can be as large as, or even larger than, the direct inhalation dose from the plume. For dry deposition, the size distribution of the particulates released in an accident is important; very small particles have small deposition velocities, leading to small ground concentrations. For wet deposition, particles of all sizes can be washed out by precipitation. If an accidental release of radioactive particulates occurs during a period of rain or snow, the subsequent resuspension inhalation dose will be much larger than it would be otherwise.

It is noted that the guidance in DOE-STD-3009-94, CN#2, Appendix A allows the analyst to ignore resuspension.

A-2.5.7 Ingestion

Fallout of particulates from a plume may contaminate water and food supplies. The uptake of radionuclides by plants and animals, and their transfer into the food chain for humans, is a very complex process and beyond the scope of this appendix. Several models have been developed and incorporated into computer models for atmospheric dispersion and consequence assessment.

Consumption of contaminated food products is not restricted to persons living near the site of an accidental release, as the food products may transported to another location for processing, and consuming in still another location. The ingestion dose must therefore be calculated separately from the other doses (from inhalation, etc.). It is not to be added to the doses from the other modes of intake unless it is clear that the receptor for the ingestion dose is the same as the receptor for the other modes of intake.

Once the amount of radioactive material ingested has been determined, the dose can be calculated by multiplying this amount by the DCF for ingestion. Tables of ingestion DCFs for a large number of radionuclides are available from both the older FGR 11/12 series as well as the ICRP 72 series. Like the inhalation DCFs, the units of the DCFs are Sv/Bq (or rem/Ci).

For calculations supporting DSA preparation, ingestion is ignored.

A-2.5.8 Cloudshine

The amount of gamma radiation (and beta, if appropriate) received by a receptor from a plume of radioactive material depends upon the location of the receptor relative to the plume. The greatest dose would be received by a receptor in the plume centerline, of course, and dose conversion factors have been developed for such a receptor. The assumptions made in deriving these DCFs are that (1) the plume is uniform and semi-infinite ("semi" because the plume extends upward from the ground, but not downward) and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide and the DCF, integrated over the duration of the plume. The doses from all the radionuclides must then be summed. Cloudshine DCFs are expressed in units of $(Sv\text{-}m^3)/(Bq\text{-}s)$.

The cloudshine doses calculated using the DCFs from Federal Guidance Report #12 are conservative because of the assumptions that the receptor is standing upright in a uniform, semi-infinite cloud. The plume, of course, is neither uniform nor semi-infinite, the receptor may not be at plume centerline (and the plume may even be elevated), the receptor may be sheltered, and the receptor may not be standing up. Each of these factors would tend to reduce the dose. Corrections for finite cloud size and distribution (Gaussian), and for receptor location off-centerline, are included in several computer models of atmospheric dispersion and consequence assessment. However, for typical MOI dose-to-an-individual calculations supporting DSA preparation, the effect of structural shielding is conservatively not taken into account.

A-2.5.9 Groundshine

The treatment of groundshine is similar to that of cloudshine. The amount of gamma radiation received by a receptor from radioactive material deposited on the ground (fallout) depends upon the location of receptor relative to the fallout. The greatest dose would be received by a receptor at the center of the fallout, of course, and dose conversion factors have been developed for such a receptor. The assumptions made in deriving groundshine DCFs are that (1) the material is uniformly distributed on the surface or in the soil for an infinite distance in every horizontal direction, and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide on (or in) the ground and the

DCF, integrated over the duration of the exposure (i.e., how long the receptor is present to receive groundshine). The groundshine doses from all the radionuclides must then be summed. The concentration to be used in the calculation is either an areal concentration (Bq/m^2), if the material is only on the surface, or a volume concentration (Bq/m^3), if mixed with the soil. Groundshine DCFs are expressed in units of either $(Sv\text{-}m^2)/(Bq\text{-}s)$ for surface contamination, or $(Sv\text{-}m^3)/(Bq\text{-}s)$ for soil contaminated down to a specified depth.

Typically, the groundshine doses calculated using these DCFs are conservative because of the assumptions that the receptor is standing upright on a uniformly contaminated, infinite plane. The fallout, of course, is neither uniform nor infinite and the receptor may not be in the middle of it. Furthermore, surface irregularities (surface roughness and uneven terrain) tend to shield the receptor, the receptor may be sheltered, and the receptor may be elevated. Each of these factors would tend to reduce the dose. Corrections for finite size and distribution of the fallout pattern, and for receptor location off-centerline, are included in several computer models of atmospheric dispersion and consequence assessment. The safety analyst may also wish to consider additional dose reduction factors associated with sheltering or surface roughness / unevenness.

In calculating groundshine doses, the time variation of the ground concentration at the receptor's location must be considered. In the early stages of plume passage, the ground concentration is increasing, the concentration reaching a peak at the end of plume passage. Resuspension of the particulates then erodes the amount of contamination. The dose received from groundshine therefore must consider not only the exposure duration of the receptor, but also the period during which the exposure is attained. Such considerations are included in several computer models of atmospheric dispersion and consequence assessment.

A-2.5.10 Skin Deposition

Doses from skin deposition are normally of short duration (a few hours) because of decontamination of the skin. The only radionuclides of importance for skin contamination are the beta emitters. Beta particles can penetrate the surface layer of dead skin cells and damage the cells directly beneath. Experiments show that for beta radiation in the 200 keV to 2 MeV range, the absorbed dose to these cells is about 0.2 rad/s for a surface contamination of 1 Ci/m^2 (Healy, 1984). Because the radiation-weighting factor for beta radiation is one (Table A-4), this equates to a dose rate of 5.4×10^{-14} $(Sv\text{-}m^2)/(Bq\text{-}s)$. This dose rate must then be integrated over the duration, T, that the material is on the skin prior to decontamination to give the skin DCF

$$DCF_{skin} = 5.4\times10^{-14}\,(1 - e^{-\lambda T}) / \lambda \qquad \text{(A-37)}$$

The dose to the exposed skin from a given beta-emitting isotope (i) for a receptor at (or under) plume centerline is

$$Dose_{i,skin} = AC_i \times V_d \times DCF_{skin} \times F \qquad \text{(A-38)}$$

where AC_i is the ground-level air concentration of this isotope, V_d is the deposition velocity to the skin (on the order of 1 cm/s or less, depending upon the particle size distribution), and F is the fraction of the plume duration that the receptor is exposed to the plume. Correction factors

need to be applied for a receptor off-centerline or sheltered. The total skin dose will be the sum of the contributions from all the beta-emitters that are deposited on the skin.

A-2.5.11 Direct (Prompt) Dose

Doses from criticalities arise from both the plume of fission products that may be released and from prompt radiation, i.e., the gamma rays and neutrons that are emitted during the brief (millisecond) energy burst(s) during the criticality spike(s). The doses from the plume of fission products are included in the discussions above and won't be repeated here.

The prompt dose depends only upon the number of fissions in the criticality, the distance to the receptor, and the amount of intervening shielding material, such as concrete. The gamma and neutron doses should be quantified using nuclear engineering principles.

Shielding is expressed in terms of the amount of intervening concrete, or the equivalent if other shielding materials are involved. In the case of gamma radiation, the dose is reduced by a factor of 2.5 for the first eight inches of concrete, a factor of 5.0 for the first foot, and a factor of 5.5 for each additional foot. For neutron radiation, the dose is reduced by a factor of 2.3 for the first eight inches of concrete, a factor of 4.6 for the first foot, and a factor of 20 for each additional foot.

Prompt dose is important for the immediate worker, i.e., one within some tens of meters from the accident, but is rarely important for persons more distant. The dose to a collocated worker at a distance of 100 m is normally small and the dose to the public is negligible.

A-2.6 Health Risks

The discussion in the following sections is added for completeness. DOE-STD-3009-94, CN#2 Appendix A requires the calculation of individual doses but not health effects.

Once doses have been calculated, the corresponding health risks can be determined. This is done by multiplying doses by stochastic risk factors. Latent Cancer Fatalities (LCFs) are the health risks of most interest. The term "latent" indicates that the estimated cancer fatalities would occur sometime in the future, within the next 50 years for adult workers, or the next 70 years for the general population, which includes children. One can also calculate latent cancer occurrences (fatal plus non-fatal), genetic effects, etc., but these are not normally evaluated in safety analyses. The stochastic risk factor depends upon the type of radiation and the organ considered.

A-2.6.1 High-LET Radiation

In the case of alpha emitters, such as Pu and U, the only organs of importance for cancer risk are the lungs, liver, and bone surface (Abrahamson, 1993). The stochastic risk factors for cancer fatalities for these organs are shown in Table A-7. For these three organs, the stochastic risk factors are linear and continuous. Earlier models, based on ICRP-26 (ICRP, 1977), used a linear-quadratic model. The new model, based on ICRP-60 (ICRP, 1991), is linear but may be

discontinuous for some radionuclides. The Abrahamson (Abrahamson, 1993) values (Table A-7) differ from the earlier ones (ICRP-26): the lung factor is about four times larger, the bone skeleton factor is about ten times smaller, and liver is about three times smaller than the earlier values. The values in Table A-7 are for high-LET radiation (alpha particles). Table A-7 does not give the stochastic risk factor for committed effective dose, as the total cancer risk should be calculated as the sum of the individual organ cancer risks [Σ (dose $\times$ stochastic factor)]. The other organs of the body do not contribute significantly to cancer risk from exposure to alpha radiation and have been ignored.

Table A-7. Stochastic Risk Factors for Alpha-Emitters (Abrahamson, 1993)

ORGAN	RISK FACTOR *(LCF/rem)*
Bone Surface	6.0×10^{-7}
Lungs	8.0×10^{-5}
Liver	1.5×10^{-5}

Example: Suppose a calculation of committed inhalation doses to a certain receptor from a release of plutonium gives a bone-surface dose of 0.353 rem, a lung dose of 0.112 rem, and a liver dose of 0.0787 rem; the effective dose (whole body) was 0.0351 rem. (The effective dose includes contributions from all organs, not just the three mentioned here.) For this individual, the LCF risk would therefore be $(0.353)(6.0 \times 10^{-7}) + (0.112)(8.0 \times 10^{-5}) + (0.0787)(1.5 \times 10^{-5}) = 1 \times 10^{-5}$ LCF. This means that only one person in 10^5 would die of cancer from this exposure. Note that although the bone dose is larger than the doses to the other organs, the lung dose is more important in terms of cancer risk, as seen in this example.

A-2.6.2 Low-LET Radiation

For low-LET radiation (beta and gamma radiation), the latent cancer risk is normally calculated from the committed effective dose, although the individual organ cancer risks could also be summed. ICRP-60 (ICRP, 1991) recommends using a stochastic risk factor of 5×10^{-4} LCF/rem (5×10^{-2} LCF/Sv) for the whole population, or 4×10^{-4} LCF/rem (4×10^{-2} LCF/Sv) for adult workers, based on the committed effective dose. (The factor for the public is higher than for adult workers because the public consists of a mixture of individuals with varying degrees of resistance to hazardous materials, including children, the elderly, and the infirm. This includes the cancer risk to all organs, unlike the treatment of alpha radiation, which considers only the three organs of Table A-7 to be important for cancer risk.) This ICRP-60 recommendation has been adopted by the Environmental Protection Agency for the evaluations of Environmental Assessments (EAs) (NEPA, 1993). Had this factor been used in the above example, the LCF risk to that individual would have been $(0.0351)(5 \times 10^{-4}) = 1.75 \times 10^{-5}$ LCF, or about 75% higher than obtained from using Table A-7 data. This low-LET risk factor is not recommended for alpha-emitters (high LET).

A-2.6.3 Acute Health Risks

Doses received in a short period (acute doses) may cause acute health risks, if large enough. A dose from gamma or neutron radiation, such as from a criticality, is the primary concern here. Table A-8 (adapted from (Turner, 1986)) summarizes the health effects associated with varying levels of gamma radiation.

Table A-8. Acute Radiation Effects for Gamma Radiation

DOSE (rad)	HEALTH EFFECT
0 -25	No detectable effect
25 - 100	Some biological damage; recovery probable
100 - 300	More damage; recovery probable but not assured
300 – 600	Fatalities occur in about half the population
> 600	Death expected

An acute, whole-body, gamma-ray dose of about 450 – 500 rad would probably be fatal to about half the population within about 30 days. This dose is known as LD_{50}, sometimes called $LD_{50/30}$, where "LD" means Lethal Dose. Because gamma radiation has a radiation-weighting factor of one (Table A-4) the doses in Table A-8 could also have been labeled in rem. Presumably, neutron doses (in rem) would give similar effects.

An acute dose from inhalation of plutonium or uranium, i.e., the dose received in a few hours or days, is normally very small. All of the isotopes of plutonium and uranium have half-lives of many years; therefore, the inhalation dose received by a person during the first few days following an acute exposure via the inhalation pathway will only be a small fraction of the lifetime dose. Accordingly, an acute health effect requires a very large amount of plutonium to be released. For example, in order for a person at a distance of about 2 km from the release site to get a dose large enough to cause pneumonitis (the first prompt health effect to occur), an airborne release of about 100 kg of respirable plutonium would be required (Peterson, 1993). Such a large release is extremely unlikely. Therefore, *acute* health effects need not be considered for releases of plutonium or uranium.

A-2.6.4 Radiation Protection

Radiation protection of the worker is governed by the As Low As Reasonable Achievable (ALARA) principle. Control of internal exposure to radionuclides is based on the limitation of the sum of current and future doses from annual intake (i.e., the committed effective dose equivalent) rather than on annual dose. If it is found that limits on committed dose have been exceeded for a worker, corrective actions are needed to limit further exposure.

The primary guides for worker annual exposure are 5 rem for effective dose equivalent, 50 rem to individual organs or tissues (except the lens of the eye), and 15 rem to the lens of the eye. Two types of derived guides are used to implement this. These are the Annual Limit on Intake (ALI) and the Derived Air Concentration (DAC). The ALI is the annual intake of a radionuclide that would result in a radiation dose to the reference man equal to the relevant primary guide. The DAC is the air concentration of a radionuclide that would result in an intake corresponding to its ALI, if breathed for a work-year (2,000 hours).

The above guidance of comparing the annual exposure limit (primary guide) with the full 50-year (or 70-year) committed effective dose received is found in several DOE and EPA documents. For dose calculations supporting DSAs, the dose should be calculated using the full fifty-year commitment, following conservative health protection and radiological practices. The newer dose conversion factor methodology and biokinetics models as described in ICRP 60, 66, and ICRP 68/72 are recommended. The older FGR guidance can be used as an alternative, should local agreements still support use of the earlier dose conversion data.

Appendix B. Software Defect Notifications

The following statement is on the RSICC web site for GENII 1.485:

> "The potential exists for a limited combination of options: specifically, only for cases of acute, atmospheric release when the "food production grid" input option is used, if "food export" is chosen, and one of the input radionuclides is tritium or carbon-14.
>
> Because tritium and carbon-14 are handled with special specific-activity models, calculations for these two radionuclides do not have the same path through the code logic. If the above combination of options is used, the food production grid is inappropriately applied to H-3 and C-14. The total amount of food input of the full 80-km circle is assumed to be contaminated with these two radionuclides, rather than just that from the selected downwind sector. The estimated dose provided by the GENII 1.485 code is too large by factors of about 10 to 20.
>
> If the user wants to combine these options, a simple input modification can be used to obtain the appropriate answer. If the food production grid file is adjusted so that non-downwind sectors have zero production, and only the sector of interest has input data, the results should be correct.
>
> The developers of GENII 1.485 have no intention at this time of making changes to the code. The code update, GENII Version 2, is scheduled to undergo formal peer review in the immediate future, and will be replacing GENII 1.485 after comment resolution is completed."

The following statement is included under Computer Software Requirements:

> Lahey F77L Version 4.10 (92%) and Microsoft QuickBASIC 3.0 (8%) were used to create the executables under DOS 3.1. They also run from a DOS window of Windows95 or WindowsNT. These executables were created in the early 1990s and may not run correctly under WindowsXP. The GENII and APPRENTICE source files were added to the package in the March 1995 update. APPRENTICE, which is written in Microsoft QuickBASIC 3.0, uses modules and subroutines from the Komputerwerk FINALLY! Modules libraries.

Appendix C. Sample Problem – Joint Frequency Distribution File

```
MACCS2 CONVERSION MET DATA

Created 03-Feb-04 VS

    8    6    1    1    0.0

  0.66    1.87  3.15    4.32  5.55    6.76  8.05    9.77

 0.00 0.00 0.02 0.01 0.07 0.07 0.02 0.03 0.02 0.00 0.02 0.05 0.03 0.00 0.02 0.02

 0.00 0.02 0.17 0.70 0.49 0.25 0.21 0.10 0.26 0.19 0.11 0.10 0.06 0.00 0.01 0.00

 0.00 0.00 0.02 0.05 0.05 0.02 0.01 0.00 0.02 0.00 0.00 0.01 0.00 0.00 0.00 0.00

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 0.00 0.02 0.40 0.73 0.96 0.13 0.02 0.06 0.33 0.18 0.19 0.01 0.00 0.00 0.00 0.00

 0.00 0.00 0.07 0.05 0.00 0.02 0.01 0.10 0.00 0.01 0.00 0.00 0.00 0.00 0.00 0.01

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 0.34 0.47 0.45 0.33 0.34 0.17 0.15 0.17 0.11 0.07 0.09 0.13 0.27 0.50 0.19 0.18

 0.49 1.47 2.79 2.48 1.12 0.30 0.07 0.03 0.10 0.18 0.33 0.14 0.06 0.08 0.08 0.17
```

0.14	0.42	3.14	2.25	1.89	0.11	0.02	0.02	0.09	0.62	0.61	0.02	0.00	0.00	0.01	0.01
0.08	0.54	3.07	2.02	2.87	0.37	0.01	0.01	0.11	0.59	0.64	0.00	0.01	0.00	0.00	0.02
0.00	0.63	2.31	0.73	0.74	0.19	0.00	0.02	0.19	0.37	0.11	0.00	0.00	0.00	0.00	0.00
0.00	0.25	1.21	0.26	0.01	0.01	0.00	0.01	0.16	0.05	0.01	0.00	0.00	0.00	0.00	0.01
0.00	0.11	0.31	0.05	0.03	0.00	0.00	0.02	0.15	0.03	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.06	0.01	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.66	0.71	0.63	0.47	0.25	0.22	0.17	0.27	0.30	0.31	0.29	0.50	0.89	1.36	0.80	0.59
1.34	1.92	1.12	0.64	0.32	0.06	0.03	0.05	0.08	0.10	0.17	0.33	0.15	0.16	0.15	0.10
0.16	0.87	1.12	0.15	0.06	0.03	0.00	0.01	0.02	0.03	0.06	0.02	0.00	0.01	0.01	0.00
0.06	0.53	1.02	0.02	0.01	0.00	0.00	0.01	0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.71	0.56	0.48	0.43	0.32	0.21	0.38	0.45	0.63	0.86	1.20	1.79	2.03	2.52	1.69	0.91
0.22	0.18	0.08	0.10	0.10	0.03	0.00	0.07	0.10	0.03	0.11	0.32	0.30	0.13	0.11	0.09
0.01	0.02	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

SEPARATION

PAGE

CFAST Computer Code Application Guidance for Documented Safety Analysis

Final Report

U.S. Department of Energy
Office of Environment, Safety and Health
1000 Independence Ave., S.W.
Washington, DC 20585-2040

June 2004

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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the CFAST computer software for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the CFAST documentation provided by the code developer. CFAST is one of six computer codes designated by DOE's Office of Environmental, Safety and Health as a toolbox code for safety analysis..

Suggestions for corrections or improvements to this document should be addressed to –

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REVISION STATUS

Page/Section	Revision	Change
1. Entire Document	1. Final Draft for Review	1. Original Issue
2. Entire Document	2. Final Report	2. Updated all sections per review comments.

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EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications (DOE, 2002b). The Consolidated Fire and Smoke Transport (CFAST) code is one of the designated toolbox codes.

CFAST is a zone-based fire model, which was developed by the National Institute of Standards and Technology. The code has been widely used in the fire protection community to support alternate design approaches, post-fire investigations and as a research tool to better understand fire phenomena. This report sanctions the use of the two NIST supported versions, CFAST 3.1.7 and CFAST 5.1.1. The report explains the advantages of both versions.

The CFAST guidance report includes the following:

(i) Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis

(ii) Code development information and SQA background

(iii) Appropriate regimes and code limitations

(iv) Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and

(v) Default input value recommendations for site-independent parameters.

Use of the information contained here, although not ensuring correct use of CFAST in each analytical context, will minimize potential user errors and the likelihood of CFAST use outside its regime of applicability.

This guidance report is supplemental in nature to documentation from the code developer such as the user's guide and model description. The DOE safety analyst should obtain a complete and up to date set of documentation from the CFAST code maintainer.

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1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25 (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and in the variability of guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its Recommendation to DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the DNFSB concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include

(i) Identification of a set of accident analysis software that is widely used in the DOE Complex, and

(ii) Issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regimes in accident analysis, default inputs, and special conditions for use.

Safety analysis software for the DOE "toolbox" status was designated by the DOE Office of Environment, Safety, and Health (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications* (see http://www.deprep.org/archive/rec/2002-1/NNSACCodes1.pdf). It includes the Consolidated Fire and Smoke Transport (CFAST) code.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in its guidance report. The code-specific document will be maintained and updated until a minimum qualification software package is completed, or until such time that it is determined to no longer be necessary to update.

The contents of this report are applicable in the interim period until measures are completed to bring CFAST into compliance with defined SQA standards. The primary objective of this guidance report is to provide information on the use of CFAST for supporting DOE safety-basis accident analysis. Specifically, the report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Overcoming known vulnerabilities and avoiding code errors
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications
- Default input value recommendations for site-independent parameters, and
- Citations of currently available SQA documentation.

Thus, this report is intended to complement existing CFAST user's documentation. The latter tends to be much broader in coverage of the full range of capabilities of CFAST and the spectrum of inputs that might be needed depending upon the application, but lack cohesive and targeted guidance for particular applications such as DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The CFAST guidance document is written using the following outline. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830 (CFR, 2001c). It provides a brief description of the fire modeling software *Consolidated Model of Fire Growth and Smoke Transport* (CFAST) and its interface software Fire Growth And Smoke Transport (FAST) (Peacock 2000). More information follows on the scope and purpose of this document. The next major section is a summary description of CFAST. A third section discusses applicable regimes for using CFAST in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, is next. Following this discussion are sections on special conditions for use of the software and software limitations. A sample case is then provided, followed by acronyms and definitions, references, and appendices. Appendix A discusses fire severity. Appendices B through I give sample problem detailed information. Appendix J discusses CFAST history. Appendix K provides an error message table for CFAST.

1.1 Background: Overview of Toolbox Software in Context of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software will be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version,

identify compliance with their organization's SQA requirements and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as "toolbox" codes (DOE, 2002b). Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

This CFAST guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

CFAST is a zone-based fire model that was developed by the National Institute of Standards and Technology (NIST). There are currently two versions of the software in general use, Version 3.1.7 (Jones, 2003; Peacock, 1993) and Version 5.1.1 (NIST, 2002). Both are available from the NIST web site http://cfast.nist.gov/.

1.3 Purpose

The CFAST code, while part of the toolbox collection of software, still may require Software Quality Assurance (SQA) upgrades prior to meeting current established standards for software. However, until these CFAST upgrades are completed, CFAST can be applied safely under the condition that the guidance contained in this and related reports is followed. Once upgrades are finalized with CFAST, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of CFAST in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

It is recognized that other computer codes besides CFAST exist that perform similar types of calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for some accident analysis applications that involve fire. The relative merits of using a different computer program or using a hand calculation for a given application is a judgment that must be made by the analyst on a case-by-case basis.

An uncontrolled fire in a nuclear facility can be a very energetic event. Severe smoke, excessive temperatures, and large thermal gradients are common. Such fires can readily breach containment barriers (glove box, ventilation ductwork and building envelope), and because of the significant thermal gradients, readily disperse radioactive material. While DOE has a good record on fire safety, an uncontrolled fire remains a dominant risk in many nuclear facilities (Shields, 2000).

To adequately evaluate the fire risk, calculations must be prepared that establish the fire severity and consequences expected for credible fire scenarios. There are a variety of analytical tools and techniques that can be implemented to accomplish this. Some of these are discussed in Appendix A. Because of the complexity of the fire phenomena, most of these tools and techniques are software based. The fire modeling software *Consolidated Fire Growth and Smoke Transport* (CFAST) is one of these tools.

In addition to the nuclear safety fire risk, worker, monetary and business interruption protection must also be addressed as part of the DOE Fire Protection Program. This program is established in two orders. DOE Order 420.1 (DOE, 2002a) requires each facility to have a program to minimize the likelihood of unacceptable fire losses or damage. DOE Order 440.1A (DOE, 1998) provides "the framework for an effective worker protection program" that includes the establishment of a "comprehensive fire protection program with the objective of providing an acceptable level of safety from fire and related hazards." For a discussion on how the DSA and Fire Hazard Analysis should be coordinated see DOE-HDBK-1163-2003 (DOE, 2003b).

The DNFSB in Tech-25 (Burns, 2000) identified the importance of trained and competent software users. The DOE Fire Protection Committee had recognized this many years prior to the inception of the DNFSB. This recognition is why the *Implementation Guide for use with DOE Orders 420.1 and 440.1 Fire Safety Program* (DOE, 1995, DOE G-420.1/B-0, DOE G-440.1/E-0) contains the following paragraph:

> A tool that may be used in the development of an FHA is a fire model, such as those developed by the National Institute of Standards and Technology, as applied by qualified fire protection engineers. However, the use of such models is predicated on their being conservative and validated. As of this date, DOE has not sanctioned the use of any one model for use in an FHA. DOE acceptance of individual models will be considered on a case-by-case basis.

During the review of this guidance report the DOE Fire Protection Committee was concerned that publication of this report would invalidate the guidance in DOE G-420.1/B-0, DOE G-440.1/E-0 (DOE, 1995). This CFAST guidance report does not replace the guidance in DOE G-

420.1/B-0, DOE G-440.1/E-0. Outside of its use to evaluate source terms, CFAST will still require the case-by-case authorization from the appropriate Authority having Jurisdiction (AHJ).

2.0 SUMMARY DESCRIPTION OF SOFTWARE

Computer-based solutions to fire models are often sought because of the complexity of fire phenomena. There are two basic fire model approaches in general use. They are the field model and the zone model. Both approaches solve the Navier-Stokes (N-S) equations for mass and energy transport. Field (or computational fluid dynamic) models solve the complete set of N-S equations using numerical methods subject only to the fire compartment boundary conditions. The solution is accomplished by descritizing the spatial regions of interest into a set of nodes or finite elements. The computer is then tasked with estimating the local conditions (e.g., temperature, pressure, and combustion products) by solving the time-averaged N-S equations for each node or element.

The zone (or control volume) fire model relies on the stratification behavior observed in most fires and represents the two layers as separate control volumes (i.e., upper layer and lower layer). Each layer is assumed to be uniform (i.e., temperature, smoke and gas concentrations are assumed to be homogeneous throughout the layer). The time-dependent fire response for each layer is predicted based on N-S equations integrated over the zones. Mass and energy exchange between the control volumes is estimated using both numerical techniques and correlations that approximate fire behavior. (For additional information on this behavior see Appendix A.)

CFAST is such a zone model. The model can accommodate 30 compartments with multiple openings between the compartments. A fire plume represents the movement of energy and mass between the lower layer and upper layer. Mass and energy can also be exchanged between the layers at the vents. Exchange between the layers resulting from wall flows is not modeled in CFAST.

CFAST was developed by NIST in the late 1980s. There are two current versions of CFAST supported by NIST. CFAST 5.1.1 (1 May 2004) is the most current version and is designed to operate on all versions of the Windows operating systems. CFAST 3.1.7 is DOS based and will run under Windows 3.1, 3.11, 95, 98, 2000 and Me. CFAST 3.1.7 is compatible with the graphical user interface (GUI) FAST.

The GUI simplifies the preparation process for initial input data files (Section 4.2) and modification of the data libraries (Section 4.1). As discussed Section 4.2 some users may find it easier to edit the input data files using WordPad after their initial assembly. Thus, FAST coupled with CFAST 3.1.7 can be used to establish the initial input data files and CFAST 5.1.1 can be used to perform the final calculations.

CFAST 5.1.1 includes modules to model corridor flow and horizontal heat transfer. It also includes tools to convert numerical results into SmokeView. SmokeView is a post-processing software tool that can be used to visualize numerical fire predictions (Forney, 2003). CFAST 5.1.1 replaces CFAST 5.1.0 as explained in Appendix J.

CFAST and FAST documentation consists of various reports that address multiple aspects of the code primarily in the form of NIST technical reports. Documentation includes:

- NIST Technical Note 1431, *A Technical Reference for CFAST: An Engineering Tool for Estimating Fire and Smoke Transport* (Jones, 2003)
- NIST Special Publication 921, 2000 Edition, *A User's Guide for FAST: Engineering Tools for Estimating Fire Growth and Smoke Transport* (Peacock, 2000)
- NIST Technical Note 1299, *CFAST, the Consolidated Model of Fire Growth and Smoke Transport* (Peacock, 1993)
- NISTIR 5486-1, *Technical Reference Guide for FPEtool Version 3.2* (Deal, 1995)
- NBSIR 85-3223, *Data Sources for Parameters Used in Predictive Modeling of Fire Growth and Smoke Spread* (Gross, 1985)

These documents are available from the NIST web site http://cfast.nist.gov/. This web site lists additional documents that may be useful to the analyst.

2.1 Program Availability and Installation

Both versions of CFAST and the Graphical User Interface (GUI) FAST may be downloaded from the NIST website at http://cfast.nist.gov/. CFAST 5.1.1 is downloaded as an executable file, which is named cfastv511.exe. When executed from the Windows desktop it will install the folders, files and programs listed in Table 2-1. CFAST 3.1.7 and FAST are also downloaded as an executable file. The file is titled fast317.exe and when executed will install the files and programs listed in Table 2-2.

Regardless of the CFAST version, the program and its associated files should be installed in a folder that is close to the top of the directory. (i.e., Keep the folder path short, C:NIST\CFAST). This will make the execution of CFAST easier.* After the appropriate executable files are installed in the "FAST" folder, the file "setupf.exe" should be run from the "start" button on the bottom left of the computer screen. If necessary, use the browse option under the run command. Follow the instructions on the screen as the program installs.

For CFAST 3.1.7 it is recommended that the analyst keep the CFAST and FAST executable files, the data files and the database files in the same folder. If not, it will be necessary to establish the path in the input data files.

---

* For CFAST 5.1.1 the setup file will automatically use the path C:\NIST\CFAST511.

Table 2-1. — Files Installed With CFAST Version 5.1.1

Installed in base folder

Name	Size	Modified
data (see right)	folder	installation date
fonts (see right)	folder	installation date
cfast.exe	1,244 KB	05/05/2004 3:34 PM
cplot.exe	600 KB	05/02/1996 3:35 PM
curve.df	4 KB	05/02/1996 12:33 PM
Hazard.tbl	1 KB	11/10/1998 6:36 PM
hv5.cf	1 KB	05/05/2004 3:47 PM
INSTALL.LOG	13 KB	installation date
limits.df	3 KB	08/01/2003 2:51 PM
Objects.df	130 KB	10/24/2001 5:11 PM
Objects.ndx	1 KB	10/24/2001 4:55 PM
readme.txt	10 KB	05/05/2004 3:47 PM
report.exe	748 KB	05/05/2004 3:35 PM
reportss.exe	728 KB	05/05/2004 3:35 PM
Thermal.df	10 KB	02/15/2001 1:20 PM
Thermal.ndx	1 KB	02/15/2001 1:20 PM
ToPanel.exe	748 KB	05/05/2004 3:36 PM
ToSmokeView.exe	388 KB	05/05/2004 3:36 PM
UNWISE.EXE	161 KB	09/28/2001 6:00 PM
Varnames.dat	2 KB	11/10/1998 6:36 PM

Installed in data folder

Name	Size	Modified
basecase.dat	2 KB	03/11/2004 2:55 PM
hhtest.dat	1 KB	09/26/2003 1:45 PM
multi.dat	5 KB	03/11/2004 2:55 PM
nistdem2.dat	3 KB	03/11/2004 2:55 PM
nistdem2.map	1 KB	03/25/2002 5:32 PM
nistdem2.plt	14 KB	03/11/2004 2:56 PM
nistdem2.smv	1 KB	03/11/2004 2:56 PM
nistdemo.dat	3 KB	03/11/2004 2:55 PM
nistdemo.map	1 KB	01/04/2002 12:13 PM
o2test.dat	1 KB	03/08/2004 2:19 PM
specieserror.dat	4 KB	03/10/2004 2:54 PM
standard.csv	84 KB	05/05/2004 4:00 PM
standard.dat	2 KB	03/02/2004 6:10 PM
standard.xls	254 KB	05/05/2004 4:00 PM
test01.dat	2 KB	03/11/2004 2:55 PM
test02.dat	2 KB	03/11/2004 2:55 PM
test03.dat	2 KB	03/11/2004 2:55 PM
test03.hi	346 KB	03/11/2004 2:56 PM
testob1.dat	2 KB	03/11/2004 2:55 PM
testob2.dat	2 KB	03/11/2004 2:55 PM
Ventlim.dat	1 KB	03/01/2004 3:34 PM

Installed in fonts folder

Name	Size	Modified
devfnt02.fnt	48 KB	11/03/1998 9:16 PM
devfnt03.fnt	48 KB	11/03/1998 9:16 PM
devfnt04.fnt	50 KB	11/03/1998 9:16 PM
devfnt05.fnt	50 KB	11/03/1998 9:16 PM
devfnt06.fnt	54 KB	11/03/1998 9:16 PM
devfnt07.fnt	52 KB	11/03/1998 9:16 PM
devfnt08.fnt	51 KB	11/03/1998 9:16 PM
devfnt09.fnt	51 KB	11/03/1998 9:16 PM
devfnt10.fnt	58 KB	11/03/1998 9:16 PM
devfnt11.fnt	56 KB	11/03/1998 9:16 PM
devfnt12.fnt	59 KB	11/03/1998 9:16 PM
devfnt13.fnt	68 KB	11/03/1998 9:16 PM
devfnt14.fnt	62 KB	11/03/1998 9:16 PM
devfnt15.fnt	77 KB	11/03/1998 9:16 PM
devfnt16.fnt	76 KB	11/03/1998 9:16 PM
devfnt17.fnt	93 KB	11/03/1998 9:16 PM
devfnt18.fnt	86 KB	11/03/1998 9:16 PM
devfnt19.fnt	77 KB	11/03/1998 9:16 PM
devfnt20.fnt	57 KB	11/03/1998 9:16 PM
devfnt21.fnt	50 KB	11/03/1998 9:16 PM
devfnt22.fnt	62 KB	11/03/1998 9:16 PM
devfnt23.fnt	52 KB	11/03/1998 9:16 PM
devfnt24.fnt	57 KB	11/03/1998 9:16 PM

Table 2-2. — Files Installed With CFAST Version 3.1.7

Name	Size	Modified	Name	Size	Modified
bintoasc.exe	345 KB	11/29/1999 11:51 AM	Draw2.exf	3 KB	04/01/1999 2:15 AM
Box.pic	4 KB	04/01/1999 2:15 AM	Draw2.pic	6 KB	04/01/1999 2:15 AM
build.exe	270 KB	04/01/1999 2:15 AM	Ecadtest.exf	1 KB	04/01/1999 2:15 AM
cedit.cfg	2 KB	04/01/1999 2:15 AM	Exf2bld.doc	3 KB	04/01/1999 2:15 AM
cfast.exe	1,707 KB	11/08/2001 4:32 PM	Exfast.dat	6 KB	10/01/1997 12:11 AM
Cfast.rsc	50 KB	11/14/2001 3:31 PM	Exftobld.exe	51 KB	04/01/1999 2:15 AM
colortes.exe	482 KB	04/01/1999 2:15 AM	Exmedium.dat	6 KB	10/01/1997 12:11 AM
compare.exe	262 KB	11/29/1999 11:51 AM	Exslow.dat	6 KB	10/01/1997 12:11 AM
compinfo.exe	258 KB	11/29/1999 11:51 AM	Exultra.dat	6 KB	10/01/1997 12:11 AM
cplot.exe	1,126 KB	11/08/2001 4:32 PM	Exwatts.dat	5 KB	10/01/1997 12:11 AM
curve.df	4 KB	04/01/1999 2:15 AM	Fast.exe	2,588 KB	11/14/2001 3:31 PM
devfnt02.fnt	12 KB	04/01/1999 2:15 AM	fast.ico	1 KB	05/14/1993 7:19 AM
devfnt03.fnt	12 KB	04/01/1999 2:15 AM	hazard.tbl	1 KB	04/01/1999 2:15 AM
devfnt04.fnt	13 KB	04/01/1999 2:15 AM	INSTALL.LOG	4 KB	08/22/2002 10:07 AM
devfnt05.fnt	13 KB	04/01/1999 2:15 AM	Objects.df	218 KB	04/01/1999 2:15 AM
devfnt06.fnt	14 KB	04/01/1999 2:15 AM	pallet.pal	1 KB	04/01/1999 2:15 AM
devfnt07.fnt	13 KB	04/01/1999 2:15 AM	Readme.txt	8 KB	11/14/2001 3:31 PM
devfnt08.fnt	13 KB	04/01/1999 2:15 AM	report.exe	1,116 KB	11/08/2001 4:32 PM
devfnt09.fnt	13 KB	04/01/1999 2:15 AM	reportg.exe	1,270 KB	11/08/2001 4:32 PM
devfnt10.fnt	15 KB	04/01/1999 2:15 AM	reportss.exe	1,096 KB	11/08/2001 4:32 PM
devfnt11.fnt	14 KB	04/01/1999 2:15 AM	romantri.fnt	9 KB	04/01/1999 2:15 AM
devfnt12.fnt	15 KB	04/01/1999 2:15 AM	system64.fnt	6 KB	04/01/1999 2:15 AM
devfnt13.fnt	17 KB	04/01/1999 2:15 AM	system72.fnt	0 KB	08/08/1997 3:28 PM
devfnt14.fnt	16 KB	04/01/1999 2:15 AM	test01.dat	2 KB	04/01/1999 2:15 AM
devfnt15.fnt	20 KB	04/01/1999 2:15 AM	test02.dat	2 KB	04/01/1999 2:15 AM
devfnt16.fnt	19 KB	04/01/1999 2:15 AM	test03.dat	2 KB	04/01/1999 2:15 AM
devfnt17.fnt	24 KB	04/01/1999 2:15 AM	test04.dat	2 KB	04/01/1999 2:15 AM
devfnt18.fnt	22 KB	04/01/1999 2:15 AM	testg1.dat	1 KB	04/01/1999 2:15 AM
devfnt19.fnt	20 KB	04/01/1999 2:15 AM	testg2.dat	4 KB	04/01/1999 2:15 AM
devfnt20.fnt	15 KB	04/01/1999 2:15 AM	testg3.dat	2 KB	04/01/1999 2:15 AM
devfnt21.fnt	13 KB	04/01/1999 2:15 AM	testg3b.pic	16 KB	04/01/1999 2:15 AM
devfnt22.fnt	16 KB	04/01/1999 2:15 AM	testg3t.pic	6 KB	04/01/1999 2:15 AM
devfnt23.fnt	13 KB	04/01/1999 2:15 AM	thermal.df	10 KB	04/01/1999 2:15 AM
devfnt24.fnt	15 KB	04/01/1999 2:15 AM	Thermal.ndx	1 KB	04/01/1999 2:15 AM
Draw1.exf	1 KB	04/01/1999 2:15 AM	UNWISE.EXE	146 KB	06/25/1999 10:55 AM
Draw1.pic	2 KB	04/01/1999 2:15 AM	Varnames.dat	2 KB	11/10/1998 5:36 PM

For CFAST 5.1.1 the default configuration is to keep the input data files (*.dat) in the data folder. CFAST will write the output files to this folder. This approach of keeping the data files in a separate folder from the executable files was introduced between the issuance of CFAST 5.0.1 and CFAST 5.1.0.

2.2 Program Execution

Either version of CFAST can be executed from the DOS command prompt. CFAST 3.1.7 may also be executed from the FAST GUI. This section will explain both methods.

2.2.1 DOS Command Prompt

Typically the command prompt can be accessed from the window desktop by clicking Start\ Programs\Accessories\Command Prompt. If the Command Prompt shortcut is not located in this

path, the user will need to establish the correct path. To simplify operation it is recommended that the analyst switch the active command prompt to the folder where CFAST is installed. This is done with the following statement:

```
CD \<path>\<folder containing CFAST.EXE>

CD \NIST\CFAST511
```

If the wrong drive device is noted in the command prompt (e.g., i:\> when c:\> is desired) attempt to change the drive by typing the desired drive letter followed by a colon (e.g., C:) followed by the return key.

The command line for CFAST is:

```
CFAST <input file> <output file> <options>
```

where:

`<input file>`: is the name of the input data file

`<output file>`: is the name of the file to which any specified text output will be written.

`<options>`: specify any output reporting or other options to control the output of the program.

The available options are described in Appendix B of *A User's Guide for FAST: Engineering Tools for Estimating Fire Growth and Smoke Transport* (Peacock, 2000). The two most useful are:

`/l` which directs that CFAST to generate an error log file named CFAST.LOG containing detailed debugging information.

`/r` which directs CFAST to includes additional variables in any text or spreadsheet output. The /r is followed by one or more of the following characters to produce the desired output:

w – include wall surface and target fluxes in the output

i – include model initial conditions and scenario description in the output

n – include "normal" printout of layer temperatures, interface height, and fire size in the output

f – include vent flows in the output

s – include layer and wall surface species concentrations in the output

t – include tenability estimates for each compartment in the output

p – include wall temperature profiles in the output

Thus, the option /rwinfstp would include the most complete spreadsheet output. A typical command line, as used for the later example problem would be:

```
CFAST CAB042.DAT CAB042.TXT /rin
```

2.2.2 FAST Graphical User Interface

The graphical user interface software FAST can be started from the DOS command prompt or by opening the file FAST.EXE in the appropriate Windows folder. To start from the DOS command prompt follow the instruction above to establish the appropriate active directory, then start FAST with the following command line

```
FAST
```

FAST will automatically generate the input file* (*.DAT file). For the sample problem presented, the analyst will then need to provide the input data, which is discussed in the next section. The reader is referred to (Peacock, 2000), for a thorough description of the FAST interface.

In addition to the interface for CFAST, the GUI FAST provides a series of estimation tools, which were derived from FIREFORM. Most of these tools are numerical solutions of empirical correlations. While they are excellent tools for exploratory evaluation, in general they are not suitable for calculations that support a DSA. If it is necessary to present results of a FAST estimation tool in a calculation that supports a DSA, the analyst should provide a citation to the correlation source document, and provide adequate analytical discussion to allow a qualified analyst to replicate the calculations without the benefit of the FAST software.

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* Within the DOE community such files sometimes will be referred to as the input deck.

3.0 APPLICABLE REGIMES IN ACCIDENT ANALYSIS

Most DOE Nuclear Facilities have experienced at least one unwanted fire (i.e., initiating frequencies vary from 0.1 to 1 fire per year). Typically these fires remain small, and cause minimal damage. These successes occur because early detection systems coupled with operator intervention result in prompt suppression, or combustible control programs limit the fire propagation. These small fires, if not extinguished, can evolve to fully involve the room of origin. Most of the time the combustibles present in a nuclear facility will not promote a fire that can lead to full room involvement; however, to fully implement this preventive feature in all locations has usually proven impractical. Thus the optimistic probability of an incipient fire leading to full room involvement is about 0.05 if no automatic sprinkler is present.

If the automatic sprinkler system or the fire compartment walls do not contain the fire it will continue to grow in size. A typical failure probability for a sprinkler system is 0.04. For fire walls the failure probability typically ranges from 0.05 to 0.2. Since the fire department success probability in a nuclear facility, given failure of the sprinkler system is problematic (i.e., 50:50) the frequency of a propagating fire in a well-managed nuclear facility (as an example for discussion) is approximately 5E-06 yr^{-1} based on the most optimistic values presented above*. (Actual probability for a particular facility will vary and detailed discussion of frequency is beyond the scope of this guidance document.) This value is above the 1.0E-6 yr^{-1} threshold for incredibility recommended in DOE-STD-3009-94 (DOE, 2000b) for conservatively calculated natural phenomena events. While this threshold frequency does not explicitly apply to in-facility accidents and thus to fire events, it establishes a value that has repeatedly been used to evaluate accident credibility. Thus, this example serves to illustrate that the severity and consequences of a propagating fire must be evaluated as part of most facility DSAs.

3.1 Fire Scenario

The general sequence of a fire is predictable. With favorable geometry, adequate combustibles and no intervention most fires will proceed through the phases shown in Figure 3-1. Ignition will occur when a kindling material is brought in contact with an ignition source. When sufficient combustible materials are present, the fire will grow exponentially until fully developed. Full development occurs when rapid fire growth stops because of limited oxygen, fuel geometry limitations, or chemical kinetic restrictions. When the combustibles are exhausted, the room temperature will start to decrease (decay) as heat escapes the fire compartment.

---

* (0.1 fires/yr)(0.05 propagates)(0.04 sprinkler fails)(0.05 wall fails)(0.5 fire department fails)

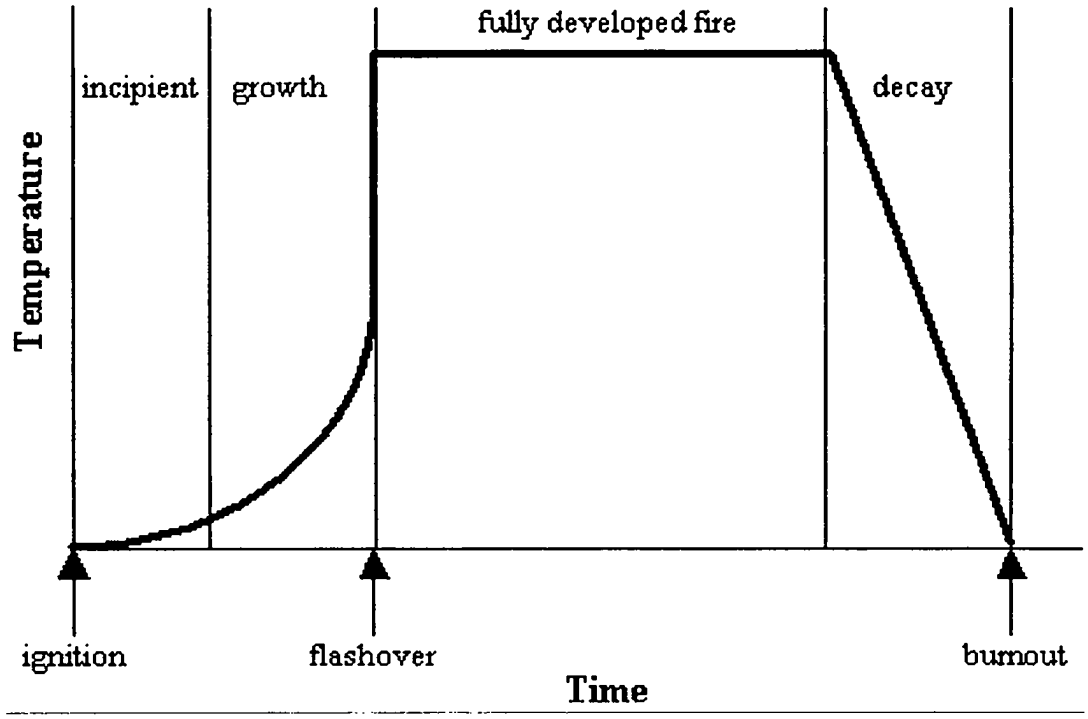

Figure 3-1. Typical Compartment Fire Curve

The consequences of a fire (e.g., bursting of a container, release of radioactive material) are strongly dependent on the container and building response to fire. The reasonably bounding responses of a building are fairly predictable. Some of the expectations are:

- Smoke migrates through a significant portion of the structure hampering emergency response and personnel evacuation.
- Ventilation systems shutdown if equipped with isolation dampers. HEPA filters become loaded and impede the exhaust flow.
- Intermediate walls (both rated and unrated) delay fire spread, but do not prevent it. Multiple room involvement occurs.
- Metal panel exterior walls open, venting smoke directly to the outside.
- Exposed structural steel fails, allowing additional venting.
- Reinforced concrete buildings maintain their configuration, thus limiting ventilation to the fire and extending the fire duration.

When evaluating the container response to fire, a model of the fire severity is necessary. This model must consider the fire conditions (e.g., heat flux, temperature as calculated by CFAST), container conditions (e.g., container strength, internal pressure as determined by structural and thermodynamic analyses) and secondary damage (e.g., impact from collapsing structures as determined by structural analyses).

3.2 Source Term

The radiological consequences are typically established using the methods discussed in the *Release Fraction Handbook* (DOE, 2000a). Since the dose from the inhalation pathway will usually dominate the overall dose, the handbook recommends that the source term be estimated from:

(1) $ST = MAR \cdot DR \cdot ARF \cdot RF \cdot LPF$

where:

- Source term (ST) is the total quantity of respirable material exiting the building (or area of interest) during the fire.
- Material-at-Risk (MAR) is the total quantity of radionuclides (in grams or curies of activity for each radionuclide) available that are subject to fire conditions.
- Damage Ratio (DR) is the fraction of the MAR actually impacted by the fire.
- Airborne Release Fraction (ARF) is the fraction of a radioactive material suspended in air as an aerosol and thus available for transport.
- Respirable Fraction (RF) "is the fraction of airborne radionuclides as particles that can be transported through air and inhaled into the human respiratory system and is commonly assumed to include particles 10-μm Aerodynamic Equivalent Diameter (AED) and less."
- Leakpath Factor (LPF) is the fraction of the radionuclides in the aerosol transported through some confinement deposition system (e.g., building rooms, ductwork) or filtration mechanism (e.g., fan filters or sand filter).

For most fire accident analyses the MAR is best defined as the maximum inventory that is permitted within the room, fire area or facility. While it is permissible to exclude material forms that are considered to be unaffected by a fire from the MAR, experience suggests that for these forms the DR is usually best set to zero for the fire release mechanism. The overall result using either approach is the same, but by assigning DR values to each combination of inventory form and release mechanism, there is the expectation that each credited form (e.g., a shipping package that is certified to withstand the postulated fire severity) is also reviewed against secondary fire events (e.g., building collapse initiated by the fire) and therefore, less likely to be overlooked.

The ARF and RF values presented in the *Release Fraction Handbook* (DOE, 2000a) are derived from discrete experiments that typically evaluated a single release mechanism. In a severe fire there may be many mechanisms occurring simultaneously. Powdered metals might be subject to entrainment by fire-induced air currents, falling because of equipment (glove box) collapse, and impact because of objects falling into the exposed fire. In addition, multiple occurrences could occur for specific mechanisms (e.g., impact of falling object on a stable powder). Aqueous solutions could be subject to boiling within the storage tank, spillage because of a tank collapse, and rapid evaporation plus splashing as the liquid sits in a diked area during the same postulated fire. Solid metals can be subject melting, dripping and burning during the same event. To

accommodate multiple mechanisms it is common to consider the ARF and RF values for each mechanism in the source term estimate.

Just as with the (ARF·RF) term, there can be multiple LPF terms applied to a single material form (e.g., room leakage, ventilation system deposition, filtration system effectiveness). Thus, their cumulative effect must be accounted for. There can be interdependence between the LPF and DR in some applications. If a shipping package is considered to leak during a fire, the leakpath effect as the material exits the packaging can be accounted for as an LPF or a DR. Based on experience, it is recommended that source term reductions related to localized conditions such as at shipping packages, and glove boxes be accounted for in the DR term. This approach allows the source term contribution from individual rooms to be readily compared. It also simplifies comparisons between the room source term and the building source term.

Based on the above discussion, Equation (1) can be generally reformatted as:

$$(2)\quad ST_{jk} = \sum_{i=1}^{n_i} \left\{ MAR_{ij} \cdot DR_{ijk} \cdot \left[(ARF \cdot RF)_{ijk} \cdot \left(\sum_{m=1}^{n_m} LPF_m \right)_{ijk} \right] \right\}$$

where: i is the MAR component in a specific form

j is the MAR component by type (e.g., Pu_{238}, Pu_{239})

k is the release mechanism

m is the filtration or deposition stage

n is the number of parameters for the form, type, mechanism or stage based on the subscript.

Thus, the source term is usually expressed in terms of an isotopic activity distribution for each release mechanism. Source term components that are associated with the same release duration can be combined, but source term components that have different release mechanisms should be kept separate to account for time-dependent variance in atmospheric dispersion for consequence assessment.

Note that the DR, but not the MAR, is shown in Equation (2) as a function of the release mechanism (k subscript), based upon the recommendation above on how to best handle the interplay between the MAR and the DR. Frequently, the DR, ARF, RF, and LPF terms are specified independently of the type, and the j subscript can be dropped from these terms as applicable.

CFAST has the potential to assist the analyst in establishing the DR and LPF terms. Selection of the proper ARF/RF may also be assisted by CFAST (e.g., a pressurize release versus not pressurized). The heat flux and temperature predictions that can be obtained using CFAST can establish possible container and building responses that aid in the specification of the DR values. The mass transport terms in CFAST can be used to help derive room and building LPF values.

To date, CFAST use by the DOE safety analysis community has primarily focused on evaluating container and building responses.

CFAST was developed to support the general fire protection community. It is intended to predict the temperatures, gas concentrations and smoke layer heights in a multi-compartment structure during a postulated fire. The zone model approach that is implemented by the software tracks the energy and mass transfer in the building that is the result of a defined fire. The software can be used to estimate the timing of specific events in the building fire performance: detector activation, sprinkler activation, and flashover. The software is also used to estimate the environmental conditions (e.g., temperature, combustion product concentrations, layer height) in the fire compartment and neighboring compartments. These conditions can then be used to assess the effect of fire on building occupants. Using CFAST to assess the stress on packages, containers and buildings that house radiological material is a reasonable extension of this use.

3.3 Radiological Consequences

Once the source term is established, the consequences to the public and workers in neighboring facilities can be estimated. For fires scenarios at facilities with relatively short distances to the site boundary, the receptor at the site boundary may be exposed to lower concentrations as a result of plume buoyancy that can cause lofting of the plume core above the receptor. Under these circumstances, higher receptor exposures can be expected downwind of the site boundary as the effects of increasing downwind plume growth progressively makes plume rise effect less significant. The touchdown point refers to the location of maximum receptor concentration. Thus, the maximally exposed individual for a lofted plume is not at the site boundary, but rather at the touchdown point. Rather than evaluating for this point, it can be more cost effective to estimate the fire consequences as a ground level release with the maximally exposed individual at the site boundary. While the results will be higher than the plume-buoyancy credited analysis, the increase may not be significant when compared to the uncertainties in the analysis and the analysis complexity.

Typically the off-site radiological consequences are expressed as the total effective dose equivalent (TEDE) at the site boundary (or other receptor location of interest) assuming a ground-level release using software codes such as MACCS (Chanin, 1998). The TEDE includes the 50-year committed effective dose equivalent (CEDE) from inhalation both during plume passage and later from resuspension, the cloudshine effective dose equivalent (EDE), the groundshine EDE, and the skin absorption EDE. This TEDE calculation does not include the ingestion CEDE from consumption of contaminated water and foodstuffs. The inhalation CEDE is usually the dominant contributor and its relationship to the source term is highlighted below.

The basic equation for the radiological consequences to an individual receptor (i.e., stationary at a specific downwind location) from the inhalation pathway during plume passage is:

$$(3)\quad \text{Receptor Inhalation CEDE} = BR \cdot \sum_{k=1}^{n_k} \left\{ \left(\frac{\chi}{Q} \right)_j \sum_{j=1}^{n_j} \left[ST_{jk}\ C_j\ IDCF_j \right] \right\}$$

where: j, k, n are as defined in Equation (2) above

BR is the breathing rate of the individual exposed to the plume of released radiological material, with typical units of m^3/s.

C_j is the specific activity of isotope j, with typical units of Ci/kg if ST is in mass units (kg) and unity if ST is in activity units (Ci).

$IDCF_j$ is the inhalation dose conversion factor for unit activity uptake of isotope j, with typical units of rem/Ci.

$(\chi/Q)_k$ is the downwind dilution factor from atmospheric transport and dispersion, which represents the time-integrated concentration at a specific downwind location that is normalized by the quantity released to the atmosphere, with typical units of s/m^3.

The inhalation CEDE as well as for TEDE is usually expressed in rem. The units for the ST and IDCF must be consistent. When developing the ST values, typical units for MAR and thus the ST are generally isotopic curies (but are also frequently isotopic grams). The corresponding IDCF values are rem per curie (or rem per isotopic gram).

When the ST value is input into the MACCS code, the MACCS output provides the TEDE values at the requested receptor locations that will include the contribution from the plume-passage inhalation CEDE as well as the contributions from resuspension inhalation CEDE, cloudshine EDE, groundshine EDE, and skin absorption EDE.

The sequence of steps that are outlined above represents the recommended approach for calculating receptor consequences. Sometimes for matters of convenience, other approaches besides direct input of the ST value into the MACCS code are used to calculate consequences. Two of these are described below. An advantage that both these approaches share is that they allow for MACCS consequence calculations to be performed independently of the source term calculations, which is a consideration when faced with a demanding schedule.

Recall that the DR, ARF, RF, and LPF terms are frequently specified independently of the type, and the j subscript can be dropped from these terms in Equation (2). Sometimes under these circumstances, an analyst uses a normalized MAR that equals the MAR divided by the total inventory mass or total inventory volume and inputs the normalized MAR into the MACCS calculation. Under these circumstances, the consequence calculations of MACCS yield normalized TEDE values that represent the receptor TEDE per unit quantity of mass or volume of respirable material that is released to the atmosphere for each release mechanism. The product of these TEDEs with the corresponding source term mass or volume (ST quantity as defined by Equation (4) below) will yield the receptor dose for each of the release mechanisms.

$$(4)\quad \left(\text{ST quantity}\right)_k = \sum_{i=1}^{n_i}\left\{\left(\text{inventory mass or volume}\right)_i \cdot DR_{ik} \cdot \left[\left(ARF \cdot RF\right)_{ik} C\left(\sum_{m=1}^{n_m} LPF_m\right)_{ik}\right]\right\}$$

and

$$(5)\quad \text{Receptor TEDE} = \sum_{k=1}^{n_k} \left\{ (\text{ST quantity})_k \, C \, (\text{normalized TEDE})_k \right\}$$

Another approach that is sometimes employed is to individually input 1-Ci values of the inventory isotopes into the MACCS code for each release mechanism to yield unit-curie TEDEs. Recall, that the release duration that is associated with each release mechanism is a variable that factors into the χ/Q value that is calculated by MACCS. So, unit-curie TEDEs must be calculated individually for the various time durations that represent the various release mechanisms. With the unit-curie approach, the following equation is used to determine the receptor consequences.

$$(6)\quad \text{Receptor TEDE} = \sum_{j=1}^{n_j} \sum_{k=1}^{n_k} \left\{ ST_{jk} \, (\text{unit TEDE})_{jk} \right\}$$

4.0 DEFAULT INPUTS & RECOMMENDATIONS

This section provides a description of the data libraries, data files and output files associated with CFAST use.

4.1 Data Libraries

CFAST uses two data libraries. The first is the thermal data file THERMAL.DF and its index file THERMAL.NDX. This library provides the typical heat transfer data used to describe walls and other objects. The analyst may use the NIST provided thermal data file; however, to ensure proper configuration control, it may be appropriate for a given application to develop an application specific thermal data library. When a modification is made to the thermal data file (or to the object data file discussed below) the analyst should delete the applicable index file. CFAST will automatically rebuild the index files.

The second data library is the object data file OBJECT. DF and its index file OBJECT.NDX. This library provides object fire definitions that can be used to represent multiple fires in addition to the main fire. At this time the development of site-specific object files has been problematic. Thus, their use in most DSA work has been avoided. Since multiple fires are a real phenomenon, further evaluation of their use is warranted.

4.2 Input Data

The data file (*.DAT) provides all the simulation data necessary for CFAST to complete each simulation. The data is arranged by keywords, which are defined in Appendix A of Jones, 2003. Specific keywords are discussed in the sample problem .The files may be modified or created using any ASCII* text editor. Appendix B provides a sample data file.

The data file may also be generated using the graphical user interface software FAST. In general it is easier to construct the initial data file using the GUI and edit an existing data file in an ASCII text editor such as WordPad. This technique also allows the analysis to circumvent some of the numerical constraints that are established on some FAST inputs (e.g., ductwork is limited to a flow area of 1 m^2). When editing the data file using WordPad, save it as a text file with a *.DAT extension.

4.3 Output Files

CFAST will provide output files in several different formats. These include the history file (*.HI), a comma delimited file (*.csv) and a text file (*.txt). The name of the history file is established by the DUMPR keyword in the CFAST data file. If a name is not established in the data file, the history file will not be generated. The history file is accessed by the routine CPlot, which is executed from the DOS command prompt. This program is described in Appendix C of

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* American Standard Code for Information Interchange.

Peacock, 2000. CPlot 5.1.1 is provided with CFAST 5.1.1, while the version provided with CFAST 3.1.7 is identified as CPlot 3.1.7.

The comma delimited file name is established by the ADUMP keyword in the CFAST data file. As with the history file, if a name is not established in the data file, the comma-delimited file will not be generated. The comma-delimited file is readily opened with common spreadsheet programs such as Microsoft Excel. The data that will be written into the comma-delimited file is established by the output option characters. These characters are the same as those specified for the *.txt file in the command line.

The text file name is established by the analyst in the command line that executes CFAST. The options for the text file are discussed above. The text file will be ASCII compatible and readily read by any ASCII editor. The analyst should take care in comparing the text file data with the history or comma-delimited files. Often the units of the text file will be different than the default units used by CFAST.

If FAST is being used to support the CFAST model, the history file and comma-delimited files can both be generated. When opening an existing data file with FAST, the output option characters in the data file will not be read. FAST will set the option to "n" which will limit the output to layer temperatures, interface height and fire size. If the analyst desires to have the comma-delimited file to contain other information, the options must be reset in FAST. Instead of the text file as discussed above, FAST will generate a file title "Lite.lst". This file contains the model initial conditions and the scenario description as well as selected data for each time step specified in the history interval. Each time a solution is initiated in FAST the Lite.lst file will be replaced. If the analyst is using FAST and wishes to retain the Lite.lst files, he or she should rename the files between each FAST solution.

4.4 Solution Method

When developing a DSA to the requirements of the 10 CFR 830 rule (CFR, 2001b), in the context of DOE-STD-94-3009 (DOE, 2000b), there is an expectation that the accident analysis modeling results will be reasonably bounding. A single fire modeling simulation or even a small set will not usually support this expectation. As discussed earlier, there are many variables associated with fire phenomena and sometimes the conservatism of the results is not necessarily intuitive. The analytical approach presented below will provide a technically appropriate approach for preparing a DSA.

Because some fire behaviors can be counter-intuitive it is strongly recommended that a fire model begin with nominal conditions, rather than forcing specific parameters to their most bounding state. When the nominal model is working successfully, the inputs can be systematically varied to demonstrate a reasonably bounding solution.

1. Establish the most likely ventilation conditions and geometry.

2. Establish a reasonably bounding HRR curve as the base condition. The total energy released should not exceed the total energy content of the combustibles that are permitted to be present.

3. Establish the room temperature profile for the above conditions.

4. Iterate the ventilation conditions (e.g., open or close doors, adjust fan operations) and geometry to maximize the upper level temperature. (See discussion on flashover below.)

5. Iterate the HRR curve to produce a Peak Heat Release Rate (PHRR) that is 50 percent higher than the base condition. The fire duration should be adjusted to avoid releasing more energy than can credibly be present. Repeat the ventilation iteration.

6. Iterate the HRR curve to produce a PHRR that is 80 percent of the base condition. The fire duration should be adjusted to avoid releasing more energy than can credibly be present. Repeat the ventilation iteration.

7. Report the most demanding time-temperature profiles developed above as sufficiently bounding temperature profiles.

The phenomenon of flashover can be accounted for using the following logic:

- Flashover is not expected if the maximum predicted upper layer temperatures resulting from the iterated ventilation conditions do not exceed 450°C. Thus, the maximum temperatures predicted in the above represent the most demanding expected.

- If the maximum predicted upper layer temperatures resulting from the iterated ventilation conditions exceed 600°C, flashover should be expected. The temperatures should be iterated to produce temperature curves that have extended high temperatures rather than very high short duration temperature peaks.*

- If the maximum predicted upper layer temperatures resulting from the iterated ventilation conditions is between 450 and 600°C, the occurrence of flashover is indeterminate. To account for the flashover threshold uncertainty the HRR curve should be increased slightly, the duration extended, or both. If the total energy released from the HRR curve (integrated value) exceeds the total energy content of the combustibles that are permitted to be present by a factor of two and the maximized predicted temperature does not exceed 600°C, the maximum temperatures predicted using the nominal HRR curve are considered representative. If the maximized predicted temperature exceeds 600°C, then that value should be used in the DSA.

Analysis Margin – In establishing the HRR and combustible loading values the confidence level of these two values should be considered. The *SFPE Engineering Guide to Performance-Based Fire Protection* (SFPE, 2000) recommends that the term sufficiently bounding may be used

---

*This approach is recommended since the fire demand is usually defined in terms of absorbed energy, which is the heat flux integrated over time. Typically, varying the boundary conditions to increase the fire exposure 5 or 10 minutes results in a nominal reduction in room temperature (~ 50°C) and heat flux, but a significant increase in the fire demand.

"when all but one parameter used for an analysis are set to best-estimate values, and the one extreme parameter is set as follows:

- "Values associated with operating expectations (e.g., combustible loading) should be taken at a minimum of 90 percent of the anticipated situation...
- "Scientific input values (e.g., [failure thresholds] and flashover temperature) should be taken at 95 percent coverage."

Example: If the best estimate HRR is considered to be 20 MW with a standard deviation of 1 MW, then the 90 percent coverage value would be:

(7) $20\,\text{MW} + (1.28 \times 1\,\text{MW}) = 21.3\,\text{MW}$

5.0 SPECIAL CONDITIONS FOR USE OF SOFTWARE

This section provides guidance on how to address the key uncertainties associated with most fire modeling predictions. The section contains explicit instructions on how to use CFAST to establish defensible and reproducible results.

5.1 Heat Release Rate

The single best metric to evaluate the severity of a fire is the Heat Release Rate (HRR). This is the quantity of energy released by the fire resulting from the combustion process. The HRR in a well-ventilated fire is proportional to its pyrolysis rate (i.e., solid combustible mass converted to vapor). These two terms are related by the heat of combustion.

$$(8) \quad \dot{Q} = \Delta H_c \dot{m}$$

Thus, if the HRR, $\dot{Q}$, and heat of combustion, ΔH_c, are known, the pyrolysis rate, $\dot{m}$, can be calculated and as long as there is adequate oxygen, the HRR can be estimated from the pyrolysis rate and the heat of combustion. When the availability of oxygen limits the combustion rate (i.e., ventilation limited) the HRR will decrease while the pyrolysis rate, depending on fire conditions, could remain constant or accelerate.

It is common practice to establish the HRR empirically. A typical HRR test result is presented in Figure 5-1. These tests are typically conducted in a free-burn (i.e., non-oxygen limited) arrangement using a calorimeter (ASTM, 1999b). For this type of test, the item in question is burned in a controlled situation where the plume flow rate and oxygen concentration can be accurately measured. This data is then used to calculate the HRR.

While empirical heat release rates for many types of residential furnishings are available, the data for materials that are common to nuclear processing facilities is very limited. To compensate for this, it is common to extrapolate HRR curves from known test data.

It is very important that the analyst using CFAST understand that CFAST does not evaluate the HRR. Rather CFAST accepts the HRR curve as an input that is reflected by three interrelated quantities mass loss rate (keyword: FMASS), Heat Release Rate (keyword: FQDOT) and heat of combustion (keyword; CHEMI). In most cases the keyword order in the data file is CHEMI, FMASS and FQDOT. The actual order is important since CFAST calculates the third parameter based on the last two parameters specified. Thus, for the most common sequence, CFAST will estimate the heat of combustion as the HRR divided by the mass loss rate as a function of time. (See Appendix B-10 of (Jones, 2003) for further discussion of this treatment.)

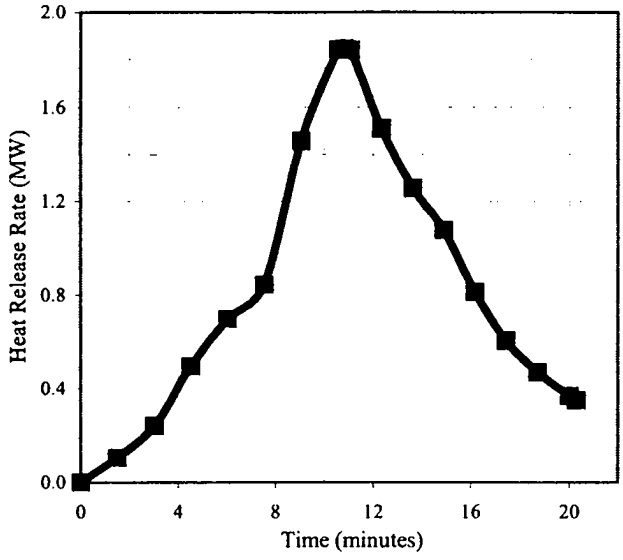

Figure 5-1 Typical HRR Curve.

CFAST uses the pyrolysis curve to represent the fire and the HRR curve to estimate the energy released. The model will limit the energy release to account for limited oxygen conditions. (See Section 3.1.2 of (Jones, 2003) for further discussion of this subject.) Because the pyrolysis curve is an input value, CFAST results do not account for increased pyrolysis due to radiative feedback from the flame or the compartment. This shortcoming can be accounted for by implementing the solution methods proposed in Section 4.4.

5.2 Performance Thresholds

There are several thresholds that are commonly used in executing fire analysis. This section will present three of the most common.

5.2.1 Secondary Ignition

The ignition process is very complex. It is influenced by the target surface finish, imposed radiation heat flux, the convective heat flux, the thermal mass, ambient environment, chemical kinetics and exposure duration. Many of these influences are not independent. In addition, most liquid and solid materials do not burn directly; rather, heat causes the materials to emit combustible vapors (e.g., pyrolysis). These vapors are the material that combust. Thus, most ignition tests focus on demonstrating the conditions that must exist to generate sufficient vapors to support ignition.

Ignition test approaches usually focus on a single ignition mode (piloted or spontaneous) and a single heat transfer mechanism (radiation or convection). Two basic ignition criteria are used in current tests, ignition temperature and critical heat flux. The ignition temperature is usually

measured at the target surface. The crucial heat flux (i.e., minimum flux to cause ignition) is measured as the total incident flux. Depending on the specific test approach the test material might only be exposed to fire conditions for a short duration (seconds to minutes).

In general, piloted ignition occurs at lower temperatures than spontaneous ignition. In addition, spontaneous ignition occurs at higher temperatures for radiant exposure when compared to convective exposure. Typical data are (DOE/EH, 2003, *Designation of Initial Safety Analysis Toolbox Codes,* Letter, US Department of Energy (March 28, 2003).

Drysdale, 1998):

Mode of heat transfer	Spontaneous ignition	Piloted ignition
Radiation	600°C	300 – 410°C
Convection	490°C	450°C

As might be expected if a target is in a severe fire environment, the heat transfer will be a mix of radiation and convection. Thus, spontaneous ignition would be expected at the convective value or below, perhaps as low as 400°C, which is in the range for piloted ignition. While specific studies have not been conducted, it is expected that this behavior exists for most other materials. Thus, for most fire modeling work, when temperature will be used as the ignition criterion, the piloted ignition temperature should be used unless specific data supporting a higher value is provided.

As mentioned earlier, most heat flux tests measure the incident heat flux. Typically these tests have little or no convective heat transfer component. The target heat flux values calculated by CFAST are the net values (i.e., incident radiation from all sources, convective flux, less reflected radiation flux). Since surface temperatures are often close to, or higher than air temperatures it is common for the convective flux to be small or negative. The test values neglect reflected radiation and re-radiation resulting from low ambient air conditions. Thus, comparing most empirical heat flux test data to the net flux data calculated by CFAST is usually not appropriate. Unless specific test data is available that is consistent with the modeled problem, the heat flux criterion for ignition should not be used.

5.2.2 Flashover

As stated above, flashover is the transition from a growing fire to a fully developed fire where all combustible items in the compartment ignite simultaneously. An upper layer room temperature of 600°C is a commonly used threshold to predict the onset of flashover; however, there is no explicit temperature at which flashover will always occur. A reasonable range for the flashover threshold is 450°C to 700°C (NFPA, 2000), however flashover has been observed to occur at gas temperatures as low as 300°C (Walton, 2002).

In preparing a fire temperature profile, if the upper-layer room temperature remains below 450°C then room temperature predictions may be assumed to be reasonably accurate. If the prediction is that the 600°C flashover threshold will be exceeded, then temperatures are again usually considered reasonable predictions. When predicted peak temperatures are in the range of 450 to 600°C, then the analysts must account for the flashover criterion uncertainty.

5.2.3 Steel failure

The critical temperature for the failure of steel is sometimes defined as the temperature at which steel has 50 percent of its strength at ambient temperature. For structural steel this is 538°C (Kodur, 2002). This does not imply that the failure temperature is 538°C. When plutonium oxide is packaged in welded containers it is common to have moisture in the container. When the container is heated this moisture will turn to steam, pressurizing the container, which can result in container burst. Depending on the moisture content this failure can occur at temperatures well below the critical temperature. It is important to investigate and understand the accident conditions and context under which a structural failure might occur when assessing the structural integrity of components during a fire.

6.0 SOFTWARE LIMITATIONS

This section describes two known weaknesses in the CFAST documentation, error messages and validation documentation. It also provides an overview of the technical limits associated with CFAST.

First, as discussed earlier, there are multiple documents that describe CFAST. At present there is no formally published comprehensive listing of error messages that CFAST or FAST might generate, however Appendix K does contain such a listing that was provided through a private communication with NIST.

Second, there is unfortunately no comprehensive publicly available listing of CFAST validation efforts. CFAST has evolved over the past 20 years and has become a well-accepted tool within the fire engineering community. This evolution process has included multiple benchmarking efforts that have compared CFAST results to controlled fire tests and real-world fires. Much of this work is published in NIST reports or peer reviewed journals. While this lack of a comprehensive listing is a known shortcoming, it is not considered to be prohibitive in using CFAST to support a DSA. As with most modeling efforts, it is the responsibility of the analyst to demonstrate that the model results are a reasonable representation of reality and that the selected controls ensure safe nuclear operations.

To address some of the fire modeling software quality assurance questions, the Nuclear Regulatory Commission (NRC) and NIST are coordinating a fire modeling benchmarking effort, *International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications* (NRC, 2002). This multi-national project is intended to share the knowledge and resources of various participating organizations to evaluate and improve the state of the art of fire models for use in nuclear power plant fire safety and fire hazard analyses. The group has completed one benchmark exercise and is in the process of developing a second. The first exercise modeled a medium sized room with a fire, which exposed a cable. The second exercise will model a large two-story structure and will evaluate both cable and steel targets.

While CFAST has some published physical operating limits such as the maximum number of rooms that can be modeled (30 per Appendix B of (Peacock, 2000)), there are few absolute limits on the input parameters (e.g., room size, HRR, physical properties). The GUI, FAST, does have some numerical limits for specific room dimensions and other parameters. These limits are not documented and in many cases are artificial. They can be bypassed by using the GUI to establish most of the input file (*.dat) and then editing the input file in WordPad. Thus, there are few if any absolute parameter limits, rather the uncertainties associated with the more extreme room geometries are greater. The user must judge the significance of these uncertainties.

One technique to minimize the uncertainties is to benchmark CFAST to a known fire experiment that is similar to the fire scenario being evaluated in CFAST. Thus, CFAST is being used to judge the effect of changing the scenario from a known test result, rather then doing an absolute prediction. The more similar the fire experiment is to the DSA fire scenario, the lower the uncertainties associated with the fire severity and consequences.

7.0 SAMPLE CALCULATIONS APPLYING SOFTWARE

This section discusses a typical fire analysis problem that is evaluated in a DSA. The analysis starts by evaluating the nominal fire, which would typically be considered the most likely scenario. It then evaluates possible variations in the scenario that could lead to increased consequences. For this and similar problems it must be recognized that the solution is iterative. Preparing a single CFAST run does not adequately model the problem. Rather, it is expected that several variations should be presented in the DSA, and that multiple iterations will need to be prepared to support the final documentation.

7.1 Description

A common room arrangement in the DOE community is a process or laboratory room that can be entered through an airlock from a long hallway. Often there is a window between the process room and the corridor, but no direct access to the corridor. The sample problem arrangement is shown in Figure 7-1 and Figure 7-2. For this sample problem the fire is limited to several trash bags containing 12 kg of contaminated polyethylene waste.

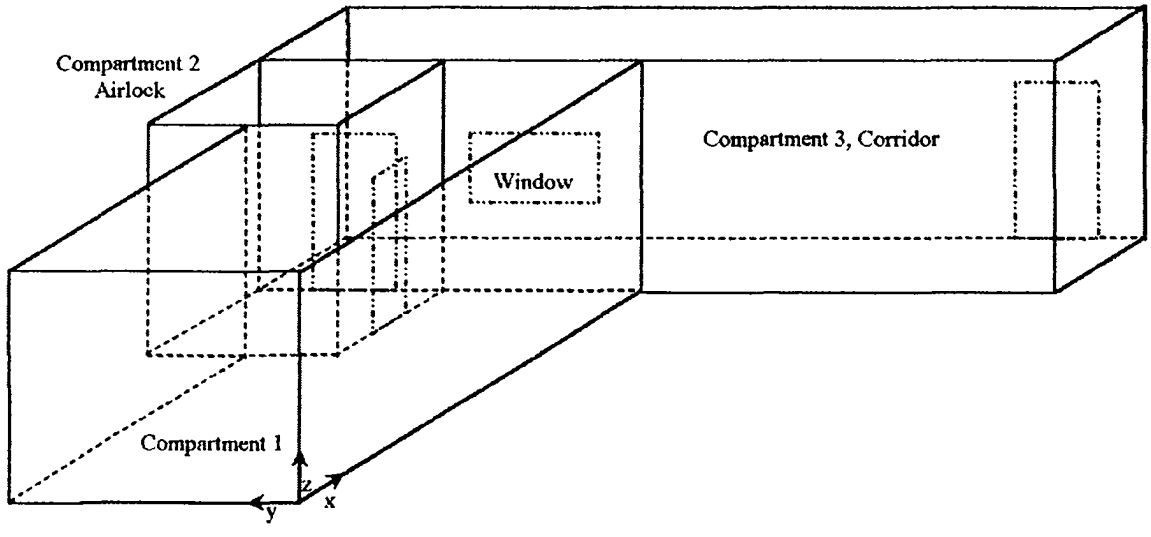

Figure 7-1. Sample Problem Arrangement – Isometric View

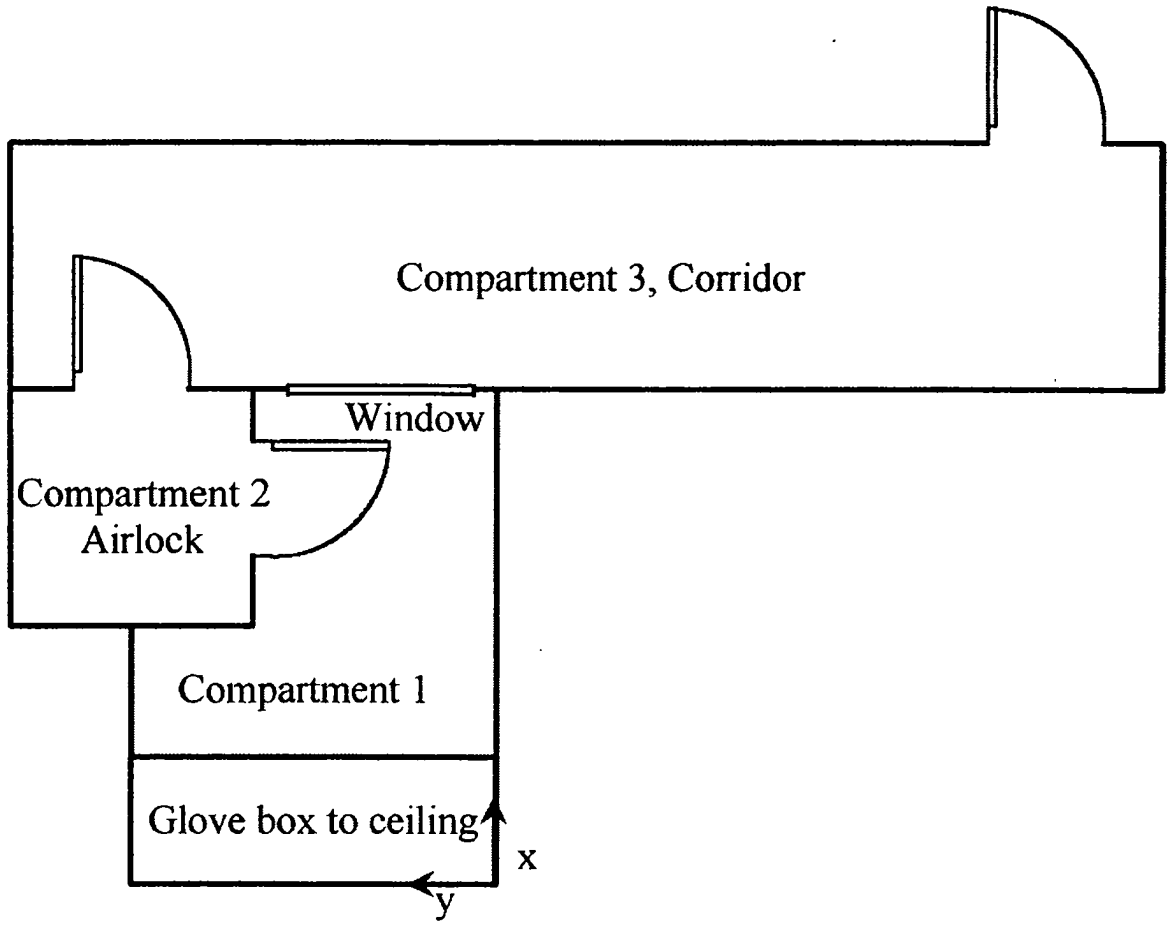

Figure 7-2. Sample Problem - Plan View

Usually the design fire starts with a description of the combustibles involved in the fire. The analyst must then postulate a reasonable HRR curve based on the material description. While there are published results for trash fires, these tests are more applicable to residential and office situations. Most of the tests involve less than 5 kg of material, burn for less than 10 minutes and have a peak heat release rate (PHRR) of 50 to 300 kW. These fires are smaller than those that could occur in a process room with several bags of waste. The polyethylene waste has a heat of combustion of 43 MJ/kg (SFPE, 2002). Thus the total available energy is about 516 MJ, or approximately 60 pounds of wood equivalent*. For this sample problem the fire is taken as a slow to medium growth fire†, with a PHRR of 500 kW. If the fire decay is linear and occurs between 900 and 1200 seconds, then the total energy released is 430 MJ. This equates to an efficiency of slightly more than 80 percent, thus the HRR is judged to be reasonably bounding.

---

* pounds of wood equivalent is an energy unit. It is equal to 8,000 Btu/pound or 19 MJ/kg.

† The growth period is taken as $Q = 0.00556\ t^2$, where the heat release rate, Q, is in kW, and the time, t, is in seconds.

7.2 Input File

This section provides a line-by-line explanation of the data file, CAB042.DAT, which is provided in Appendix B. The order of the discussion is based on the windows that are established in FAST. The headers in this section are based on the window title bars in FAST. Additional information for each keyword can be found in Appendix A of (Peacock, 2000), and Appendix B of (Jones, 2003). The file was initially constructed using the FAST GUI. Once the steady-state, no-fire data file (Appendix C) was successfully executed the data file was modified using WordPad to that shown in Appendix B. Keywords that begin with the symbol "#" are comments and do not affect the results. Where there are multiple entries for the same keyword (e.g., HVENT, CVENT) only a single data file line is presented.

7.2.1 Desktop Information

VERSN specifies the version of the CFAST model for which the input data file was prepared and an optional user defined title for the file. When using the FAST interface, the version number is automatically assigned for the corresponding CFAST version.

```
VERSN     3BASE CASE FOR EXAMPLE - FIRE
#VERSN 3 BASE CASE FOR EXAMPLE - FIRE
```

7.2.2 Model Input/Output

TIMES, in units of seconds, are the simulation time, print interval, history interval and display interval followed by the copy count.

```
TIMES    2710      10      10      20       0
```

The simulation time is a required input that has a maximum value of 86400 seconds. The print interval is the time interval between each printing of the output values. If omitted or less than or equal to zero, no printing of the output values will occur. The history interval is the time interval between each writing of the output to the history file. Documentation ((Peacock, 2000), Section A.3) states that this value must be zero if no history file is to be used; however, non-specification of this parameter leads to no spreadsheet file output (i.e., even if no history output file is to be generated, the history file is still "used" to generate the spreadsheet output file). The display interval and copy count pertain to the graphical display.

DUMPR gives the location and name of the history file output.

```
DUMPR CAB042.HI
```

History file is an optional input. If omitted, the file will not be generated. Note that, in order to obtain a history file, this parameter must be specified and the history interval must be set to a non-zero number. NOTE: As FAST is a DOS based program, the DOS naming conventions apply.

ADUMP (or ADUMPF as identified in the documentation, (Peacock, 2000), Section A.3) gives the location and name of the spreadsheet (output) file and a specification of the type of output

written to the spreadsheet file (n = normal, f = flow field, w = targets and walls, s = species, p = wall temperatures profiles).

```
ADUMP CAB042.CSV NFS
```

The spreadsheet file is an optional input. If omitted, the file will not be generated. Note that in order to obtain a spreadsheet file, this parameter must be specified and the history interval must be set to a non-zero number. Normal output is the default setting for type of output. It appears that the settings are usually not loaded from this line, thus whenever a new file is loaded the output is set to Normal. If it is desired to produce additional outputs they must be manually specified for each execution of the file. This is accomplished within FAST by selecting the filename icon in the environment section of the overview window. Next, select the *Spreadsheet* text button and then check the radio button(s) for the desired output. Click "OK", then specify the path and filename for the spreadsheet output file. Specifying a *.CSV or *.TXT file creates a comma delimited file that can then be opened with a spreadsheet program (e.g., Excel). NOTE: As FAST is a DOS based program, the DOS naming convention applies.

THRMF specifies the input file provides the location and name of the thermal database. The thermal database specifies the thermo-physical properties of the enclosing surfaces and targets by specifying the thermal conductivity, specific heat, emissivity, density, and thickness of specific materials that are then identified as enclosing surfaces or targets in the structure settings.

```
THRMF WSMSTH04.DF
```

The default thermal database file as provided by NIST is initially THERMAL.DF (not THERMAL.TPF or THERMAL.DAT as identified in (Peacock, 2000), Section A.6). An alternate thermal database file can be entered in the configuration file. For analyses that support a DSA it is recommended that a site-specific or facility specific database file be established. For the sample problem the database selected is titled WSMSTH04.DF. This approach was used to ensure that the physical property information in the database was traceable to a source document.

7.2.3 Ambient Conditions

TAMB specifies the initial the internal ambient temperature (K), internal ambient pressure (Pa) and station elevation (m) of the location at which the ambient temperature and pressure are measured.

```
TAMB  293.150         101300.  0.000000
```

EAMB specifies the initial external ambient temperature (K), internal ambient pressure (Pa) and station elevation (m) of the point at which the ambient temperature and pressure are measured.

```
EAMB  293.150         101300.  0.000000
```

Documentation ((Peacock, 2000), Section A.4) identifies the default ambient pressure as 101300 Pa and the default ambient temperature as 300 K. However, it appears that the default ambient temperature is 293.15 K.

7.2.4 Compartment (Descriptions)

The size and location of every compartment in the structure must be described. In a structure with *n* compartments, *n+1* denotes outside.

HI/F is the absolute height (in meters) of the floor of the compartment with respect to the station elevation and is specified when defining each compartment. HI/F is a required input. The default setting is zero. A structure with *n* compartments will have *n* data entries for this parameter. Since there are three compartments for the sample problem there are three numerical entries for the Compartment Description keywords.

```
HI/F   0.000000 0.000000 0.000000
```

WIDTH specifies the width (from left wall to right wall [y], in meters) of each compartment. (See Figure 7-3.) As with the HI/F keyword and the remaining keywords in this section a data file with *n* compartments will have *n* data entries.

```
WIDTH   3.0000   2.00000   3.00000
```

DEPTH specifies the depth (from rear wall forward [x], in meters) of each compartment. (See Figure 7-3.)

```
DEPTH   3.0000   2.00000   15.0000
```

HEIGH specifies the height [z] (in meters) of each compartment. (See Figure 7-3.)

```
HEIGH   2.4400   2.44000   2.44000
```

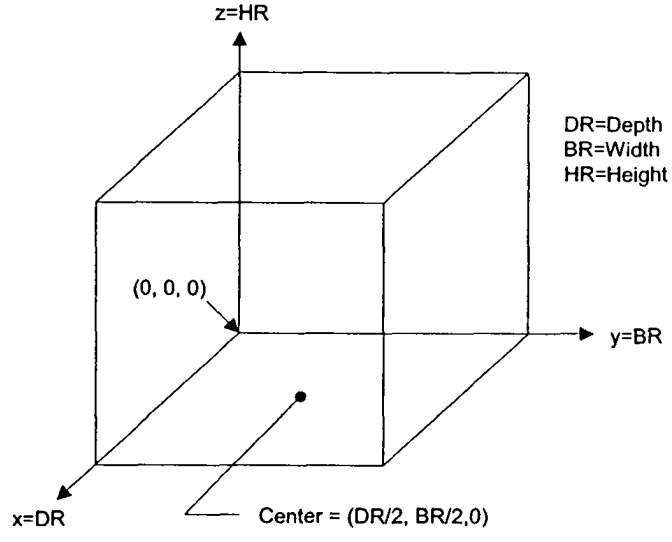

Figure 7-3. Orientation

CEILI specifies the name of the material accessed from the thermal database file for the ceiling of each compartment.

```
CEILI GYPSUM    GYPSUM    GYPSUM
#CEILI GYPSUM    GYPSUM    GYPSUM
```

WALLS specifies the name of the material accessed from the thermal database file for the walls of each compartment.

```
WALLS GYPSUM    GYPSUM    GYPSUM
#WALLS GYPSUM    GYPSUM    GYPSUM
```

FLOOR specifies the name of the material accessed from the thermal database file for the floor of each compartment.

```
FLOOR CONC003   CONC003   CONC003
#FLOOR CONC003   CONC003   CONC003
```

7.2.5 Horizontal Flow

HVENT specifies natural flow horizontal vents. The first three integers specify the "From Compartment", "To Compartment", and the sequential vent number (i.e., from Compartment 1 to Compartment 2 - Vent number 1 for the line below). The next three of numbers define the opening width, soffit height and sill height (m) of the vent. For the line presented below, the door width is 0.91 meters, with a 2.13 meter height and a sill even with the bottom of the floor. The next parameter defines the wind coefficient, and the remaining two establish the horizontal distance between the centerline of the vent and the respective reference point in the "From" and "To" compartments.

```
HVENT  1  2  1 0.910000  2.130000 0.000000 0.000000
   0.000000 0.000000
```

It is possible to define a total of four (4) horizontal flow connections between any pair of compartments. Location of the connection (i.e., sill height, soffit height) is given with respect to the floor of the "from" compartment.

CVENT specifies the opening/closing parameter for the natural flow horizontal vents. As with the HVENT keyword, the first three integers define the compartments and the vent number. The remaining values are the opening/closing parameters corresponding to each point on the specified fire timeline. The default value of one corresponds to an open vent and a fractional value represents the ratio of the opening (i.e., 0.5 would specify a vent which is halfway open). The height of the soffit and sill are not affected by this keyword. The time increments corresponding to these opening/closing factors are specified in FTIME below.

```
CVENT  1  2  1        0.00000        0.00000        0.00000
   0.00000        0.00000        0.00000        0.00000
   0.00000        0.00000        0.00000        0.00000
   0.00000        0.00000        0.00000        0.00000
   0.00000        0.00000        0.00000        0.00000
   0.00000
```

7.2.6 Ventilation System Settings

MVDCT specifies a duct that exists between two defined nodes. The first two values define the nodes. The next three establish the duct length (m), diameter (m) and absolute roughness (m). The remaining values describe the inlet flow coefficient, inlet area (m^2), outlet flow coefficient and outlet area (m^2).

```
MVDCT  1  2  20.0000 0.120000 0.000150000  2.00000 0.120000
   4.000000 0.120000
```

MVFAN specifies the location of a fan in the ventilation network and the fan curve. The first two values are the nodes that the fan is connected to. The third and fourth values are the minimum and maximum pressures (Pa) respectively. Below the minimum pressure the fan flow is assumed to be constant. Above the maximum pressure the fan flow is assumed to stop

```
MVFAN  2  3 0.000000  500.000  0.038 0.00000 0.00000
   0.000000 0.000000
```

The remaining five values specify the fan curve as:

(9) $F = A_1 + A_2\Delta p + A_3\Delta p^2 + A_4\Delta p^3 + A_5\Delta p^4$

where: F is the flow [m^3/s]

A_i is the respective flow coefficient

Δp is the pressure increase across the fan [Pa]

MVOPN specifies a connection between a compartment and the ventilation system network. The first value is the compartment number and the second is the node number. (Note: For this sample problem compartment number 4 is the outside.) The opening orientation is specified as horizontal (H) or vertical (V). The remaining values represent the height of the duct above the floor (m) and the area of the opening into the compartment (m^2).

```
MVOPN  1  1 V  1.00000 0.100000

MVOPN  4  3 H  10.0000 0.400000
```

INELV specifies the height of a ventilation node with respect to the height of the reference datum. The first value specifies the node number; the second the elevation (m).

```
INELV  2  1.00000
```

7.2.7 Main Fire Specifications

CHEMI specifies the parameters for fire kinetics as follows: the molar weight (molecular weight of the fuel vapor used for conversion to ppm), relative humidity (%), lower oxygen limit (%), heat of combustion (J/kg), initial fuel temperature (K), gaseous ignition temperature (K), and radiative fraction.

```
CHEMI  28.0000  50.0000  12.0000 4.00000E+007  293.150
   393.150 0.300000
```

The molar weight (28.0) is the value for polyethylene (SFPE, 2002). The default when using FAST is 16.0. The relative humidity (50%) was assigned based on the FAST default value of 50 percent. (Note: Relative humidity is specified within the environment settings.)

The lower oxygen limit (12%) is applicable only to Type 2 fires (see LFBT below). A Type 2 fire models the condition where the quantity of air entering the fire compartment is constrained by the ventilation openings. Under such conditions the HRR will be limited and excess pyrolysis gases will occur. The oxygen concentration threshold for this condition is in the range of 8 to 15 percent by volume (Babrauskas, 1992). FAST has a default value of 10 percent. The 12 percent value used in the sample problem has been accepted as good practice by the *International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications* (NRC, 2002).

The net heat of combustion for polyethylene is 43 MJ/kg (SFPE, 2002). It has been rounded down to 40 MJ/kg since trash is seldom a uniform material. The default heat of combustion for FAST, which is based on wood, is 1.95E+07 J/kg (not 5.0E+07 as indicated in Peacock, 2000, Section A.10).

The initial fuel temperature (293.15 K) was selected from the initial room condition of 20°C. This value is consistent with the FAST default initial fuel temperature.

The gaseous ignition temperature (393.15 K) was set at 100 K higher than the initial fuel temperature. The default value in FAST is 100 K higher than the initial fuel temperature. There is sometimes discussion that the gaseous ignition temperature should be set at the spontaneous or autoignition temperature (AIT) of the pyrolysis gases. In addition to the information previously discussed in Section 5.2.1 there are two additional shortcomings to this: (1) the pyrolysis gases are seldom well understood, (2) if an ignition source exists (e.g., spark, brand, hot object) then ignition could occur at a temperature below the AIT. Polyethylene is known to decompose into propane, propene, ethane, ethene, butene, hexene-1 and butene-1 (Beyler, 2002). The flashpoint and AIT for these materials, where available, range from 138 to 193 K and 658 to 745 K, respectively (Kanury, 2002). The 393.15 K value is above the flashpoint value, but below the AIT for the available data.

The HRR from a fire is the total energy release rate, which consists of both radiation and convective terms. Typically, the radiation term is 20 to 40 percent of the total energy release rate (Karlsson, 2000). The radiative fraction (0.3) is the midpoint of this range.

LFBO is the compartment of fire origin (i.e., Compartment 1).

```
LFBO 1
```

LFBT is the type of fire (0 = Off, 1 = Unconstrained, 2 = Constrained/Constrained with Flashover)

```
LFBT 2
```

CJET indicates for which surfaces convective heating will be determined. Setting selections are *OFF*, *CEILING*, *WALLS* and *ALL*.

```
CJET ALL
```

FPOS defines the position of the fire (X, Y, Z). Note: -1.0 indicates position is centered on that axis.

```
FPOS -1.00000 -1.00000 0.000000
```

Where: X is the position of the fire (in meters) as a distance from the rear wall of the compartment (See Figure 7-3 for orientation)

Y is the position of the fire (in meters) as a distance from the left wall of the compartment

Z is the height of the fire above the floor (in meters).

FTIME specifies the times that correspond to the pyrolysis and heat release rate curves. Because the 0.0 time is not listed in this keyword, there is one numeric entry less than in the fire descriptor keywords (e.g., FMASS). The units of time are seconds.

```
FTIME        50.000       100.000       150.000
   200.000      250.000       300.000       350.000
   400.000      450.000       500.000       550.000
   600.000      650.000       700.000       800.000
   900.000     1000.000      1100.000      1200.000
```

Initial entry of this curve specifies the mass loss rate, heat release rate, and if applicable the heat of combustion curve (see discussion below on over specifying fire curves). It also specifies the time step for various other parameters (CVENT, HCR, HCN, etc.). Note that after initial entry, any adjustment to this curve will affect all the time-related curves.

FMASS specifies the mass loss rate (e.g., fuel pyrolysis rate) corresponding to each point of the specified fire. The units of the mass loss rate are kg/s.

```
FMASS   0.000E+000  4.861E-004  1.944E-003  4.375E-003
   7.778E-003  1.215E-002  1.250E-002  1.250E-002  1.250E-
   002  1.250E-002  1.250E-002  1.250E-002  1.250E-002
   1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.167E-
   002  5.833E-003  0.000E+000
```

FQDOT specifies the heat release rate corresponding to each point of the specified fire. The units of the heat release rate are Watts.

```
FQDOT   0.000E+000  1.944E+004  7.778E+004  1.750E+005
   3.111E+005  4.861E+005  5.000E+005  5.000E+005
   5.000E+005  5.000E+005  5.000E+005  5.000E+005
   5.000E+005  5.000E+005  5.000E+005  5.000E+005
   5.000E+005  4.667E+005  2.333E+005  0.000E+000
```

Over specifying Fire Curves: Since the heat of combustion, heat release rate, and mass loss rate are inter-related, it is possible to over-specify the fire curve. The FAST GUI editor accounts for this by using the two most recently entered to calculate the third parameter. If CFAST is executed from the DOS command prompt the model will use the mass loss rate and the HRR. The heat of combustion will not be reflected in the simulation.

HCR specifies the hydrogen to carbon ratio (kg/kg) corresponding to each point of the specified fire timeline. Polyethylene is C_2H_4, thus the hydrogen to carbon ratio is 0.167. The default value when using FAST for this ratio is 0.08.

```
HCR        0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000
```

7.2.8 Graphics

The remaining keywords (e.g., SELECT, DEVICE, etc.) support the run time graphics associated with CFAST. The reader is directed to Jones, 2003, for a description of these keywords

7.3 Output Files

The Input File, CAB042.DAT, which is discussed above and presented in Appendix B directs CFAST to prepare two output files. In addition, a third output file can be created if CFAST is executed from the DOS command line. Each of these files is discussed below.

7.3.1 Spreadsheet File

The comma delimited spreadsheet file is CAB042.CSV. It contains the normal (n) outputs (layer temperatures, interface height, and fire size), the vent flows (f) and the species concentrations (s). The specific entries, and their respective units, are listed in Appendix H. With the exception of the HRR values, which were generated from the history file, all of the plots presented in this section are based on the spreadsheet files.

7.3.2 History File

The history file name is CAB042.HI. For the sample problem the size of this file should be about 6093 kB. The file is accessed by the routine CPlot, which was discussed earlier. The spreadsheet file contains most of the data that is in the history file, however there is some important information that is not exported to the spreadsheet file. While the spreadsheet file contains the main fire HRR, it does not provide the HRR for the other rooms.

The HRR for the three compartments and the outside were obtained from the history file using CPlot.

7.3.3 Text File

When CFAST is executed from the DOS prompt with the command line

```
CFAST CAB042.DAT CAB043.TXT /rinfs
```

a text file is generated. As stated previously the name of the data file associated with this command line is "CAB042.DAT." The name of the text file is "CAB043.TXT." The options selected by this line direct that the text file should contain the model initial conditions and scenario description (i), the standard output data (n), the vent flow data (f), and the layer species concentrations (s). Appendix G provides the *.txt file for the sample problem base case where only the initial conditions were requested.

7.4 Sample Results

The base case results are presented graphically in Figure 7-4 through Figure 7-9. The spreadsheet data for this case is summarized in Appendix H. The data for layer height (Figure 7-6), room pressure (Figure 7-6), and oxygen content (Figure 7-9) are plotted directly from the respective spreadsheet columns. The temperatures were converted from K to °C prior to preparing Figure 7-4. The flows, which are presented in Figure 7-7, were derived by combining the four respective mass flow values for each opening. Where there were multiple openings between two rooms, the net flow for each opening was combined. For example, for flow through opening 1 from compartment 2 to compartment 1:

$$(10)\quad \mathrm{Flow}_{\mathrm{net},2\text{-}1,1} = \mathrm{Flow}_{1-2,\mathrm{upper,in}} - \mathrm{Flow}_{1-2,\mathrm{upper,out}} + \mathrm{Flow}_{1-2,\mathrm{lower,in}} - \mathrm{Flow}_{1-2,\mathrm{lower,out}}$$

The net flow from compartment 2 to compartment 1 is:

$$(11)\quad \mathrm{Flow}_{\mathrm{net},2\text{-}1} = \mathrm{Flow}_{\mathrm{net},2\text{-}1,1} + \mathrm{Flow}_{\mathrm{net},2\text{-}1,2} + \mathrm{Flow}_{\mathrm{net},2\text{-}1,3}$$

The HRR data for compartment 1 may be obtained from the spreadsheet (CAB042.CSV) or the history file (CAB042.HI). The HRR values for compartment 2, 3, and the outside are not available in the spreadsheet (CAB042.CSV). For this scenario, since the HRR values in the remaining compartments are negligible, this data would normally be sufficient. However the HRR results for these compartments are not negligible for CAB043.DAT, so the method to obtain them is presented here.

From the DOS command prompt start the program CPlot with the following entry:

```
CPLOT
```

When prompted from CPlot, enter:

```
File
```

This will direct CPlot to access the appropriate history file. Enter the respective file name

```
CAB042.HI
```

Prompt CPlot to read the appropriate data with the command:

```
ADD
```

CPlot will then request the keyword name, which is HEAT. Once entered indicate the fire compartment: 1. Repeat this for compartments 2, 3 and 4. When the data has been read into memory it may be saved to an ASCII file with the following command:

```
SAVE
```

When prompted, provide the appropriate file name. This file can be imported into Microsoft Excel and plotted as shown in Figure 7-8.

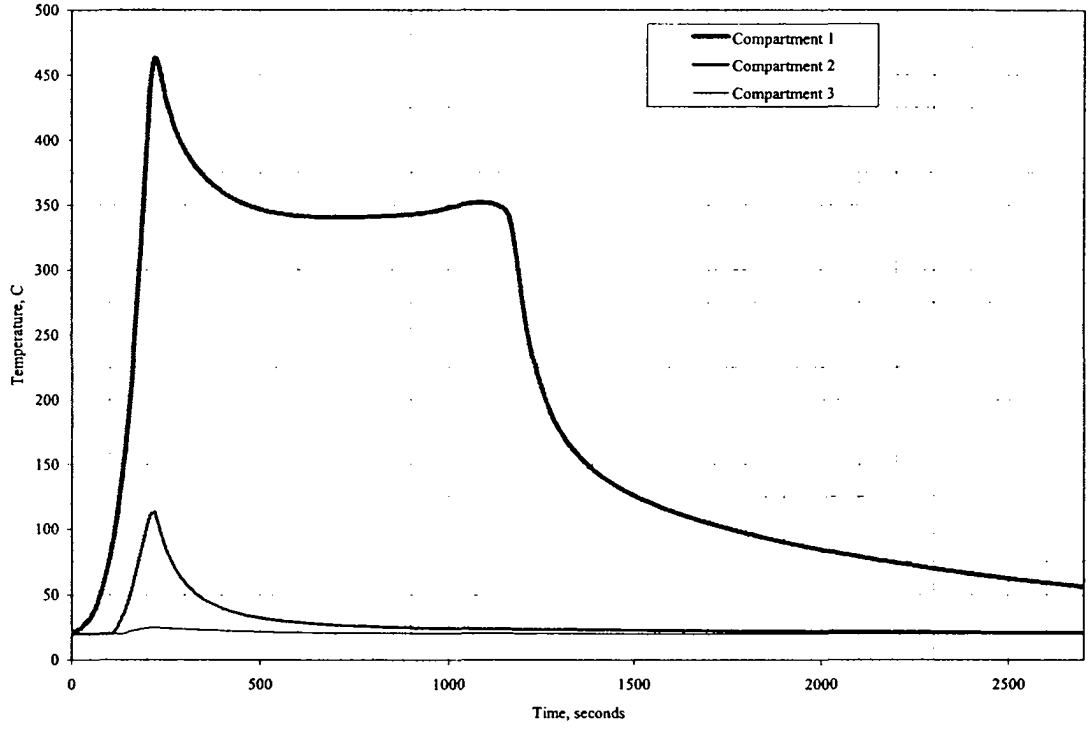

Figure 7-4. Upper Layer Temperatures For Base Case (CAB042.DAT)

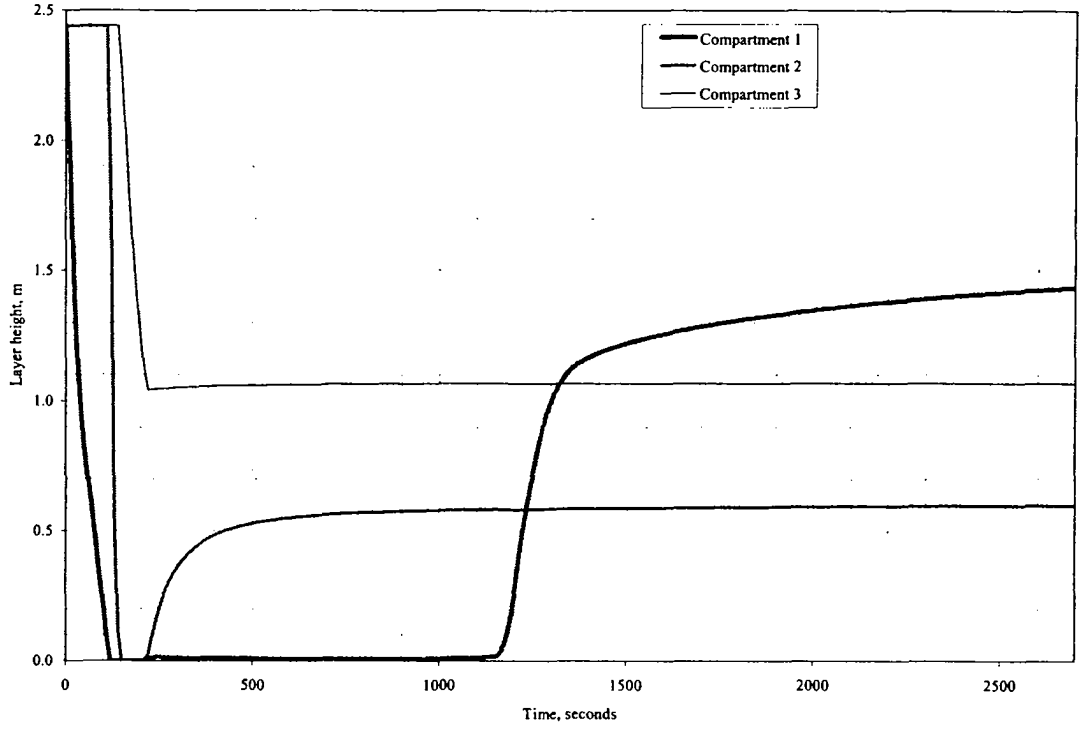

Figure 7-5. Layer Heights For Base Case (CAB042.DAT)

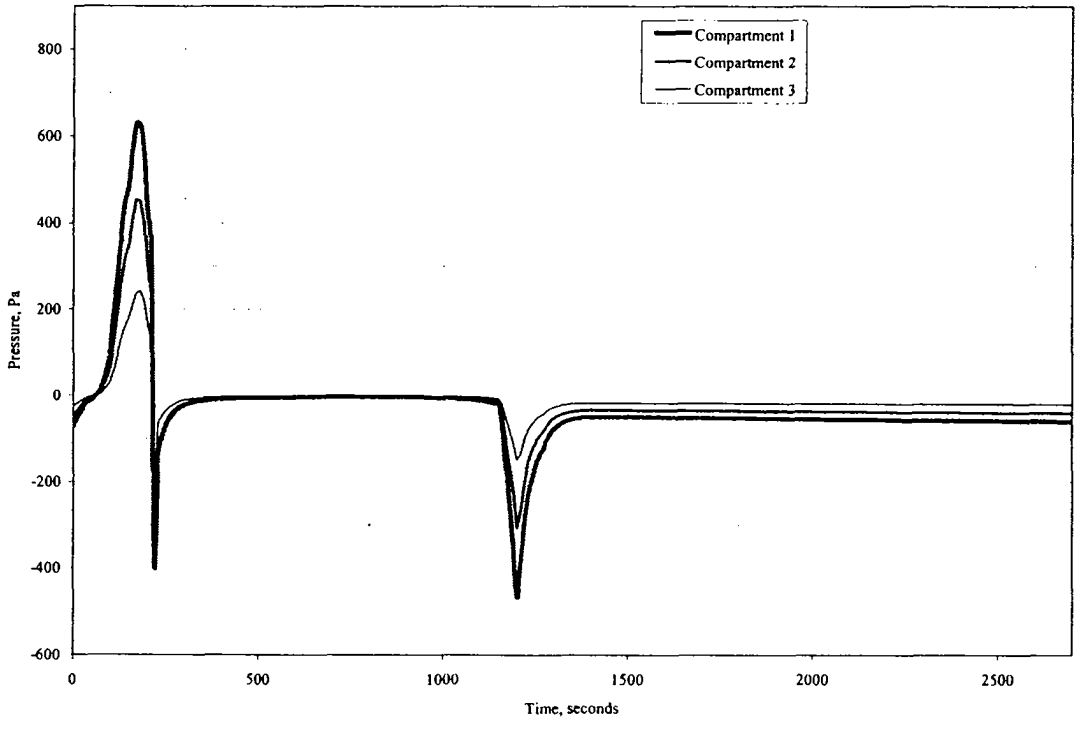

Figure 7-6. Room Pressures For Base Case (CAB042.DAT)

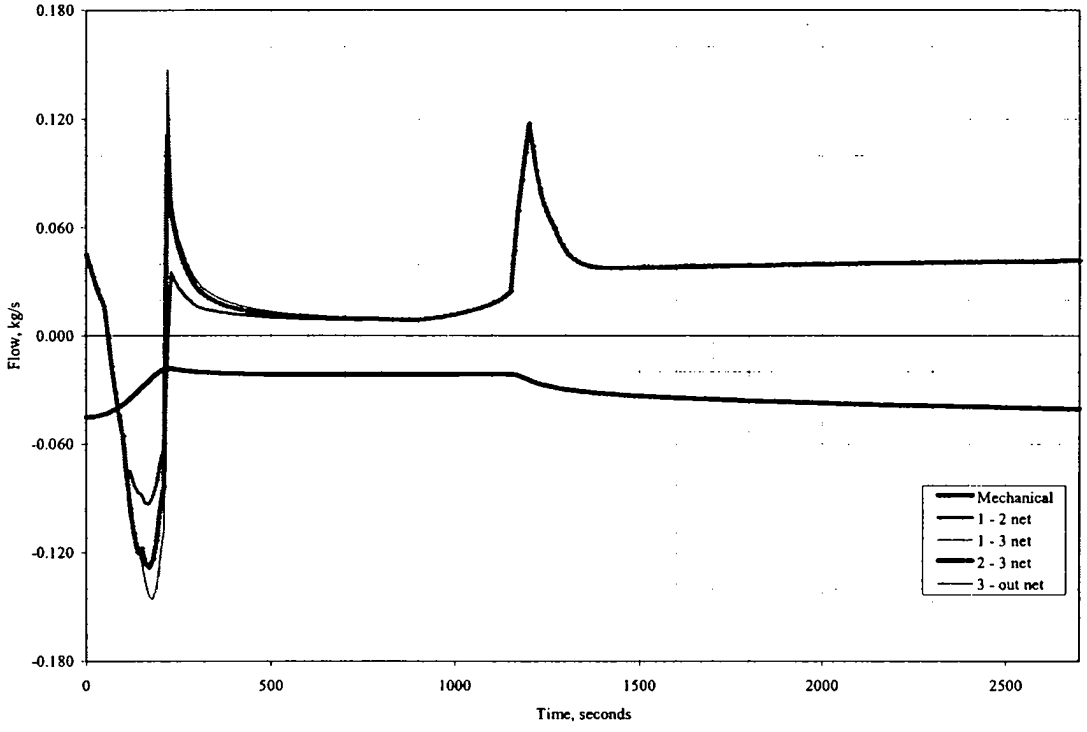

Figure 7-7. Ventilation Flows For Base Case (CAB042.DAT)

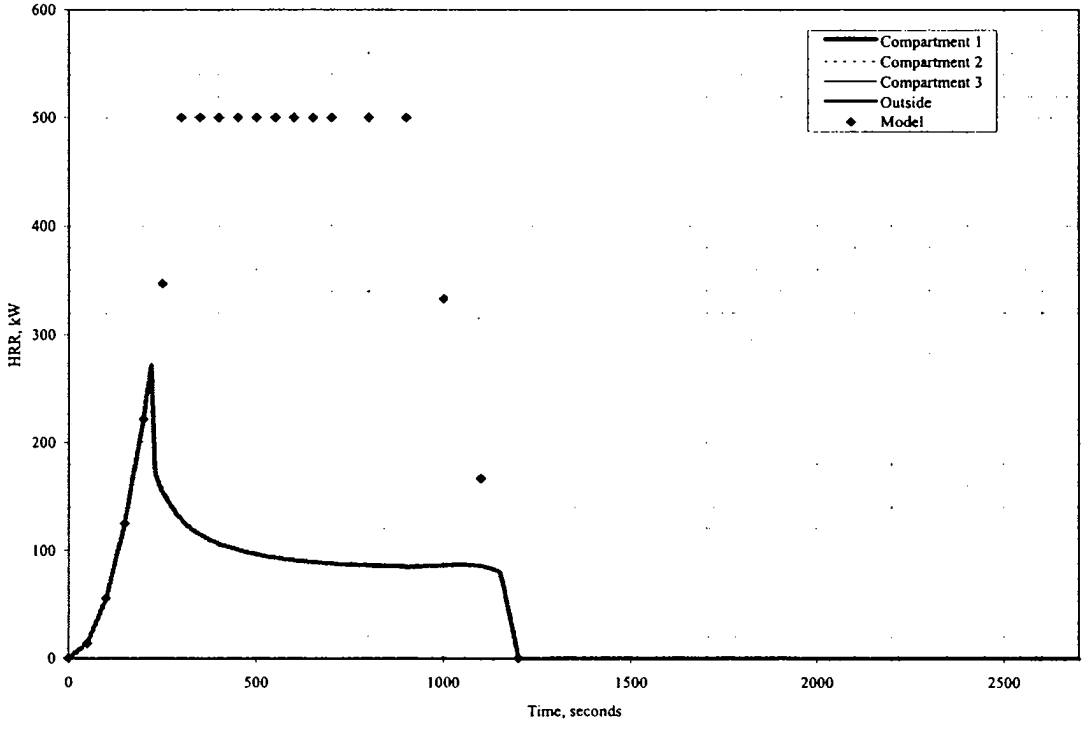

Figure 7-8. Heat Release Rates For Base Case (CAB042.DAT)

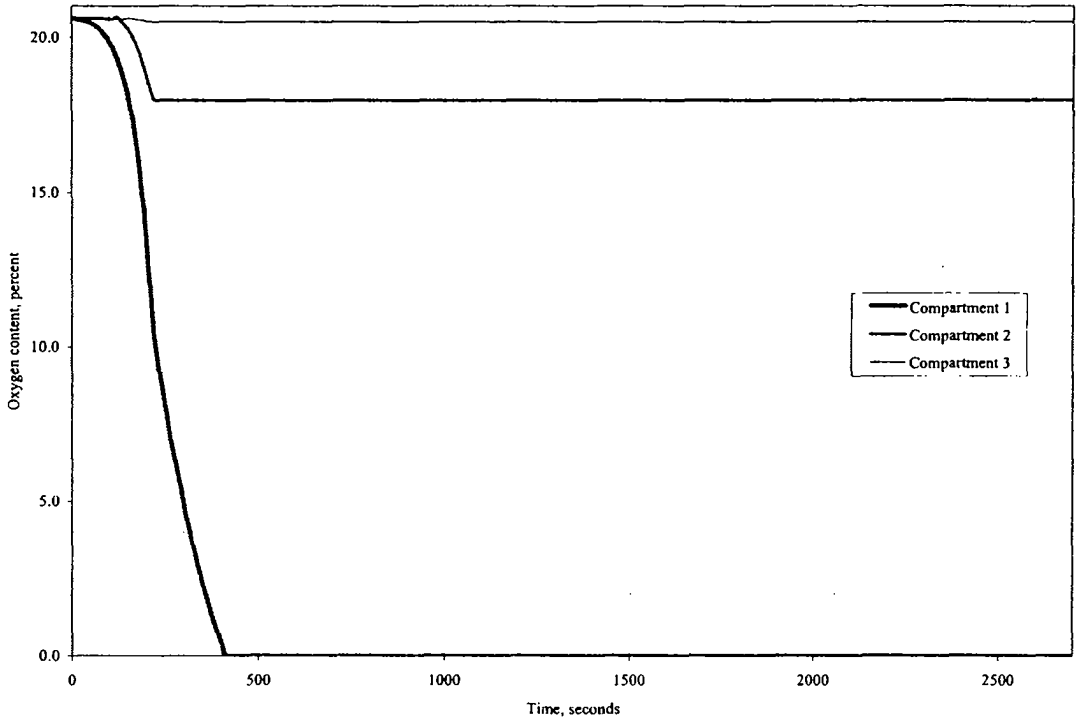

Figure 7-9. Oxygen Contents For Base Case (CAB042.DAT)

In addition to the base case (CAB042.DAT), there are several additional data files in the appendices. These include a no-fire case (Appendix C), which is a good diagnostic tool, and a case that involves breaking of the window between compartment 1 and 3 (Appendix D). Such breakage can occur during a fire where the temperature difference between the center of a glass pane and the glass, which is embedded in the window frame, exceeds 70°C (NFPA, 2001). These cases represent a subset of the potential scenarios that must be evaluated in establishing the most severe fire descriptions using the solution method presented in Section 4.4.

7.5 Discussion

Since the upper layer temperature in compartment 1, as shown in Figure 7-4, exceeds 450°C, there is the potential that flashover could occur. However for this particular scenario since the temperature does not exceed 600°C, flashover may not necessarily occur. Since the temperature is below 800°C and the high-temperature duration is less than 30 minutes (1800 seconds), material that is in shipping containers that are certified to 10 CFR 71.73(CFR, 2001a) will not be released (i.e., DR = 0). The integrity of steel containers that will not pressurize and are not in direct flame contact will also not be compromised. The room temperatures are such that storage containers that may contain moisture will require a structural analysis to determine if they will fail.

Figure 7-5 provides the layer heights for each compartment. For compartment 1 (process room) and compartment 2 (airlock) the layer height drops to the floor about 2 minutes after the fire starts. Such conditions will prevent operators from safely entering to manually suppress the fire. The layer height in the corridor (approximately 1 meter at 3.5 minutes) will limit operator actions

in compartment 3 (corridor). The conclusion, based solely on the temperature and layer height profiles, is that there is little a facility occupant can do to safely intervene in the scenario unless equipped with turnout gear.

Figure 7-6 presents the room pressures for the three compartments. At the start of the fire the pressures were slightly negative for each room as compared with ambient. At 60 seconds into the fire the pressures reverse. This occurs because of thermal expansion as the fire heats the air in compartment 1. The pressure peaks in all three compartments at 170 seconds. These pressures indicate that a flow reversal occurs in all of the compartments. This reversal lasts until 220 seconds. Following the initial flow reversal, the decrease in fire HRR allows the room atmosphere to cool, thus creating a thermal contraction that pulls air into the room. This repeats at the end of the HRR curve.

The flow rates in Figure 7-7 mirror the pressure behaviors in Figure 7-6. Initially flow is from compartment 3, through compartment 2 and into compartment 1 where it is exhausted through the mechanical ventilation system. As the fire HRR increases the mechanical exhaust will decrease. For this scenario the ventilation system moves air out of compartment 1 throughout the entire scenario.

Figure 7-8 provides the HRR curves for the three fire compartments, the outside, and the model input file. Early in the fire the predicted HRR fire in compartment 1 follows the model input. At about 220 seconds the HRR rapidly drops. This is fairly typical for fire compartments with limited ventilation. As can be seen in Figure 7-9 this coincides with the oxygen level in the upper layer of compartment 1 reaching 10.4 percent. As represented in CFAST, the mass loss rate will continue at the model input rate, but the HRR will be limited by the available oxygen. This effect continues until the predicted HRR curve intersects with the decay portion of the input HRR curve.

Figure 7-9 presents the oxygen content in the three compartments. The oxygen concentration in the upper layer of compartment 1 decreases to zero at 420 seconds. The concentration in the upper layer of the airlock decreases to 18 percent. For compartment 3 the upper layer concentration decreases to 20.5 percent.

It is possible to predict the leakpath factor (LPF) using the CFAST results. To do this explicitly is a straightforward, but time consuming process. A simplified method is presented in Appendix I. The estimate is based on the following assumptions:

1. All of the contamination is released into compartment 1 at the start of the fire.

2. Any contamination exiting compartment 1 goes directly outside. (This avoids the need to track concentrations in compartments 2 and 3.)

3. Once contamination leaves compartment 1, it does not reenter compartment 1.

4. The contamination is uniformly distributed in a layer.

Figure 7-10 shows the total contamination as a percent of the original release. The figure also provides the contamination that travels through the mechanical ventilation system, and

presumably is trapped on a filter. From this figure it is implied that the LPF is no greater than 0.42.

The temperature predictions for data file CAB043.DAT (Appendix D) are provided in Figure 7-11. The only difference between this case and the base case (CAB042.DAT) is the window between compartment 1 and compartment 3, which is assumed to fail at 700 seconds. The timing of the window failure was determined iteratively with the intent of maximizing the temperature in compartment 1. Immediately after this postulated event, the upper layer temperatures in compartment 1 and compartment 3 rise. The temperature in compartment 1 reaches 608°C, while in compartment 3 the temperature is predicted to be 530°C. Thus, for compartment 1 flashover (via a backdraft) is expected. Thus, the MAR for this scenario would include any radiological material that could be in compartment 3, in addition to the material in compartment 1.

The HRR rate also significantly increases after window failure as shown in Figure 7-12. In this scenario flames are also predicted in compartment 3. The flames in compartment 3 will last for about 2 minutes. Based on these results, ignition of some materials in compartment 3 would be expected. Thus, the DSA would need to address a multi-room fire, which would be more severe than is presented in this sample problem. (i.e., The sample problem neglects combustibles outside of compartment 1.)

The severity of the fire associated with CAB043.DAT is very severe. The damage ratio for most containers should be taken as unity unless a mechanistic structural model is developed. In addition to the thermal loads, the temperatures are sufficiently high to initiate failure of structural steel. As such, glove boxes may tip and spill their contents. If radiological material is in powder form several release mechanisms will exist (e.g., pressurized release from storage container failure, spillage when glove box supports fail, and air entrainment). In addition, lamps and similar devices that are hung from the ceiling or wall may fall and impact power that is exposed.

CFAST 3.1.7 room representations are limited to rectangular parallelepipeds. Thus, when presenting a model involving a non-rectangular room a compromise must be made: balance the free room volume and the wall surface area. In addition, if the contents of a room are significant (e.g., glove box), the effective room volume may be substantially less than the space that the room displaces. Accounting for these effects explicitly in CFAST is difficult. To account for non-rectangular geometries, non-uniform wall construction, and large building contents, a sensitivity analysis approach is recommended. This can be accomplished by bracketing the expected condition with two similar models. If the conclusions of the bracketing models are similar, then the need to demonstrate that a specific model explicitly represents the facility is alleviated. The data file CAB044.DAT (Appendix E) provides an alternate model to the base case in CAB042.DAT. For this case the compartment depth is reduced from 3 to 2 meters.

As with the base case (CAB042.DAT) the upper layer temperature in compartment 1, as shown in Figure 7-13, exceeds 450°C. In terms of timing, this high temperature occurs earlier for the reduced-volume model, although the difference is not significant. The HRR reduction limitation occurs earlier for the reduced-volume model as shown in Figure 7-14. There is also a brief recovery after the initial drop, although the overall effect is minimal.

The data file CAB045.DAT (Appendix F) uses an alternate HRR curve as the input. In this case, the PHRR is increased from 500 kW to 750 kW. The temperature and HRR predictions for this data file are presented in Figure 7-15 and Figure 7-16. There is no significant difference in the conclusions for this high PHRR scenario as compared with the base case.

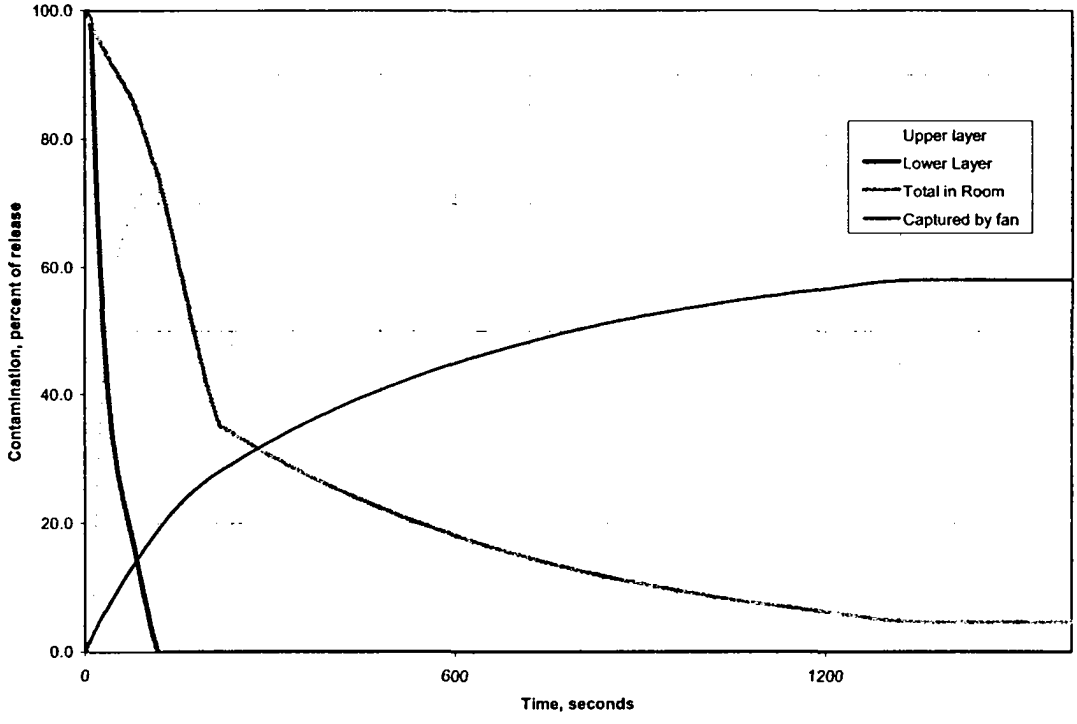

Figure 7-10. Contamination Location For Base Case (CAB042.DAT)

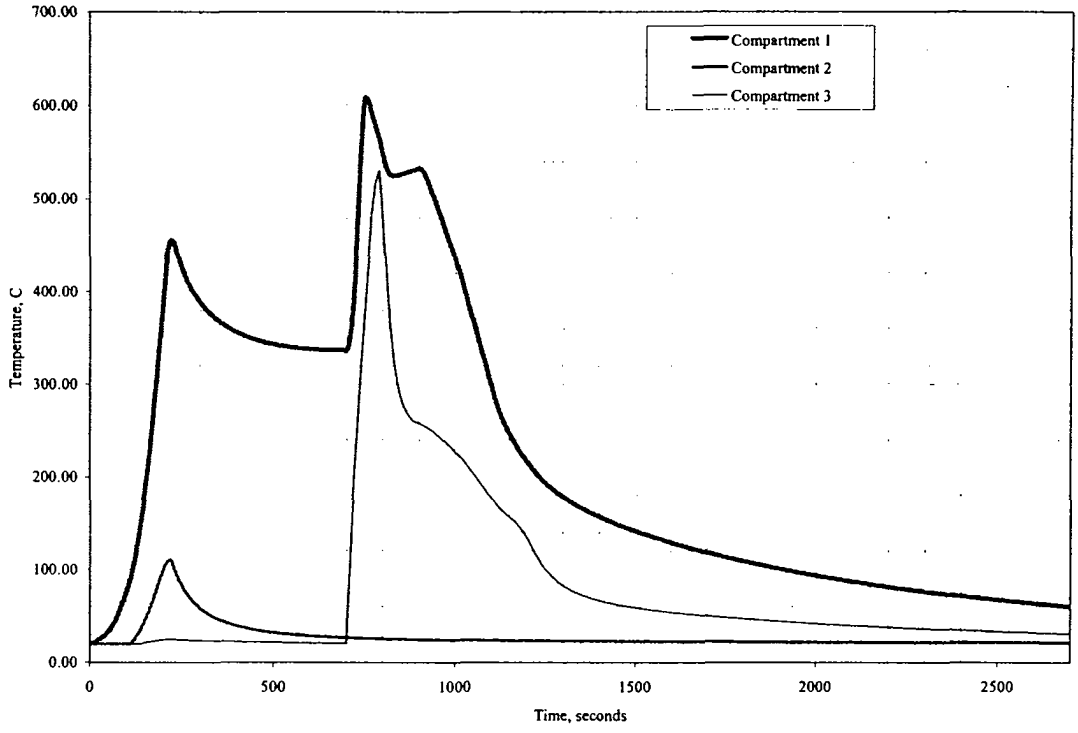

Figure 7-11. Upper Layer Temperatures For Window Failure Fire (CAB043.DAT)

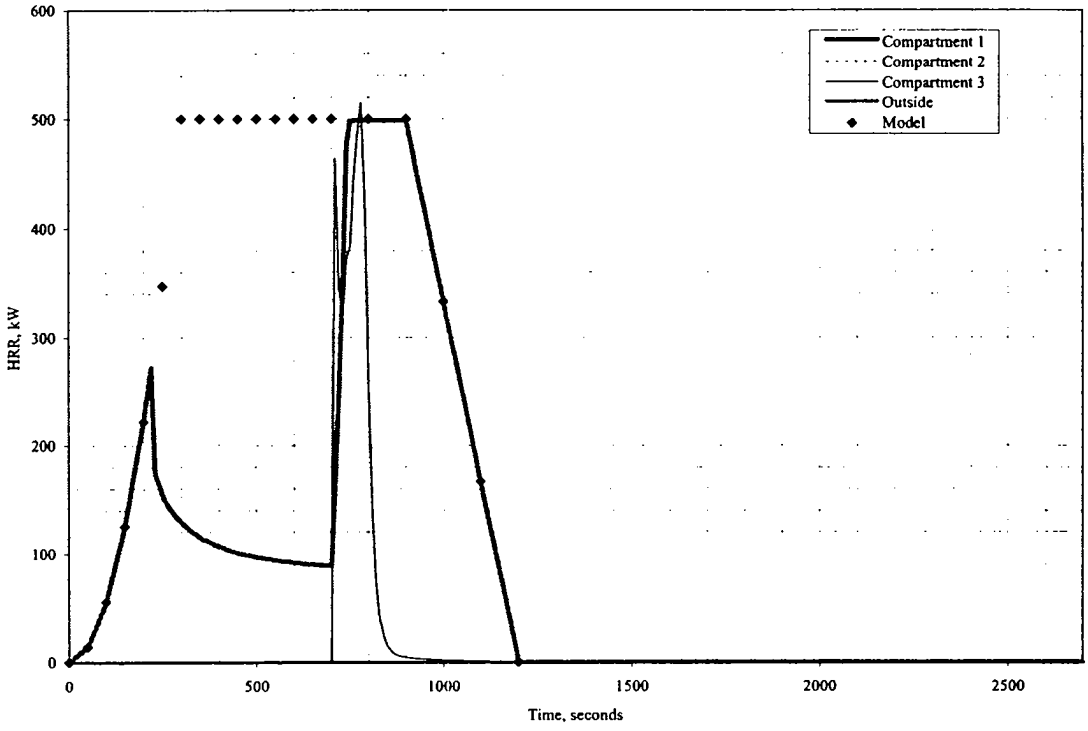

Figure 7-12. Heat Release Rates For Window Failure Fire (CAB043.DAT)

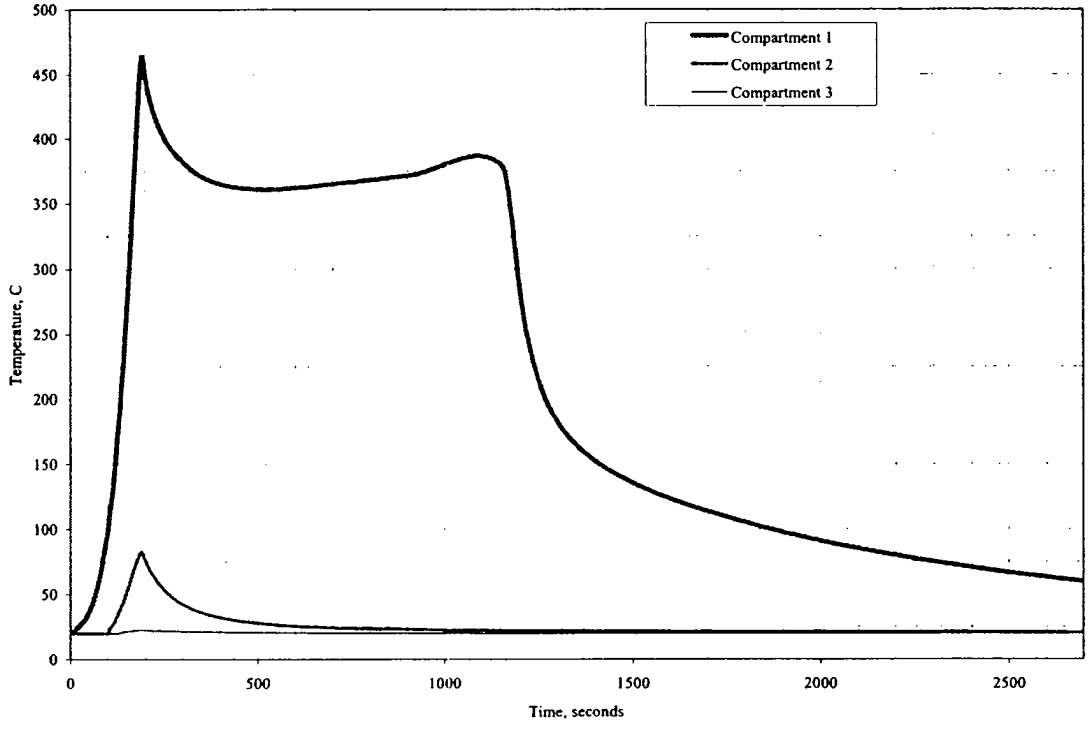

Figure 7-13. Upper Layer Temperatures For Reduced Room Size (CAB044.DAT)

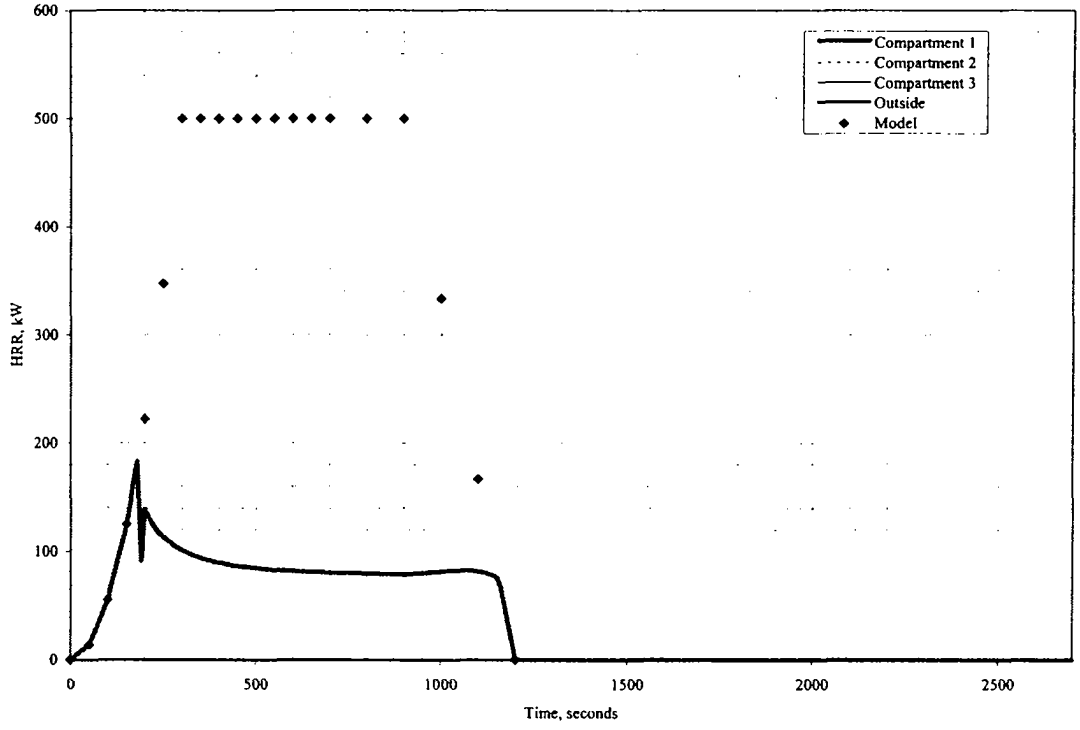

Figure 7-14. Heat Release Rates For Reduced Room Size (CAB044.DAT)

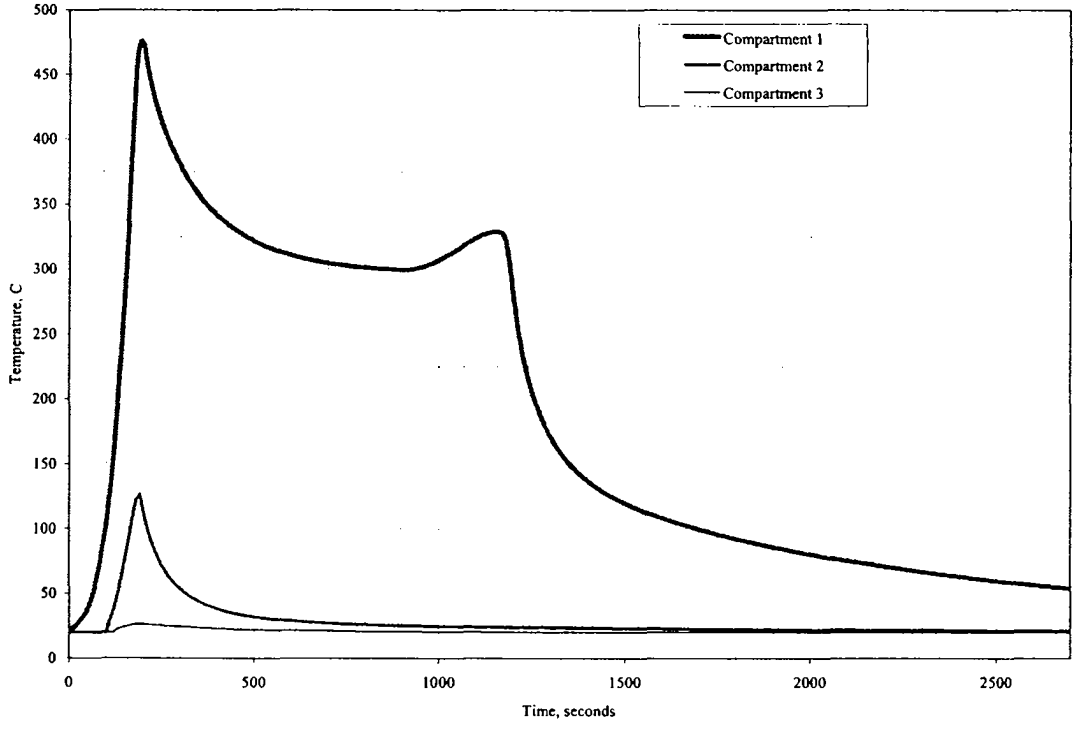

Figure 7-15. Upper Layer Temperatures For 750kw Fire (CAB045.DAT)

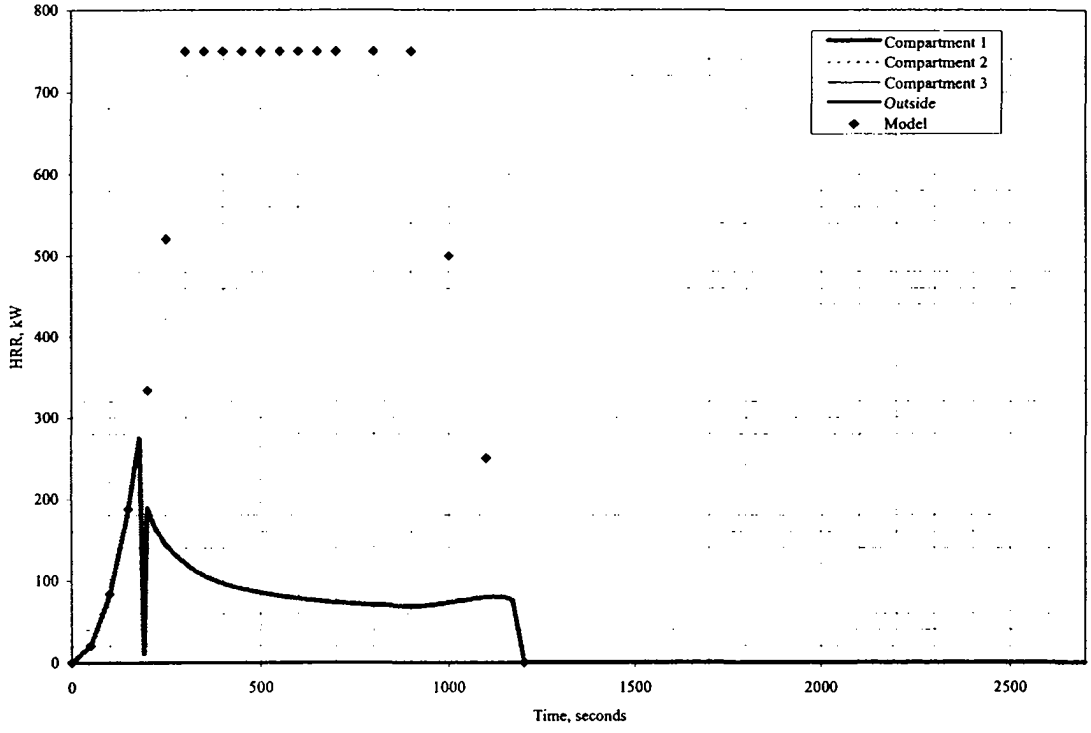

Figure 7-16. Heat Release Rates For 750kw Fire (CAB045.DAT)

8.0 ACRONYMS AND DEFINITIONS

ACRONYMS:

AHJ	Authority Having Jurisdiction
ALOHA	Areal Locations of Hazardous Atmospheres (designated toolbox software)
ANSI	American National Standards Institute
ARF	Airborne Release Fraction
ARR	Airborne Release Rate
BR	Breathing Rate
CEDE	Committed Effective Dose Equivalent (see definition below)
CFAST	Consolidated Fire and Smoke Transport Model (designated toolbox software)
CFR	Code of Federal Regulations
DBA	Design Basis Accident
DCF	Dose Conversion Factor
DNFSB	Defense Nuclear Facilities Safety Board
DoD	Department of Defense
DOE	Department of Energy
DR	Damage Ratio
DSA	Documented Safety Analysis
EFCOG	Energy Facility Contractors Group
EH	DOE Office of Environment, Safety and Health
EM	DOE Office of Environmental Management
EPIcode	Emergency Prediction Information code (designated toolbox software)
GENII	Generalized Environmental Radiation Dosimetry Software System - Hanford Dosimetry System (Generation II) (designated toolbox software)
ICRP	International Commission for Radiological Protection
IDCF	Inhalation Dose Conversion Factor
IEEE	Institute of Electrical and Electronics Engineers
IP	Implementation Plan
ISO	International Organization for Standardization
LPF	Leak Path Factor
MACCS2	MELCOR Accident Consequence Code System 2 (designated toolbox software)
MAR	Material at Risk
MELCOR	Methods for Estimation of Leakages and Consequences of Releases (designated toolbox software)
NIST	National Institute of Standards and Technology
NNSA	National Nuclear Security Administration
NRC	Nuclear Regulatory Commission
RF	Respirable Fraction
SASG	Safety Analysis Software Group (see definition below)
SQA	Software Quality Assurance
ST	Source Term
TEDE	Total Effective Dose Equivalent (see definition below)
V&V	Verification and Validation
WSMS	Washington Safety Management Solutions

Selected Terms and Definitions

Committed Dose Equivalent ($H_{T,50}$) – The dose equivalent calculated to be received by a tissue or organ over a 50-year period after the intake of a radionuclide into the body. It does not include contributions from radiation sources external to the body. Committed dose equivalent is expressed in units of rem (or sievert) (1 rem = 0.01 sievert).

Committed Effective Dose Equivalent (CEDE) – The sum of the committed dose equivalents ($HT,_{50}$) over a fifty-year period to various organs or tissues in the body, each multiplied by the appropriate weighting factor (w_T) -- that is $H_{E,50} = \Sigma\, w_T\, H_{T,50}$. CEDE is applicable to exposure from internally deposited radionuclides.

Piloted ignition – Ignition of combustible gases or vapors by a pilot source of ignition (ASTM, 1999a).

Safety Analysis Software Group (SASG) – A group of technical experts formed by the Deputy Secretary in October 2000 in response to Technical Report 25 issued by the Defense Nuclear Facilities Safety Board (DNFSF). This group is responsible for determining the safety analysis and instrument and control (I&C) software needs to be fixed or replaced, establishing plans and cost estimates for remedial work, providing recommendations for permanent storage of the software and coordinating with the Nuclear Regulatory Commission on code assessment as appropriate.

Spontaneous ignition – Unpiloted ignition caused by an internal exothermic reaction (ASTM, 1999a).

Toolbox Codes – A small number of standard computer models (codes) supporting DOE safety analysis, having widespread use, and of appropriate qualification that are maintained, managed, and distributed by a central source. Toolbox codes meet minimum quality assurance criteria. They may be applied to support 10 CFR 830 DSAs provided the application domain and input parameters are valid. In addition to public domain software, commercial or proprietary software may also be considered. In addition to safety analysis software, design codes may also be included if there is a benefit to maintain centralized control of the codes [modified from DOE N 411.1].

Total Effective Dose Equivalent (TEDE) – The sum of the deep dose equivalent (from external exposure) and the committed effective dose equivalent (from internal exposure). Note that the TEDE is equivalent to the EDE. For purposes of compliance, deep dose equivalent to the whole body may be used as effective dose equivalent for external exposures.

9.0 REFERENCES

ASTM, 1998, *Standard Guide for Documenting Computer Software for Fire Models*, ASTM. E 1472-92, West Conshohocken, PA (1998).

ASTM, 1999a, *Standard Terminology of Fire Standards*, American Society of Testing and Metals, ASTM E-176, West Conshohocken, PA (1999).

ASTM, 1999b, *Standard Test Method for Heat and Visible Smoke Release Rates for Materials and Products using an Oxygen Consumption Calorimeter*, ASTM. E-1354-99, West Conshohocken, PA (1999).

Babrauskas, 1992, Vytenis Babrauskas, "Effect of Environmental Variables" in *Heat Release in Fires*, Elsevier Applied Science, New York, NY (1992).

Beyler, 2002, Craig L. Beyler, Marcelo M. Hirschler, "Thermal Decomposition of Polymers" in the *SFPE Handbook of Fire Protection Engineering,* National Fire Protection Association, Quincy, MA (2002).

Burns, 2000, Thomas Burns, Matthew Forsbacka, and Charles R. Martin, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities,* DNFSB/TECH-25, Defense Nuclear Facility Safety Board, Washington, DC (January 2000).

CFR, 2001a, "Hypothetical Accident Conditions" in *Packaging and Transportation of Radioactive Material*, 10CFR71.73 (2001).

CFR, 2001b, *Nuclear Safety Management*, Department of Energy, 10 CFR 830, Washington, DC (January 1, 2001).

CFR, 2001c, 10 CFR Part 830, Nuclear Safety Management Rule, Code of Federal Regulations, Office of the Federal Register, Washington, DC (2001).

Chanin, 1998, D. Chanin and M. Young, *Code Manual for MACCS2: User's Guide, Volume 1,* NUREG/CR-6613, SAND97-0594, U.S. Nuclear Regulatory Commission and U.S. Department of Energy, Washington, DC (May 1998).

Deal, 1995, Deal, Scot, *Technical Reference Guide for FPEtool Version 3.2,* NISTIR 5486-1, National Institute of Standards and Technology, Building and Fire Research Laboratory, Gaithersburg, MD (April 1995).

DNFSB, 2000, *Defense Nuclear Facilities Safety Board, Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities*, Technical Report DNFSB/TECH-25, (January 2000).

DNFSB, 2002, *Recommendation 2002-1, Quality Assurance for Safety-Related Software*, Defense Nuclear Facilities Safety Board, Washington, DC (September 2002).

DOE, 1995, *Implementation Guide for use with DOE Orders 420.1 and 440.1 Fire Safety Program*, DOE G-420.1/B-0, DOE G-440.1/E-0, Department of Energy, Washington, DC (September 30, 1995).

DOE, 1998, *Worker Protection Management for DOE Federal and Contractor Employees*, DOE O 440.1A, Department of Energy, Washington, DC (March 27, 1998)..

DOE, 2000a, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities, Volume 1-Analysis of Experimental Data*, DOE-HDBK-3010-94, Change 1, Department of Energy, Washington, DC (March 2000) .

DOE, 2000b, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports*, DOE-STD-3009-94, Change Notice No. 1, Department of Energy, (January 2000).

DOE, 2002a, *Facility Safety*, DOE O 420.1A, Department of Energy, Washington, DC (May 20, 2002).

DOE 2002b, *Selection of Computer Codes for DOE Safety Analysis Applications*, Department of Energy, National Nuclear Security Agency - Defense Programs Technical Report, (May 2002).

DOE, 2003a, Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation *2002-1: Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, US Department of Energy, Washington, DC (February 28, 2003).

DOE, 2003b, *Integration of Multiple Hazard Analysis Requirements and Activities,* DOE-HDBK-1163-2003, US Department of Energy, Washington, DC. (October 2003).

DOE, 2003c, *Software Quality Assurance Improvement Plan: Format and Content for Code Guidance Reports,* US Department of Energy, Washington, DC. (August 2003).

DOE/EH, 2003, *Designation of Initial Safety Analysis Toolbox Codes*, Letter, US Department of Energy (March 28, 2003).

Drysdale, 1998, Dougal Drysdale, *An Introduction to Fire Dynamics*, John Wiley & Sons, New York, NY (1998).

Forney, 2003, Glenn P. Forney and Kevin B. McGrattan, *User's Guide for SmokeView Version 3.1 – A Tool for Visualizing Fire Dynamics Simulation Data,* NISTIR 6980, Gaithersburg, MD. U. S. Department of Commerce, National Institute of Standards and Technology (April 2003).

Gross, 1985, Daniel Gross, *Data Sources for Parameters Used in Predictive Modeling of Fire Growth and Smoke Spread,* NBSIR 85-3223, U. S. Department of Commerce, Center for Fire Research, Gaithersburg, MD (September 1985).

Jones, 2003, Walter W. Jones, Glenn P. Forney, Richard D. Peacock and Paul A. Reneke, *A Technical Reference for CFAST: An Engineering Tool for Estimating Fire and Smoke Transport*, NIST TN 1431, National Institute of Standards and Technology, Gaithersburg, MD. (April).

Kanury, 2002, A. Murty Kanury, *Ignition of Liquid Fuels,* "SFPE Handbook of Fire Protection Engineering", National Fire Protection Association, Quincy, MA (2002).

Karlsson, 2000, Björn Karlsson, and James G. Quintiere, *Enclosure Fire Dynamics*, CRC Press, New York, NY (2000).

Kodur, 2002, V. K. R. Kodur and T. Z. Harmathy, *Properties of Building Materials*, "SFPE Handbook of Fire Protection Engineering", National Fire Protection Association, Quincy, MA (2002).

NFPA, 2000, *Guide on Methods for Evaluating Potential for Room Flashover,* NFPA 555, National Fire Protection Association, Quincy, MA (2000).

NFPA, 2001, *Guide for Fire and Explosion Investigations*, NFPA 921, National Fire Protection Association, Quincy, MA (2001).

NIST, 2002, CFAST Version 5 Update, National Institute of Standards and Technology, Gaithersburg, MD, http://cfast.nist.gov/documents/V5Update.pdf. (August 2002)

NRC, 2002, *Evaluation of Fire Models for Nuclear Power Plant Applications: Cable Tray Fires*, NUREG-1758, Office of Nuclear Regulatory Research, Division of Risk Analysis and Applications, US Nuclear Regulatory Commission, Washington, DC (2002).

Peacock, 1993, R. D. Peacock, Paul A. Reneke, Walter W. Jones, Rebecca M. Portier, and Glenn P. Forney, *CFAST, the Consolidated Model of Fire Growth and Smoke Transport*, NIST Technical Note 1299, National Institute of Standards and Technology, Gaithersburg, MD (February 1993).

Peacock, 2000, R. D. Peacock, Paul A. Reneke, Richard W. Bukowski, and Glenn P. Forney, *A User's Guide for FAST: Engineering Tools for Estimating Fire Growth and Smoke Transport,* NIST Special Publication 921, 2000 edition, National Institute of Standards and Technology, Gaithersburg, MD (March 2000).

SFPE, 2000, *SFPE Engineering Guide to Performance-Based Fire Protection*, National Fire Protection Association, Quincy, MA (2000).

SFPE, 2002, *Heats of Combustion and Related Properties of Plastics, Table C.3*, "SFPE Handbook of Fire Protection Engineering", National Fire Protection Association, Quincy, MA (2002).

Shields, 2000, William M. Shields, Farid Bamdad, and Ajit K. Gwal, *Fire Protection at Defense Nuclear Facilities*, DNFSB/TECH-27, Defense Nuclear Facility Safety Board, Washington, DC (June 2000).

Walton, 2002, William D., Walton and Philip H. Thomas, *Estimating Temperatures in Compartment Fires,* "SFPE Handbook of Fire Protection Engineering", National Fire Protection Association, Quincy, MA (2002).

Appendix A Fire Severity

Fire severity has historically been defined as the room average temperature as a function of time. This approach was developed in the early 1920s based on testing by Ingberg.[1] Based on this approach, a building with a combustible contents equivalent to 10 pounds of wood equivalent* would be expected to have an equivalent fire severity of 1 hour as defined in ASTM E-119.[2] If the loading were 20-psf, the equivalent severity would be 2-hours. The fire protection community still sometimes uses this approach as a fire severity metric[3] and for most fire-resistant construction materials the simplification provides reasonable results. (i.e., For a given structural element, the maximum internal temperature at the critical depth does not depend significantly on the temporal variation of the heat flux penetrating the element.) For metals and surfaces that are covered with metal, which are the more common situation in safety evaluations, the method is not appropriate and an alternate severity metric should be applied.[4] Thus, for most DSA work fire severity predications should be developed based on engineering fundamentals.

In defining the fire severity within a fire compartment the effect of the ventilation must be understood. The nominal effect is illustrated in Figure A-1. For relatively low ventilation rates, the temperature in the fire compartment decreases with decreasing ventilation. This occurs because the less air entering the compartment, the lower the combustion rate (i.e., chemical energy released in the compartment by combustion processes). Under such conditions the fire is described as ventilation limited and the energy release will be limited to approximately 3 MJ per kg of air entering the compartment.[5] As the ventilation rate is increased there is an optimum combustion state where the temperature is maximized. For flow rates above this optimum rate, the room temperature, and hence the fire severity, is lower. This lower severity occurs because the excess airflow tends to dilute the hot fire gases.

Fires occurring in an enclosure exhibit the interaction of several complicated phenomena. As shown Figure A-2 energy exits the compartment through the enclosure perimeter (walls, ceiling and floor), by convection with the combustion products through the door and other openings. Fresh air will enter the compartment through open doors, windows, ventilation systems and other leak paths. This fresh air will be relatively cool and will then to move towards the floor. The fire will tend to draw in this cooler air, thus supporting continued combustion and will pump combustion products and heated air towards the ceiling in a well-defined plume. The development of two distinct layers occurs in many fire enclosure fires, where the upper layer is relatively hot. Mass enters the hot layer via the fire plume and exits through doors and other openings. The lower layer is relatively cool and is maintained by the in flow of fresh air and the loss via the fire plume. With the exception of the plume, there is usually little exchange between the layers except where countercurrent flow is occurring at the enclosure boundaries.

The height of the interface between the two layers is dependent on the combustion rate, the room ventilation (forced and natural) and the enclosure heat transfer properties. The greater the

---

* pounds of wood equivalent is an energy unit. It is equal to 8,000 Btu/pound or 19 MJ/kg.

combustion rate, the lower the interface height will descend. If the interface height descends to contain the fire, the combustion rate in the compartment could decrease, however the pyrolysis rate will likely be unaffected. Under such conditions the excess pyrolate will often burn outside the compartment. (e.g., The luminous flames often observed above windows and doors).

Error! Not a valid link.

Figure A-1. Ventilation Effect On Fire Conditions

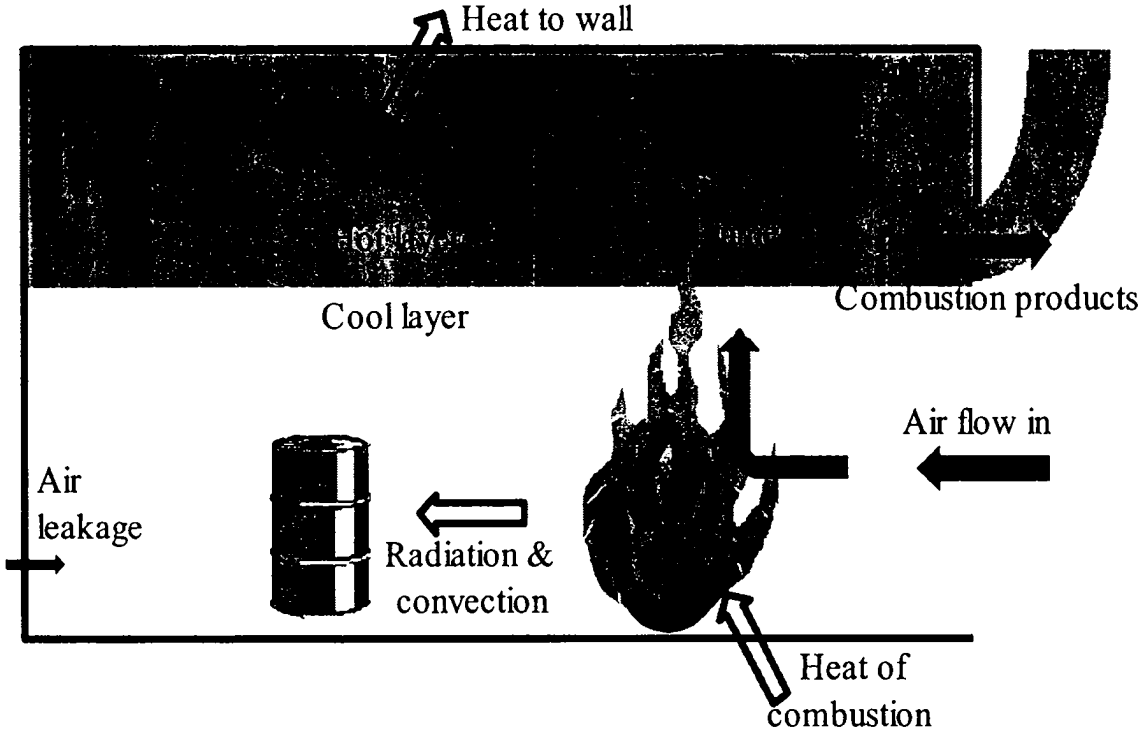

Figure A-2. Energy And Mass Flow Diagram For Compartment Fire

The above discussion did not introduce the concept of multiple fire sources in the compartment. There are several mechanisms that can lead to ignition of secondary fires in the enclosure. Two will be presented. The first is ignition by thermal heating between the first burning object and a second "fuel package." There are many publications that discuss this ignition mechanism.[6] This will be the dominant propagation mechanism early in the fire prior to flashover, and in large rooms where flashover, backdraft and similar rapid ignition behaviors do not occur.

Flashover is the other predominate ignition mechanism. It is defined as "the rapid transition to a state of total surface involvement in a fire of combustible materials within an enclosure."[7] It is essentially a thermal instability phenomenon. There are multiple criteria that have been defined to predict flashover. These criteria will be discussed in a later section. The behavior of a compartment fire prior to flashover is very different from that observed after flashover. Prior to

flashover the fuel type and geometry usually limit the combustion rate. In a post-flashover fire the combustion rate is limited by the ventilation rate. During the fully developed portion of a post-flashover the average air temperature in the enclosure is typically 700 to 1200°C. In addition there will be regions in the room where combustion is occurring. In these localized areas flame temperatures will occur. These temperatures may range from 900 to 1500°C.[8, 9] Any DSA efforts should be careful to not confuse the widely published average room temperatures with the flame temperatures.

Appendix A Works Cited

1 Ingberg, S. H., "Tests of the Severity of Building Fires," in *Quarterly National Fire Protection Association*, Vol. 22 (1928) pp 43-61.

2 *Standard Test Methods for Fire Tests of Building Construction and Materials*. 1998. West Conshohocken, PA: American Society of Testing and Metals, ASTM E-119.

3 Campbell, John A. 1997. "Confinement of fire in Buildings" in the *Fire Protection Handbook, 18th Ed.* Quincy: MA. National Fire Protection Association.

4 Harmathy, T. Z. 1993. *Fire Safety Design and Concrete*. New York. John Wiley & Sons, Inc.

5 Walton, William D., and Philip H. Thomas. 2002. "Estimating Temperatures in Compartment Fires" in the *SFPE Handbook of Fire Protection Engineering*. Quincy, MA: National Fire Protection Association.

6 *Guide on Methods for Evaluating Potential for Room Flashover*. 2000. Quincy, MA: National Fire Protection Association. NFPA 555.

7 *Standard Terminology of Fire Standards*. 1999. West Conshohocken, PA: American Society of Testing and Metals, ASTM E-176.

8 Beyler, Craig L. 2002. "Fire Hazard Calculations for Large, Open Hydrocarbon Fires" in the *SFPE Handbook of Fire Protection Engineering*. Quincy, MA: National Fire Protection Association.

9 Tien, C. L., K. Y. Lee, and A. J. Stretton. 2002. "Radiation Heat Transfer" in the *SFPE Handbook of Fire Protection Engineering*. Quincy, MA: National Fire Protection Association.

Appendix B Example Problem Input Data

BASE Case Fire (CAB042.DAT)

```
VERSN    3BASE CASE FOR EXAMPLE - FIRE
#VERSN 3 BASE CASE FOR EXAMPLE - FIRE
TIMES   2710     10     10     20      0
DUMPR CAB042.HI
ADUMP CAB042.CSV NFS
TAMB  293.150        101300. 0.000000
EAMB  293.150        101300. 0.000000
THRMF WSMSTH04.DF
HI/F  0.000000 0.000000 0.000000
WIDTH  3.0000  2.00000  3.00000
DEPTH  3.0000  2.00000  15.0000
HEIGH  2.4400  2.44000  2.44000
CEILI GYPSUM   GYPSUM   GYPSUM
WALLS GYPSUM   GYPSUM   GYPSUM
FLOOR CONC003  CONC003  CONC003
#CEILI GYPSUM   GYPSUM   GYPSUM
#WALLS GYPSUM   GYPSUM   GYPSUM
#FLOOR CONC003  CONC003  CONC003
HVENT  1  2  1 0.910000  2.130000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  1  2  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  1  3  3 1.20000  1.80000  0.90000 0.000000 0.000000 0.000000
CVENT  1  3  3       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  3  4  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
MVDCT  1  2  20.0000 0.120000 0.000150000  2.00000 0.120000 4.000000 0.120000
MVFAN  2  3 0.000000  500.000  0.038 0.00000 0.00000 0.000000 0.000000
MVOPN  1  1 V  1.00000 0.100000
MVOPN  4  3 H  10.0000 0.400000
INELV  2  1.00000
CHEMI  28.0000  50.0000  12.0000 4.00000E+007  293.150  393.150 0.300000
LFBO 1
LFBT 2
CJET ALL
FPOS -1.00000 -1.00000 0.000000
FTIME        50.000       100.000       150.000       200.000       250.000
    300.000       350.000       400.000       450.000       500.000       550.000
```

```
    600.000       650.000       700.000       800.000       900.000      1000.000
    1100.000      1200.000
FMASS   0.000E+000  3.472E-004  1.389E-003  3.125E-003  5.556E-003  8.681E-003
    1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002
    1.250E-002  1.250E-002  1.250E-002  1.250E-002  8.333E-003  4.167E-003  0.000E+000
FQDOT   0.000E+000  1.389E+004  5.556E+004  1.250E+005  2.222E+005  3.472E+005
    5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005
    5.000E+005  5.000E+005  5.000E+005  5.000E+005  3.333E+005  1.667E+005  0.000E+000
HCR       0.1670000     0.1670000     0.1670000     0.1670000     0.1670000
    0.1670000     0.1670000     0.1670000     0.1670000     0.1670000     0.1670000
    0.1670000     0.1670000     0.1670000     0.1670000     0.1670000     0.1670000
    0.1670000     0.1670000     0.1670000
SELECT 1 2 3
#GRAPHICS ON
DEVICE 1
WINDOW    0.    0. -100. 1280. 1024. 1100.
LABEL  1  970.  960.    0. 1231. 1005.   10. 15 00:00:00 0.00  0.00
GRAPH  1  100.   50.    0.  600.  475.   10. 3 TIME HEIGHT
GRAPH  2  100.  550.    0.  600.  940.   10. 3 TIME CELSIUS
GRAPH  3  720.   50.    0. 1250.  475.   10. 3 TIME FIRE_SIZE(kW)
GRAPH  4  720.  550.    0. 1250.  940.   10. 3 TIME O|D2|O()
HEAT   0 0 0 0 3   1 U
HEAT   0 0 0 0 3   2 U
HEAT   0 0 0 0 3   3 U
TEMPE  0 0 0 0 2   1 U
TEMPE  0 0 0 0 2   2 U
TEMPE  0 0 0 0 2   3 U
INTER  0 0 0 0 1   1 U
INTER  0 0 0 0 1   2 U
INTER  0 0 0 0 1   3 U
O2     0 0 0 0 4   1 U
O2     0 0 0 0 4   2 U
O2     0 0 0 0 4   3 U
```

Appendix C Example Problem Input Data

No-Fire Solution (CAB041.DAT)

```
 VERSN    3BASE CASE FOR EXAMPLE - NO FIRE
#VERSN 3 BASE CASE FOR EXAMPLE - NO FIRE
TIMES   2710     10     10     20      0
DUMPR CAB041.HI
ADUMP CAB041.CSV NFS
TAMB  293.150        101300. 0.000000
EAMB  293.150        101300. 0.000000
THRMF WSMSTH04.DF
HI/F  0.000000 0.000000 0.000000
WIDTH  3.0000  2.00000  3.00000
DEPTH  3.0000  2.00000  15.0000
HEIGH  2.5000  2.44000  2.44000
CEILI GYPSUM   GYPSUM   GYPSUM
WALLS GYPSUM   GYPSUM   GYPSUM
FLOOR CONC003  CONC003  CONC003
#CEILI GYPSUM   GYPSUM   GYPSUM
#WALLS GYPSUM   GYPSUM   GYPSUM
#FLOOR CONC003  CONC003  CONC003
HVENT  1  2  1 0.910000  2.130000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  1  2  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  1  3  3 1.20000  1.80000  0.90000 0.000000 0.000000 0.000000
CVENT  1  3  3       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  2  3  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
MVDCT  1  2  20.0000 0.120000 0.000150000  2.00000 0.120000 4.000000 0.120000
MVFAN  2  3 0.000000  500.000  0.038 0.00000 0.00000 0.000000 0.000000
MVOPN  1  1 V  1.00000 0.100000
MVOPN  4  3 H  10.0000 0.400000
INELV  2  1.00000
CHEMI  28.0000  50.0000  12.0000 4.00000E+007  293.150  393.150 0.300000
LFBO 1
LFBT 2
CJET ALL
FPOS -1.00000 -1.00000 0.000000
```

```
FTIME         50.000        100.000        150.000        200.000        250.000
     300.000        350.000        400.000        450.000        500.000        550.000
     600.000        650.000        700.000        800.000        900.000       1000.000
     1100.000       1200.000
FMASS    0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000
     0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000
     0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000
FQDOT    0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000
     0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000
     0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000  0.000E+000
HCR         0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
     0.1670000      0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
     0.1670000      0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
     0.1670000      0.1670000      0.1670000
SELECT 1 2 3
#GRAPHICS ON
DEVICE 1
WINDOW     0.     0. -100. 1280. 1024. 1100.
LABEL   1  970.   960.     0. 1231. 1005.    10. 15 00:00:00 0.00  0.00
GRAPH   1  100.    50.     0.  600.  475.    10. 3 TIME HEIGHT
GRAPH   2  100.   550.     0.  600.  940.    10. 3 TIME CELSIUS
GRAPH   3  720.    50.     0. 1250.  475.    10. 3 TIME FIRE_SIZE(kW)
GRAPH   4  720.   550.     0. 1250.  940.    10. 3 TIME O|D2|O()
HEAT    0 0 0 0 3    1 U
HEAT    0 0 0 0 3    2 U
HEAT    0 0 0 0 3    3 U
TEMPE   0 0 0 0 2    1 U
TEMPE   0 0 0 0 2    2 U
TEMPE   0 0 0 0 2    3 U
INTER   0 0 0 0 1    1 U
INTER   0 0 0 0 1    2 U
INTER   0 0 0 0 1    3 U
O2      0 0 0 0 4    1 U
O2      0 0 0 0 4    2 U
O2      0 0 0 0 4    3 U
```

Appendix D Example Problem Input Data

Window Failure Fire (CAB043.DAT)

```
VERSN    3BASE CASE FOR EXAMPLE - WINDOW BREAKS
#VERSN 3 BASE CASE FOR EXAMPLE - WINDOW BREAKS
TIMES   2710     10     10     20      0
DUMPR CAB043.HI
ADUMP CAB043.CSV NFS
TAMB  293.150        101300. 0.000000
EAMB  293.150        101300. 0.000000
THRMF WSMSTH04.DF
HI/F  0.000000 0.000000 0.000000
WIDTH  3.0000  2.00000  3.00000
DEPTH  3.0000  2.00000  15.0000
HEIGH  2.4400  2.44000  2.44000
CEILI GYPSUM   GYPSUM   GYPSUM
WALLS GYPSUM   GYPSUM   GYPSUM
FLOOR CONC003  CONC003  CONC003
#CEILI GYPSUM   GYPSUM   GYPSUM
#WALLS GYPSUM   GYPSUM   GYPSUM
#FLOOR CONC003  CONC003  CONC003
HVENT  1  2  1 0.910000  2.130000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  1  2  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  1  3  3 1.20000  1.80000  0.90000 0.000000 0.000000 0.000000
CVENT  1  3  3       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  2  3  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
MVDCT  1  2  20.0000 0.120000 0.000150000  2.00000 0.120000 4.000000 0.120000
MVFAN  2  3 0.000000  500.000  0.038 0.00000 0.00000 0.000000 0.000000
MVOPN  1  1 V  1.00000 0.100000
MVOPN  4  3 H  10.0000 0.400000
INELV  2  1.00000
CHEMI  28.0000  50.0000  12.0000 4.00000E+007  293.150  393.150 0.300000
LFBO 1
LFBT 2
CJET ALL
FPOS -1.00000 -1.00000 0.000000
```

```
FTIME         50.000       100.000       150.000       200.000       250.000
     300.000       350.000       400.000       450.000       500.000       550.000
     600.000       650.000       700.000       800.000       900.000      1000.000
     1100.000      1200.000
FMASS   0.000E+000  3.472E-004  1.389E-003  3.125E-003  5.556E-003  8.681E-003
     1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002
     1.250E-002  1.250E-002  1.250E-002  1.250E-002  8.333E-003  4.167E-003  0.000E+000
FQDOT   0.000E+000  1.389E+004  5.556E+004  1.250E+005  2.222E+005  3.472E+005
     5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005
     5.000E+005  5.000E+005  5.000E+005  5.000E+005  3.333E+005  1.667E+005  0.000E+000
HCR        0.1670000     0.1670000     0.1670000     0.1670000     0.1670000
     0.1670000     0.1670000     0.1670000     0.1670000     0.1670000     0.1670000
     0.1670000     0.1670000     0.1670000     0.1670000     0.1670000     0.1670000
     0.1670000     0.1670000     0.1670000
SELECT 1 2 3
#GRAPHICS ON
DEVICE 1
WINDOW    0.    0. -100. 1280. 1024. 1100.
LABEL  1  970.  960.    0. 1231. 1005.   10. 15 00:00:00 0.00  0.00
GRAPH  1  100.   50.    0.  600.  475.   10. 3 TIME HEIGHT
GRAPH  2  100.  550.    0.  600.  940.   10. 3 TIME CELSIUS
GRAPH  3  720.   50.    0. 1250.  475.   10. 3 TIME FIRE_SIZE(kW)
GRAPH  4  720.  550.    0. 1250.  940.   10. 3 TIME O|D2|O()
HEAT   0 0 0 0 3   1 U
HEAT   0 0 0 0 3   2 U
HEAT   0 0 0 0 3   3 U
TEMPE  0 0 0 0 2   1 U
TEMPE  0 0 0 0 2   2 U
TEMPE  0 0 0 0 2   3 U
INTER  0 0 0 0 1   1 U
INTER  0 0 0 0 1   2 U
INTER  0 0 0 0 1   3 U
O2     0 0 0 0 4   1 U
O2     0 0 0 0 4   2 U
O2     0 0 0 0 4   3 U
```

Appendix E Example Problem Input Data

Reduced Room Size Fire (CAB044.DAT)

```
VERSN    3BASE CASE FOR EXAMPLE - REDUCED VOLUME
#VERSN 3 BASE CASE FOR EXAMPLE - REDUCED VOLUME
TIMES   2710     10     10     20      0
DUMPR CAB044.HI
ADUMP CAB044.CSV NFS
TAMB  293.150        101300. 0.000000
EAMB  293.150        101300. 0.000000
THRMF WSMSTH04.DF
HI/F  0.000000 0.000000 0.000000
WIDTH  3.0000  2.00000  3.00000
DEPTH  2.0000  2.00000  15.0000
HEIGH  2.4400  2.44000  2.44000
CEILI GYPSUM   GYPSUM   GYPSUM
WALLS GYPSUM   GYPSUM   GYPSUM
FLOOR CONC003  CONC003  CONC003
#CEILI GYPSUM   GYPSUM   GYPSUM
#WALLS GYPSUM   GYPSUM   GYPSUM
#FLOOR CONC003  CONC003  CONC003
HVENT  1  2  1 0.910000  2.130000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  1  2  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  1  3  3 1.20000  1.80000  0.90000 0.000000 0.000000 0.000000
CVENT  1  3  3       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  3  4  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
MVDCT  1  2  20.0000 0.120000 0.000150000  2.00000 0.120000 4.000000 0.120000
MVFAN  2  3 0.000000  500.000  0.038 0.00000 0.00000 0.000000 0.000000
MVOPN  1  1 V  1.00000 0.100000
MVOPN  4  3 H  10.0000 0.400000
INELV  2  1.00000
CHEMI  28.0000  50.0000  12.0000 4.00000E+007  293.150  393.150 0.300000
LFBO 1
LFBT 2
CJET ALL
FPOS -1.00000 -1.00000 0.000000
```

```
FTIME         50.000        100.000        150.000        200.000        250.000
    300.000        350.000        400.000        450.000        500.000        550.000
    600.000        650.000        700.000        800.000        900.000       1000.000
    1100.000       1200.000
FMASS   0.000E+000  3.472E-004  1.389E-003  3.125E-003  5.556E-003  8.681E-003
    1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002  1.250E-002
    1.250E-002  1.250E-002  1.250E-002  1.250E-002  8.333E-003  4.167E-003  0.000E+000
FQDOT   0.000E+000  1.389E+004  5.556E+004  1.250E+005  2.222E+005  3.472E+005
    5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005  5.000E+005
    5.000E+005  5.000E+005  5.000E+005  5.000E+005  3.333E+005  1.667E+005  0.000E+000
HCR        0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000
SELECT 1 2 3
#GRAPHICS ON
DEVICE 1
WINDOW    0.    0. -100. 1280. 1024. 1100.
LABEL  1  970.  960.    0. 1231. 1005.   10. 15 00:00:00 0.00  0.00
GRAPH  1  100.   50.    0.  600.  475.   10. 3 TIME HEIGHT
GRAPH  2  100.  550.    0.  600.  940.   10. 3 TIME CELSIUS
GRAPH  3  720.   50.    0. 1250.  475.   10. 3 TIME FIRE_SIZE(kW)
GRAPH  4  720.  550.    0. 1250.  940.   10. 3 TIME O|D2|O()
HEAT   0 0 0 0 3   1 U
HEAT   0 0 0 0 3   2 U
HEAT   0 0 0 0 3   3 U
TEMPE  0 0 0 0 2   1 U
TEMPE  0 0 0 0 2   2 U
TEMPE  0 0 0 0 2   3 U
INTER  0 0 0 0 1   1 U
INTER  0 0 0 0 1   2 U
INTER  0 0 0 0 1   3 U
O2     0 0 0 0 4   1 U
O2     0 0 0 0 4   2 U
O2     0 0 0 0 4   3 U
```

Appendix F Example Problem Input Data

750 kW Fire (CAB045.DAT)

```
VERSN    3BASE CASE FOR EXAMPLE - HIGH FIRE
#VERSN 3 BASE CASE FOR EXAMPLE - HIGH FIRE
TIMES   2710     10     10     20      0
DUMPR CAB045.HI
ADUMP CAB045.CSV NFS
TAMB  293.150        101300. 0.000000
EAMB  293.150        101300. 0.000000
THRMF WSMSTH04.DF
HI/F  0.000000 0.000000 0.000000
WIDTH  3.0000  2.00000  3.00000
DEPTH  3.0000  2.00000  15.0000
HEIGH  2.4400  2.44000  2.44000
CEILI GYPSUM   GYPSUM   GYPSUM
WALLS GYPSUM   GYPSUM   GYPSUM
FLOOR CONC003  CONC003  CONC003
#CEILI GYPSUM   GYPSUM   GYPSUM
#WALLS GYPSUM   GYPSUM   GYPSUM
#FLOOR CONC003  CONC003  CONC003
HVENT  1  2  1 0.910000  2.130000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  1  2  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  1  2  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  1  3  3 1.20000  1.80000  0.90000 0.000000 0.000000 0.000000
CVENT  1  3  3       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  2  3  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  2  3  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
HVENT  3  4  1 0.910000  2.13000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  1       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000       0.00000       0.00000       0.00000
    0.00000       0.00000       0.00000
HVENT  3  4  2 0.910000 0.0095000 0.000000 0.000000 0.000000 0.000000
CVENT  3  4  2       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000       1.00000       1.00000       1.00000
    1.00000       1.00000       1.00000
MVDCT  1  2  20.0000 0.120000 0.000150000  2.00000 0.120000 4.000000 0.120000
MVFAN  2  3 0.000000  500.000  0.038 0.00000 0.00000 0.000000 0.000000
MVOPN  1  1 V  1.00000 0.100000
MVOPN  4  3 H  10.0000 0.400000
INELV  2  1.00000
CHEMI  28.0000  50.0000  12.0000 4.00000E+007  293.150  393.150 0.300000
LFBO 1
LFBT 2
CJET ALL
FPOS -1.00000 -1.00000 0.000000
```

```
FTIME         50.000        100.000        150.000        200.000        250.000
    300.000        350.000        400.000        450.000        500.000        550.000
    600.000        650.000        700.000        800.000        900.000       1000.000
    1100.000       1200.000
FMASS    0.000E+000  5.208E-004  2.083E-003  4.688E-003  8.333E-003  1.302E-002
    1.875E-002  1.875E-002  1.875E-002  1.875E-002  1.875E-002  1.875E-002  1.875E-002
    1.875E-002  1.875E-002  1.875E-002  1.875E-002  1.250E-002  6.250E-003  0.000E+000
FQDOT    0.000E+000  2.083E+004  8.333E+004  1.875E+005  3.333E+005  5.208E+005
    7.500E+005  7.500E+005  7.500E+005  7.500E+005  7.500E+005  7.500E+005  7.500E+005
    7.500E+005  7.500E+005  7.500E+005  7.500E+005  5.000E+005  2.500E+005  0.000E+000
HCR        0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000      0.1670000      0.1670000      0.1670000
    0.1670000      0.1670000      0.1670000
SELECT 1 2 3
#GRAPHICS ON
DEVICE 1
WINDOW     0.     0. -100. 1280. 1024. 1100.
LABEL   1  970.   960.     0. 1231. 1005.   10. 15 00:00:00 0.00  0.00
GRAPH   1  100.    50.     0.  600.  475.   10. 3 TIME HEIGHT
GRAPH   2  100.   550.     0.  600.  940.   10. 3 TIME CELSIUS
GRAPH   3  720.    50.     0. 1250.  475.   10. 3 TIME FIRE_SIZE(kW)
GRAPH   4  720.   550.     0. 1250.  940.   10. 3 TIME O|D2|O()
HEAT    0 0 0 0 3    1 U
HEAT    0 0 0 0 3    2 U
HEAT    0 0 0 0 3    3 U
TEMPE   0 0 0 0 2    1 U
TEMPE   0 0 0 0 2    2 U
TEMPE   0 0 0 0 2    3 U
INTER   0 0 0 0 1    1 U
INTER   0 0 0 0 1    2 U
INTER   0 0 0 0 1    3 U
O2      0 0 0 0 4    1 U
O2      0 0 0 0 4    2 U
O2      0 0 0 0 4    3 U
```

Appendix G Example Problem Text File Results

Base Case Fire (CAB042.TXT)

```
**      CFAST  Version   3.1.7  Run  8/28/ 2      **
**                                                **
**             A contribution of the              **
** National Institute of Standards and Technology **
**             Gaithersburg, MD  20899            **
**             Not subject to Copyright           **
**                                                **
**        DOS/4GW Memory Manager Copyright (c)    **
**             Rational System, Inc (1993)        **

CFAST Version    3.1.7     BASE CASE FOR EXAMPLE - FIRE

Data file is cab042.dat    (Checksum 00000000)


OVERVIEW


Compartments    Doors, ...    Ceil. Vents, ...    MV Connects

   3               7             0                   2

Simulation     Print       History     Restart
Time           Interval    Interval    Interval
(s)            (s)         (s)         (s)

  2710          10          10          0

Ceiling jet is on for all
History file is CAB042.HI


AMBIENT CONDITIONS

Interior       Interior       Exterior       Exterior       Station        Wind           Wind           Wind
Temperature    Pressure       Temperature    Pressure       Elevation      Speed          Ref. Height    Power
(K)            (Pa)           (K)             (Pa)          (m)            (m/s)           (m)

   293.          101300.         293.          101300.         0.00          0.0            10.0           0.16
```

COMPARTMENTS

Compartment	Width (m)	Depth (m)	Height (m)	Area (m^2)	Volume (m^3)	Ceiling Height (m)	Floor Height (m)
1	3.00	3.00	2.44	9.00	21.96	2.44	0.00
2	2.00	2.00	2.44	4.00	9.76	2.44	0.00
3	3.00	15.00	2.44	45.00	109.80	2.44	0.00

VENT CONNECTIONS

Horizontal Natural Flow Connections (Doors, Windows, ...)

From Compartment	To Compartment	Vent Number (m)	Width (m)	Sill Height (m)	Soffit Height (m)	Abs. Sill (m)	Abs. Soffit (m)	Area (m^2)
1	2	1	0.91	0.00	2.13	0.00	2.13	1.94
1	2	2	0.91	0.00	0.01	0.00	0.01	0.01
1	3	3	1.20	0.90	1.80	0.90	1.80	1.08
2	3	1	0.91	0.00	2.13	0.00	2.13	1.94
2	3	2	0.91	0.00	0.01	0.00	0.01	0.01
3	Outside	1	0.91	0.00	2.13	0.00	2.13	1.94
3	Outside	2	0.91	0.00	0.01	0.00	0.01	0.01

There are no vertical natural flow connections

Mechanical Flow Connections (Fans, Ducts, ...)

Connections and Ducts

System	From	From Elev. (m)	To	To Elev. (m)	Length (m)	Area (m^2)	Rough (mm)
1	Comp 1	1.00	Node 1	1.00		0.10	
	Node 1	1.00	Node 2	1.00	20.00	0.09	0.00

Fans

System	From	From Elev. (m)	To	To Elev. (m)	Fan Number	Minimum (Pa)	Maximum (Pa)	Fan Curve	
1	Node 2	1.00	Node 3	10.00	1	0.00	500.00	3.80E-02	0.00E+00
0.00E+00	0.00E+00	0.00E+00							
	Node 3	10.00	Outside	10.00		0.40			

THERMAL PROPERTIES

Compartment	Ceiling	Wall	Floor
1	GYPSUM	GYPSUM	CONC003
2	GYPSUM	GYPSUM	CONC003
3	GYPSUM	GYPSUM	CONC003

Thermal data base used: WSMSTH04.DF

Name	Conductivity	Specific heat	Density	Thickness	Emissivity	HCL B's (1->5)			
GYPSUM	0.200	1.000E+03	700.	1.600E-02	0.900	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00									
CONC003	1.75	1.000E+03	2.200E+03	0.152	0.940	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00									

TARGETS

Target	Compartment	Position (x, y, z)			Direction (x, y, z)			Material	
1	1	1.50	1.50	0.00	0.00	0.00	1.00	CONC003	Floor, compartment 1
2	2	1.00	1.00	0.00	0.00	0.00	1.00	CONC003	Floor, compartment 2
3	3	7.50	1.50	0.00	0.00	0.00	1.00	CONC003	Floor, compartment 3

FIRES

Name: Main Fire

Compartment	Fire Type		Position (x,y,z)			Relative Humidity		Lower O2 Limit		Pyrolysis Temperature			
1	Constrained		1.50	1.50	0.00	50.0		12.00		293.			
Time (s)	Fmass (kg/s)	Hcomb (J/kg)	Fqdot (W)	Fhigh (m)		C/CO2 (kg/kg)	CO/CO2 (kg/kg)	H/C (kg/kg)	O/C (kg/kg)	HCN (kg/kg)	HCL (kg/kg)		
0.	0.00E+00	4.00E+07	0.00E+00	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
50.	3.47E-04	4.00E+07	1.39E+04	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
100.	1.39E-03	4.00E+07	5.56E+04	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
150.	3.13E-03	4.00E+07	1.25E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
200.	5.56E-03	4.00E+07	2.22E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
250.	8.68E-03	4.00E+07	3.47E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
300.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
350.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
400.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
450.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
500.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
550.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
600.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
650.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
700.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
800.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
900.	1.25E-02	4.00E+07	5.00E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
1000.	8.33E-03	4.00E+07	3.33E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
1100.	4.17E-03	4.00E+07	1.67E+05	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		
1200.	0.00E+00	4.00E+07	0.00E+00	0.00E+00		0.00E+00	0.00E+00	0.33	0.00E+00	0.00E+00	0.00E+00		

Appendix H Example Problem Comma-Delimitated Entries

Base Case Fire (CAB042.CSV)

Output Parameter	Spreadsheet Output Selection	Units	Description
TIME	Normal	seconds	Time
Upper Layer Temp(1)	Normal	K	Upper layer temperature in compartment 1
Lower Layer Temp(1)	Normal	K	Lower layer temperature in compartment 1
Layer Height(1)	Normal	m	Height from floor to bottom of upper layer in compartment 1
Upper Layer Volume(1)	Normal	m^3	Volume of upper layer in compartment 1
Pressure(1)	Normal	Pa	Gauge pressure in compartment 1
Ambient Target(1)	Normal	W/m^2	Undefined
Floor Target(1)	Normal	W/m^2	Undefined
Upper Layer Temp(2)	Normal	K	Upper layer temperature in compartment 2
Lower Layer Temp(2)	Normal	K	Lower layer temperature in compartment 2
Layer Height(2)	Normal	m	Height from floor to bottom of upper layer in compartment 2
Upper Layer Volume(2)	Normal	m^3	Volume of upper layer in compartment 2
Pressure(2)	Normal	Pa	Gauge pressure in compartment 2
Ambient Target(2)	Normal	W/m^2	Undefined
Floor Target(2)	Normal	W/m^2	Undefined
Upper Layer Temp(3)	Normal	K	Upper layer temperature in compartment 3
Lower Layer Temp(3)	Normal	K	Lower layer temperature in compartment 3
Layer Height(3)	Normal	m	Height from floor to bottom of upper layer in compartment 3
Upper Layer Volume(3)	Normal	m^3	Volume of upper layer in compartment 3
Pressure(3)	Normal	Pa	Gauge pressure in compartment 3
Ambient Target(3)	Normal	W/m^2	Undefined
Floor Target(3)	Normal	W/m^2	Undefined
Main Plume Flow	Normal	kg/s	Plume mass flow rate for main fire
Main Pyrolysis Rate	Normal	kg/s	Fuel mass loss rate for main fire
Main Fire Size	Normal	W	Heat release rate (HRR)
Main Flame Height	Normal	m	Flame height
Main Convec. Size	Normal	W	Flame convection energy
Upper N2(1)	Species	%	mass concentration of nitrogen in the upper layer of compartment 1
Upper O2(1)	Species	%	mass concentration of oxygen in the upper layer of compartment 1
Upper CO2(1)	Species	%	mass concentration of carbon dioxide in the upper layer of compartment 1
Upper CO(1)	Species	ppm	mass concentration of carbon monoxide in the upper layer of compartment 1
Upper HCN(1)	Species	ppm	mass concentration of hydrogen cyanide in the upper layer of compartment 1
Upper HCL(1)	Species	ppm	mass concentration of hydrogen chloride in the upper layer of compartment 1
Upper TUHC(1)	Species	%	mass concentration of total unburned hydrocarbons in the upper layer of compartment 1
Upper H2O(1)	Species	%	mass concentration of water in the upper layer of compartment 1
Upper OD(1)	Species	m^{-1}	mass concentration of soot in the upper layer of compartment 1
HCl c(1)	Species	mg/m^2	Undefined
HCl uw(1)	Species	mg/m^2	Undefined
HCl lw(1)	Species	mg/m^2	Undefined
HCl f(1)	Species	mg/m^2	Undefined
Upper N2(2)	Species	%	
Upper O2(2)	Species	%	
Upper CO2(2)	Species	%	
Upper CO(2)	Species	ppm	
Upper HCN(2)	Species	ppm	
Upper HCL(2)	Species	ppm	
Upper TUHC(2)	Species	%	
Upper H2O(2)	Species	%	
Upper OD(2)	Species	m^{-1}	
HCl c(2)	Species	mg/m^2	
HCl uw(2)	Species	mg/m^2	
HCl lw(2)	Species	mg/m^2	
HCl f(2)	Species	mg/m^2	

Output Parameter	Spreadsheet Output Selection	Units	Description
Upper N2(3)	Species	%	
Upper O2(3)	Species	%	
Upper CO2(3)	Species	%	
Upper CO(3)	Species	ppm	
Upper HCN(3)	Species	ppm	
Upper HCL(3)	Species	ppm	
Upper TUHC(3)	Species	%	
Upper H2O(3)	Species	%	
Upper OD(3)	Species	m^{-1}	
HCl c(3)	Species	mg/m^2	
HCl uw(3)	Species	mg/m^2	
HCl lw(3)	Species	mg/m^2	
HCl f(3)	Species	mg/m^2	
Lower N2(1)	Species	%	mass concentration of nitrogen in the lower layer of compartment 1
Lower O2(1)	Species	%	mass concentration of oxygen in the lower layer of compartment 1
Lower CO2(1)	Species	%	mass concentration of carbon dioxide in the lower layer of compartment 1
Lower CO(1)	Species	ppm	mass concentration of carbon monoxide in the lower layer of compartment 1
Lower HCN(1)	Species	ppm	mass concentration of hydrogen cyanide in the lower layer of compartment 1
Lower HCL(1)	Species	ppm	mass concentration of hydrogen chloride in the lower layer of compartment 1
Lower TUHC(1)	Species	%	mass concentration of total unburned hydrocarbons in lower layer
Lower H2O(1)	Species	%	mass concentration of water in the lower layer of compartment 1
Lower OD(1)	Species	m^{-1}	mass concentration of soot in the lower layer of compartment 1
HCl c(1)	Species	mg/m^2	Undefined
HCl uw(1)	Species	mg/m^2	Undefined
HCl lw(1)	Species	mg/m^2	Undefined
HCl f(1)	Species	mg/m^2	Undefined
Lower N2(2)	Species	%	
Lower O2(2)	Species	%	
Lower CO2(2)	Species	%	
Lower CO(2)	Species	ppm	
Lower HCN(2)	Species	ppm	
Lower HCL(2)	Species	ppm	
Lower TUHC(2)	Species	%	
Lower H2O(2)	Species	%	
Lower OD(2)	Species	m^{-1}	
HCl c(2)	Species	mg/m^2	
HCl uw(2)	Species	mg/m^2	
HCl lw(2)	Species	mg/m^2	
HCl f(2)	Species	mg/m^2	
Lower N2(3)	Species	%	
Lower O2(3)	Species	%	
Lower CO2(3)	Species	%	
Lower CO(3)	Species	ppm	
Lower HCN(3)	Species	ppm	
Lower HCL(3)	Species	ppm	
Lower TUHC(3)	Species	%	
Lower H2O(3)	Species	%	
Lower OD(3)	Species	m^{-1}	
HCl c(3)	Species	mg/m^2	
HCl uw(3)	Species	mg/m^2	
HCl lw(3)	Species	mg/m^2	
HCl f(3)	Species	mg/m^2	
Upper Inflow 1- 2(1)	Flow Field	kg/s	mass flow rate into upper layer of compartment 1 from compartment 2 for vent 1.

Output Parameter	Spreadsheet Output Selection	Units	Description
Upper Outflow 1- 2(1)	Flow Field	kg/s	mass flow rate out of the upper layer of compartment 1 to compartment 2 for vent 1.
Lower Inflow 1- 2(1)	Flow Field	kg/s	mass flow rate into lower layer of compartment 1 from compartment 2 for vent 1.
Lower Outflow 1- 2(1)	Flow Field	kg/s	mass flow rate out of the lower layer of compartment 1 to compartment 2 for vent 1.
Mixing to Upper 1- 2(1)	Flow Field	kg/s	
Mixing to Lower 1- 2(1)	Flow Field	kg/s	
Upper Inflow 1- 2(2)	Flow Field	kg/s	
Upper Outflow 1- 2(2)	Flow Field	kg/s	
Lower Inflow 1- 2(2)	Flow Field	kg/s	
Lower Outflow 1- 2(2)	Flow Field	kg/s	
Mixing to Upper 1- 2(2)	Flow Field	kg/s	
Mixing to Lower 1- 2(2)	Flow Field	kg/s	
Upper Inflow 1- 3(3)	Flow Field	kg/s	
Upper Outflow 1- 3(3)	Flow Field	kg/s	
Lower Inflow 1- 3(3)	Flow Field	kg/s	
Lower Outflow 1- 3(3)	Flow Field	kg/s	
Mixing to Upper 1- 3(3)	Flow Field	kg/s	
Mixing to Lower 1- 3(3)	Flow Field	kg/s	
MV Upper Inflow 5	Flow Field	kg/s	
MV Upper Outflow 5	Flow Field	kg/s	
MV Lower Inflow 5	Flow Field	kg/s	
MV Lower Outflow 5	Flow Field	kg/s	
Upper Inflow 2- 1(1)	Flow Field	kg/s	
Upper Outflow 2- 1(1)	Flow Field	kg/s	
Lower Inflow 2- 1(1)	Flow Field	kg/s	
Lower Outflow 2- 1(1)	Flow Field	kg/s	
Mixing to Upper 2- 1(1)	Flow Field	kg/s	
Mixing to Lower 2- 1(1)	Flow Field	kg/s	
Upper Inflow 2- 1(2)	Flow Field	kg/s	
Upper Outflow 2- 1(2)	Flow Field	kg/s	
Lower Inflow 2- 1(2)	Flow Field	kg/s	
Lower Outflow 2- 1(2)	Flow Field	kg/s	
Mixing to Upper 2- 1(2)	Flow Field	kg/s	
Mixing to Lower 2- 1(2)	Flow Field	kg/s	
Upper Inflow 2- 3(1)	Flow Field	kg/s	
Upper Outflow 2- 3(1)	Flow Field	kg/s	
Lower Inflow 2- 3(1)	Flow Field	kg/s	
Lower Outflow 2- 3(1)	Flow Field	kg/s	
Mixing to Upper 2- 3(1)	Flow Field	kg/s	
Mixing to Lower 2- 3(1)	Flow Field	kg/s	
Upper Inflow 2- 3(2)	Flow Field	kg/s	
Upper Outflow 2- 3(2)	Flow Field	kg/s	
Lower Inflow 2- 3(2)	Flow Field	kg/s	
Lower Outflow 2- 3(2)	Flow Field	kg/s	
Mixing to Upper 2- 3(2)	Flow Field	kg/s	
Mixing to Lower 2- 3(2)	Flow Field	kg/s	
Upper Inflow 3- 1(3)	Flow Field	kg/s	
Upper Outflow 3- 1(3)	Flow Field	kg/s	
Lower Inflow 3- 1(3)	Flow Field	kg/s	
Lower Outflow 3- 1(3)	Flow Field	kg/s	
Mixing to Upper 3- 1(3)	Flow Field	kg/s	
Mixing to Lower 3- 1(3)	Flow Field	kg/s	
Upper Inflow 3- 2(1)	Flow Field	kg/s	
Upper Outflow 3- 2(1)	Flow Field	kg/s	
Lower Inflow 3- 2(1)	Flow Field	kg/s	
Lower Outflow 3- 2(1)	Flow Field	kg/s	
Mixing to Upper 3- 2(1)	Flow Field	kg/s	

Output Parameter	Spreadsheet Output Selection	Units	Description
Mixing to Lower 3- 2(1)	Flow Field	kg/s	
Upper Inflow 3- 2(2)	Flow Field	kg/s	
Upper Outflow 3- 2(2)	Flow Field	kg/s	
Lower Inflow 3- 2(2)	Flow Field	kg/s	
Lower Outflow 3- 2(2)	Flow Field	kg/s	
Mixing to Upper 3- 2(2)	Flow Field	kg/s	
Mixing to Lower 3- 2(2)	Flow Field	kg/s	
Upper Inflow 3-Outside(1)	Flow Field	kg/s	
Upper Outflow 3-Outside(1)	Flow Field	kg/s	
Lower Inflow 3-Outside(1)	Flow Field	kg/s	
Lower Outflow 3-Outside(1)	Flow Field	kg/s	
Upper Inflow 3-Outside(2)	Flow Field	kg/s	
Upper Outflow 3-Outside(2)	Flow Field	kg/s	
Lower Inflow 3-Outside(2)	Flow Field	kg/s	
Lower Outflow 3-Outside(2)	Flow Field	kg/s	

Appendix I Example Problem Leak Path Estimate Spreadsheet

BASE CASE Fire (CAB042.xls)

Mass flow calculation for a contaminate

	A	B	C	D	E	F	G	H
1	Time (s)	Mass flow (kg/s)						
2	TIME	Main Plume Flow	Upper fan	Lower fan	Upper inflow	Lower inflow	Mixing upper to lower	Mixing lower to upper
3	0	0.00E+00	0.0000	-0.0454	0.0000	0.0454	0.0000	0.0000
4	10	5.48E-01	0.0000	-0.0451	0.0000	0.0390	0.0000	0.0000
5	20	3.98E-01	0.0000	-0.0448	0.0000	0.0324	0.0000	0.0000
6	30	2.79E-01	0.0000	-0.0445	0.0000	0.0260	0.0000	0.0000
7	40	2.01E-01	-0.0253	-0.0187	0.0000	0.0208	0.0000	0.0000
8	50	1.54E-01	-0.0435	0.0000	0.0000	0.0163	0.0000	0.0000
9	60	1.27E-01	-0.0428	0.0000	0.0000	-0.0014	0.0000	0.0000
10	70	1.13E-01	-0.0418	0.0000	0.0000	-0.0171	0.0000	0.0000
11	80	1.06E-01	-0.0406	0.0000	0.0000	-0.0314	0.0000	0.0000
12	90	8.96E-02	-0.0393	0.0000	0.0000	-0.0443	0.0000	0.0000
13	100	7.75E-02	-0.0380	0.0000	0.0000	-0.0555	0.0000	0.0000
14	110	5.58E-02	-0.0365	0.0000	0.0000	-0.0765	0.0000	0.0000
15	120	2.08E-03	-0.0348	0.0000	-0.0692	-0.0060	0.0000	0.0000
273	2700	0.00E+00	0.0000	-0.0404	0.0000	0.0418	0.0000	0.0000

	A	I	J	K	L	M	N
1	Time (s)	Temperature (K)		Densities (kg/m^3)		Layer Volumes (m^3)	
2	TIME	Upper	Lower	Upper	Lower	Upper	Lower
3	0	293.2	293.2	1.189	1.189	0.0	22.0
4	10	295.0	293.2	1.181	1.189	4.1	17.8
5	20	297.0	293.2	1.174	1.189	8.2	13.8
6	30	299.5	293.2	1.164	1.189	11.1	10.8
7	40	302.6	293.3	1.152	1.189	13.2	8.8
8	50	306.2	293.3	1.139	1.188	14.5	7.4
9	60	311.3	293.4	1.120	1.188	15.7	6.3
10	70	318.8	293.5	1.094	1.188	16.7	5.3
11	80	327.9	293.7	1.063	1.187	17.8	4.1
12	90	338.4	294.0	1.030	1.186	18.9	3.0
13	100	350.3	294.4	0.995	1.184	20.1	1.9
14	110	364.5	295.0	0.956	1.181	21.2	0.8
15	120	382.5	297.8	0.911	1.171	22.0	0.0
273	2700	329.2	310.4	1.059	1.123	9.0	12.9

Mass flow calculation for a contaminate (con't)

	A	O	P	Q	R	S	T	U
1	Time (s)	Volume flow (m^3/s)						
2	TIME	Plume lower to upper	Upper fan	Lower fan	Upper inflow	Lower inflow	Mixing upper to lower	Mixing lower to upper
3	0	0.0000	0.0000	-0.0382	0.0000	0.0000	0.0000	0.0000
4	10	0.4611	0.0000	-0.0379	0.0000	0.0000	0.0000	0.0000
5	20	0.3351	0.0000	-0.0377	0.0000	0.0000	0.0000	0.0000
6	30	0.2348	0.0000	-0.0374	0.0000	0.0000	0.0000	0.0000
7	40	0.1689	-0.0219	-0.0157	0.0000	0.0000	0.0000	0.0000
8	50	0.1293	-0.0382	0.0000	0.0000	0.0000	0.0000	0.0000
9	60	0.1065	-0.0382	0.0000	0.0000	-0.0012	0.0000	0.0000
10	70	0.0950	-0.0382	0.0000	0.0000	-0.0144	0.0000	0.0000
11	80	0.0892	-0.0382	0.0000	0.0000	-0.0265	0.0000	0.0000
12	90	0.0756	-0.0382	0.0000	0.0000	-0.0373	0.0000	0.0000
13	100	0.0654	-0.0382	0.0000	0.0000	-0.0469	0.0000	0.0000
14	110	0.0472	-0.0382	0.0000	0.0000	-0.0647	0.0000	0.0000
15	120	0.0018	-0.0382	0.0000	-0.0759	-0.0051	0.0000	0.0000
273	2700	0.0000	0.0000	-0.0360	0.0000	0.0000	0.0000	0.0000

	A	V	W	X	Y	Z	AA	AB	AC
1	Time (s)	Contaminate mass (kg)			Contaminate concentration (kg/m^3)		Mass collected at fan (kg)		
2	TIME	Upper layer	Lower Layer	Total in Room	Upper	Lower	Upper	Lower	Sum
3	0	0.0	100.0	100.0	0.00	4.55	0.0	0.0	0.0
4	10	0.0	98.3	98.3	0.00	5.51	0.0	-2.1	-2.1
5	20	25.4	70.7	96.2	3.11	5.13	0.0	-4.0	-4.0
6	30	42.6	51.6	94.2	3.84	4.76	0.0	-5.8	-5.8
7	40	53.8	38.7	92.5	4.08	4.40	-0.9	-6.5	-7.4
8	50	60.3	30.5	90.9	4.15	4.12	-2.5	-6.5	-9.0
9	60	64.1	25.2	89.3	4.09	4.00	-4.0	-6.5	-10.5
10	70	66.8	20.9	87.7	4.00	3.97	-5.6	-6.5	-12.1
11	80	69.0	16.6	85.6	3.87	4.00	-7.0	-6.5	-13.5
12	90	71.1	11.9	83.0	3.75	3.96	-8.5	-6.5	-15.0
13	100	72.7	7.5	80.1	3.62	3.93	-9.9	-6.5	-16.4
14	110	73.8	3.1	76.9	3.49	3.89	-11.2	-6.5	-17.7
15	120	74.3	0.0	74.3	3.39	0.00	-12.5	-6.5	-19.0
273	2700	4.7	0.0	4.7	0.52	0.00	-51.6	-6.5	58.1

Equations for mass flow calculation for a contaminate

	A	B	C	D	E	F	G	H
1	Time (s)	Mass flow (kg/s)						
2	TIME	Main Plume Flow	Upper fan	Lower fan	Upper inflow	Lower inflow	Mixing upper to lower	Mixing lower to upper
3	0	0.00E+00	0.0000	-0.0454	0.0000	0.0454	0.0000	0.0000
4	10	5.48E-01	0.0000	-0.0451	0.0000	0.0390	0.0000	0.0000
5	20	3.98E-01	0.0000	-0.0448	0.0000	0.0324	0.0000	0.0000
6	30	2.79E-01	0.0000	-0.0445	0.0000	0.0260	0.0000	0.0000
7	40	2.01E-01	-0.0253	-0.0187	0.0000	0.0208	0.0000	0.0000
8	50	1.54E-01	-0.0435	0.0000	0.0000	0.0163	0.0000	0.0000
9	60	1.27E-01	-0.0428	0.0000	0.0000	-0.0014	0.0000	0.0000
10	70	1.13E-01	-0.0418	0.0000	0.0000	-0.0171	0.0000	0.0000
11	80	1.06E-01	-0.0406	0.0000	0.0000	-0.0314	0.0000	0.0000
12	90	8.96E-02	-0.0393	0.0000	0.0000	-0.0443	0.0000	0.0000
13	100	7.75E-02	-0.0380	0.0000	0.0000	-0.0555	0.0000	0.0000
14	110	5.58E-02	-0.0365	0.0000	0.0000	-0.0765	0.0000	0.0000
15	120	2.08E-03	-0.0348	0.0000	-0.0692	-0.0060	0.0000	0.0000
273	2700	0.00E+00	0.0000	-0.0404	0.0000	0.0418	0.0000	0.0000

	A	I	J	K	L	M	N
1	Time (s)	Temperature (K)		Densities (kg/m^3)		Layer Volumes (m^3)	
2	TIME	Upper	Lower	Upper	Lower	Upper	Lower
3	0	293.2	293.2	=348.59/I3	=348.59/J3	0.0	=21.96-M3
4	10	295.0	293.2	=348.59/I4	=348.59/J4	4.1	=21.96-M4
5	20	297.0	293.2	=348.59/I5	=348.59/J5	8.2	=21.96-M5
6	30	299.5	293.2	=348.59/I6	=348.59/J6	11.1	=21.96-M6
7	40	302.6	293.3	=348.59/I7	=348.59/J7	13.2	=21.96-M7
8	50	306.2	293.3	=348.59/I8	=348.59/J8	14.5	=21.96-M8
9	60	311.3	293.4	=348.59/I9	=348.59/J9	15.7	=21.96-M9
10	70	318.8	293.5	=348.59/I10	=348.59/J10	16.7	=21.96-M10
11	80	327.9	293.7	=348.59/I11	=348.59/J11	17.8	=21.96-M11
12	90	338.4	294.0	=348.59/I12	=348.59/J12	18.9	=21.96-M12
13	100	350.3	294.4	=348.59/I13	=348.59/J13	20.1	=21.96-M13
14	110	364.5	295.0	=348.59/I14	=348.59/J14	21.2	=21.96-M14
15	120	382.5	297.8	=348.59/I15	=348.59/J15	22.0	=21.96-M15
273	2700	329.2	310.4	=348.59/I273	=348.59/J273	9.0	=21.96-M273

	A	O	P	Q	R	S	T	U
1	Time (s)	Volume flow (m^3/s)						
2	TIME	Plume lower to upper	Upper fan	Lower fan	Upper inflow	Lower inflow	Mixing upper to lower	Mixing lower to upper
3	0	=B3/L3	=C3/K3	=D3/L3	=IF(E3>0,0,E3)/K3	=IF(F3>0,0,F3)/L3	=G3/K3	=H3/L3
4	10	=B4/L4	=C4/K4	=D4/L4	=IF(E4>0,0,E4)/K4	=IF(F4>0,0,F4)/L4	=G4/K4	=H4/L4
5	20	=B5/L5	=C5/K5	=D5/L5	=IF(E5>0,0,E5)/K5	=IF(F5>0,0,F5)/L5	=G5/K5	=H5/L5
6	30	=B6/L6	=C6/K6	=D6/L6	=IF(E6>0,0,E6)/K6	=IF(F6>0,0,F6)/L6	=G6/K6	=H6/L6
7	40	=B7/L7	=C7/K7	=D7/L7	=IF(E7>0,0,E7)/K7	=IF(F7>0,0,F7)/L7	=G7/K7	=H7/L7
8	50	=B8/L8	=C8/K8	=D8/L8	=IF(E8>0,0,E8)/K8	=IF(F8>0,0,F8)/L8	=G8/K8	=H8/L8
9	60	=B9/L9	=C9/K9	=D9/L9	=IF(E9>0,0,E9)/K9	=IF(F9>0,0,F9)/L9	=G9/K9	=H9/L9
10	70	=B10/L10	=C10/K10	=D10/L10	=IF(E10>0,0,E10)/K10	=IF(F10>0,0,F10)/L10	=G10/K10	=H10/L10
11	80	=B11/L11	=C11/K11	=D11/L11	=IF(E11>0,0,E11)/K11	=IF(F11>0,0,F11)/L11	=G11/K11	=H11/L11
12	90	=B12/L12	=C12/K12	=D12/L12	=IF(E12>0,0,E12)/K12	=IF(F12>0,0,F12)/L12	=G12/K12	=H12/L12
13	100	=B13/L13	=C13/K13	=D13/L13	=IF(E13>0,0,E13)/K13	=IF(F13>0,0,F13)/L13	=G13/K13	=H13/L13
14	110	=B14/L14	=C14/K14	=D14/L14	=IF(E14>0,0,E14)/K14	=IF(F14>0,0,F14)/L14	=G14/K14	=H14/L14
15	120	=B15/L15	=C15/K15	=D15/L15	=IF(E15>0,0,E15)/K15	=IF(F15>0,0,F15)/L15	=G15/K15	=H15/L15
273	2700	=B273/L273	=C273/K273	=D273/L273	=IF(E273>0,0,E273)/K273	=IF(F273>0,0,F273)/L273	=G273/K273	=H273/L273

	A	V	W	X	Y	Z	AA	AB	AC
1	Time (s)	Contaminate mass (kg)			Contaminate concentration (kg/m^3)		Mass collected at fan (kg)		
2	TIME	Upper layer	Lower Layer	Total in Room	Upper	Lower	Upper	Lower	Sum
3	0	0	100	=SUM(V3:W3)	=IF(M3=0,0,V3/M3)	=IF(N3=0,0,W3/N3)	0	0	=-SUM(AA3:AB3)
4	10	=IF(V3+(Y3*(P3+R3-T3)+Z3*(U3+O3))*10<=0,0,V3+(Y3*(P3+R3-T3)+Z3*(U3+O3))*10)	=IF(W3+(Z3*(Q3+S3-O3-U3)+T3*Y3)*10<=0,0,W3+(Z3*(Q3+S3-O3-U3)+T3*Y3)*10)	=SUM(V4:W4)	=IF(M4=0,0,V4/M4)	=IF(N4=0,0,W4/N4)	=Y4*P4*10+AA3	=Z4*Q4*10+AB3	=-SUM(AA4:AB4)
5	20	=IF(V4+(Y4*(P4+R4-T4)+Z4*(U4+O4))*10<=0,0,V4+(Y4*(P4+R4-T4)+Z4*(U4+O4))*10)	=IF(W4+(Z4*(Q4+S4-O4-U4)+T4*Y4)*10<=0,0,W4+(Z4*(Q4+S4-O4-U4)+T4*Y4)*10)	=SUM(V5:W5)	=IF(M5=0,0,V5/M5)	=IF(N5=0,0,W5/N5)	=Y5*P5*10+AA4	=Z5*Q5*10+AB4	=-SUM(AA5:AB5)
6	30	=IF(V5+(Y5*(P5+R5-T5)+Z5*(U5+O5))*10<=0,0,V5+(Y5*(P5+R5-T5)+Z5*(U5+O5))*10)	=IF(W5+(Z5*(Q5+S5-O5-U5)+T5*Y5)*10<=0,0,W5+(Z5*(Q5+S5-O5-U5)+T5*Y5)*10)	=SUM(V6:W6)	=IF(M6=0,0,V6/M6)	=IF(N6=0,0,W6/N6)	=Y6*P6*10+AA5	=Z6*Q6*10+AB5	=-SUM(AA6:AB6)
7	40	=IF(V6+(Y6*(P6+R6-T6)+Z6*(U6+O6))*10<=0,0,V6+(Y6*(P6+R6-T6)+Z6*(U6+O6))*10)	=IF(W6+(Z6*(Q6+S6-O6-U6)+T6*Y6)*10<=0,0,W6+(Z6*(Q6+S6-O6-U6)+T6*Y6)*10)	=SUM(V7:W7)	=IF(M7=0,0,V7/M7)	=IF(N7=0,0,W7/N7)	=Y7*P7*10+AA6	=Z7*Q7*10+AB6	=-SUM(AA7:AB7)
8	50	=IF(V7+(Y7*(P7+R7-T7)+Z7*(U7+O7))*10<=0,0,V7+(Y7*(P7+R7-T7)+Z7*(U7+O7))*10)	=IF(W7+(Z7*(Q7+S7-O7-U7)+T7*Y7)*10<=0,0,W7+(Z7*(Q7+S7-O7-U7)+T7*Y7)*10)	=SUM(V8:W8)	=IF(M8=0,0,V8/M8)	=IF(N8=0,0,W8/N8)	=Y8*P8*10+AA7	=Z8*Q8*10+AB7	=-SUM(AA8:AB8)
9	60	=IF(V8+(Y8*(P8+R8-T8)+Z8*(U8+O8))*10<=0,0,V8+(Y8*(P8+R8-T8)+Z8*(U8+O8))*10)	=IF(W8+(Z8*(Q8+S8-O8-U8)+T8*Y8)*10<=0,0,W8+(Z8*(Q8+S8-O8-U8)+T8*Y8)*10)	=SUM(V9:W9)	=IF(M9=0,0,V9/M9)	=IF(N9=0,0,W9/N9)	=Y9*P9*10+AA8	=Z9*Q9*10+AB8	=-SUM(AA9:AB9)

	A	V	W	X	Y	Z	AA	AB	AC
10	70	=IF(V9+(Y9*(P9+R9-T9)+Z9*(U9+O9))*10<=0,0,V9+(Y9*(P9+R9-T9)+Z9*(U9+O9))*10)	=IF(W9+(Z9*(Q9+S9-O9-U9)+T9*Y9)*10<=0,0,W9+(Z9*(Q9+S9-O9-U9)+T9*Y9)*10)	=SUM(V10:W10)	=IF(M10=0,0,V10/M10)	=IF(N10=0,0,W10/N10)	=Y10*P10*10+AA9	=Z10*Q10*10+AB9	=-SUM(AA10:AB10)
11	80	=IF(V10+(Y10*(P10+R10-T10)+Z10*(U10+O10))*10<=0,0,V10+(Y10*(P10+R10-T10)+Z10*(U10+O10))*10)	=IF(W10+(Z10*(Q10+S10-O10-U10)+T10*Y10)*10<=0,0,W10+(Z10*(Q10+S10-O10-U10)+T10*Y10)*10)	=SUM(V11:W11)	=IF(M11=0,0,V11/M11)	=IF(N11=0,0,W11/N11)	=Y11*P11*10+AA10	=Z11*Q11*10+AB10	=-SUM(AA11:AB11)
12	90	=IF(V11+(Y11*(P11+R11-T11)+Z11*(U11+O11))*10<=0,0,V11+(Y11*(P11+R11-T11)+Z11*(U11+O11))*10)	=IF(W11+(Z11*(Q11+S11-O11-U11)+T11*Y11)*10<=0,0,W11+(Z11*(Q11+S11-O11-U11)+T11*Y11)*10)	=SUM(V12:W12)	=IF(M12=0,0,V12/M12)	=IF(N12=0,0,W12/N12)	=Y12*P12*10+AA11	=Z12*Q12*10+AB11	=-SUM(AA12:AB12)
13	100	=IF(V12+(Y12*(P12+R12-T12)+Z12*(U12+O12))*10<=0,0,V12+(Y12*(P12+R12-T12)+Z12*(U12+O12))*10)	=IF(W12+(Z12*(Q12+S12-O12-U12)+T12*Y12)*10<=0,0,W12+(Z12*(Q12+S12-O12-U12)+T12*Y12)*10)	=SUM(V13:W13)	=IF(M13=0,0,V13/M13)	=IF(N13=0,0,W13/N13)	=Y13*P13*10+AA12	=Z13*Q13*10+AB12	=-SUM(AA13:AB13)
14	110	=IF(V13+(Y13*(P13+R13-T13)+Z13*(U13+O13))*10<=0,0,V13+(Y13*(P13+R13-T13)+Z13*(U13+O13))*10)	=IF(W13+(Z13*(Q13+S13-O13-U13)+T13*Y13)*10<=0,0,W13+(Z13*(Q13+S13-O13-U13)+T13*Y13)*10)	=SUM(V14:W14)	=IF(M14=0,0,V14/M14)	=IF(N14=0,0,W14/N14)	=Y14*P14*10+AA13	=Z14*Q14*10+AB13	=-SUM(AA14:AB14)

	A	V	W	X	Y	Z	AA	AB	AC
15	120	=IF(V14+(Y14*(P14+R14-T14)+Z14*(U14+O14))*10<=0,0,V14+(Y14*(P14+R14-T14)+Z14*(U14+O14))*10)	=IF(W14+(Z14*(Q14+S14-O14-U14)+T14*Y14)*10<=0,0,W14+(Z14*(Q14+S14-O14-U14)+T14*Y14)*10)	=SUM(V15:W15)	=IF(M15=0,0,V15/M15)	=IF(N15=0,0,W15/N15)	=Y15*P15*10+AA14	=Z15*Q15*10+AB14	=-SUM(AA15:AB15)
273	2700	=IF(V272+(Y272*(P272+R272-T272)+Z272*(U272+O272))*10<=0,0,V272+(Y272*(P272+R272-T272)+Z272*(U272+O272))*10)	=IF(W272+(Z272*(Q272+S272-O272-U272)+T272*Y272)*10<=0,0,W272+(Z272*(Q272+S272-O272-U272)+T272*Y272)*10)	=SUM(V273:W273)	=IF(M273=0,0,V273/M273)	=IF(N273=0,0,W273/N273)	=Y273*P273*10+AA272	=Z273*Q273*10+AB272	=-SUM(AA273:AB273)

Appendix J CFAST History Summary

The information presented in this Appendix is reproduced from the website http://cfast.nist.gov/versionhistory.html (May 10, 2004).

Version 5.1.1 (May 1, 2004)

There was an error in the HCR (hydrogen/carbon ratio) calculation. It introduced about a 6% error into the pyroloysis calculation. [Note: This only applies to calculations made using Version 5.1.0.*]

Version 5.1.0 (March 1, 2004)

In version 5.0 and earlier, the oxygen calculation used the oxygen to fuel ratio, whereas the technical reference manual states that it uses the oxygen to carbon ratio. The model now matches the guide.

Version 5.0.1 (May 7, 2003)

Flow was not being **reported** correctly in some cases. The calculation was correct, but the output from cfast (/rf) was not updated when a vent opening decreased to zero.

The vertical flow calculation has been fixed. The symptom is that it the pressure in a compartment connected by VVENT was never updated.

Version 5.0 (11/1/2001)

The number of points in a time history has been increased. This is to allow editing of the examples, which default to 21 intervals.

Fix a printout error: the size of the fire was reported incorrectly in some cases. The calculation was done correctly, but the output from Report and ReportSS was incorrect. The problem occurs if there are two fires in a compartment, with one of them in the upper layer, and one in the lower layer. Once again, the report was incorrect, but the value used in subsequent calculations was correct.

The workspace for the solver was not dimensioned correctly, so CFAST could not do 30 compartments. This has been fixed.

(These fixes have been done in 3.1.7 as well and there is an update package available on the website to implement the update.)

Version 4.0.1 (3/1/00)

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* Based on private communication with the NIST Subject Matter Expert for CFAST.

This release runs as an application under the Windows series of operating systems.

New phenomena: horizontal heat conduction (wall/wall) (HHEAT), horizontal smoke flow in corridors (HALL), variable geometry for compartments (ROOMA, ROOMH).

Fonts must be in the "font" directory off the "bin" folder.

Version 3.1.6 (11/1/99)

This is the last full GUI (FAST).
Add "constrained/with flashover" to FAST as a fire type (note, this is not carried into CFAST!)

Version 3.1.5 (4/1/99)

The program Build is included, along with sample files and documentation, which can be used to generate ".pic" files for the VIEW command.
Reportss has been fixed to include target temperatures in the output.
New phenomena: single zone switch (single layer model).

Version 3.1.4 (7/1/98)

Fix compatibility between FAST and CFAST. The history files were not compatible

Version 3.1.3 (4/1/98)

Fix fonts for FAST (remove wddraw from an explicit include in fast and fastlite), file naming error in the spreadsheet output, incorrect entrainment when the fire is in the upper layer and eliminate heat conduction thru the ceiling/floor connection to the outside (nputp)

Version 3.1.2 (1/1/98)

Fix boundary condition for vertical flow to the outside.
New phenomena: vertical heat flow.

Version 3.1.1 (10/1/97)

Fix font interface for metawindows. The fortran-c interface could sometimes cause a page fault. Fonts are now names devfntnn.fnt where nn=1 to 24 (4 is the default). Note that font changes used in labels are permanent for the session, so the bracket |Hnn .... |H04 should be used. Removed O(n**2) data structures (about 40 arrays). Added a non-rectangular room option - roomhgt, roomarea are the key words.

Wind - wind now applies to vents rather than rooms (couldn't do from vs back) - effect of wind was zero for ground floor rooms. wind induced pressure rise is now calculated at the average of the floor and ceiling elevation Initialize inside and outside pressure and temperature to the same lapse rate.

Output warning for excessive number of small time steps (set in solver.ini) (DTCHEK).

Add BLACK option to have atmosphere behave as a blackbody Note: rework SHAFT option to use only 3 equations per room. Modify hybrid code to conform to new FDS heat loss algorithm

Version 3.0 (1/3/96)

New user interface for CEdit. Add flame height calculation to report and flame spread algorithm to the model. New module, reportss, which uses the same format as report, but puts the output into a spread sheet (ascii delimited text) output format. Added reporting option for wall and target heat flux printout. New output options are /r:winfstp. W is now wall and target heat fluxes and P is now wall temperature profiles.

New phenomena added: ceiling/floor heat transfer for inter-compartment heat transfer, CFAST keyword CFCON. and heat transfer to targets. Multiple objects in a desired position, orientation, and material.

Program calculation of object temperature and impinging heat fluxes can be printed. CFAST keyword is TARGET.

Improved stability of mechanical ventilation routines so that solution converges over a wider range of input values.

Modules in the release: cfast (main model), fast (gui data editor), cplot (plotting package), report (report utility), reportss utility to generate spread sheet format, reportg to provide graphics playback, bintoasc to convert binary history files to ascii text files, compare to compare two separate cfast runs (using ascii text files) and compinfo to summarize output from compare .

Version 2.1.1/ H1.2 "fix on fail" update (1/1/95)

Fixed optional ceiling jet calculation to not take into account lower wall surfaces. Too much energy was lost through the lower wall.

Corrected EXITT and SURVIVAL to access the layer interface height correctly. Prior to this fix, layer depth was always zero, making smoke detection (by detectors or "smell") inoperable.

Fixed thermal properties in several example data files to be consistent with current THERMAL.DF file.

Version 2.0.1 H 1.2 (7/1/94) This release did not get a new number!

Corrected write of vertical vent information to .DAT file in CEDIT. For large vent area, old format would merge two fields together resulting in read errors with the model. Tightened differential equation solver tolerances to correct calculated species

concentrations for one test case. This may make the model run slower when conditions are rapidly changing, but the answers should be more correct.

Corrected interaction between fire size and plume entrainment. Before the fix, CFAST calculated plume entrainment via a two step process:

1) Determine the plume entrainment in FIRPLM via McCaffrey's method using the fire size unconstrained by the available oxygen.

2) Once the actual fire size is calculated from the available oxygen in CHEMIE, a new estimate for the plume entrainment is determined by a simple linear correction. Since the plume entrainment is not a linear function of the fire size and the fire size depends on the oxygen entrained, this simple process can lead to an inconsistency between the fire size (calculated from the unconstrained plume entrainment) and the new estimate of the plume entrainment. For very large fires where the fire size is limited by the amount of oxygen entrained, this can lead to significant differences between the calculated fire size and the amount of oxygen actually available for the combustion. The fix is a simple one: when the fire is limited by the available oxygen entrained into the plume, the plume entrainment and fire size are both re-calculated by calling FIRPLM and CHEMIE a second time to get a better estimate of the actual oxygen available (and thus the actual fire size).

Version 2.0.1 (2/13/94) - H 1.2

Corrected flow through horizontal openings (VVENT). In some test cases (where significant flow occurred from upper room to lower room), model would calculate extremely low temperatures in the lower room. Corrected species mass balance. For very large fires in small rooms, species mass fractions would not sum to unity when fire became oxygen limited. Printed output file is now placed in the data subdirectory along with the input data file.

Version 2.0 (August 23, 1993)

Code restructured for future addition of a flame spread model. Consolidated calculation of hazardous conditions (and colors for plotting of them). Added a new THERMAL.DF file taken from Incorpera and DeWitt. New conduction routine. New convection routine. Use Watcom Fortran compiler. Printout routine has been totally rewritten to provide additional information with a consistent format.

Version 1.6.2 (December 1, 1992)

Implement a faster initialization routine, and better selection rules for vertical flow. We now use the Pharlap memory expander which supports more display drivers. Mechanical ventilation is now tightly coupled with vertical and horizontal flow routines.

Version 1.5 (June, 1, 1992)

Added object specification (heat loss, ...), a more robust ODE solver (DASSL), restructured code to include physical interface routines for each physical phenomenon, and CEdit support for all modeling features.

Version 1.4 (February 1, 1992)

Added multiple fires, history file compression, extended memory, vertical flow, multiwall radiation model, distributed mechanical ventilation ducts, ceiling jet and 3D positioning of fires. The number of compartments was increased to 15.

CFAST Version 1.0 (May 1, 1990)

An amalgam of FAST 18.5 and CCFM -- functionally equivalent to FAST but more modular like CCFM.

FAST version 18.5 (May 1, 1990) HAZARD version 1.1 FAST version 18.3 (July 1988) HAZARD I version 1.0

Appendix K Error Messages

	Error No.	Error Message
	-11	ERROR IN RESID
	0	< Dassl error
1	1	Not an allowed fire type. (NPUTP)
2	2	Object no. XXX is in room XXX beyond the limit XXX rooms defined (NPUTP)
3	3	INTERNAL ERROR IN NPUTQ - RESTART OUT OF BOUNDS (NPUTQ)
4	4	No configuration and no data file (CFAST)
5	7	Error reading restart file (DREADIN)
6	6	Display area over written in view file read (DISPLAYC)
7	7	Error in accessing dump file (DUMPER)
8	-11	GASLOAD - Non numeric Token for display pointer (GASLOAD)
9	-11	GASLOAD - a pointer to a compartment must be a number (GASLOAD)
10	-11	GASLOAD - a pointer to a compartment must be a number (GASLOAD)
11	-11	GASLOAD - a layer must be specified (GASLOAD)
12	-11	HCLTRAN - H2O out of range (HCLTRAN)
13	-11	HVFRIC - I greater than 20 (HVFRIC)
14	14	HVINIT - Interior node has too many or too few connections (HVINIT)
15	15	LOADUP - Invalid number (LOADUP)
16	16	OFFSET - Node range exceeded for HVAC (OFFSET)
17	-11	RAD2 - Singular matrix (RAD2)
18	-11	RAD4 - Singular matrix (RAD4)
19	7	PACKOT - Overwrite, input and index = (WRITEOT)
20	20	UPDOBJ - Incorrectly defined object type (UPDOBJ)
21	21	INITTARG - Failure of target initialization (INITTARG)
22	22	NPUTP - Failure in nputp (NPUTP)
23	23	NPUTQ - Ignition criteria incorrect (NPUTQ)
24	24	NPUTQ - Invalid DETECTOR specification - room X is not a valid (NPUTQ)
25	25	NPUTQ - DETACT keyword must have at least 2 parameters (NPUTQ)
26	26	NPUTQ - Failure CFCON keyword (NPUTQ)
27	27	NPUTQ - Failure in SHAFT keyword (NPUTQ)
28	28	NPUTQ - Failure in TARGET keyword (NPUTQ)
29	29	NPUTQ - Failure in TARG keyword (NPUTQ)
30	30	OPENOBJ - Objects database file ',A,' does not exist. (NPUTOB)
31	31	GETOBJ - Error in object definition in database (NPUTOB)
32	32	GETOBJ - Specified unsupported type. (NPUTOB)
33	33	GETOBJ - Too many targets (NPUTOB)
34	34	GETOBJ - Fatal error: too many flamespread type objects (NPUTOB)
35	35	SETFSM - Normal to the wall incorrectly defined (NPUTOB)
36	36	OPNTPF - Thermophysical properties file XXX does not exist. (NPUTT)
37	37	GETTTP - Failure in thermal physical properties definition. (NPUTT)
38	38	RSETVNTS - Adding too many time points. (RSETVNTS)
41	41	CFCON used to specify the outside. This is not an allowable specification.