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NSRD-10: Leak Path Factor Guidance Using MELCOR

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Abstract

Estimates of the source term from a U.S. Department of Energy (DOE) nuclear facility requires that the analysts know how to apply the simulation tools used, such as the MELCOR code, particularly for a complicated facility that may include an air ventilation system and other active systems that can influence the environmental pathway of the materials released. DOE has designated MELCOR 1.8.5, an unsupported version, as a DOE ToolBox code in its Central Registry, which includes a leak-path-factor guidance report written in 2004 that did not include experimental validation data. To continue to use this MELCOR version requires additional verification and validations, which may not be feasible from a project cost standpoint. Instead, the recent MELCOR should be used. Without any developer support and lack of experimental data validation, it is difficult to convince regulators that the calculated source term from the DOE facility is accurate and defensible.

This research replaces the obsolete version in the 2004 DOE leak path factor guidance report by using MELCOR 2.1 (the latest version of MELCOR with continuing modeling development and user support) and by including applicable experimental data from the reactor safety arena and from applicable experimental data used in the DOE-HDBK-3010. This research provides best practice values used in MELCOR 2.1 specifically for the leak path determination. With these enhancements, the revised leak-path-guidance report should provide confidence to the DOE safety analyst who would be using MELCOR as a source-term determination tool for mitigated accident evaluations.

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NOMENCLATURE

ACE	Advanced Containment Experiment
AED	Aerodynamic equivalent diameter
AMMD	Aerodynamic mass mean diameter
ARF	Airborne release fraction
BMC	Battle Model Containment
CCF	Countercurrent flow
CF	Control function
CFAST	Consolidated model of Fire And Smoke Transport code
CFD	Computational Fluid Dynamics
CVH	Control volume hydrodynamics
CSTF	Containment System Test Facility
DOE	U.S. Department of Energy
DR	Damage ratio
DSA	Document Safety Analysis
DUO	Depleted uranium oxide
EDF	External data file
EOS	Equation of state
FD	Fluid dynamics
FFF	Five-Factor Formula
FP	Fission product
Fuego	SNL SIERRA 3-dimensional Fluid Mechanics Code
GMND	Geometric mean number diameter
GMMD	Geometric mass mean diameter
GSD	Geometric standard deviation
HEPA	High-efficiency particulate air
hr	Hour
HS	Heat structure
HVAC	Heat and ventilation air conditioning
IC	Integrated Code
INEL	Idaho National Engineering Laboratory
ITAR	International Traffic in Arms Regulations
JAERI	Japan Atomic Energy Research Institute
LACE	Light water reactor Aerosol Containment Experiments
LES	Large-eddy simulation
LLNL	Lawrence Livermore National Laboratory
LPF	Leak path factor
MAEROS	A multisectional, multicomponent aerosol dynamics code
MAR	Material-at-risk
MMD	Mass mean diameter
mph	Miles per hour
MJ	million joule
NCG	Non-condensable gas
NNSS	Nevada Nuclear Safety Site
NRC	Nuclear Regulatory Commission

NSRD	Nuclear Safety Research and Development
OECD	Organization for Economic Co-operation and Development
PARE	Pressurized airborne release equipment
PART	Pressurized airborne release tank
PNL	Pacific Northwest Laboratory
PWR	Pressure water reactor
QA	Quality Assurance
RANS	Reynolds averaging of the Navier Stokes equations
RF	Respirable fraction
RN	Radionuclide
SB	Safety basis
SNAP	Symbolic Nuclear Analysis Package
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory
STORM	Simplified Test on Resuspension Mechanism
ST	Source term
TBP	Tributyl phosphine
TF	Tabular function
V&V	Verification and validation

Symbols

a	Sound speed
A	Surface area
C_p	Pressure coefficient
D	Diameter
E	Energy
F_{rad}	Fraction of energy lost to thermal radiation
i	impulse
$\bar{i}$	Scaled impulse
m	mass
n	exponent
P	Pressure
$\bar{P}$	Scaled pressure
q_r	Radiation power flux
Q	Heat release rate
R	Standoff distance
$\bar{R}$	Scaled distance
T	Temperature
t	Time
u	Velocity
γ	Ratio of specific heat
α	Fire intensity coefficient
ΔP	Pressure drop
ϵ_{gas}	Emissivity of gas
ρ	Density

σ	Stephan-Boltzmann constant
Ψ	Parameter defined in Equation (4-8)

Subscript

0	Ambient
a	aerosol
F	Fuel
g	Geometric
r	Reflected
s	Side on
exp	Explosion
v	ventilation

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1 INTRODUCTION

MELCOR is developed at Sandia National Laboratories (SNL) for the Nuclear Regulatory Commission (NRC). Although the name “MELCOR” is occasionally and incorrectly said to be an acronym for “Methods for Estimation of Leakages and Consequence of Releases,” it is actually a portmanteau derived from “MELting CORE.” MELCOR has been widely used domestically and internationally for nuclear reactor accident analyses. Recently SNL has published three volumes of MELCOR manuals [Humphries 2015a-c].

MELCOR was developed to facilitate probabilistic risk assessments for nuclear power installations. Assessing risk requires characterization of release event to the environment by determining the following: timing, magnitude, composition, energy, and aerosol size distribution of hazardous material released from the facility. MELCOR employs various models to determine the transportation, agglomeration, and deposition of hazardous materials throughout the facilities to characterize the environmental source term. Given these available models MELCOR can be applied to non-reactor facilities, such as source-term characterization for nuclear and non-nuclear facilities. At the U.S. Department of Energy (DOE) complex, a concern is the release of radioactive airborne materials (such as PuO_2) from a nuclear explosive, waste, or process facilities as a result of accident conditions such as spills, fires, or explosions (i.e., from an explosive or combustible gas such as hydrogen or natural gas). To estimate the source term for a given facility, MELCOR is often used by safety basis (SB) analysts at DOE facilities to perform the leak path factor (LPF) calculation, where LPF is a term in the five-factor formula for determining source term [DOE 1994] (see Chapter 2 for this formula). These calculations enable analysts to estimate the release fraction of the concerned material from inside of the facility to the environment via any leak path, such as door gaps, penetrations, door opening during evacuation, or opening due to an energetic accident event.

Unlike many safety analysis codes that are specifically designed only for nuclear reactor applications, MELCOR is a modular computer code that allows users to select specific packages for their specific applications (i.e., LPF calculations), without any issue regarding reactor-specific modeling packages. To assist the usage of MELCOR for LPF determination for the DOE complex, DOE has designated MELCOR as a DOE/EH Toolbox Code in the Central Registry. With that designation, and in conjunction with the quality assurance (QA) program, a MELCOR LPF guidance report was written in 2004 [DOE 2004] (referred to herein as 2004 report) and provided in the Central Registry. However, the MELCOR version listed in the Toolbox Tool in the Central Registry is version 1.8.5, which is no longer supported by SNL (i.e., no new model development, testing, or issue correction). In addition, many of the safety analysts in the DOE safety basis community have used MELCOR 1.8.6 (also currently unsupported by SNL) with an independent verification and validation procedure to comply with the DOE quality assurance program for many years. There was no subsequent report written for the latest versions of MELCOR, i.e., MELCOR 2.1. In addition, the 2004 MELCOR LPF guidance report above did not include validations for LPF applications. Code validations, such as from experiment data of reactor applications and from DOE-HDBK-3010, can provide QA for code development and applications.

Normally, an SB analyst relies on the example problems provided in the 2004 report to conduct verification and validation (V&V) for the MELCOR version that they use. In particular, there is an example problem with size restriction in MELCOR 1.8.5 that causes many analysts to go with another version of MELCOR, namely MELCOR 1.8.6. While conducting the V&V on MELCOR 1.8.6, Sanchez, et.al [Sanchez 2007] reported issues with the 2004 report example problems and discrepancies in the results. With these issues, analysts had to perform additional V&V to convince regulators of their intent to use a more recent version of MELCOR. This additional V&V effort increased costs for the analyst's project. Currently, only MELCOR 2.0 or higher versions are supported by SNL. Additionally, unlike reactor safety applications where SNL has developed a set of best practices inputs and suggestions for using MELCOR, there are no best practices inputs and suggestions for using MELCOR for LPF determination available, except a set of specific guidance provided in the 2004 report. Thus, SB analysts must know MELCOR well in order to perform an accurate LPF calculation. The use of the reactor-specific best practices may not be appropriate for non-reactor applications. Therefore, SNL provides best practices applicable to LPF application in Chapter 4 of this report. In Chapter 2, we discuss a review of the 2004 report, which includes other LPF literature reviews currently available. In Chapter 3, MELCOR is validated for LPF applications, along with discussions of the reactor experiment assessment SNL conducted for possible applications to LPF.

The remainder of this chapter describes the MELCOR code version difference, and provides a brief description of MELCOR code packages that are applicable for LPF applications.

1.1 Code Version Difference

Starting with Version 2.0 and beyond, MELCOR is developed in FORTRAN 95. The use of FORTRAN 95 allows MELCOR to continue its development in the future in terms of extensibility and maintainability. All previous versions of MELCOR were developed in FORTRAN 77 (obsolete), which is no longer supported by many FORTRAN compilers currently available today. Most of our development work is done in Visual Studio TM and Intel Fortran compiler TM in the Windows TM environment.

Another major difference between Version 2.0 and 1.8.6 is the code architecture, even though most of the 1.8.6 algorithms were kept intact. The original Version 2.0 was developed using the object-oriented approach in terms of input and calculated variables (using different levels: program [MELGEN, MELCOR], package [CVH, FL, etc.], and object [CV_ID, etc.] levels) and storage spaces (dynamically allocated memory). Thus this difference contributed to the input format change between these two versions. Version 1.8.6 and previous versions used numbers as the unique identification for an input card or a set of cards. Figure 1-1 shows a comparison of the input format between the two versions. As shown in this figure, MELCOR 2.1 uses the "block input" format, which requires a "INPUT" card for the designation of a package input, then followed by "_ID". Therefore, the input format starting in Version 2.0 is called "block input".

To help the user transition to this new format, a converter, SNAP, which stands for Symbolic Nuclear Analysis Package developed by Applied Programming Technology, Inc. for the NRC (see Figure 1-2), allows the conversion from an input developed in version 1.8.6 (or 1.8.5 deck without COR input) to Version 2 or higher. SNAP incorporates a set of various plug-ins specific

to the code application desired; therefore, the MELCOR plug-in is required to perform input conversions. SNAP can also be used for post-processing and visualization. Editing tools from SNAP can also provide additional simulation needs.

<pre> * Comments common to MELGEN and MELCOR * *FOR* MELGEN TITLE Test RUNONLY NM RESTARTFILE tmiarest OUTPUTFILE tmioutg DIAGFILE tmdiagg DTIME 0.1 CRATOUT R*I*F cvhinput FLO0100 cv101-cv102 101 102 1.5 1.5 ... FLO0200 cv103-cv104 103 104 1.22 1.22 ... R*I*F hsininput R*I*F rsininput R*I*F otherinput . *FOR* MELCOR TITLE Test RUNONLY NM RESTARTFILE tmiarest OUTPUTFILE tmioutg DIAGFILE tmdiagg MESSAGEFILE tmmes PLOTFILE tmiplot CPULEFT 30.0 CPULIM 36000.0 CRATOUT NOCOPY RESTART 0 TIME1 0.0 5.0 0.0001 500.0 2.0 500.0 TIME2 1000.0 10.0 0.0001 1000.0 5.0 1000.0 TEND 6000.0 R*I*F scinput PLOT000 RN1-ADEP-1-10-1.30001 PLOTabc.....RN1-ADEP-1-9-1.30001 .. PLOTxyz RN1-ADEP-1-10-1.30001 . </pre>	<pre> ! Comments common to MELGEN and MELCOR ! MEG_DIAGFILE tmdiagg MEL_DIAGFILE tmdiagg MEG_OUTPUTFILE tmioutg MEL_OUTPUTFILE tmioutg MEG_RESTARTFILE tmiarest MEL_RESTARTFILE tmiarest NNCYCLE 0 PLOTFILE tmiplot.ptf MESSAGEFILE tmmes Program MELGEN !* Block: EXEC data ***** EXEC_INPUT EXEC_TITLE "Test" ! Title of the calculation EXEC_RUNONLY NM EXEC_DTIME 0.1 !* END EXEC ***** INCLUDE cvhinput FL_INPUT FL_ID 'cv101-cv102' 1 ! FL_FT '101' '102' 1.5 1.5 ... FL_ID 'cv103-cv104' 2 FL_FT '103' '104' 1.22 1.22 ... INCLUDE hsininput INCLUDE rsininput INCLUDE otherinput ... END Program MELGEN data ! Program MELCOR !* Block: MEX (Exec) data ***** EXEC_INPUT EXEC_TITLE "Test" ! Title of the calculation EXEC_RUNONLY NM EXEC_TIME 2 ! NUMBER TIME DTMAX DTMIN DTEST DTPLT DTRST DCRST 1 0.0 5.0 0.0001 500.0 2.0 500.0 0.1E+11 2 1000.0 10.0 0.0001 1000.0 5.0 1000.0 0.1E+11 EXEC_CPULEFT 30.0 EXEC_CPULIM 36000.0 EXEC_TEND 6000.0 EXEC_NOCOPY EXEC_PLOT 3 1 RN1-ADEP(HS30001,LHS,U02,TOT) 2 RN1-ADEP(HS30001,LHS,LA,TOT) 3 RN1-ADEP(HS30001,LHS,U02,TOT) !* END MEX (Exec) ***** INCLUDE scinput END Program MELCOR data </pre>
--	--

Figure 1-1. Difference in Input Format between MELCOR 1.8.6 and MELCOR 2.1.

1.2 Features Useful for LPF Analyses

SNL has made a decision to develop new models only in MELCOR 2.0, preventing the duplication of efforts across various versions and code standards, and permitting focused resource allocations. Table 1-1 describes the MELCOR packages and models that may be of interest to the safety basis community for use in the LPF analyses. As shown in this table, a number of packages should be included in the LPF calculation. RN, CVH, and FL packages are the major packages utilized for the LPF analyses, since the RN package tracks the radionuclides and aerosol, and both CVH and FL define the thermal conditions of the problem. FL is also used to track the release of the radionuclide and aerosol to the environment. Also shown in this table are the number of models available for use in the LPF calculations. Significant improvement in the aerosol deposition model has been added to MELCOR, namely the abilities to disable the aerosol deposition model, and to model the turbulent deposition in pipes and ducts (including bends in ventilation systems (see Table 1-1 for the model limitation).

Table 1-1 MELCOR Packages and Models Useful for LPF Analyses

Package	Description/Comments
EXEC	Main control of various processing tasks and control of the overall calculation sequence. Sensitivity coefficients of many package models can be redefined in MELGEN or changed at any restart via MELCOR input. Common block feature, which is designated in the input as starting with “(((name block” and ending with “)))” can be used to allow a single input file to simulate a number of different runs. The name block can be included during execution of the MELGEN/MELCOR calculations or included in the beginning of the input file. The use

	of the common blocks is extremely useful for sensitivity studies.
NCG	For consistency with the rest of the table, define each term, namely NCG, before explaining its usage. The NCG (non-Condensable Gas) package is used to define the gases in the control volumes.
CVH/FL	The CVH/FL (Control Volume Hydrodynamics/Flow Paths) package use time-independent volume for the environment, which prevent aerosols from being drawn back into the facility. A large environment volume (10^{10} m^3) may be too large, since its energy and mass may dilute any actual mass and energy errors in the problem. Therefore, it is recommended to use a reasonable size volume. MELCOR 1.8.6 users may find it difficult to use the new CVH inputs to define the thermodynamic condition of the volume. To ease this problem, an alternative input, CV_THERM, restores some features as in MELCOR 1.8.6. In addition, FL_MACCS input in FL package serves as the designated data set that can be provided for the consequence code MACCS, since MACCS requires data on fluid flows and radionuclide transport to the environment.
HS	The HS (Heat Structures) package allows the model of heat transfer surfaces in the facility as well as for any aerosol deposition or condensation of the water.
RN	The RN (Radionuclide Behavior) package is the most important package for the LPF analysis, because this package tracks and models much of the physics for the aerosols and radionuclides modeled. A new input, RN1_VISUAL, enables the extraction of aerosol information (such as aerosol section and deposition masses) as a function of time to store in files for post-processing, using “ResultsViewer” to display graphically or use SNAP utility or another graphic program to discuss the results.
CF/TF	Both the control function (CF) and tabular function (TF) packages provide a way to control the problem as well as to read and write data for the problems.
EDF	The EDF (External Data File) provides a way to read or write a large amount of data that can be input to MELCOR, or that MELCOR can write out for plotting or inputs to other applications.
Models	Description/Comments
Counter-current flow (CCF) model	A new stratified counter-current flow of gases in a flow path was developed (see FL package input – FL_CCF). User input is available to allow coupling of flows in two paths through momentum exchange, using Epstein-Kenton correlations. This model can be used for modeling counter-current flow in a fire condition, but it is limited for the horizontal flow only.
Critical Flow	CVH package provides an option to select the critical flow in the atmosphere, when two-phase flow may be important. This input card, CVH_ATMCS, is provided. Additionally, the user can print out the sound speed of the flow using CVH_CSTBL.
Aerosol deposition model deactivation flag	RN1_ADFG input in the RN package permits disabling a particular aerosol deposition model – such as a gravitational, diffusive or thermophoresis aerosol settling model. This allows the users to determine which deposition model has the effect on the results.
Turbulent Aerosol Deposition	RN1_TURB input in the RN package allows the modeling of the turbulent aerosol deposition in pipe or duct that contains gas flows in the turbulent regime. Deposition in bends, venturi, and contraction of the pipe or duct transitions can also be captured. Because many of the benchmarks done for this model are from the reactor applications, cautions should be used when applying this model for the LPF application.
Filters	Filter models within the RN2 inputs in the RN package are flexible enough to permit the user to model a variety of aerosol or vapor filters in deposition, flow, and degradation phenomena, because many of the filter inputs can be modeled using control function logic. (See Chapter 4 on best practices for the detailed usage of this model.)
Sprays	The SPR package was developed for the containment spray in the reactor containment. Because of the generality of the spray inputs, this spray model can be used to simulate the fire sprinkler system to reduce the thermal condition of control volumes and can be used to scrub radionuclides/aerosols to minimize the LPF value. (See Chapter 4 on best practices for the detailed usage of this model.)

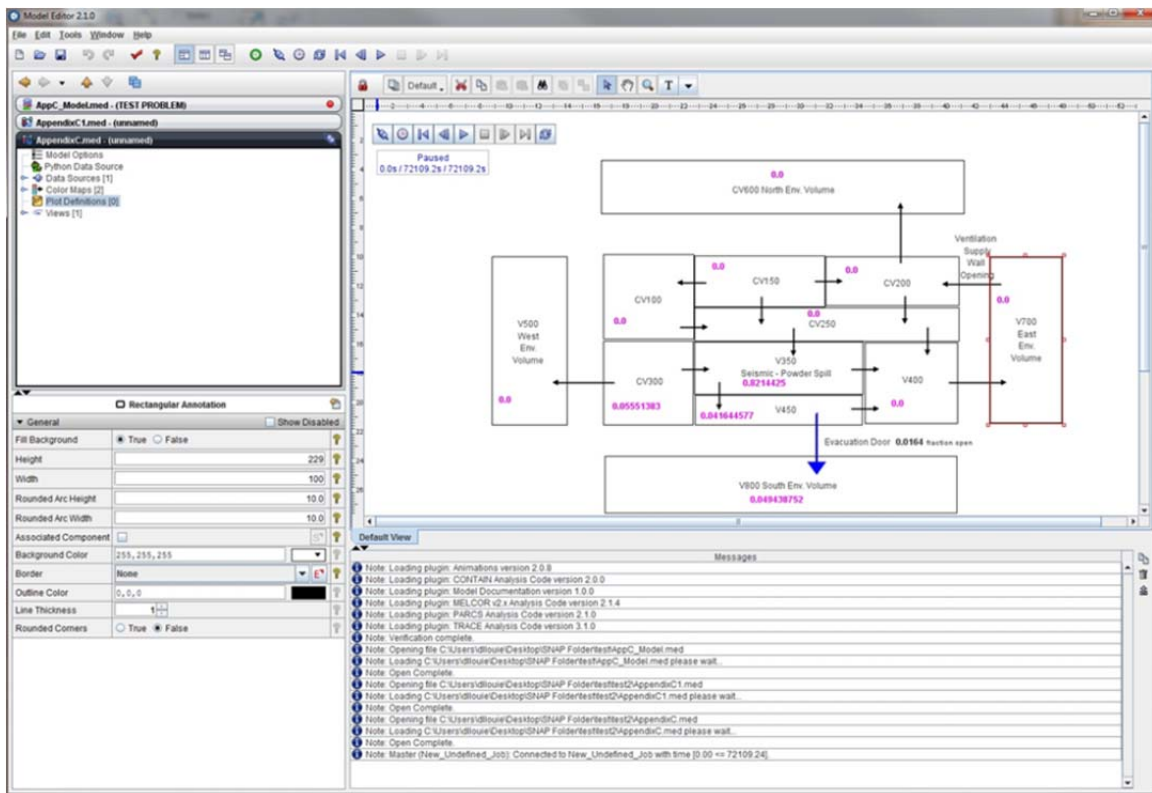


Figure 1-2. Typical SNAP Simulation.

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2 LPF LITERATURE REVIEW

To provide a better understanding of leak path factor (LPF), we will first describe the importance of the LPF from the source term analysis perspective, and the associated major accidents that can influence LPF (see DOE-HDBK-3010 [DOE 1994]).

Source term analysis often starts with the five-factor formula for the source term (ST):

$$ST = MAR \times DR \times ARF \times RF \times LPF \quad (2-1)$$

where MAR (material-at-risk) represents the materials of concern. DR (damage ratio) represents the fraction of MAR that involves in the accident as material affected. ARF (airborne release fraction) represents the fraction of material affected that results in airborne as the suspended material. RF (respirable fraction) represents the fraction of ARF that the particulate (or aerosol) is within $< 10 \mu\text{m}$; and LPF represents the fraction of the suspended material that is released out of a facility. For outdoor or open air, LPF is equal to 1.

The significance of Equation (2-1) is the magnitude of the individual terms in the equation. A high MAR value will increase the source term. The rest of the terms as factors in this equation contain a value between zero and one.

The magnitude of ARF and RF values depends on the initial event or accident involved. Many of these values may be found in DOE-HDBK-3010.

As shown in Equation (2-1), LPF cannot be obtained from DOE-HDBK-3010, because it is a strong function of the energy source, leak, and flow paths within the facility, and all facilities may not be built in the same way. Furthermore, the release characteristics of all postulated accidents are not the same. An LPF value less than 1 includes a credit given for any attenuation of the airborne aerosol within the facility. This attenuation is greatly dependent upon the initial accident event. The major accident events found across the DOE complex include explosion, fire, inadvertent criticality, and spill. Earthquakes can induce many of these accident events, such as explosion and fire. These phenomena can influence the value of LPF and are discussed in the following section.

High attenuation of aerosols would reduce the significant amount of aerosol release from a facility. This attenuation is influenced by many factors, one of which is the confinement barrier. Figure 2-1 shows a three-tier barrier confinement system for a facility with an active ventilation system. As shown in this figure, Zone 1 is the first barrier of defense from the release. Once it is compromised, the second barrier should provide the attenuation. The exterior structure is the last defense. In this three-tier barrier confinement system, active ventilation plays a significant role in preventing aerosols from escaping because of the air flow direction as shown in Figure 2-1. Many active ventilation systems do contain a filtering subsystem that captures much of the particulates in the exhaust stream. Thus, the filter subsystem is important to minimize the release of the particulates. Once these barriers are identified, the question remains how these barriers could be compromised, allowing the aerosol to escape through open pathways. These pathways can be man-made or result from the accident events. Earthquake and explosions can induce cracks in the concrete barriers which can provide an open path. Not all facilities within the DOE complex contain the three-tier barrier system. A one-tier barrier facility would yield a high LPF value for a given event in comparison to a three-tier barrier facility.

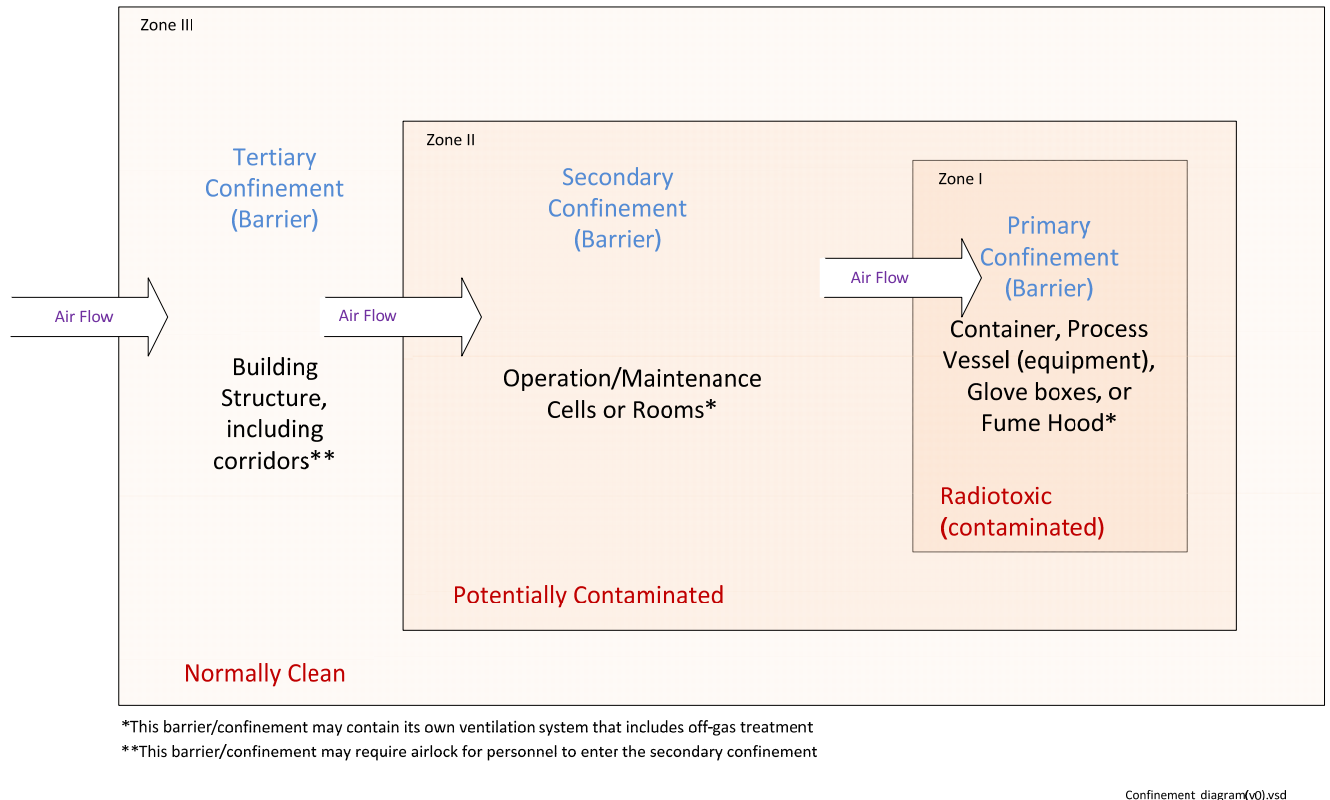


Figure 2-1. Three-Tier Confinement Zones with Active Ventilation System in a Facility with Radioactive or Toxic Materials.

Besides providing the initial release of aerosols within the facility, the initiating event can also influence the attenuation of the aerosol through leak path and distance of travel in the facility. For example, explosions can damage internal structure and exterior structure of the facility. Once this exterior structure is compromised, an open pathway is provided for the aerosol to escape. In addition, explosions may blow out the ventilation system as well as the filtering systems, which can provide a direct path for the aerosols to escape through exhaust of the ventilation or stack, as well as create sufficient energy to force airborne material to other confinement zones or the environment. On the other hand, because of the energy involved, a spill event inside a facility may not have sufficient energy for the suspended aerosols to escape. An external source of flows, such as winds outside the facility or the movement of personnel being evacuated could influence aerosols to escape. A fire accident is unique because it tends to last longer than explosion accidents, but the overall energy output from a fire may exceed that of an explosion. The duration is greatly dependent upon the amount of combustible and oxygen available. If a fire occurs in a room, for example, the heat from the fire rises to the top of the room, which allows a hot gas layer to build up. This layer grows downward until it reaches an opening to escape, allowing the cooler air to enter. This exchange may cause the hot gas layer to sink until the hot gas layer grows again when fire energy is being deposited into this layer. Thus this cycle may influence the transport of the aerosol in the fire.

2.1 Review of LPF Application Documents

To estimate the LPF for a given facility, hand calculations and computer simulations are used to estimate the attenuation of the aerosols through leak paths within the facility. Code simulations are necessary since the details are needed for the accident scenarios and the transport within the facility [Jordan 2003]. For example, the In-Facility Transport Working Group conducted a code review on in-facility transport code review [Spore 1996] to a number of codes, including MELCOR, CONTAIN, FIRAC, GASFLOW, and KBERT. Code such as CONTAIN has been used for LPF determination [Jessen 2011, Ma 2006]. The latest version of CONTAIN 2.0 was last published in 1997 [Murata 1997], and it is no longer supported by SNL. The FATE code, which has been developed by Fauske & Associates, can also be used for analyzing LPF [Plys 2005]. Other code, such as FSSIM was used for U.S. Navy applications for determining LPF as well [Floyd 2004].

Use of MELCOR for LPF applications in the DOE complex began well before MELCOR 1.8.5 was included in the DOE Central Registry. LANL used MELCOR for analyzing their facilities [Bond 1999, Leonard 1998, Letellier 1999, Shaffer 1999]. The facilities at LANL that used MELCOR for their LPF analyses include: TA-55, the Waste Characterization Reduction and Repackaging Facility, the Decontamination and Volume Reduction System Facility, the Chemistry and Metallurgy Research Replacement Facility, and the Beryllium Technology Facility. Other sites began to use MELCOR for their in-facility transport analysis [Ashley 2007, Hawkley 2010]. Other facilities outside of LANL which have used MELCOR include: the Plutonium Facility at Lawrence Livermore National Laboratory (LLNL), the Device Assembly Facility and G Tunnel at the Nevada Nuclear Safety Site (NNSS), Assembly cells at Pantex, and K Area Spent Fuel Storage Facility at Savannah River National Laboratory (SRNL) [Louie, 2016].

In this section, we will summarize several important references that are applicable for this guidance report:

- Previous MELCOR guidance report [DOE 2004] – Although this report documents the use of MELCOR 1.8.5 and information about the modeling using MELCOR 1.8.5, the review of this report is appropriate and useful for default values for LPF calculations.
- LA-UR-03-7945 [Jordan 2003] – This report contains a lot of the information about LPF, aerosol physics, and derivations on LPF analyses, even though the report is written specifically for LANL facilities.
- MELCOR 2.1 Manuals [Humphries 2015a-b] – These are the current published MELCOR 2.1 manuals on theories and usages. A review of these documents provides additional insights about MELCOR 2.1's capability, besides the version differences identified in the previous chapter.
- SAND2009-1701 [Power 2009] – Power reviews the literatures on aerosol deposition and plugging, since these mechanisms are important in terms reducing the value of LPF.

2.1.1 Review of Previous MELCOR Guidance Report

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. This report specified software quality assurance (QA) requirements for safety-related software and also created a Central Registry by designating software approved for safety analysis of DOE defense nuclear facilities. Since MELCOR (version 1.8.5) was included in the Central Registry, a MELCOR LPF guidance report [DOE 2004] was subsequently published to satisfy the requirements of TECH-25. The Accident Phenomenology and Consequence Methodology Evaluation Program at DOE issued the MELCOR LPF Guidance Report, which contained the following objectives for using MELCOR:

- Baseline, accident analysis calculations of LPF
- Scoping analysis in the initial design of facilities or back-fit modification of existing facilities
- Emergency planning for workers
- Confirmatory calculations for evaluating mitigative and preventive safety controls

Table 2-1 describes the review of the previous MELCOR guidance report that was used for version 1.8.5. This research will revise this reference to update MELCOR to version 2.1. In terms of performance, MELCOR 1.8.5 used single precision arithmetic while MELCOR 2.1 uses exclusively double-precision arithmetic which allows better calculation accuracy. As indicated in Table 2-1, there was a need for a software requirements document, software design document and test case description and validation report specific for LPF. MELCOR is a generalized system code, which is developed for severe nuclear reactor accident analyses. However, because it is modularized in nature, it can be used to model LPF for nuclear and non-nuclear facilities. For LPF, the validation with experiments that are applicable for LPF should be done. Thus, this research will include assessments with known experiments applicable for LPF analyses.

Table 2-1. Review of MELCOR 1.8.5 LPF Guidance Report [DOE 2004]

Area	Comments and Suggestions
<i>MELCOR description</i>	It describes MELCOR 1.8.5, which became obsolete
<i>Five-Factor Formula</i>	No comments
<i>Default Input and Recommendation</i> Suggests to include cracks of the structures in seismic events Models door gaps Evacuation	This phenomenon is discussed further in the aerosol physics section. It is important phenomenon to be modeled in LPF analyses, particularly for a nuclear facility as shown in Figure 2-1 since exterior doors contain gaps to allow inflows to maintain the intent of the ventilation system. We will review the door gap data provided in this report. MELCOR 2.1 contains control functions that can be used to model the open and close of the doors for evacuation purposes.

Area	Comments and Suggestions
MELCOR 1.8.5 specific input requirements	Many of the specific input requirements no longer apply for MELCOR 2.1. For example, a recommended 10^{10} m ³ for the environment is no longer needed because MELCOR 2.1 contains time-independent volume that could be used to model the environment. This reference recommended the use of 1 g/cc for modeling aerosol density; however, this density is for water. Therefore, when a dried condition is modeled, it may not truly represent the density of the aerosol. In this case, the actual density should be used.
<i>Sample problems for MELCOR</i>	The data for pressure drop for a range of wind speeds will be verified. We have conducted verification tests (in terms of version-to-version comparison) using the sample problems provided in this report for MELCOR 1.8.5, 1.8.6 and 2.1. We also added additional verification problems to the sample problem sets.
<i>MELCOR limitation</i>	This report pointed out a number of improvement needs for MELCOR 1.8.5, including those specified for LPF applications. Since then, the MELCOR Quality Assurance (QA) program was strengthened by a QA plan to track code changes, user bug reporting, code-review, code documentation (see Table 2-3 for details) and code configuration management. This research will provide a number of validation tests with known experiments and analytical calculations specifically for LPF applications. This research will provide a list of best practices to use MELCOR for LPF applications.

2.1.2 Review of LA-UR-03-7945

As shown in Table 2-2, LA-UR-03-7945 covers a wide range of information about the use of MELCOR for LPF analyses. Although this report is dedicated to LANL's nuclear facility safety, the information covered in this report can be applicable to many sites in the DOE complex. This report also references other aerosol in-transport codes, such as CONTAIN, FIRAC and GASFLOW. Although the spray model (SPR package) in MELCOR 2.1 allows the removal of aerosol by water spray droplets, the usage as a sprinkler system as documented in this table has not been widely used by the safety basis analysts in the DOE complex, because removal of airborne material by water droplets from the sprinkler system has not been credited to provide a safety function. The sprinkler system has only been credited for its fire suppression or control capability. Chapter 4 of this report provides suggestions how to use this SPR model for modeling sprinkler systems for aerosol removal, if this safety function needs to be modeled and credited.

Table 2-2. Review of LA-UR-03-7945 [Jordan 2003]

Area	Comments and Suggestions
<i>Aerosol physics related to LPF</i>	This report includes a summary of aerosol attenuation phenomena, including fire sprinkler system and filters as attenuation methods. This will be addressed in the aerosol physics section below.
<i>Gas and vapor</i>	This topic will not be discussed further in this NSRD-10 report.
<i>Analytical LPF approach</i>	This NSRD-10 report includes these analytical analyses (Table 2-3 for more details for the RN package to be analyzed).
<i>LPF analysis using MELCOR</i>	Although MELCOR 2.1 does not have solid combustibles as a part of the Burn package, the powerful feature of the control function models (CF package) in MELCOR allows the user to model the solid combustible efficiently. A demonstration of this model will be included in this NSRD-10 report.
Lack of hot gas layer	This report includes the inadequacy of MELCOR 1.8.5 for modeling stratified hot gas layer in the fire scenarios. This is still true for MELCOR 2.1. A user still has to model this hot layer using the technique described in LA-UR-03-7945 (see also Section 3.3.1).

Area	Comments and Suggestions
Lack of counter-current flow (CCF) model	This is not true for MELCOR 2.1. A CCF model has been implemented in the FL package. Similarly, this report states the requirement of fire code analysis for the input of the MELCOR calculations.
Small, suspended material models in MELCOR	The MELCOR 1.8.5 models described in this report tend to use “1” g aerosol mass as the initial source term for calculating LPF. Once LPF is obtained, the result is scaled back to the initial suspended material involved in the accident. The use of such small mass by the authors and most safety analysts in the DOE complex is to yield conservative LPF values to minimize agglomeration and deposition [Siebe 2007]. However, this approach may undermine the aerosol physics, particularly for agglomeration, which may not be scaled linearly. In addition, because of the ability to disable the desired aerosol physics, we suggest modelling initial suspended material from the source terms when using MELCOR 2.1 for LPF analyses (see the aerosol physics section for more details).

2.1.3 Review of MELCOR 2.1 Manuals for LPF Applications

As shown in Table 2-3, MELCOR 2.1 includes a number of significant model improvements over MELCOR 1.8.5. Additional improvements not in the MELCOR assessment report [Humphries 2015c] include aerosol resuspension model from surfaces, tracking deposited mass in sectional quantity rather than a lump sum value, realistic pump models, improvement of the calculation numeric, no restriction of the number of CVH volumes, and modelling flow path. These four packages, as shown in Table 2-3, are the most important packages to be included in a LPF calculation. Other packages such as the HS package can be used to provide deposition surfaces and heat sinks.

Table 2-3. Selected Review of MELCOR 2.1 Manuals for LPF [Humphries 2015a-c]

Area	Comments and Suggestions
CVH package	Significant improvements went into MELCOR 2.1 over MELCOR 1.8.5 for this package, such as the atmosphere sound speed model (adopted from CONTAIN), time-independent volume (use for modeling environment), and specified-property volume.
FL Package	Some improvements include CCF model, flow blockage, and MACCS interfaces.
RN Package	Significant improvement went into MELCOR 2.1 over MELCOR 1.8.5 – essentially there is no restriction on number of radionuclide classes to be modeled, normalization of RN inventories, and treatment of MAEROS aerosol coefficients in terms of temperature and pressure. The aerosol filter model has been extended to allow specification of decontamination factor (DF) by particle size as well as by class. Each DF can be represented by a constant or control function. Beginning in MELCOR 2.1, many of the aerosol physics models can be turned off for individual mechanisms to allow specific aerosol testing. This turn-off feature is included for aerosol deposition and agglomeration. Turbulent deposition model has also been implemented from a recently published resuspension model from SAND2015-6119 (see Table 2-4).
CF Package	One of the powerful models in MELCOR is the control function (CF) package. This package allows the users to model different phenomenological conditions associated with the accident scenario, control volumes, or flow paths. For example, opening and closing of the doors for evacuation can be modeled using CF. In MELCOR 2.1, the CF Formula allows to program a formula which may represent a reaction, an energy function, a pump curve, or an algebraic equation. For example, a reaction of solid combustible and oxygen can be modeled (e.g., to model a fire temperature grows/decay profile) using CF.

2.2 Important Aerosol Physics Review

As shown in the LPF section, the attenuation of aerosols is greatly dependent on the leak path and traveling distance. This attenuation relies strongly on the particle interaction and transport physics. Aerosol transport is greatly dependent on the air flow that carries the aerosols as inertia forces. The magnitude of this air flow is a strong function of the initial accident conditions (or release characteristics) and other external conditions that could influence the direction of the flow. Aerodynamic drag on a particle can be determined based on the viscosity of the air, the diameter of the particle being dragged, and the particle velocity relative to the air flow. This can be modelled through the use of the Stokes number, which often refers to the ratio of the stopping distance of the particle to the characteristic dimension of the path that could cause the particle to change direction. This change of direction often refers to deposition. Because the Stokes number is a strong function of the particle size, as the particle grows in size due to particle interaction phenomena, such as agglomeration (or coagulation), this number becomes large. The cutoff value of the Stokes number can be an influence on the ratio of the particle settling velocity over the drag velocity. This cutoff is unique for a given aerosol size and the characteristic length of the particle path traveled.

During transport through leak path, deposition can occur. This deposition can create partial and complete plugging in a leak path as for the high-efficiency particulate air (HEPA) filters. This plugging, as a form of deposition, has been identified to be important particularly if the leak path opening is small, such as cracks in a concrete wall in an earthquake event, or a door gap if sufficient aerosol mass is presented. Turbulent deposition can be enhanced if the Reynolds number is in the turbulent flow regime. On the other hand, resuspension can occur if the entrainment force is sufficient enough to cause the deposited aerosols to re-suspend back into the air stream.

Table 2-4 shows the current aerosol physics being modeled in MELCOR 2.1. As shown in this table, agglomeration and deposition models are included in MELCOR 2.1 (see [Humphries 2015c]). The addition of these new models, such as resuspension is included in the latest version of MELCOR 2.1. Plugging models have not been implemented in MELCOR 2.1; however, the simulation of plugging using CF can be done, similar to that for plugging and pressure loss for HEPA filter modeling.

Table 2-4. Aerosol Physics Important for Validation in MELCOR 2.1

Physics	Comments and Suggestions
<i>Agglomeration</i>	It is important to validate this model because it identifies the degree of the aerosol interaction during the initial release from an accident.
<i>Deposition</i>	A number of deposition models have been included in MELCOR (gravitational, diffusive, and thermophoresis). Although MELCOR 2.1 allows the user to turn off one to all three of these deposition mechanisms, we will assess if one or more of these deposition models can be validated using experimental data. In addition, MELCOR 2.1 contains turbulent deposition models that are only available for heat structure surfaces (non-pool surfaces). Turbulent deposition models can be validated through experimental data for high Reynolds number regime and straight pipes, including bend geometry. Impaction can be considered as deposition.
<i>Plugging</i>	Currently MELCOR 2.1 does not contain plugging models. Consideration of plugging in LPF analyses may not be conservative in terms of the release.

Physics	Comments and Suggestions
<i>Resuspension</i>	MELCOR 2.1 contains a resuspension model from SAND2015-6119 [Young 2015] using the force balance between aerodynamic forces and adhesive forces to the surfaces. This simple model is a function of wall shear stress, friction factor, gas velocity, and surface roughness. The validation of this model is important, particularly if sufficient flow exists to entrain the deposited aerosol to the air stream. Thus the NSRD-10 research will include the resuspension validation.

Plugging as shown in Table 2-4 is a special form of deposition. In order to plug a leak path, sufficient aerosols must exist. Thus, plugging and deposition literature reviews are provided in [Power 2009] (see Table 2-5). Powers [Power 2009] summarized the aerosol deposition and plugging from a number of experiments and analyses in the open literature before 2009. In terms of plugging, he described the small cracks in concrete, capillary, orifice, slots and gaskets in the range of the widths in tenths of millimeters or so. From that, the Stoke number, which often refers to the ratio of the stopping distance of the particle to the characteristic dimension of the path that could cause the particle to change direction, is used for measuring the deposition in an aerosol flow stream. A large number of correlations and equations are presented in [Power 2009]. It also includes both laminar and turbulent flow deposition models. A large number of tables from the experiments are also included. This reference is very useful in the development of future models for implementation of deposition models into MELCOR, since it provides experimental data and models that could be used for validation and benchmark purposes. As shown in Table 2-4, no plugging model is currently implemented in MELCOR 2.1.

Table 2-5. Review of SAND2009-1701 for Aerosol Deposition and Plugging Models [Power 2009]

Topic	Comments and Suggestions
Leak pathway	This reference discusses the aerosol transport through capillary, orifice, slot, concrete crack, and gasket leak as a leak path for deposition, and subject to plugging. A number of correlations and derivations are provided for these pathways in this reference.
Plugging experiments	This reference describes (a) the capillary experiments from Mitchell and his coworkers, Nelson and Johnson, Rockwell Tests, depleted uranium dioxide flows by Sutters; (b) orifice experiments from Sutters, and Mitchells; (c) slot from Lewis tests, Mosely, Liu and Nazaroff; (d) concrete crack experiments from van de Vate, Gelain and Vendel; and (e) effects of geometrical shape experiments from Carrie and Modera, Morewitz, Watanabe, Hilliard and Postma.
Turbulent deposition data	These references also include turbulent deposition data from various experiments and model derivations from Friedlander and Johnstone, Montgomery and Corn, Wells and Chamberlain, Liu and Agarwal, El-Shobokshy, Lee and Gieseke, Shimade, Sehmel, Postma and Schwendiman, Ilori, Muyschondt, and Forney and Spielman.
Theory on deposition	In addition, Powers provides a number of models in simulating particles entering leak pathways that lead to deposition and plugging. He covers flows in laminar to turbulent regimes, including the effect of shape of the ducting. He also describes the deposition model by Chen Yu Method using multiple mechanisms: inertial, diffusion and gravitational. He also discusses models related to particle bounce off from the surfaces.

2.3 Summary and Conclusions

This chapter summarized the processes involved in determining LPF for the facility, depending on the zoning of the confinement barriers, accident conditions, and aerosol mass size. The following conclusions can be drawn from this research and further examined:

- The latest version of MELCOR is required for the LPF analysis, since MELCOR 2.1 has many thermal-hydraulic and aerosol physics improvements over MELCOR 1.8.5, and it is the current version supported by SNL.
- “Best Practices” recommend the following:
 - Using initial suspended material with agglomeration and/or deposition disabled for simulation instead of using “1” g mass to allow scaling evaluations.
 - Beginning with MELCOR 2.0, it is not recommended to model a large environment volume in the order of 10^{10} m^3 . The use of a time-independent volume feature eliminates this need.
 - Using the counter-current flow (CCF) model in the FL package to better represent the counter-current situation in fire scenarios (representing hot and cold temperature layers and circulation of air within these layers). This new model is an improvement over MELCOR 1.8.5.
 - Using new filter models in MELCOR 2.1 for modeling the HEPA filter conditions experienced in accident situations (see Chapter 4 for more details).
 - Using the SPR package to model the water fire sprinkler system (see Chapter 4 for more details).
 - Using control functions to model solid combustible burn for fire scenarios, since advance features of CF models are available in MELCOR 2.1 as an alternative method to fire codes such as CFAST (Consolidated model of Fire And Smoke Transport) to generate the heat energy data (see Chapter 3 on a MELCOR simulation for fire scenarios).
- The following important aerosol physics models need to be validated through the use of experimental data and analytical models:
 - Agglomeration
 - Deposition
 - Resuspension

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3 MELCOR VERIFICATION AND VALIDATION

Verification and validation (V&V) for any computer code, such as MELCOR, must be performed to increase the confidence level for using the code for various applications. As mentioned before, MELCOR is developed primarily for analyzing severe accidents. We have written a MELCOR assessment report specifically for this application, which includes verification assessment and experimental validations. To apply MELCOR for LPF applications, a review of these reactor-specified assessments are needed. Note that the V&V of MAEROS (A multisectional, multicomponent aerosol dynamics code) aerosol physics model in MELCOR can be assessed in reactor applications since it was developed in 1980s. In this chapter, we will discuss whether these assessments are applicable or not. To be consistent with the MELCOR 1.8.5 guidance report [DOE 2004], we will include the verification cases described in the 1.8.5 report. See Appendix A for more details. In addition, we will include a number of experimental validations using the experiments described in DOE-HDBK-3010 [DOE 1994].

This chapter is divided into four sections. The first section describes the applicability of the reactor experiment validations for MELCOR. The second section describes the selected experimental data and results from the Handbook for MELCOR validations. The third section discusses the fire-specified experimental validations and comparison to a fire code listed in the DOE registry and an aerosol-specified model validation. The last section provides summaries and conclusions for this V&V.

3.1 Discussion on Reactor Experiment Applicability

Validation of the MELCOR code is very important for the U.S. Nuclear Regulatory Commission (NRC). The NRC must provide an analytical severe accident tool to support its regulatory decisions for the operating nuclear power plants and for certifying new and advanced reactor designs [Salay 2015]. To validate MELCOR, NRC is participating internationally in a number of collaborative research and experimental programs, such as the Cooperative Severe Accident Research Program (CSARP) and the MELCOR Code Assessment Program (MCAP). These international collaborations result in further collaborative experimental programs that can be used to validate the new model development and assessment of MELCOR. These experimental programs include separate effect tests, integral tests and actual accidents. Table 3-1 identifies the experiment types. As shown in this table, among all three types of experiments, only separate effects experiments may be applicable for DOE facilities and integral experiments may be applicable if conducted for releases within the containment. Figure 3-1 shows the reactor experiments available that have been used to validate MELCOR. As shown in this figure, the experiments are categorized by the physics examined, such as radionuclide or aerosol (RN) transport, core heat-up and degradation, thermal-hydraulics in the primary coolant system (PCS), containment, and ex-vessel phenomena. Other than actual accidents, the rest of the experiments are considered to be separate effects and integral tests, because they are only examining particular parts of the reactors or parts of the multi-physics encountered in an accident; some of these experiment types, in particular those involving RN, in the containment may have applicability to DOE facilities. However, many of these experiments are specified for reactor cores and/or for the reactor coolant systems (RCSs), which may not be found at the DOE facilities, except in the research reactors. Also, there are recent validation experiments, primarily

for the separate effect tests that may be applicable for validating MELCOR. In this report, we attempt to provide a suite of experiments and analytical validations for MELCOR 2.1, so we will summarize first the applicable reactor experiments that were documented in the MELCOR assessment report. Then, we will summarize any analytical validations that can be used to benchmark MELCOR, some of which came from the MELCOR assessment report [Humphries 2015c]. Finally, we will summarize any new experiments and analytical validations that are applicable to DOE facilities.

Table 3-1. Reactor Experiment Types

Experiment Type	Description	Applicable to DOE LPF Application
Separate Effect	This experiment focuses on an individual physical process, which minimizes the combined effects of multiple physical processes. However, it may not be possible to design a single experiment that only observes a single process or physical phenomenon. Thus the separate effects tests often ignore the importance of coupling between processes that are inherent in real world applications.	Yes, since it only deals with a single process. Even though the experiment may be tailored for reactor applications, a single process validation may easily determine its applicability to DOE facilities.
Integral	This experiment examines the relationship between coupled processes and physical phenomena of multi-physics such as fluid dynamics and aerosol transports with the entire accident sequence.	No, if these experiments were involved with the reactor core, which leads to transport and releases. On the other hand, if the tests are conducted for containment, then they may be applicable for DOE LPF.
Actual Reactor Accident	This is not an experiment, but rather the actual accident that may limit the data collection which can be used to validate MELCOR. However, some assumptions for the missing data may be necessary for the code validation to be conducted.	No. The actual accidents of the reactors may not be applicable for DOE facilities because the amount of materials, temperatures and sequences are much different than that in the DOE non-reactor facility.

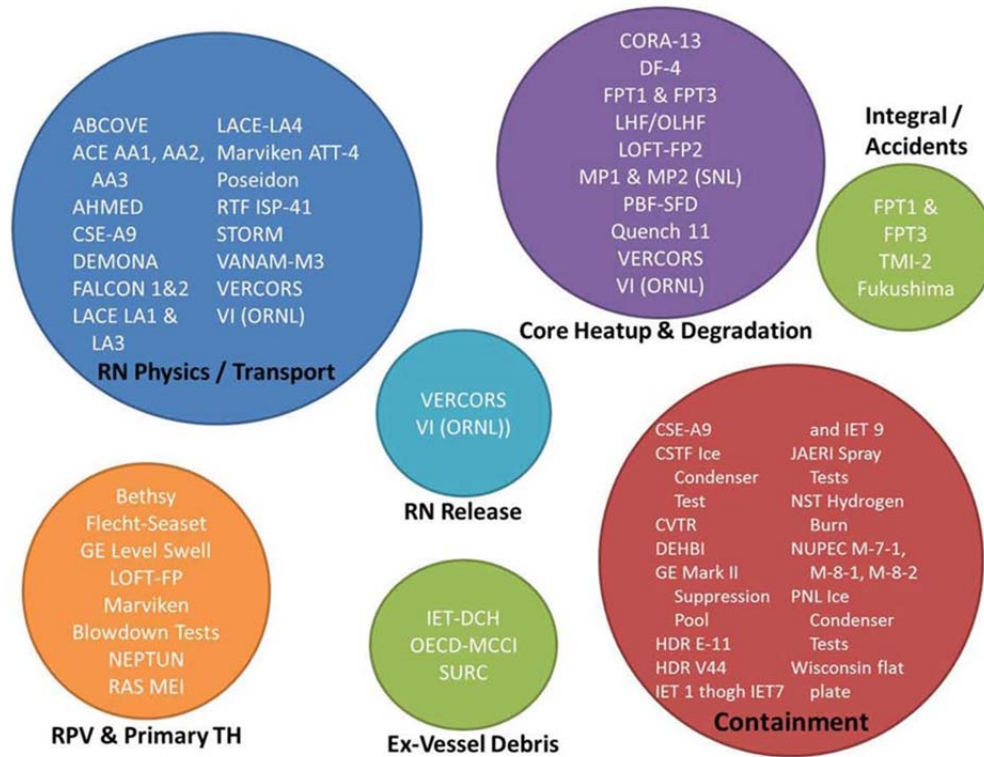


Figure 3-1. Experiments and Accidents Used for Validating MELCOR [Humphries 2015c].

3.1.1 Reactor Type Experiments

Reactor experiments are very important for MELCOR, since these experiments can be used to validate individual and multiple physics packages in MELCOR (see Figure 3-1). Even though many of the experiments may be directly related to the reactors, particularly in the area of severe reactor accidents, these experiments, nonetheless, provide validations of the code. For those experiments directly involved with the reactor core heat-up and degradation, they will not be applicable for DOE non-reactor nuclear facilities. Similarly, the experiments related to ex-vessel debris as shown in Figure 3-1 will not be applicable for DOE nuclear facilities. Experiments such as RN physics and transport may be applicable for DOE nuclear facilities, since RN in MELCOR deals with both radionuclides and aerosol physics/transport. As shown in this figure, some reactor experiments generally deal with thermal hydraulics in a large volume and multiple volumes, engineered safety features such as water sprays or ice condenser, and pool scrubbing and hydrogen ignition. Only those experiments for thermal hydraulic, hydrogen ignition and water spray may be useful for DOE facilities where differential thermal conditions, hydrogen combustion and the use of water sprinklers for fire-fighting events can occur. In general, most experiments that cover a number of physics, such as thermal-hydraulics and aerosol physics/transport, could be important to LPF determinations, since heat and flow determines the conditions for the aerosol flows as well as the aerosol physics such as the rate of deposition and resuspension. When those reactor experiments deal with significant amount of MAR and extreme conditions as in core-melt, then these experiments may not be applicable for DOE

facilities. Nonetheless, these experimental validations will contribute greatly to the confidence of using MELCOR for LPF determination.

Note that not all experiments listed in Figure 3-1 are included in the MELCOR 2.1 assessment report [Humphries 2015c]. Here we identify the reactor experiments that can be used to validate a range of conditions found in potential accidents related to DOE facilities for LPF determinations. For example, explosions and fires are generally considered as energetic scenarios in terms of impulse and high energy/temperatures. Table 3-2 shows the review of the reactor experiments in the assessment report. This table provides a brief description of the experiment and the important physics being validated. In addition, the table provides whether or not the experiment is applicable for LPF determination uses at DOE facilities in terms of the accident types that are closely represented (i.e., explosions, fires and spills). Note, no result is shown in this table or in the text. The reader should consult the assessment report for details.

Table 3-2 Review of Reactor Experiments from MELCOR 2.1 Assessment Report

Experiment	Important Physics	Brief Description	Applicable to DOE LPF Application
<i>ABCOVE AB5 and AB6</i>	Thermal hydraulics and aerosol physics	These tests are designed to observe sodium spray fire. Since MELCOR does not model sodium fire currently, these tests are used to study the aerosol physics within a single volume. The test volume for the experiment is done in the CSTF ^a . AB5, a single-component aerosol test, includes a test temperature of 552 K with 445 g/s aerosol generated (MMD/GSD ^a =50 $\mu\text{m}/1.5$). AB6, a co-agglomeration of two aerosol components test, includes a test temperature of 438 K, with at least 78 g/s aerosol generated (MMD/GSD=0.5-54 $\mu\text{m}/1.5-2$).	Yes. Since these experiments are related to fire, the resulting aerosols are generally generated during the reaction. This experiment may be applicable for fire scenarios with aerosol releases encountered in DOE facilities, even though sodium spray fire may not occur at a DOE facility.
<i>ACE Pool Scrubbing</i>	Thermal hydraulics and aerosol physics	This test is designed to capture FP ^a aerosols being scrubbed in a suppression pool in the containment. The test is a part of the ACE ^a experiments.	No. Pool scrubbing of aerosols may not be important in DOE facilities.
<i>AHMED</i>	Thermal hydraulics and aerosol physics	This test is conducted at AHMED ^a facility to provide data for hygroscopic and non-hygroscopic aerosol behavior in a single and multi- component under controlled temperature and humidity (22%, 82% and 98%) conditions. It also examines the settling effects in several humidity levels. Test volume is 1.81 m ³ with sedimentation area of 1.27 m ² . Aerosol is NaOH (with AMMD ^a /GSD=2.4 $\mu\text{m}/1.64$) and the test pressure is at 1 atmosphere. It is considered a separate effect test.	Yes. Although NaOH as an aerosol may not be commonly found in DOE facilities, the test provides the results of hygroscopic behavior of aerosol, particularly during a fire situation with a water sprinkler being activated.
<i>Bethsy 6.9c</i>	Thermal hydraulics	This test is an integral test for studying the RCS thermal hydraulics. The Bethsy experimental facility is used to model PWR core and primary coolant system.	No. DOE facilities do not have RCS.
<i>CSE Spray A9</i>	Thermal hydraulics and aerosol physics	This test is designed to examine the aerosol removal by water spray. Test volume of 595 m ³ with surface to volume ratio of 0.958/m is used. The spray droplet size (MMD/GSD=1220 $\mu\text{m}/1.5$), nozzle number of 12 with spray rate of 9.135 l/s and spray volume of 8694 liters, and fission product concentrations of 2 to 100 mg/m ³ in the test volume initially are in the experiment. The interest here is uranium aerosol, which could be analogous to PuO ₂ .	Yes. Water spray in MELCOR can be used to represent water sprinklers commonly found in most DOE facilities. If the aerosol scrubbing is considered in the analysis, this test may be applicable.
<i>CORA-13</i>	Core heat-up and degradation	This test is conducted at the CORA facility as the ISP ^a -31. It models a core and pressurizer.	No. Core effects may not be applicable at DOE non-reactor facilities.

Experiment	Important Physics	Brief Description	Applicable to DOE LPF Application
<i>DEMONA-B3</i>	Thermal hydraulics and aerosol physics	This test is designed to study the effect of steam condensation on aerosol settling. The test was performed at the BMC ^a facility in Frankfurt, Germany. This facility is highly compartmentalized. SnO ₂ is the aerosol that is injected, along with air and steam.	Yes. Even though the humidity level for the test is very high, the effect of the fog in the air influencing the depletion of the aerosol is studied. High humidity can occur in a DOE facility when the water sprinkler is activated or steam may be present as part of the accident scenario.
<i>GE Swell</i>	RCS thermal hydraulics	This test is designed to study the effect of large vessel blowdown and bubbly pools. This test was conducted at the General Electric Large Blowdown Vessel Test facility.	No. The blowdown effects on pool level swell may not be applicable to a DOE facility.
<i>JAERI Spray</i>	Containment thermal-hydraulic	Water spray tests were conducted at the JAERI ^a to study the effect of the pressure suppression through condensation by sprays.	No. However, if the water sprinkler system is used to credit the pressure reduction during a fire event, then this test may be applicable for DOE facility. This pressure reduction may reduce the source term out of the facility.
<i>LACE LA-4</i>	Thermal hydraulics and aerosol physics	As a part of the LACE ^a project, this experiment is to study overlapping injection of soluble and non-soluble aerosols. This experiment was conducted in the same CSTF as for the ABCOVE experiment above. CsOH (0.949 g/s) and MnO (0.757 g/s) aerosols are injected, while steam (0.45 kg/s before aerosol injection to 0.025 kg/s after) is injected into the CSTF. The timing of the injections varies. CsOH has 1.35-2.22/1.81-1.80 AMMD/GSD and MnO has 1.82-2.43/2.56-1.70 AMMD/GSD. Drainage due to steam condensation is considered.	Yes. Although CsOH is used as a hygroscopic aerosol with steam, the MnO, as non-soluble aerosol, may be applicable when a water sprinkler is active in the DOE facilities; or when steam explosions are postulated (e.g., a furnace cooled by water).
<i>LOFT LP-FP-2</i>	Core heat-up and degradation	This test was conducted at Loss-of-Fluid Test facility at INEL ^a . The facility is a 50-megawatt thermal, volumetrically scaled PWR ^a system. The purpose of this test is to capture the fission product release, transport, and deposition in the core and the PCS. It is considered an integral test.	No. Core effects may not be applicable at DOE non-reactor facilities.
<i>Marviken Critical Flow</i>	RCS thermal hydraulics	This test examines the critical flow from pipes, nozzles, safety relief valves and vessels. The test was conducted at the Marviken facility in Sweden. The blowdown vessel is a full-size reactor vessel measuring at 5.2 m diameter, 22 m high with a volume of 425 m ³ . The blowdown of steam/water at 5 MPa is considered.	Yes. This separate effect test is used to validate the blowdown of a high-pressure water/steam vessel/pipe. This may be applicable when a process vessel containing water, which is being heated externally, has been ruptured in a DOE facility.
<i>Marviken ATT-4</i>	Thermal hydraulics and aerosol physics	This test is a part of the large-scale aerosol transport tests (ATTs) that were conducted at the Marviken facility. This test is designed to study FP transport in the RCS. FPs (I ₂ , CsI, CsOH, Te, Ag and Mn) along with various gases that were injected at various time/time periods. This test allows the study of the deposition mechanisms, including turbulent deposition. Various sizes of the aerosols are used in the simulation, since the experiment did not provide any size distribution.	Yes. Although this integral test focused on the FP transport within the RCS with various gas compositions, the test is excellent for validating aerosol physics and transport, including the turbulent deposition model in MELCOR.
<i>NTS Hydrogen Burn</i>	Containment thermal-	This test is designed to study the hydrogen burn completeness in a hydrogen dewar located at the Nevada	Yes. Hydrogen burn is possible at DOE facilities,

Experiment	Important Physics	Brief Description	Applicable to DOE LPF Application
	hydraulic	Test Site. The dewar is a spherical steel vessel with an inner diameter of 15.85 m, which has a design pressure of 0.7 MPa. A number of runs were conducted based on the gas mixture of H ₂ (5.3-12.9%) and (4.2-28.3%) steam.	particularly when hydrogen gas is used in a process or a waste facility that contains hydrogen as by-product due to radiation or decomposition.
NUPEC	Containment thermal-hydraulic	This test was conducted at the Nuclear Power Engineering Corporation facility, simulating 1/4-scale containment. This experiment examines the pressure response, temperature distribution and stratification and hydrogen mixing in the multi-compartments with steam injection and containment spray actuation. This facility is a domed cylinder 10.8 m in diameter and 17.4 m high (1310 m ³) with 28 compartments, 25 being interconnected. Since this is a thermal-hydraulics test, the helium gas was used as a surrogate for hydrogen also released from the RCS during an accident. Both steam and helium gases are introduced to the facility to simulate the overpressure of the containment.	Yes. Although this test is designed to study the overpressure in a containment of a reactor due to accident, the thermal-hydraulics associated with condensation of steam and containment spray may be applicable during a fire scenario in which a water sprinkler is used to suppress fire accidents.
PHEBUS FPT-1,3	Core heat-up and degradation	These integral tests are part of series of in-pile source term tests conducted at PHEBUS facility at Cadarache, France. Both tests consist of an in-pile fuel bundle assembly and upper plenum region, an external circuit including a steam generator, connecting lines and a containment section. However, the FPT-3 test included a steam-poor environment and a control rod.	No. Core effects may not be applicable at DOE non-reactor facilities
POEIDON	Thermal hydraulics and aerosol physics	This test is designed to provide insight into pool scrubbing phenomena and to identify/correct any existing deficiencies in the model of scrubbing. The test was conducted using the POSEIDON loop and associated aerosol generation system DRAGON, which allows the aerosol flowing through a pool to determine the decontamination factor.	No. Pool scrubbing is not a consideration in a DOE nuclear facility. However, many exhaust systems, including in the glovebox or residual storage tanks, may include a way to capture contaminant.
STORM SR-11	Thermal hydraulics and aerosol physics	This test is designed to provide the aerosol deposition (i.e., thermophoresis and eddy impaction) and resuspension (under a stepwise increasing flow rate) in pipes, which was conducted at the STORM ^a facility. This test is ISP ^a No.40, which is based on the STORM SR-11. The test section is a straight pipe 5.0 m long with a 6.3-cm inner diameter. In the first part of the test, aerosols (SnO ₂ and CsOH) are injected into the pipe and allowed to deposit. The aerosol flow rate is $\sim 3.83 \times 10^{-4}$ kg/s at 0.43 μ m geometric mean diameter and a 1.7 GSD. The second phase is to allow the deposited aerosol to resuspend via high gas velocities. In this assessment report, only the deposition phase was simulated and validated	Yes. Although the test was conducted in a pipe, the deposition phenomena are being captured. Therefore, the SnO ₂ results may be applicable for DOE facilities with energetic accidents, such as explosions or high flow conditions of the accidents. In addition, the resuspension phase of the test may be important to DOE facilities, since this test can validate the resuspension model in MELCOR.
CCI Tests	Ex-vessel phenomena	These tests are part of the OECD ^a -sponsored melt coolability and concrete interaction program to resolve any ex-vessel coolability issues.	No. Corium-concrete interactions are not issues in DOE facilities.

^a CSTF = Containment Systems Test Facility located at the Hanford Engineering Development Laboratory, FP=fission product, AMMD=aerodynamic mass mean diameter, MMD = mass mean diameter, GSD=geometric standard deviation, ACE=Advanced Containment Experiment, AHMED=Aerosol and Heat Transfer Measurement Device, ISP=International special problem, BMC=Battelle Model Containment, JAERI=Japan Atomic Energy Research Institute, INEL=Idaho National Engineering Laboratory, PWR=pressurized water reactor, OECD=Organization for Economic Co-operation and Development, LACE=Light water reactor Aerosol Containment Experiments Project, STORM=Simplified Test on Resuspension Mechanism.

3.1.2 Analytical Validations

In addition to the experiments, analytical validation is a good way to benchmark MELCOR specified physics models. These analytical validations are designed to test thermal hydraulics of

the code, including heat conduction and convection models. These validations are generally applicable to DOE facilities. Table 3-3 provides a review of the analytical validation problems included in the MELCOR 2.1 assessment report. This table provides a very brief description of the MELCOR problem and the intended physics MELCOR addresses. In addition, a comment addresses the applicability to the DOE facilities. Note that the current MELCOR 2.1 assessment report does not include any aerosol analytical validation, which is important for LPF determinations at DOE facilities. Therefore, the next section describes an analytical validation problem for aerosol physics.

Table 3-3. Review of MELCOR 2.1 Assessment Report on Analytical Validation

Physics Phenomena	Analytical Validation Description and Comments
Saturated liquid depressurization	A two-volume problem is constructed for this validation. Volume 1 contains saturated water at high pressure, which is connected via a flow path to another volume containing only a low-pressure, steam environment and a heat structure. This problem tests many thermal-hydraulic (CVH, FL and CVT) packages and heat structure (HS) packages. Although this problem is designed for validating the MELCOR models for the blowdown of the reactor pressure vessel into the containment, the ability for MELCOR to treat steam, water, and blowdown phenomena at high and low pressures should indicate that MELCOR should be able to model many accident conditions of flows, including in liquid flows in the DOE facilities.
Adiabatic flow of hydrogen	A two-volume problem is constructed to study the gas flow from a high-pressure volume to a low-pressure volume. This problem validates the CVH, FL and non-condensable gas (NCG) packages. This problem is a classical force-driven gas flow that can be found in the DOE facilities. No hydrogen deflagration is modeled.
Transport heat flow in a semi-finite solid with convective boundary conditions	A single volume problem is constructed to validate the HS package. Both steel and concrete are used in the materials of the HS with the peak temperatures in 600 K and below. A 10-meter thick heat structure simulates the semi-infinite solid in the analytical solution. This problem should be capable of validating a wide range of heat sinks commonly found at DOE facilities.
Cooling of rectangular and annular heat structures in a fluid	A single volume problem is constructed to validate the HS package. Two HS geometries are tested: rectangular and cylindrical structures. The heat structure is initially at 1000 K and is being cooled by the fluid at 500 K. The gradual cooling by the fluid lasts to 10 seconds. Although the initial HS temperature is relatively high, which may not be commonly found in accident conditions in DOE facilities, this problem demonstrates the ability for the HS package to model cooling of very hot structures.
Self-initialization of steady-state radial temperature distributions in annular	A single volume problem is constructed to validate the HS package in terms of a heat structure lying between two different fluids at different temperatures – one is higher than the other. The HS has an annular geometry. The left side is facing at a fluid at 600 K and the right side is facing at a fluid at 550 K. This problem models both steady state and transient conditions. The temperature range of this problem can be found in

structures	fire accident conditions within a DOE facility.
Establishment of flow in a pipe	A two-volume problem is constructed to model the liquid flow between two volumes. It is used to validate the CVH and FL physics packages via gravitational head. This problem can be used to simulate the tank flow under a gravitational head for the water sprinkler system or other process vessels within a DOE facility.

3.1.3 Experiments and Analytical Validation not in MELCOR 2.1 Assessment Report

As described in the previous two sections, a number of experiment and analytical validations can be applicable and used for validating MELCOR for LPF analyses. This section provides more recent experiments and analytical validations for aerosol physics and transports that can be added for this research. As shown in the analytical validation section, the current MELCOR 2.1 assessment report does not include any analytical validations for aerosol physics. This deficiency is addressed by the simple analytical aerosol problem, which will be discussed later. In recent years, there have been a number of simple, separate effect experiments for reactors. One of them is to study the aerosol physics based on the thermal condition inside a box with one hot surface and one cool surface, which is called the DIANA test at the Paul Scherrer Institute in Switzerland. This experiment will be described later. As mentioned earlier, not all experiments described in Figure 3-1 or in Table 3-2 are included or partially included in the current version of the MELCOR 2.1 assessment report [Humphries 2015b]. For example, as shown in Table 3-2, the STORM SR-11 experiment was included in the report, but only the deposition phase was evaluated. The resuspension phase should be included. Therefore, Section 3.3 will describe this experiment, including the results of resuspension phase simulation. In addition, the LACE-3 experiment can be useful for validating the aerosol deposition, including turbulent deposition. This experiment will be discussed briefly here. Note that the tests described in this section have not been included in the assessment report. However, as a part of the on-going assessment supported by NRC, all the experiments and analytical problems described in this section, except the resuspension phase of the STORM SR-11 experiment, were funded by the NRC assessment project. Note that no result is documented for those on-going assessments supported by NRC in this report. Only the descriptions of the experiments are provided here, since the validations are provided in the upcoming MELCOR assessment report which will be published in the near future.

3.1.3.1 Simple Aerosol Analytical Problem

In this simple problem, Room 1, containing a uniformly distributed 1 g aerosol, is connected to Room 2, which is larger [Jordan 2003] (see Figure 3-2). With the flow area of 0.01 m^2 , the flow rate is constant. This test validates the aerosol settling and aerosol transport through the flow path with an analytical solution. Note that there is no input deck available, so a new input deck will be developed in MELCOR 2.1, rather than MELCOR 1.8.5 as implied in the reference document [Jordan 2003].

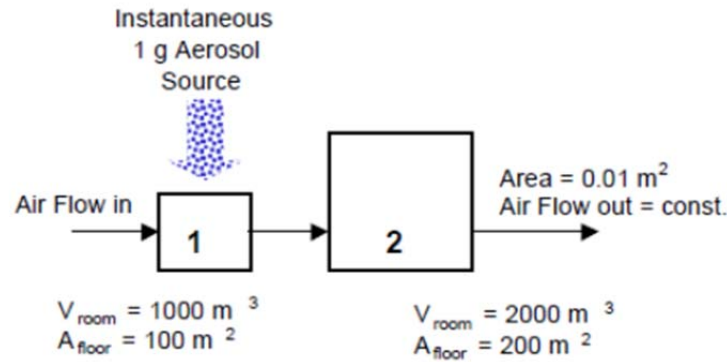
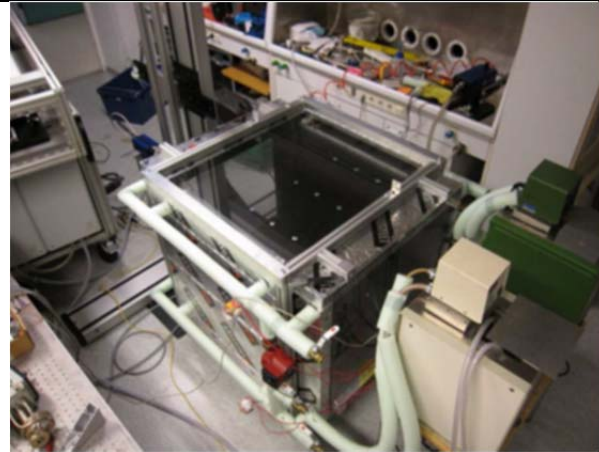


Figure 3-2. Simple Analytical Aerosol Physics Problem [Jordan 2003].

3.1.3.2 DIANA Aerosol Experiment

This separate effect experiment is designed to study the simple aerosol physics, primarily the thermophoresis deposition. This experiment was conducted at the Differentially Heated Cavity with Aerosol in Turbulent Natural Convection (DIANA) facility at the Paul Scherrer Institute. Table 3-4 shows the photo and the brief description of the experiment.

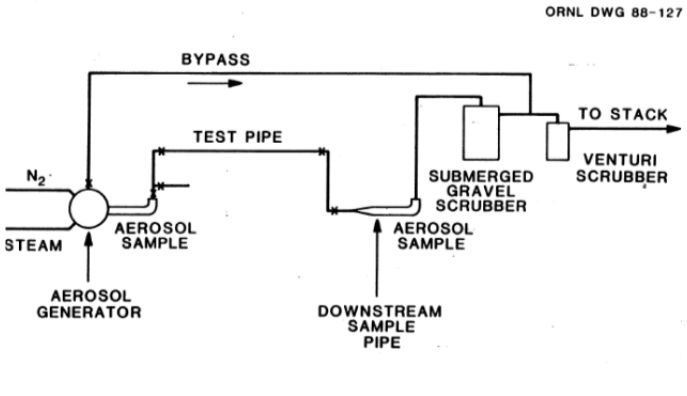
Table 3-4. DIANA Aerosol Experiment [Kalilainen 2015]

	Description [Kalilainen 2015a] • It has two vertical isothermal aluminum walls and four adiabatic glass walls (~700mm cube) in a cube measuring 0.7x0.7x0.7 m – 0.343 m³. • There is a 50 mm interspace between insulator and hot/cold wall, insulator and bottom glass and two top glass plates. Also front and back walls consist of double glass with interspace 200 mm. Polyurethane plates were used as temperature insulators – black painted on polyurethane plates facing the cavity. • Water is used to warm and cool walls. • Heat difference between walls must remain below 50K • Fluid: air, $\Delta T = 57^\circ\text{C} - 18^\circ\text{C} = 39^\circ\text{C}$, Rayleigh number ~ 109 turbulent flow. • Measurement: flow field and gas temperature. • Particle deposition rates using monodisperse SiO₂ particles with diameters 1 μm and 2.5 μm
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3.1.3.3 LACE-LA3 Experiment

In addition to LACE LA-4 as shown in Table 3-2, the LACE project includes the LA-3 experiment [Wright 1988], which is intended to determine the retention and behavior of aerosols flowing in a pipe. Turbulent deposition can be measured. The summary of the LA-3 series experiment and test description is given in Table 3-5. This experiment may be applicable for DOE facilities, where piping connected to the environment is important for the potential release during an energetic accident.

Table 3-5. LACE LA-3 Experiment and Description

Apparatus	Description
 ORN L DWG 88-127	The LA-3 series apparatus includes an aerosol generation section, a test pipe section, and an aerosol sampling section: • MnO and CsOH are used as aerosols which are injected into the test pipe with different fluid velocities and mass ratio of MnO/CsOH – LA3A (77 m/s, 5.0), LA3B (25 m/s, 7.5), and LA3C (24 m/s, 1.4). Carrier gases, such as He, Ar, N₂ and steam were used. • The test pipe was a 29-m long of 63-mm ID carbon steel pipe containing 6 90-degree bends. • The total deposited mass of CsOH and MnO are reported in pipe sections as well as those transported out of the pipe sections for all three tests.

3.2 DOE-HDBK-3010 Experiments

This section provides the validation studies for MELCOR 2.1 using the experiments listed in the Handbook. We identify that the powder release experiments conducted in the Radioactive Aerosol Release Tank (RART) facility at Pacific Northwest Laboratories (PNL) are appropriate to test the aerosol physics models in MELCOR. In these experiments, both free fall (gravitational) spill [Sutter 1981] and pressurized [Sutter 1983] releases were conducted inside RART. In the spill case, a beaker is turned over to simulate the free fall spill. The use of a rupture disk to release the powder in a chamber under various pressures is used for the pressurized release case. In addition, we will include a gasoline pool fire experiment conducted at PNL as well at the RART facility [Sutter 1973]. Our main objective in this section is to validate MELCOR using the Handbook experiments. However, we also use MELCOR to substantiate the experimental results described in this section, since MELCOR contains a detailed aerosol physics model as described in the previous chapter. These simulations can be also applied to the NSRD-11 project [Louie 2016] to substantiate data in DOE-HDBK-3010 [DOE 1994].

In this section, we will first describe the free fall spill experiment [Sutter 1981], MELCOR simulations, and discussion of the results and comparison to the experimental data. Then we will describe the pressurized release experiments [Sutter 1983], MELCOR simulations, and discussion of the results and comparison to the experimental data. In the last experiment, we will evaluate the aerosol release during a fire and during resuspension conditions in the gasoline pool fire experiment in a wind tunnel [Sutter 1973]. Because MELCOR currently does not contain any entrainment model to predict the release of contaminant during a fire (alternatively, control functions can be used to simulate this entrainment), we rely on the previous computational fluid dynamic (CFD) work done for this experiment in Year 1 of this NSR&D project [Louie 2015]. The selected input decks described in this section will be listed in Appendix B of this report. Note that all MELCOR calculations are done using Revision 8018 of MELCOR 2.1 code.

3.2.1 Free Fall Spill Experiment

As previously described, the free fall spill experiment was conducted in RART facility at PNL in early 1980s [Sutter 1981]. Figure 3-3 shows the free fall spill experiment apparatus in a RART enclosure. As shown in this figure, this enclosure is made of stainless steel, approximately 3 m high and 2.9 m in diameter, with a volume of $\sim 20 \text{ m}^3$. In this experiment, a 1-liter beaker containing the aerosol material is positioned near the center ceiling of the enclosure. The spill heights of approximately 3 m and 1 m were deployed. Also shown in this figure are the sampling equipment specification and locations. The four high-volume samplers and one cascade impactor, each equipped with appropriate glass fiber filters. The filter has a dimension of 8" (20.32 cm) by 10" (25.4 cm) with 99.9% efficiency for $0.3 \mu\text{m}$ particles. In this experiment setup, both liquid (uranyl nitrate hexahydrate) and solid powders (i.e., TiO_2 and depleted uranium oxide) were used as the test materials.

In this section, we are only examining the use of TiO_2 powders. Table 3-6 shows the additional experimental data for the sampling and the characteristic of the TiO_2 powders used in the experiment. As shown in this table, the mass mean diameter (MMD) of $1.7 \mu\text{m}$ and the GSD of 2 for TiO_2 powder were identified in the experiment [Sutter 1981]. In addition, the spill experiment report [Sutter 1981] provided the source material distribution for this powder (see Table 3-7).

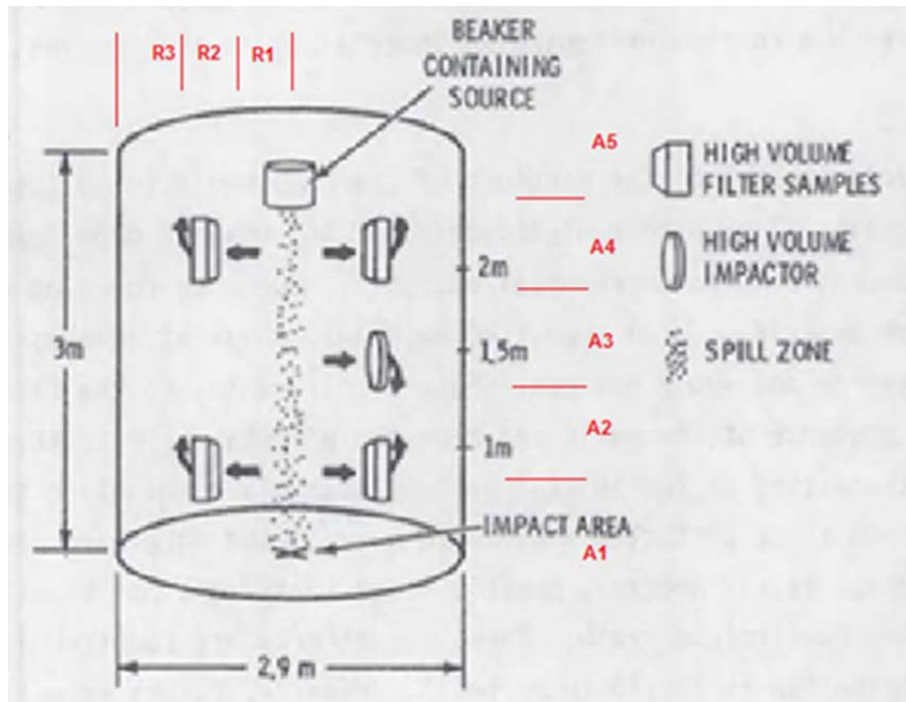


Figure 3-3. Free Fall Spill Experiment Apparatus [Sutter 1981].
(Red is the ring (R#) and Axial height (A#) for the MELCOR model in Table 3-8).

Table 3-6. Additional Experimental Data [Sutter 1981]

Parameter	Experiment
High volume filters	4
Dimension	20.32 cm × 25.4 cm
Sampling rate	1.4 m ³ /min
Impactor	1
Sampling rate	0.56 m ³ /min
Aerosol	
Density	4260 (kg/m ³)
Mass mean diameter (MMD)	1.7 (μm)
Geometric standard deviation (GSD)	2

Table 3-7. Source Powder Particle Size Distribution for TiO₂

Size (μm)	Measured Cumulative Mass Percent
20	98
10	97
8	96
6	94
4	88
2	60
1	16
0.8	11

3.2.1.1 MELCOR Simulations

In modeling the free fall spill experiment, we have used three MELCOR nodalizations to represent the RART volume: 1-volume, 5-volume and 15-volume (see Table 3-8 for the dimensions for the volume(s) represented). Figure 3-4 shows the 15-volume MELCOR nodalization for this experiment. The 5-volume nodalization is to combine the radial volumes of the 15-volume model. Similarly, the 1-volume nodalization is to combine all 15 volumes of the 15-volume model. As shown in this figure, the yellow-shaded volume represents the beaker volume where the source powder is located. The blue-shaded volumes are the environmental volumes for the sampling collection, and the recirculation flow back into the RART volume. These environment volumes are modeled as time-independent, with the height the same as the connected volume(s) of the RART volume(s). The specific flow rates for the sampling used are shown in Table 3-6. As shown in Figure 3-3, the samplings are located near the outer wall of the RART volume. For the 1-volume model (denoted as 1V), all three sampling locations are within the single control volume that models the RART. For the 5-volume model (denoted as 5V), only the middle three volumes are connected to the sampling according to the elevations as shown in

Figure 3-3. For the 15-volume model (denoted as 15V), the samplings are connected according to Figure 3-4. In the next section, we describe the model assumptions for this experiment.

Table 3-8. MELCOR Nodalization Models Used

Nodalization	Radius (m), R# and Height (m), A#
1-Volume – 1 axial segment and 1 radial segment	R1 = 1.45 m A1 = 3 m
5-Volume – 5 axial segments and 1 radial segment	R1 = 1.45 m, A1=0.75 m, A2 ^A =0.5 m, A3 ^B =0.5 m, A4 ^C =0.5 m, A5=0.75 m
15-Volume – 5 axial segments and 3 radial segment	R1=0.5, R2=0.5, R3=0.45 A1=0.75 m, A2 ^A =0.5 m, A3 ^B =0.5 m, A4 ^C =0.5 m, A5=0.75 m

^A Filter 1 and 2 sampling locations within this height

^B Impactor sampling location within this height

^C Filter 4 and 5 sampling location within this height

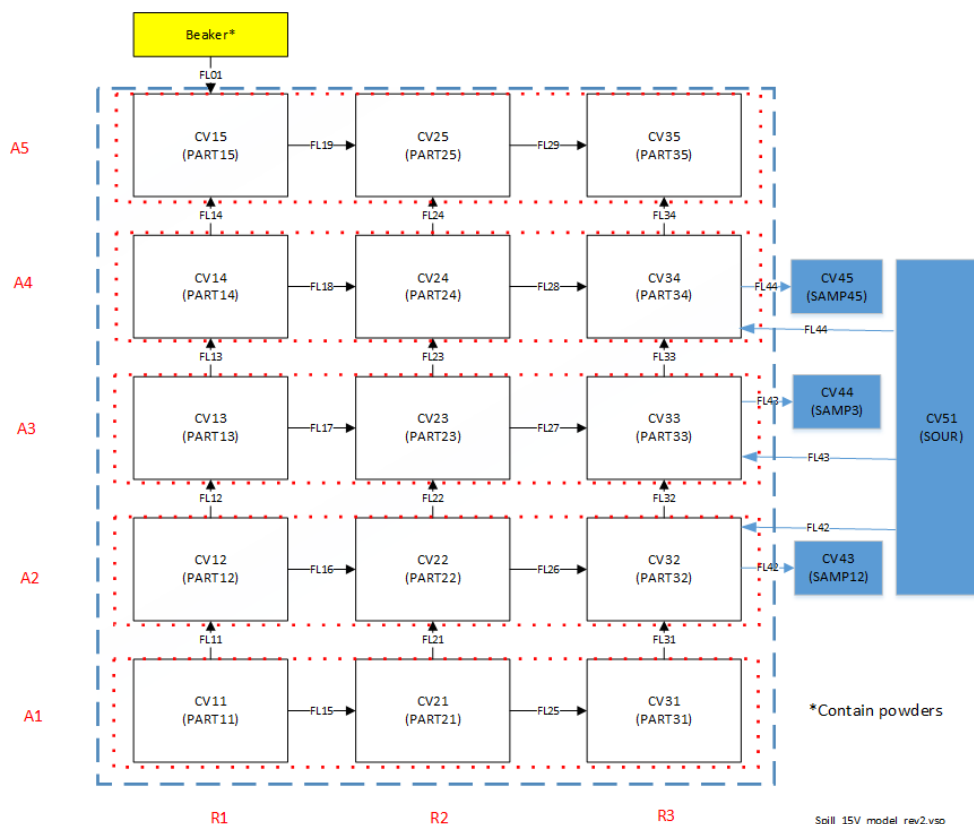


Figure 3-4. MELCOR 15-Volume Nodalization Diagram for Gravitational Spill.
(with Model Representation for the 1V in blue dash and 5V in Red dash Models and R# and A#, see Table 3-8)

3.2.1.2 Model Assumptions

This section describes the model assumptions for this spill experiment. For the aerosol source material for the beaker volume, we sourced 1 g, 25 g, 100 g, 450 g or 1000 g of TiO₂ into the

beaker using a tabular function with the assumption of the total source mass is in the atmosphere of the beaker within 0.05 seconds. Additional aerosol models are assumed:

1. Tuning the MELCOR model requires a step to ensure that the 15V model would not yield any artificial flow due to the gravity head, if all control volumes were initialized the same pressures. Figure 3-5 shows the flow oscillation if all volumes are set to the same pressure. As shown in this figure, a lack of pressure adjustment to the control volumes will introduce artificial flows (oscillation in about ± 0.03 kg/s) into the simulation which is not realistic. With the static head as shown in Figure 3-6, the flow oscillation magnitude for this model is significantly reduced to about $\pm 10^{-9}$ kg/s as shown in Figure 3-7. If one exercises the steady state simulations, the new model should only require two seconds or less to reach to a steady state according to Figure 3-7. Without establishing steady state, the maximum flow introduced is in the order of 10^{-9} kg/s, which is very small. Therefore, the MELCOR simulations described herein are conducted without conducting steady state calculations.
2. Source material is treated according to Table 3-9. As shown in this table, we chose to use a lognormal distribution with a mean diameter and a GSD approach as described in RN1_AS01 record, rather than a tabular form similar to that of Table 3-6. To establish this approach, a comparison between this approach and use of the sectional mass fraction approach was conducted for the 1V nodalization as shown in Section 3.2.1.3. In the parametric study, we chose to vary the value of mean diameter, rather than use the tabular values according to Table 3-7. Initially, we treat the mean diameter in Table 3-9 as AMMD. In the experiment report [Sutter 1981], the authors describe $1.7 \mu\text{m}$ of mean diameter as a GMMD and further discuss the relationship between AMMD and GMMD by the ratio of the square root of aerosol density with water density. We then understood the meaning of the mean diameter of the source materials in the experiment report. More discussions on the different diameter usage are in Chapter 4 of this report.
3. Thermal dynamic effect: In MELCOR, aerosol does not interact with the hydrodynamic materials, except through condensation. All aerosols are assumed to be trace quantity. To model the spill scenario in MELCOR, a fluid flow must be introduced. To do that, CFD results (SNL's SIERRA 3-dimensional fluid mechanics code, Fuego) on the same experiment are simulated in a separate NSRD project [Louie 2016].
4. Interpretation of the aerosol results from MELCOR.
 - a. For the cases when the sampling flow rate is active, the total aerosol in the sampling volumes (CV43, CV44 and CV45) for the 15-volume model is assumed.
 - b. For the cases when the sampling flow is inactive (no sample), the total aerosol in the RART volume is assumed to be the aerosol result. Note that we

introduced a slightly higher pressure for PARE volume 1.0101E5 Pa, instead of 1.01E5 Pa for the RART volume(s).

Table 3-9. Aerosol Source Assumptions for the Free Fall Spill Experiment

Model	Value	Comments
Aerosol source	TiO ₂ Mass: 1, 25, 100, 450 and 1000 g	We sourced the aerosol as an aerosol source, using CE class in RN1_AS record and using RN1_AS01 record.
Density (kg/m ³)	4260.0	
Diameter range (μm)	0.8 to 50.0	We used default 10 sections, but the minimum diameter was chosen to be 0.8 μm instead of 0.1 μm to agree with the smallest reported value in Table 3-7.
Aerosol Distribution	Log normal	
Mean diameter (m)	3.51E-06	This diameter is calculated as the aerodynamic mass mean diameter (AMMD) as described in Equation (4-11), where the geometric mass mean diameter (GMMD) as 1.7 μm
GSD	2.0	

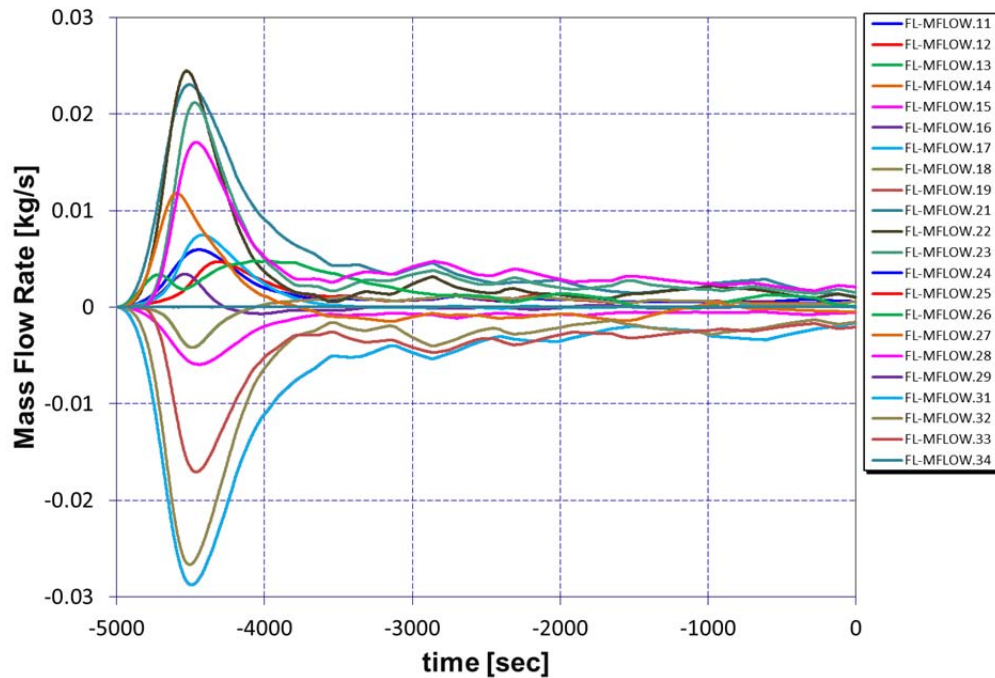


Figure 3-5. Flow Oscillations for Control Volumes with Same Pressures for the 15V Model.

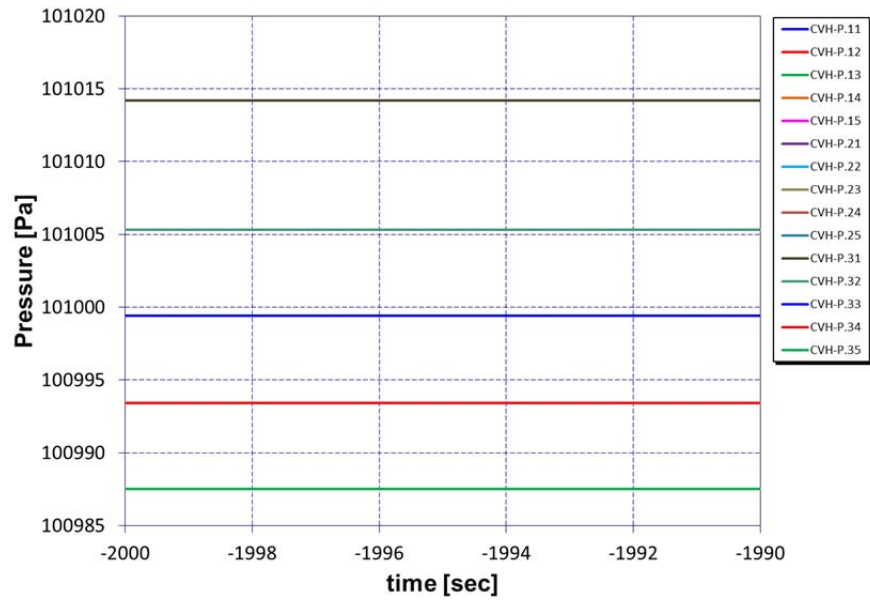


Figure 3-6. Pressure Adjustment for the 15V Model.

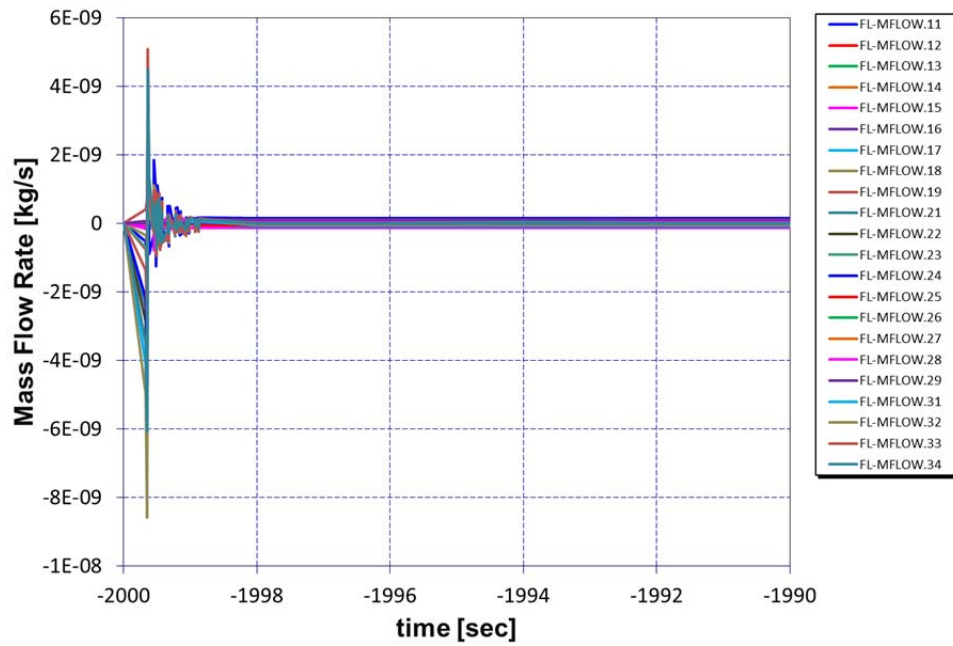


Figure 3-7. Flow Oscillations After Pressure Adjustment for the 15V Model.

Table 3-10. Sectional Mass Fraction Assumption*

Section No.	Mass Fraction
1	0.11
2	0.05
3	0.44
4	0.28
5	0.06
6	0.02
7	0.01
8	0.01
9	0.01
10	0.01

*based on Table 3-7, and assuming the values for sections 9 and 10.

3.2.1.3 Discussions of MELCOR Results

In the simulations of this experiment, we conducted a parametric study for the three MELCOR nodalization models, and designated the base case as aerosol data shown in Table 3-9. We ran the simulations out to 30 minutes of the experiment. As discussed in the previous section on the calculational assumption, we chose the use of the lognormal distribution with a mean diameter and GSD approach for the study (see Figure 3-8), rather than the sectional mass fraction method (see Table 3-10). As shown in Figure 3-8, the comparison of the results of the two approaches is very similar. Thus it is justifiable to use the former approach for the analysis. Figure 3-9 shows the average weight percent airborne versus the source size. As shown in this figure, we add a 1 g simulation to iterate the concept of 1 g used in the past (see Chapter 2 for more details). As shown in this figure, there are several cases that we have performed, including the use of 1V, 5V and 15V nodalization models. In addition, we conducted cases with no sampling flow (Assumption 4b in Section 3.2.1.3). Figure 3-10 shows the base case for the 1V model. Figure 3-11 compares the base case and no sample flow case for the 5V model. Because the aerosols in MELCOR do not influence the hydrodynamic materials (i.e., air), the introduction of the aerosol simply drops to the floor via the gravitational force. The introduction of the sampling flow (Assumption 4a in Section 3.2.1.3) into the RART volume may influence the aerosol behavior as shown in Figure 3-11.

For the 15V model, we utilized the CFD results from the Fuego code simulation of 50 psig (0.34 MPa) case described in the NSRD-11 project [Louie 2016]. Figure 3-12 shows the sampling pulling flow reaching near the center of the RART volume at 50 s. Figure 3-13 shows the Fuego calculated fluid velocity component in x, y and z coordinate as U, V and W velocities, respectively. To include these velocities in our 15V model, we took the first 50 seconds of the W velocities to remove any influence of the sampling flow in the simulation. In addition, as shown in Figure 3-4, the positive direction of FL01 is pointed downward. To use the W velocity results from Fuego, we needed to change the sign of the results, because the flow path direction is opposite to that of the Fuego simulation. As described in [Louie 2016], the Fuego simulation

only applies to 10^8 particles, which is a small fraction of the actual 100 g (in order of 10^{13} particles) of TiO_2 . To count for the all initial aerosol mass used in the experiment, we multiplied the W velocity from Fuego by 100 since the Fuego calculation only simulated a small fraction of the actual mass. Figure 3-14 shows the comparison of the base case and the addition of Fuego W velocity flow case for the 15V model.

In terms of the comparing to the experimental data as shown in Figure 3-9, without addition of fluid velocity introduction to the RART, no base case can obtain results closer to the data, since aerosol in MELCOR does not affect any fluid dynamic. The use of 1V and 5V may overestimate the dispersal effect of the spill powder to the cross section of RART area. With a larger particle size, the results seem to be closer to the data. Note that the data indicates that there is no effect of the mass being introduced into the RART volume at 3 m. As shown in this figure, using a 1-g estimate to perform spill simulation may yield results significantly different (several MELCOR data points lay outside of the displayed y axis range). The use of the Fuego fluid velocities may enhance the results closer to the experiment data as shown in this figure. The weighing factor in a Fuego case is to account for the difference in mass simulated, since a higher mass should influence stronger than the small mass, such as 1 g. So the weighing factors used for Case F with weighing factor in Figure 3-9 are 0.01 for 1 g, 0.25 for 25 g, 1 for 100 g, 4.5 for 450 g and 10 for 1000 g cases. A confirmation run was conducted to turn off the gravitational settling for the larger mass cases in Case F. The results indicate that the ARF% has increased from 0.0009 to 0.00249 and 0.0004 to 0.0117 for 450g and 1000g, respectively. In comparison to the results from the 1 g case for Case F, it shows 0.0498 for Case F. This demonstrates that it is not necessary to model releases assuming 1 g aerosol and linearly extrapolate to the actual mass. As indicated in Chapter 2 and Chapter 4, the agglomeration behavior is not linear.

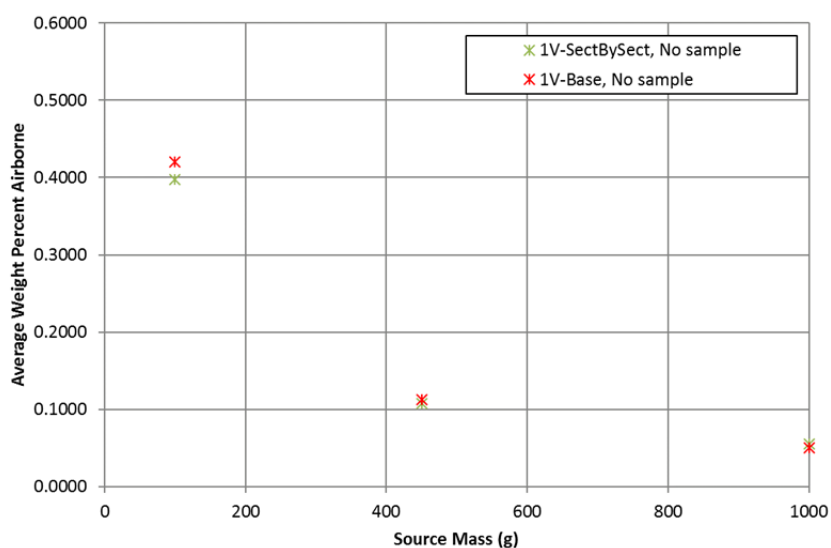


Figure 3-8. Comparison of Aerosol Source Method Used for 1V Nodalization Model in MELCOR.
SectBySect – using Table 3-10 and Base – using Table 3-9.

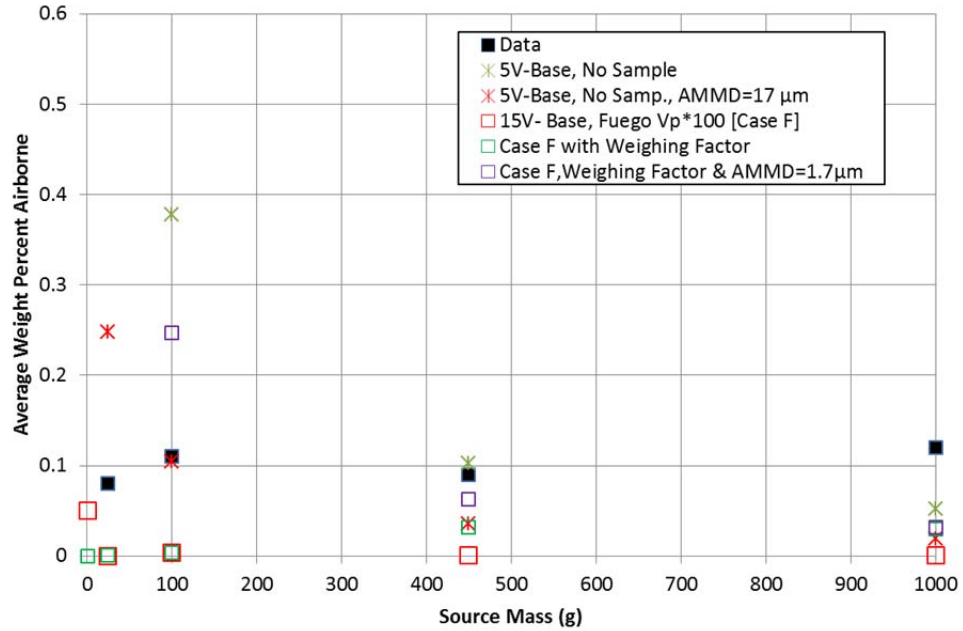


Figure 3-9. MELCOR Results for Free Fall Spill of TiO_2 at 3 m.

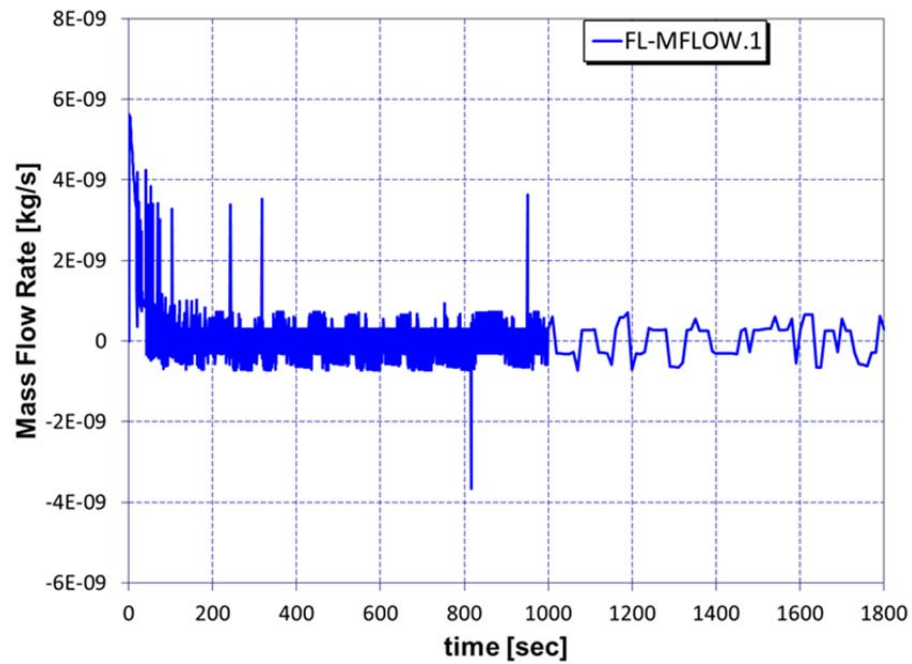


Figure 3-10. 1V Model Base Case – Beaker to RART Mass Flow.

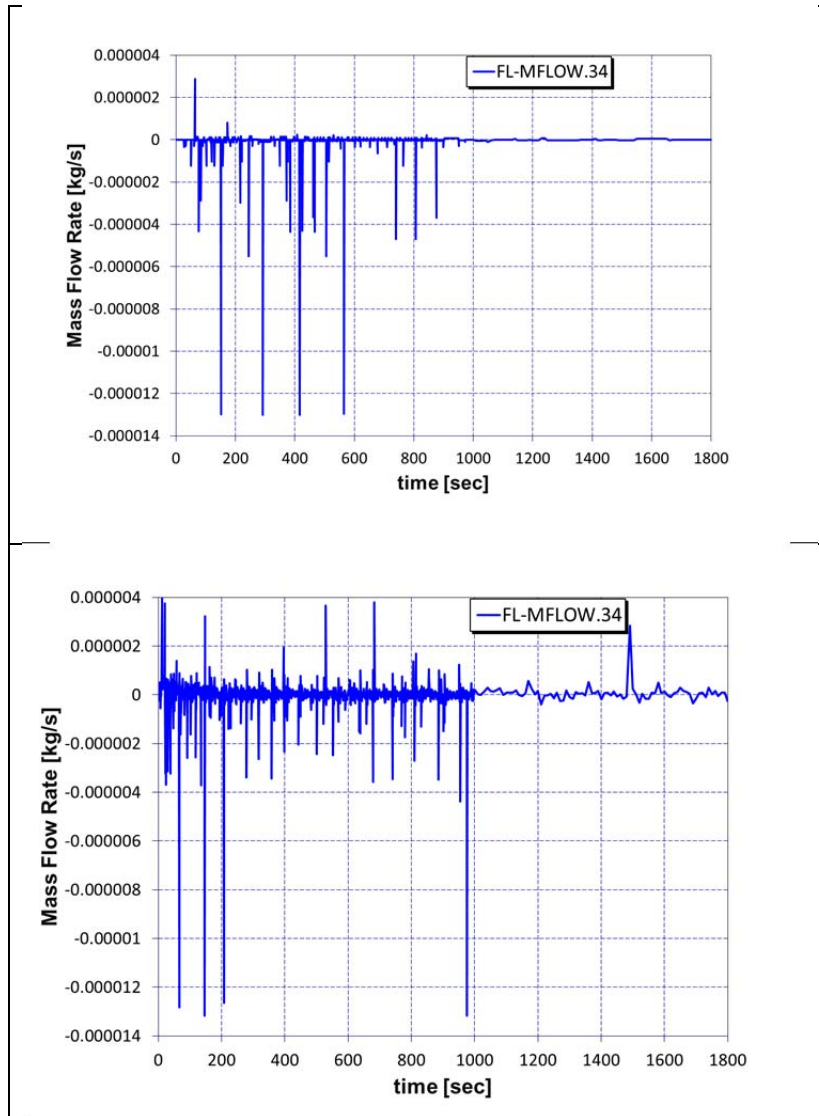


Figure 3-11. 5V Model RART Mass Flow Between Two Upper Volumes
No sample flow Case (top), Base Case (bottom).

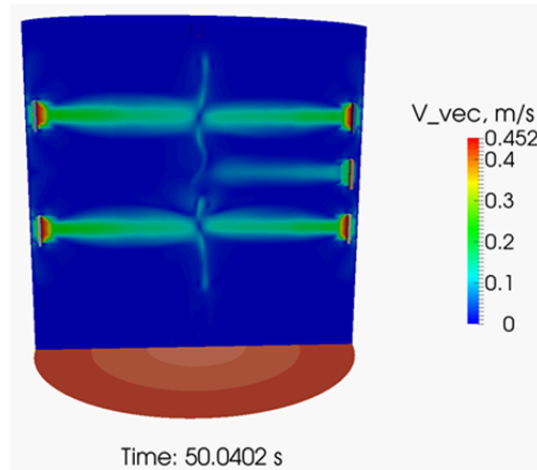


Figure 3-12. Sampling Flows Predicted by Fuego for the Gravitational Spill Experiment [Louie 2016].

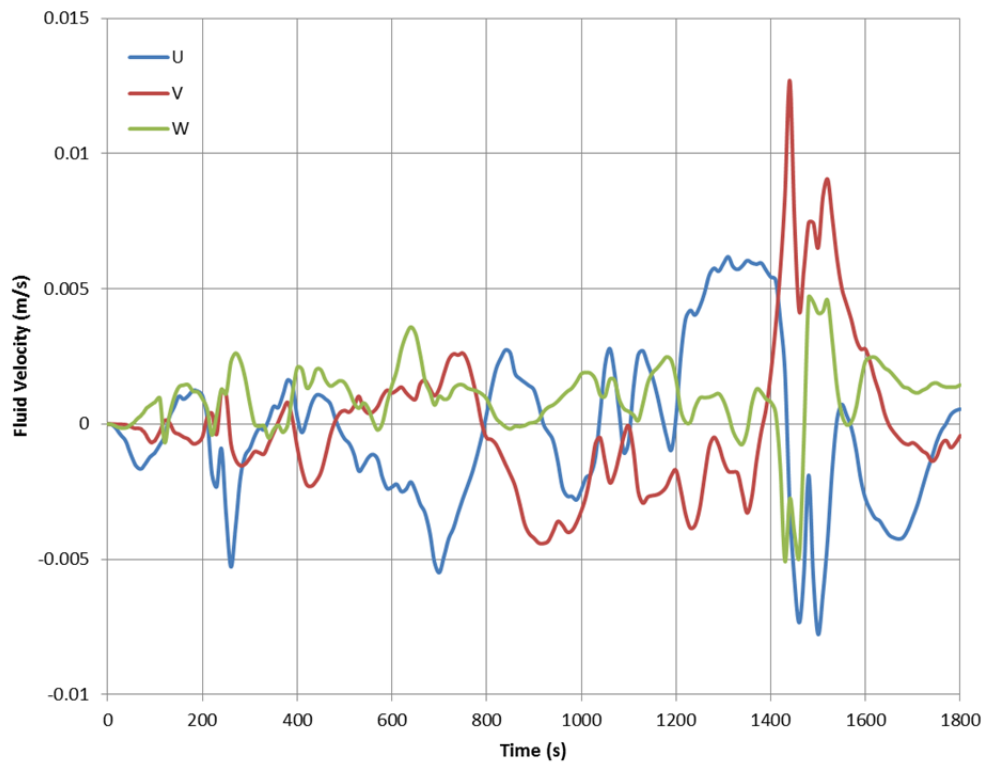


Figure 3-13. Fuego Fluid Velocities in 3-Dimensional (U in x, V in y and W in Z coordinates at the RART Point (Center, 2.6 m from floor) for Gravitational Spill Experiment [Louie 2016].

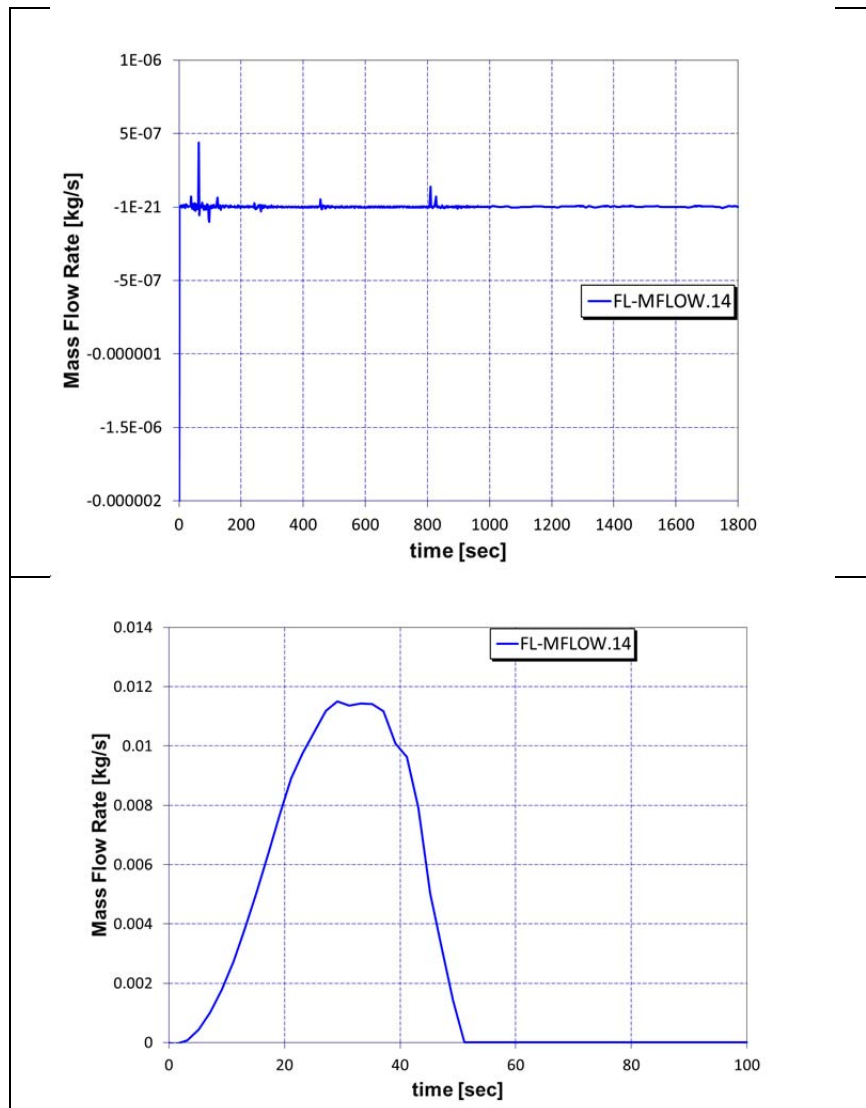


Figure 3-14. 15V RART Mass Flow Between Two Inner Upper Volumes: Base Case (top), Fuego Flow (bottom).

In addition to the airborne release estimate, additional results can be compared. For example, MELCOR tends to deposit more in the inner ring, and progress lower outward. It is similar to the experiment report which shows the inner ring (R1) or center of the RART floor has a larger deposit than the outer rings. However, Fuego predicts slightly different behavior, showing that the middle ring (R2) has the largest particle deposition which is not shown here (see NSRD-11 report [Louie 2016]). This could be due to several factors. One is that Fuego does not currently model agglomeration, which may underestimate settling because the larger particles settle faster than the smaller particles. On the other hand, the sampling flow modeled in Fuego actually pulls flows and particles near the outermost ring rather than the middle ring (R2). Therefore, the middle ring (R2) floor results in largest deposition

3.2.2 Pressurized Release Experiment

Unlike in the use of a beaker in the free fall spill experiment described in the previous section, an experimental chamber called the Pressurized Airborne Release Equipment (PARE) was designed to hold the aerosol materials using a rupture disk to simulate the pressurized release. PARE has a volume of 812 cm³ for the aerosols, and an additional 50 cm³ for the dome shaped rupture disk region (see Figure 3-15 for the PARE schematics). The overall pressurized release experiment with PARE and PART is shown in Figure 3-16. In this section, we first describe the MELCOR models used, then the model assumptions and the discussions of the MELCOR results.

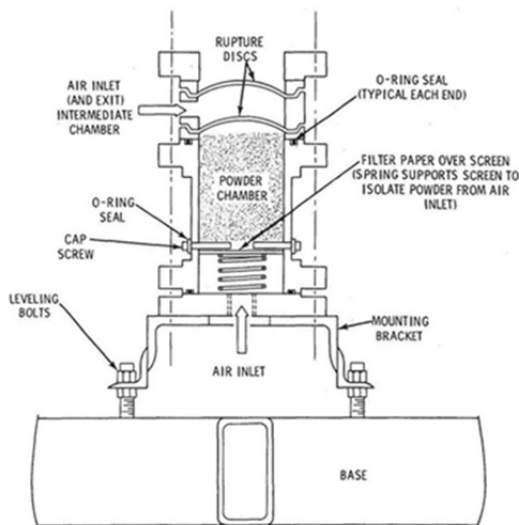


Figure 3-15. PARE Schematics for the Pressurized Release Experiments [Sutter 1983].

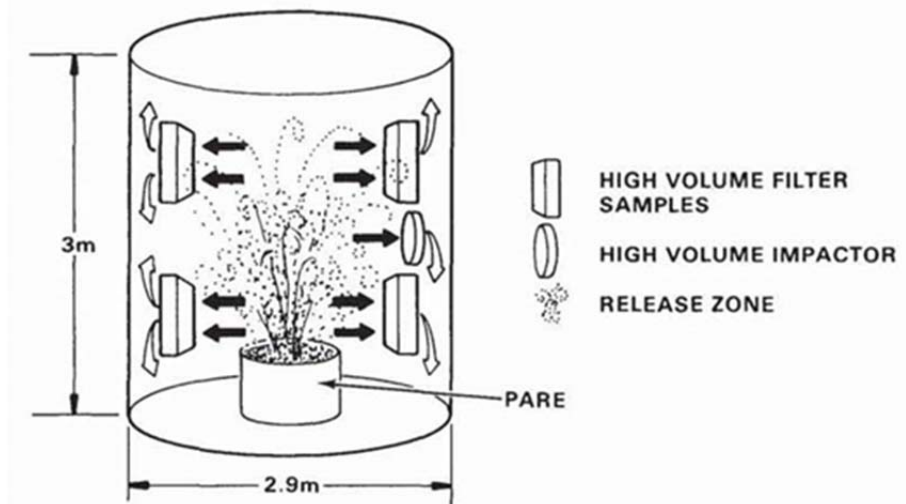


Figure 3-16. Experiment Apparatus for the Pressurized Release Experiments [Sutter 1983].

3.2.2.1 MELCOR Simulations

Similar to the spill case as described in the previous section, a 15-volume MELCOR nodalization model was developed. Similarly, 1-volume and 5-volume MELCOR models were also

developed for the pressurized release test (see Table 3-8). The only difference between the models from the spill case is the placement of the PARE and its connection to the RART volumes – at the floor versus at the ceiling in the spill case.

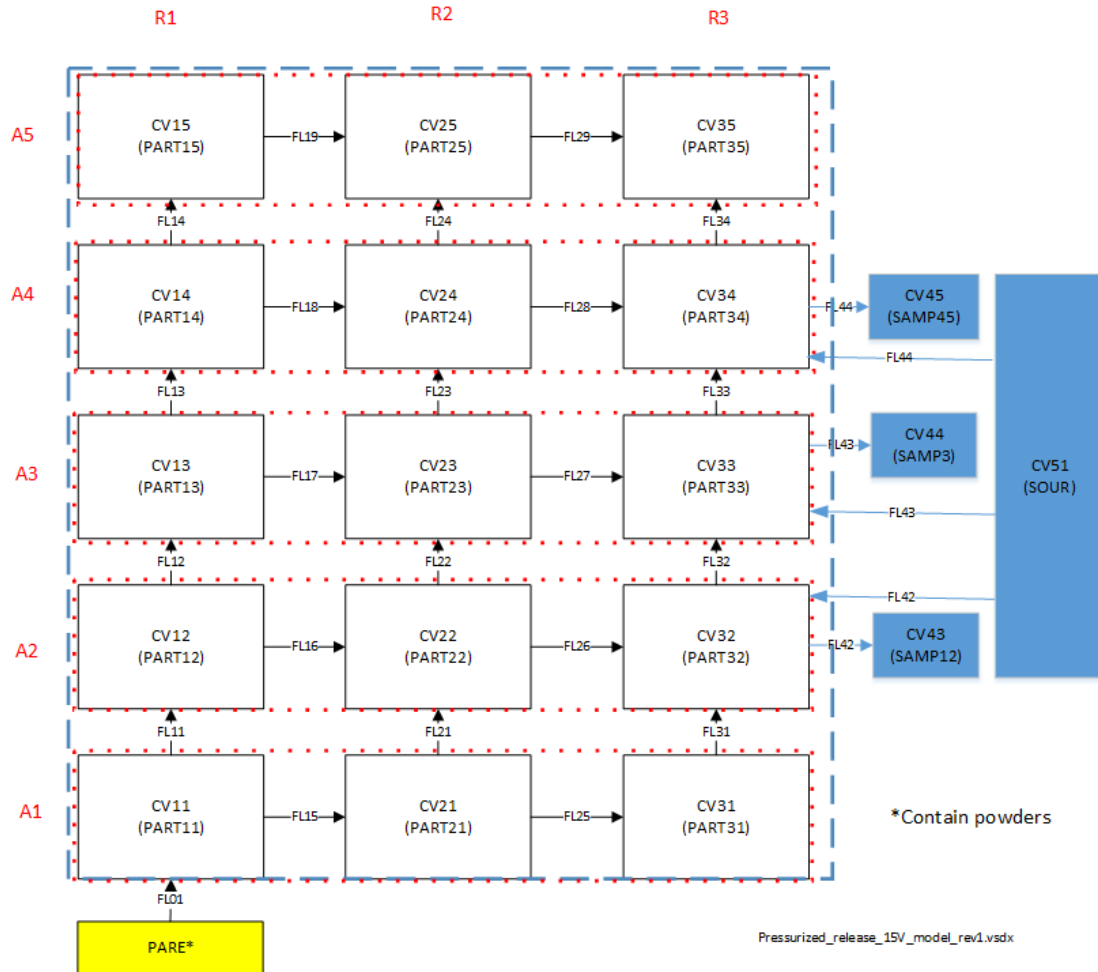


Figure 3-17. MELCOR 15-Volume Nodalization Model for Pressurized Releases.
(with Model Representation for the 1V in blue dash and 5V in Red dash Models and R# and A#, see Table 3-8)

3.2.2.2 Model Assumptions

For this experiment, we utilized the similar model assumptions described in the spill case – Table 3-6, Table 3-8, and Table 3-9 for the aerosol sources, the diameters and sampling rates, and nodalization models. In addition, we modeled the PARE initial condition of the specific pressure and a 1 g, 100 g and 350 g of TiO₂. To simulate the rupture disk opening between the PARE and RART volumes, we assumed the opening of a rupture disk of < 0.001 s. This is similar to that was used by the Fuego code [Louie 2016]. As shown in Table 3-11, the corresponding temperatures are calculated based on the ideal gas law. This is necessary; otherwise, the expansion of gases into a lower pressure volume, RART may cause the calculated atmosphere temperature below freezing. The provided temperatures in the table would prevent this. Similar

to the spill case, the interpretation of the MELCOR results for no sampling flow is the use of the RART volume(s) data for atmosphere aerosol masses. For the sampling flow cases, the total aerosol mass in the sampling volumes are taken to be compared with the experimental data.

Table 3-11. Simulated PARE's Pressure with Temperature Cases

Pressure Psig (MPa)	Temperature (K)
50 (0.345)	980
250 (1.72)	4900
500 (3.45)	9800

3.2.2.3 Discussions of MELCOR Results

In the MELCOR calculations, we utilized all three MELCOR nodalization models as previously described in the spill case (1V, 5V and 15V). The base case is assumed the AMMD of 3.51 μm with GSD of 2.0. Figure 3-18 shows the MELCOR results for the pressurized release of TiO_2 powder experiment for several PARE pressures – 50 psig (0.34 MPa), 250 psig (1.72 MPa) and 500 psig (3.4 MPa). As shown in this figure, only the 1V and 15V results are listed for MELCOR, since 5V results only yielded faster settling because the volumes are smaller compared to the 1V model. In MELCOR, aerosol physics is based on the concentration of the aerosol in a volume. In addition, the stacking volume arrangement in the 5V case will result in substantiate settling because the pressure remains high in the bottommost volume, because the arrangement does not allow recirculation. The 15V model is better suited for the experiment if the model is tuned correctly to minimize the artificial flow due to pressure gradient. Since we are unaware of the existence of information about the aerosol released out of PARE, using the aerosol size in Table 3-6 may not be adequate since this table describes the initial particle size measurement. It does not truly describe when the powder is pressurized in PARE. The powder in the pressurized condition may press together to form an aggregate (in a larger particle). Increasing the AMMD size to 17 and 24 μm compared well with data. Note that the sampling rate prescribed in the experiments may introduce more mixing than in the static air situation. Thus without sampling, the airborne release results from MELCOR requires smaller AMMD values, because without flow, only gravity is acted on the powder and eventually all particles will settle. In MELCOR, aerosol does not interact with air if the flow is nearly still. Therefore, gravitational settling is the only mechanism existing to allow aerosol to settle. To remain airborne, the smaller particle may take longer to settle. In addition, the experimental data indicate that the effect of agglomeration is not linear as shown in this figure. So using 1 g suspended material for all LPF calculations and extrapolated back to the initial suspended material may not be realistic. Figure 3-19 shows the turbulent deposition predicted in MELCOR. The values are much smaller as expected. Thus, the use of the results from CFD codes may be required to rescale the ARF results. Although the capability of the CFD code for higher pressure cases, such as 250 psig (1.72 MPa) are shown in the NSRD-11 project [Louie 2016], additional CFD simulations are required to estimate the turbulent deposition onto the ceiling of RART.

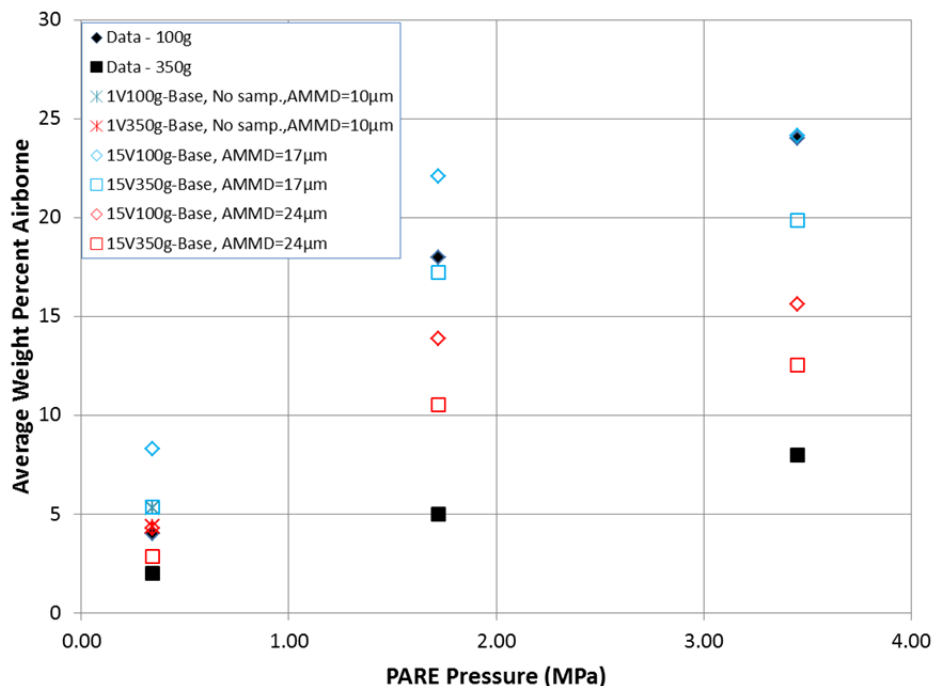


Figure 3-18. MELCOR Results for Pressurized Powder Release of TiO_2 in RART.

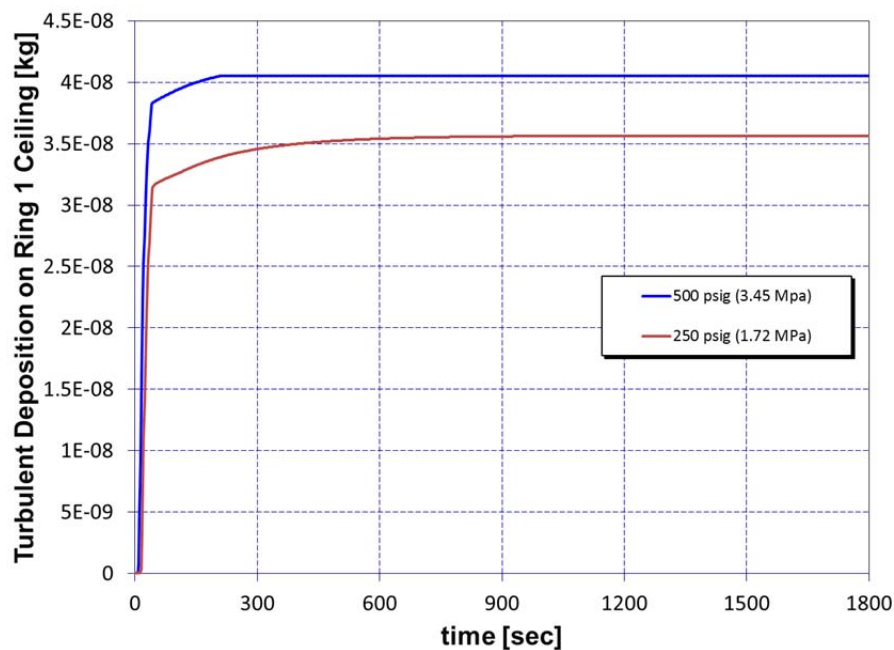


Figure 3-19. Turbulent Deposition Results for Higher Pressure Cases.

3.2.3 Gasoline Pool Fire Experiment

This section describes a MELCOR 2.1 simulation of a gasoline pool fire experiment conducted in a wind tunnel attached to the Radioactive Aerosol Release Tank (RART) located in Richland, Washington as documented in the experimental report, BNWL-1732 [Mishima 1973]. Figure

3-20 shows the schematic of the wind tunnel experiment. The experiments conducted in this facility were intended to study the radioactive release from serious transportation accidents such as a gasoline fire resulting in a container breach. In these experiments, UO_2 is used instead, but it could be used to simulate a plutonium release. To simulate the effect of winds, the experiments were done inside the wind tunnel. As shown in this figure, the wind is drawn into the wind tunnel from the left and flown over the burner tray where the fire and contaminant are located. The tunnel segment is long, but no specification is given before entering the building at the right. In the last duct section, filter samplings are collected at the two 4-inch openings. At the same section, an 8-stage impactor was located under the duct through 0.5-inch stainless steel tube inserted at the bottom of the duct to measure the size of the particle collected. A nominal sampling rate of one cubic foot per minute on all sample equipment is used. A large number of tests were conducted in this configuration. We chose the SA-17 test, because the experimental data are well documented, and it is on a stainless steel tray, instead of other surfaces (such as soil and paved road) that may not be easily modeled.

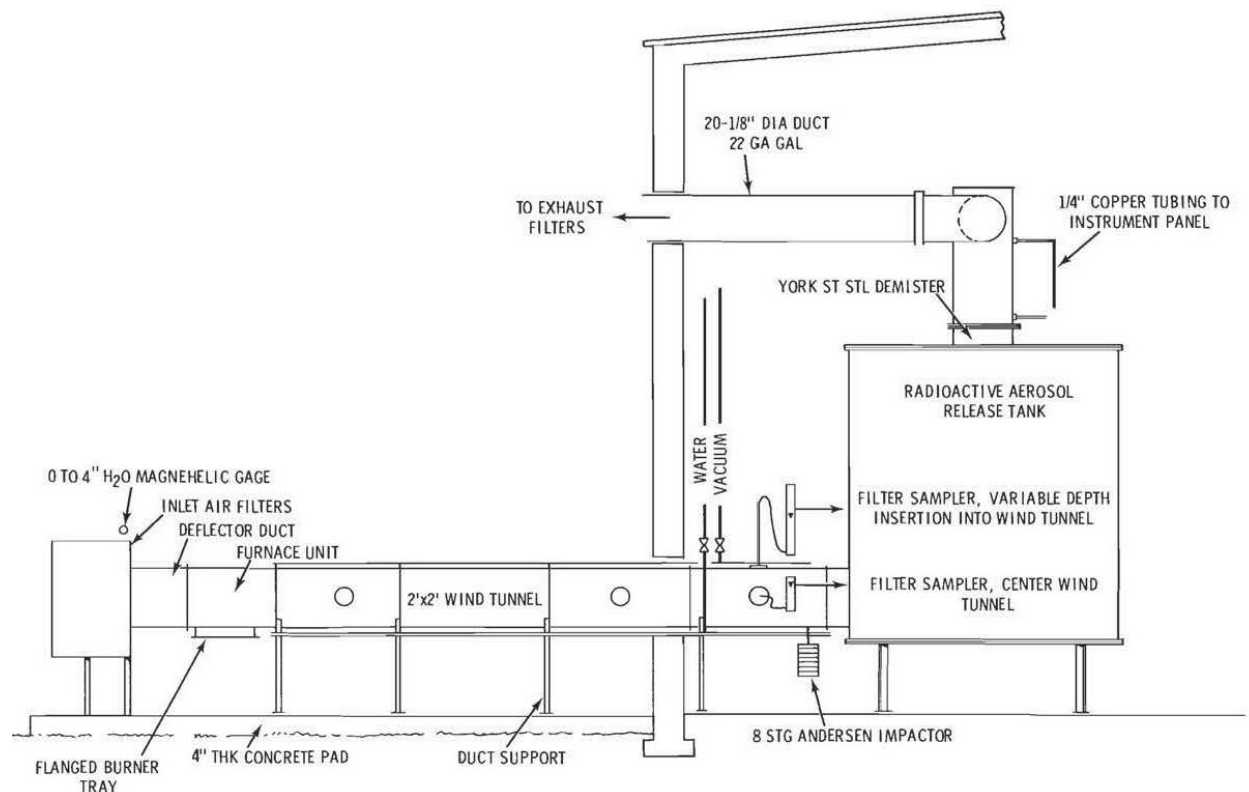


Figure 3-20. Gasoline Pool Fire Tests in Wind Tunnel at RART Facility [Mishima 1973].

3.2.3.1 Experimental Data

The test to be used in the validation is SA-17 [Mishima 1973]. There are two parts to this test. In part “a” the measurement is for the fire. In part “b” the test was conducted after the fire and lasted about 4.8 hours. Thus part “b” is considered as the resuspension phase of the experiment. In both parts, the steady wind speed is supplied. The specifications for this test are given in Table 3-12. The initial UO_2 mass of 19.5 g with the initial particle distribution is shown in Figure 3-21. The maximum wind velocity of 1.79 m/s (4 mph) is indicated in the table. In this

test, the UO_2 powder is sprinkled onto the pan (tray) before a gallon of gasoline is poured onto the surface via a 0.5-inch stainless steel tube with a 90° bend entering the top of the furnace section. In the test, there is no thermocouple data or thermal data provided. The aerosol specific data is given in the following section.

Table 3-12. Experiment SA-17 Test Specifications [Mishima 1973]

Parameter	Values
Stainless steel tray that contains gasoline and UO_2 powder (see Figure 3-21 for the initial size)	
Diameter, meter (inches)	0.3810 (15)
Deep, meter (inches)	0.0508 (2)
Calculated area, m^2	0.114
Wind tunnel dimension, assumed stainless steel	
Height, meter (inches)	0.6096 (24)
Width, meter (inches)	0.6096 (24)
Assumed length, meter (inches)	2.4384 (96)
Assumed tunnel thickness, meter (inches)	0.00508 (0.2)
Combustible	
Gasoline, cubic meters (gallon)	3.7854E-3 (1)
Calculated mass*, kg	3.293
Burn time, minutes	9
Temperature, C	1000
Uranium dioxide is sprinkled to the pan before pouring the gasoline (see Figure 3-21 for the initial size distribution)	
Initial mass used**, grams	19.5
Wind from the tunnel	
Speed**, m/s (mph)	<1.79 (4)
Initial ambient conditions	
Relative humidity in %	37
Pressure, Pa (inches)	101600 (30)
Temperature, K ($^\circ\text{F}$)	289.26 (61)

*Gasoline density of 3.49 kg/m^3 was used

**Throughout the report, discrepancy was identified. We believe that this mass value used is correct.

***Based on the value listed for this test in Table III of the experimental report.

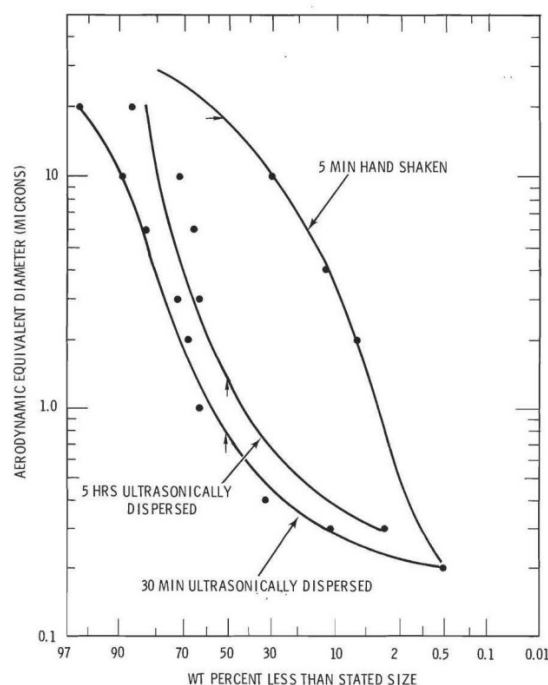


Figure 3-21. Ball-Milled Size Distribution of UO_2 Used in Experiments [Mishima 1973].

3.2.3.2 Aerosol Data

The sampling in the experiment is measured at the wind tunnel downstream at the entrance of the RART facility as shown in Figure 3-20. The locations of the sampling in the wind tunnel cross sectional duct, which consists of a movable filter, fixed filter and an impactor probe is shown in Figure 3-22. As shown in this figure, the movable filter is connected to a 3" flanged opening located near the top of the duct. The mixed filter is also connected to a 3" flanged opening located at the center of the duct, and the impactor probe is connected to a 0.5' opening through a tube.

Table 3-13 shows the results of the SA-17 test. Note that the SA-17a data in this table are for the airborne release fraction that is measured during the fire. Thus the UO_2 release is considered to be entrained during the fire. As concluded in our Year 1 final report [Louie 2015], the dominant mechanism for the particle entrainment is due to boiling of the gasoline. In this report the boiling entrained much of the contaminants early in the fire. For the baseline case, boiling accounts for about 6% of the total aerosol according to Table 4-18 in the Year 1 final report [Louie 2015]. Note that the evaporation induced entrainment mechanism has a very small contribution to the airborne release determination.

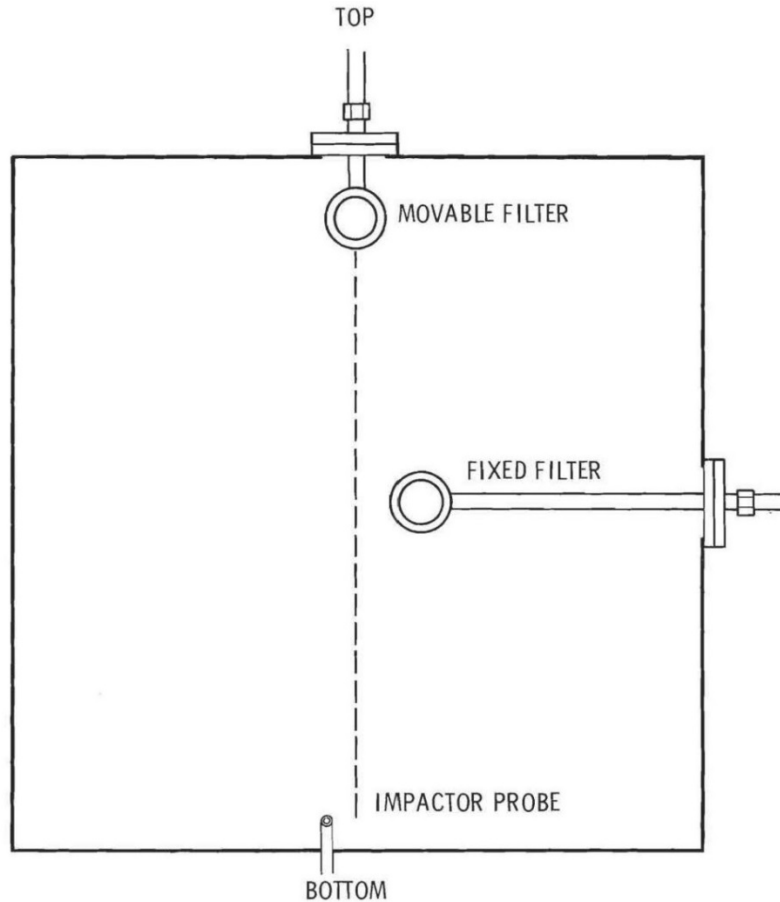


Figure 3-22. Wind Tunnel Sampling System [Mishima 1973].

Table 3-13. Measured Aerosol Results for SA-17 Test [Mishima 1973]

Parameter		Value
SA-17a	Weight % of source airborne	0.12
	Weight % < 10 μm	66
	Time collected, hours	0.12
SA-17b	Weight % of source airborne	0.09
	Weight % < 10 μm	83
	Time collected, hours	4.8

Results from Fuego analyses are used to input to MELCOR in this section, since MELCOR does not have any fire entrainment model currently. MELCOR requires the user to supply the amount of UO_2 entrained during the fire, and during resuspension. Based on the CFD simulation results reported in the Year 1 final report [Louie 2015], it is assumed that only 6% of the 19.5 g of UO_2 is released during the fire, and the remainder of 94% will remain on the tray.

3.2.3.3 MELCOR Fire Model

In this section, we validate MELCOR for modeling fire scenarios, in terms of the aerosol physics since the experiment did not provide any thermal data to compare (see Appendix B.1 for the MELCOR input model). Only a single aerosol datum for each part of the experiment is described in Section 3.2.3.2. In this experiment, a gallon of gasoline burns until all fuel has been exhausted (about 9 minutes). Because gasoline is a combination of octane and butane, one can assume either one of the hydrocarbons. We chose octane, which has a chemical formula of C_8H_{18} . For a complete reaction (burn), the following reaction yields:



The reaction creates the combustion energy of 444.3×10^5 J/kg. One gallon of gasoline is equivalent to 3.78541×10^{-3} m³. Using a typical gasoline density of 870 kg/m³, then a gallon contains 3.29 kg of gasoline. According to Figure 3-11.2 of [NFPA 1995], a gasoline burn velocity is estimated to be ~ 4 mm/min. The gasoline mass flux is given by this velocity times the gasoline density which yields 0.058 kg/m²-s. Since the stainless steel pan has a diameter of 15 inches (38.1 cm), the gasoline mass consumption rate is 6.613×10^{-3} kg/s. It would take about 498 s to consume 1 gallon of gasoline (see Appendix C.1 for the calculation). In comparison to the experiment of 540 s for the duration of the fire, we assume a fire curve with a ramp and decay of 25 s (see Chapter 4 on the details of the fire modeling). Based on the combustion energy given above, then the combustion power is 293.8 kW. If we assume thermal radiation loss of 35% to the heat structures, then 190.97 kW will heat up the atmosphere through both H₂O and CO₂. The 35% of the remaining combustion power (102.83 kW) will be sourced to the heat structures.

Based on the molecular weight of octane, 114 kg/k-mole, the corresponding mass of oxygen consumed and the gas byproducts (water and carbon dioxide) can be calculated according the above reaction:

- Oxygen consumption rate of 0.023 kg/s
- Water vapor production rate of 0.009397 kg/s
- Carbon dioxide production rate of 0.02 kg/s

Note that Appendix C.1 describes the calculation sheet for the estimate of the gas flow and thermal radiation fraction and other information related to this MELCOR calculation.

In the aerosol simulation, which only considers the UO₂ contaminant, no incomplete smoke product from the gasoline fire is modeled. The addition of smoke may influence the aerosol physics (see Appendix A for a verification problem in modeling the smoke in a fire scenario). Using the aerosol distribution from the experiment, and the percentage entrained by the boiling mechanism of 6% (and 94% remaining in the tray), the following assumptions are made for the simulation.

- 6% of 19.5 g UO₂ will be sourced into the lower tunnel volume from 0 second to 9 minutes.

- 94% of 19.5 g UO₂ will be sourced into the tray or pan before the start of the resuspension phase.
- All initial particle distribution and particle size range by 10 bins (default) would be used:
 - An assumed mass distribution to the 10 bins is given in Table 3-14. This table is based on the appropriate fit to all data in Figure 3-21.
 - The minimum diameter is 0.1E-6 m and maximum diameter is 50.0E-6 m with an aerosol density of 10900 kg/m³.

Table 3-14. Assumed Mass Fraction in Bins

Bin #	Mass Fraction
1	0.008086
2	0.051213
3	0.09973
4	0.107817
5	0.161725
6	0.161725
7	0.107817
8	0.107817
9	0.086253
10	0.107817

Figure 3-23 shows the MELCOR nodalization model used for this experiment. As shown in this figure, the wind tunnel is divided into upper and lower parts with three horizontal segments. The first segment is 2 feet long (60.96 cm) and the second/third segments are 3 feet long (91.44 cm). The cross section of the wind tunnel is 2 feet (60.96 cm) by 2 feet (60.96 cm). To simulate the wind flow, we use a constant flow rate in Flow path 01 and 02 as shown in this figure. A total of four time-independent volumes are modeled. Three of them are shown in this figure – one (CV01) adds as a source representing the facility upstream of the fire’s location, and two (CV100 and CV101) act as sinks for wind passing out of the facility. Both CV100 and CV101 are the aerosol sample collection volumes. The fourth one (CV999) is used for the heat transfer purpose for the heat structures, which model the walls of the wind tunnel, since heat is generated in the problem.

The simulation is divided into three key phases for modeling purposes. The first phase is the steady-state portion of the analysis. This phase allows for the conditions to stabilize throughout the facility prior to the ignition of the fire. Additionally, due to limited modeling procedures in MELCOR, the fraction of UO₂ which is not suspended during the fire stage, 94%, is initialized in the atmosphere of the tray control volume, CV06. During the steady-state phase, this aerosol mass largely settles out of the atmosphere onto the tray. FL03 permits unidirectional flow from the wind tunnel to CV06 to allow CV06 to equilibrate to the pressure experienced in CV10. We assumed 2000 s for establishing the steady state.

The second phase of the experiment captures the duration of the fire. With the ignition of the fire at time zero, the energy and gas sources and sinks are modeled as well as an aerosol source rate representing 6% of the UO_2 mass is sourced into CV10, the fire source volume. The fire ends at about 5 min. Finally, during the third stage of the experiment FL04 is opened. Similar to the FL01 and FL02, a user-specified velocity is provided for FL04 to generate the anticipated velocity over the tray. This velocity corresponds with the velocity which should have been observed in CV10. Aerosols settled on the tray modeled in CV06 may be suspended if the corresponding control volume velocity is supportive. FL05 allows for any suspended aerosols released from the tray to be transported to the wind tunnel control volumes.

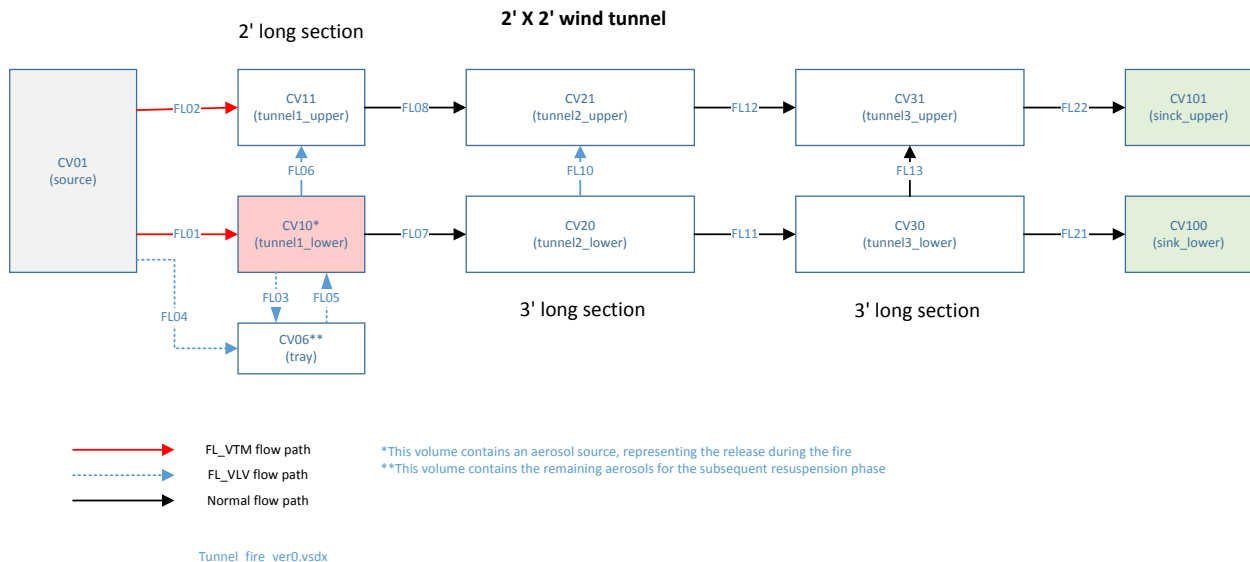


Figure 3-23. MELCOR 2.1 Model for the Gasoline Pool Fire Experiment.

3.2.3.4 Results and Discussions

Using the MELCOR model as described in the previous section, a simulation was conducted from -2000 s to 2000 s, using revision 8018 of MELCOR 2.1. The time from -2000 to 0 seconds were intended to allow the aerosol to settle onto the tray for the resuspension portion of the simulation, since the experiment did collect the resuspension aerosol after the fire was gone. Figure 3-24 shows the source flows into the wind tunnel. As shown in this figure, only the tunnel flow starts in -400 s to establish the steady-state flow in the tunnel, while the flow toward the tray is off until the fire ended and resuspension phase starts at ~500 s. Figure 3-25 shows the UO_2 airborne mass in the tray volume. As shown in this figure, the aerosol mass sourced into the tray volume is being settled closer to zero kg near time zero seconds before the fire starts. Figure 3-26 shows the pressures in the volumes. As shown in Figure 3-26, the pressure drops across the tunnel seem reasonable.

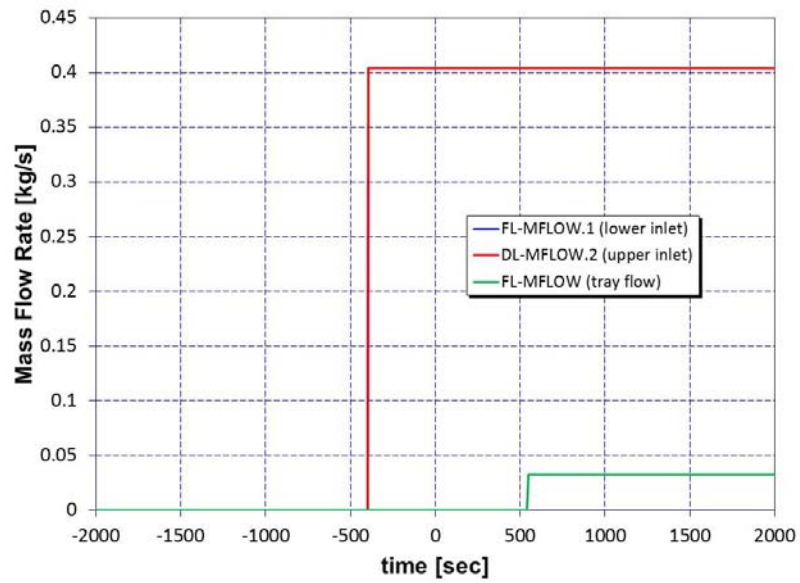


Figure 3-24. Flows in the Front Section of Tunnel.

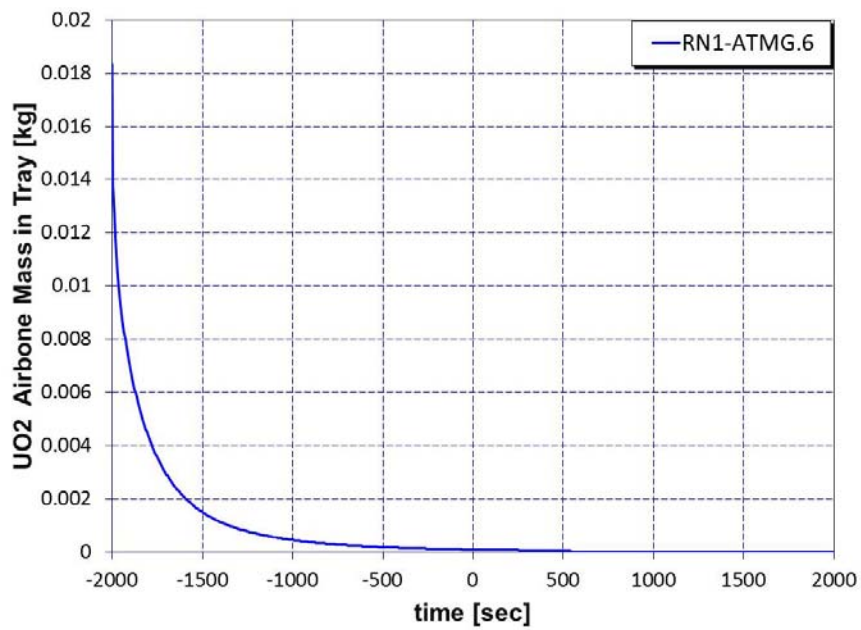


Figure 3-25. UO₂ Airborne Masses.

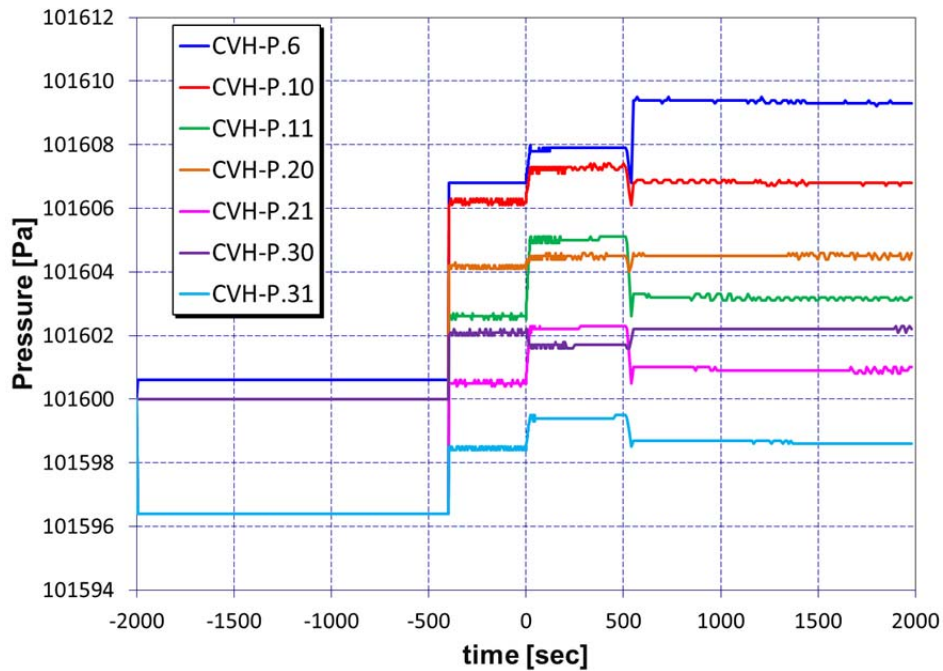


Figure 3-26. Gas Pressures in Volumes.

In terms of the fire, an assumed fire curve is used (see Figure 3-27 for the fire curve shape control function). Figure 3-28 shows the reaction gas flow rates for the fire. All these gas flow rates are modeled as input to the CV10 as the gas source and sink. Additionally, the combustion energy is added to the volume as well. Figure 3-29 and Figure 3-30 show the control volume velocity and airborne aerosol mass of UO_2 in the problem, respectively. As shown in Figure 3-29, the tunnel volume flow increases during the fire. At the end of the fire, the tray flow begins. As shown in Figure 3-30, aerosols start to release into the sink volumes (CV100 and CV101) during the fire. The release reduces as the fire ends. This also indicates that there was no resuspension of settled aerosol from the tray after the fire (see Figure 3-31). Appendix C.1 shows the critical diameter calculation on the gas velocity that is required to suspend the deposited aerosols in this simulation. Given a gas velocity in the tray control volume less than 2 m/s, the minimal critical diameter is on the order of mm. The largest aerosol diameter size modeled in this simulation is 50 μm . Therefore, no aerosol suspension is calculated. In terms of comparing to the experimental data, Table 3-15 shows the comparison. As shown in the table, the only comparison to the experiment is the release during fire, since there is no resuspension predicted. If the release from the MELCOR calculation is adjusted with the fraction of the sampling area to the tunnel area, then the ARF is similar.

In closing, this simulation does show that MELCOR can be used to model a fire accident. With the aid of the CFD code results on the entrainment during the fire, MELCOR results agree with

the experiment data. However, suspension from the burn debris from the tray is not replicated well using settled aerosols as a simulant for the UO_2 residing within the tray along with burn residue.

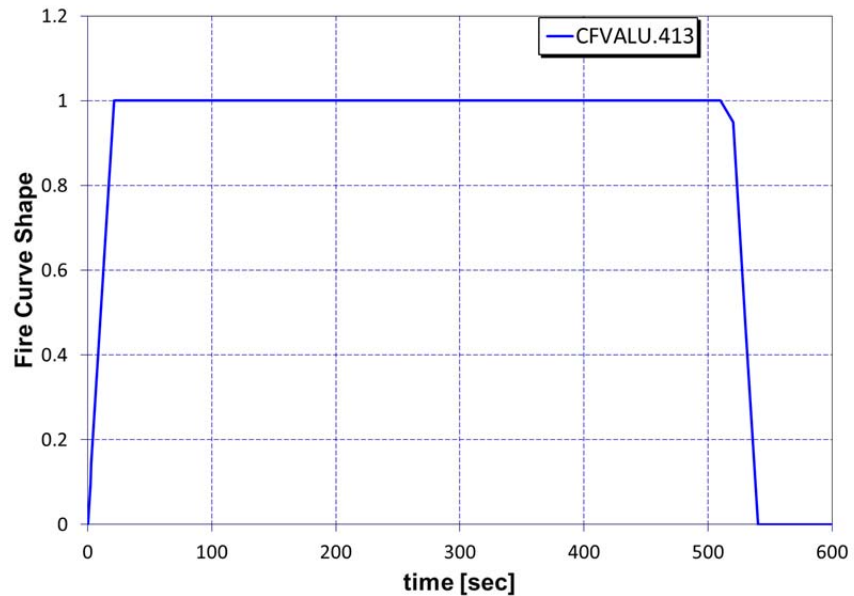


Figure 3-27. Fire Curve Shape.

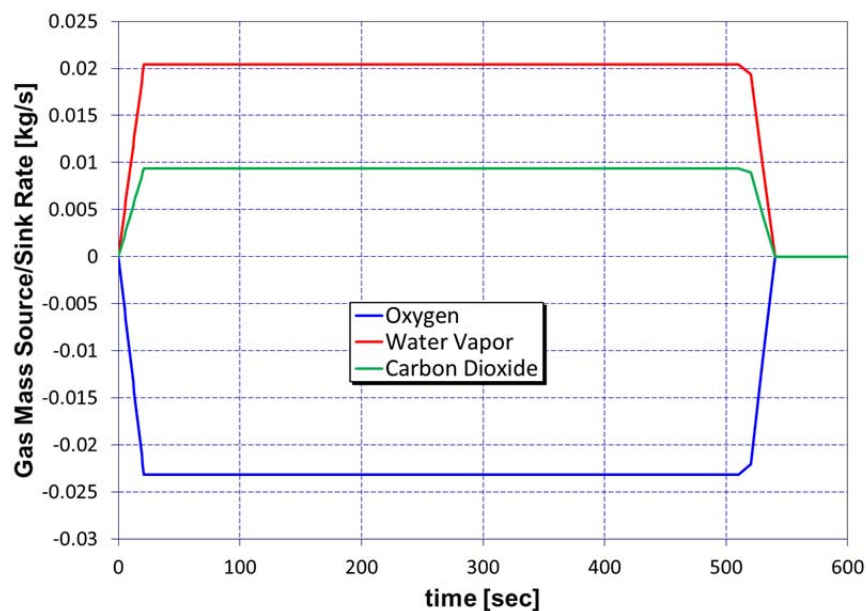


Figure 3-28. Fire Reaction and Products Source/Sink Mass Rates.

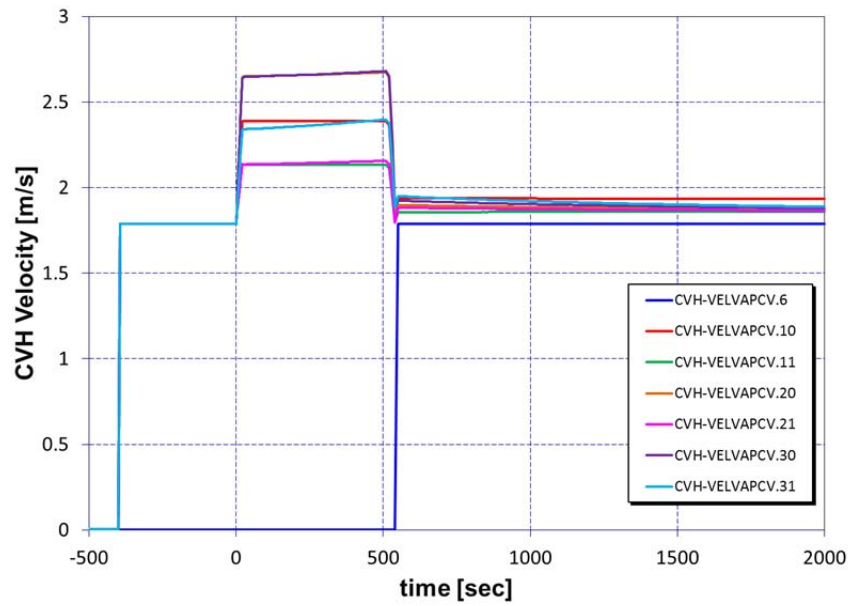


Figure 3-29. Control Volume Vapor Velocities (0 to ~500 s Fire).

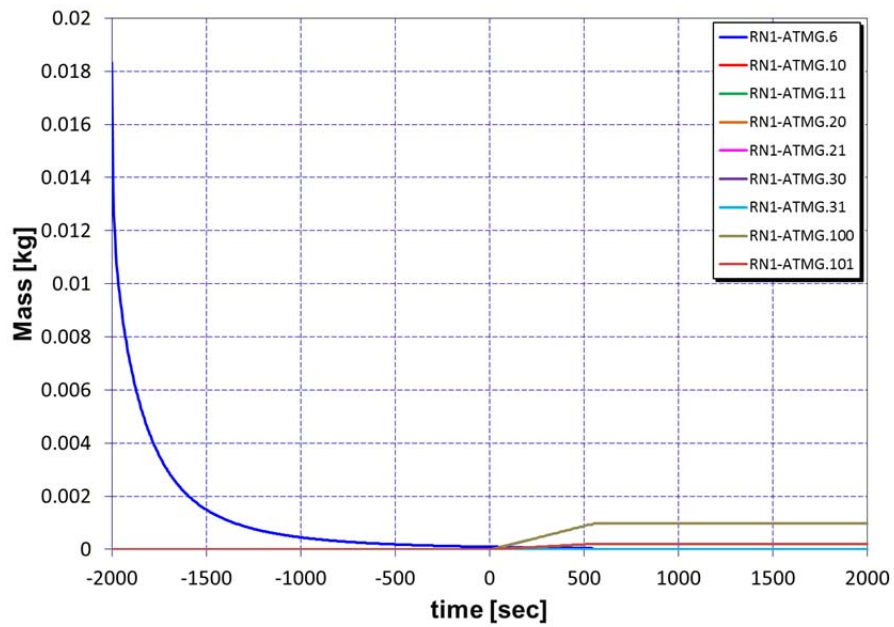


Figure 3-30. UO₂ Airborne Aerosols.

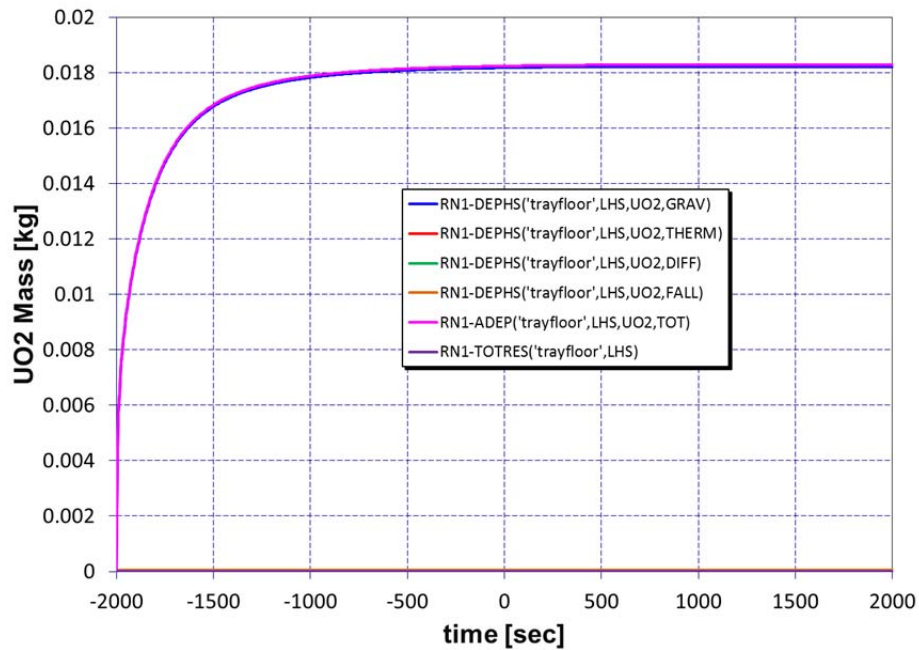


Figure 3-31. Aerosol Deposition and Resuspension in Tray Volume.

Table 3-15. Aerosol Result Summary for Gasoline Pool Fire

Experimental Data	MELCOR 2.1
During Fire – ARF=0.0012 Mass=2.34E-05 kg	During Fire – ARF= 0.0606 1.1836E-03 kg (Adjust to total area of the sampling*) Mass=2.94E-05 kg
During Resuspension- ARF=9.0E-4 Mass=1.755E-05 kg	During Resuspension (after fire gone) ARF=0.0 Mass=0.0 kg

*Total sampling cross section fraction to the wind tunnel cross section area of 0.025

3.3 Other Validations

In addition to the gasoline fire validation as described in the Handbook section above, other fire experiment validations are also included here. Although MELCOR is not a fire code, such as CFAST [Peacock 2016], the control function package allows the user to impose mass and energy rates to simulate aspects of a fire through user logics. The thermodynamics of the MELCOR simulation can then be compared to fire codes, such as CFAST, to determine whether modeling is sufficient to be extended to aerosol dynamics.

The previous section present efforts to validate the MELCOR aerosol physics models using the Handbook data. To further validate the recently added aerosol resuspension model, we included a reactor experiment, which was identified in Section 3.1. We chose the STORM-SR11 test

because it includes both deposition and resuspension phases. Unlike the gasoline pool fire as described in the previous section, the suspension of the burn residue may be difficult to characterize. In the STORM experiment, the aerosol deposited will be resuspended due to increased flow velocity. Thus, this experiment may be better characterized, and thus modeled by MELCOR.

This section provides the MELCOR validation for a fire experiment from the CFAST validation document [Peacock 2016] and the STORM-SR11 experiment [NEA 1998].

3.3.1 LLNL Enclosure Fire Experiment (T9 and T11)

In 1986, Lawrence Livermore National Laboratory (LLNL) studied the effects of ventilation on enclosure tests [Peacock 2016]. The enclosure was 6 m long, 4 m wide and 4.5 m high. It contains a methane rock burner located at the center of the enclosure floor. The burner is 0.23 m height and 0.57 m in diameter. Figure 3-32 shows the layout of this enclosure. As shown in this figure, there are two inlet ducts, which seem to be located near the top and bottom of the enclosure. The dimensions are not specified for the inlet ducts. The exhaust duct is dimensioned to be 0.65 m by 0.65 m near the top of the enclosure. For some tests, an upper plenum is used. As shown in this figure, the exhaust duct is powered, so that it draws the air out of the enclosure during the fire. A door with the dimension as shown in this figure is used for certain tests. The size of the fire is from 50 kW to 400 kW. The ventilation mass flow rate of 100 to 500 g/s is used.

The experiments do not describe the construction of the enclosure, besides the dimension. Therefore, the information about the walls and ceiling/floor structures is based on the information from CFAST (see Section 3.3.1.1 below). The principal reaction for the combustion of methane gas is given by:



For this experiment, we assume that the fuel mass fraction that results in carbon particle generations during combustion is ignored, since this simulation is targeted for the thermal-hydraulic results, rather than aerosol results.

3.3.1.1 Experiment Data

We identified two tests from the LLNL enclosure experiments to model with MELCOR: Test 9 and Test 11. Both tests use full compartment and low inlet duct. The ventilation flow exists, so that the modeling of CH₄ in the reaction is not required since the depletion of oxygen may not be possible. The locations of the thermal couples in the experiments such that there are five thermal couples near the top, middle or lower sections of the enclosure. The experimental data for Test 9 and Test 11 is provided in Table 3-16 and Table 3-17, respectively. As shown in these tables, the air exhaust flow, fuel flow rate, oxygen and carbon dioxide fractions, the pressure drop, and the average five thermocouple temperatures in the upper, middle and lower enclosure. As indicated before, no detailed information about the thermocouple locations is given.

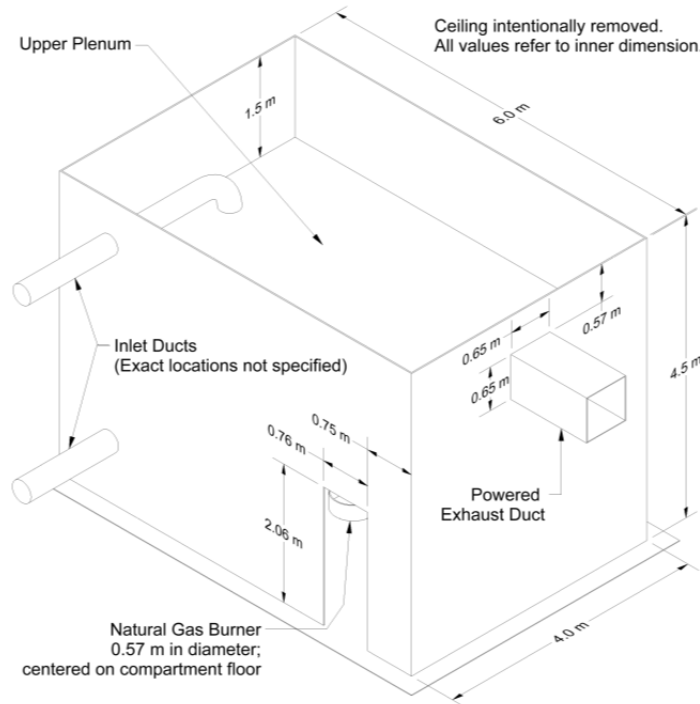


Figure 3-32. Layout of the LLNL Enclosure Experiments [Peacock 2016].

Table 3-16. Experimental Data for Test 9*

Time (s)	Air Flow (kg/s)	Fuel Flow (kg.s)	O ₂ Fraction	ΔP (Pa)	CO ₂ Fraction	West Upper TC (K)	West Middle TC (K)	West Bottom TC (K)
0	0.565	0.0	0.208	-398	0.0005	302.15	302.15	302.15
500	0.491	0.0041	0.185	-297	0.0140	399.15	386.15	332.15
1000	0.474	0.0040	0.1822	-292	0.0156	413.15	398.15	339.15
2000	0.463	0.0042	0.1809	-287	0.0159	425.15	413.15	346.15
3000	0.464	0.0039	0.1824	-278	0.0154	427.15	413.15	399.15
4000	0.461	0.0040	0.1819	-261	0.0157	434.15	419.15	405.15

*Obtained from https://github.com/firemodels/cfast/blob/master/Validation/LLNL_Enclosure/Experimental_Data/LLNL_09.csv. The constant fire power of 200 kW is used.

Table 3-17. Experimental Data for Test 11*

Time (s)	Air Flow (kg/s)	Fuel Flow (kg.s)	O ₂ Fraction	ΔP (Pa)	CO ₂ Fraction	West Upper TC (K)	West Middle TC (K)	West Bottom TC (K)
0	0.240	0.0	0.2098	-75	0.0004	292.15	292.15	292.15
500	0.222	0.0040	0.1705	-42	0.0220	408.15	394.15	339.15
1000	0.221	0.0040	0.1546	-39	0.0289	422.15	408.15	349.15
2000	0.210	0.0040	0.1486	-45	0.0325	437.15	421.15	360.15
3000	0.207	0.0040	0.1473	-38	0.0326	444.15	429.15	366.15
4000	0.204	0.0040	0.1460	-31	0.0335	452.15	436.15	373.15

*Obtained from https://github.com/firemodels/cfast/blob/master/Validation/LLNL_Enclosure/Experimental_Data/LLNL_11.csv. The constant fire power of 200 kW is used.

3.3.1.2 MELCOR Model

The development of the MELCOR model was done in stages. First, the appropriate number of volumes to capture the temperatures of the fire was needed. Initially, only three axial volumes were modeled, and resulted in high temperature near the bottom of the enclosure, which was incorrect. The hot gas should be located near ceiling of the enclosure. To provide natural recirculation, the 9-volume model was used (see MELCOR input model in Appendix B.2). Figure 3-33 shows the 9-volume model for this enclosure experiment. As shown in this figure, a flow path models the inlet plenum to the enclosure, and a flow path that goes to the exhaust fan in the upper layers of the enclosure. The reason for breaking the enclosure into three equal regions is the thermocouple layout in the enclosure, even though the exact location is not known. So each upper, middle, and lower region contains the average results of 5 thermocouples. The fire is located at the center floor. In each axial region, three concentric volumes, starting from an inner, middle and outer volumes, are shown in this figure with dimension. Therefore, when the fire starts in a rock burner at the center of the floor, the high gas would rise in the center to the upper region and move out toward the exhaust fan (see Figure 3-32).

In terms of the heat structures, the walls, floor and ceiling of the enclosure are modeled as heat sinks. Since there is no wall thickness information from the experiment provided, we utilized the information from the CFAST validation report [Peacock 2016]. In addition, the inlet flow area is taken from what CFAST used in the simulation as 0.018 m^2 , which is a leakage area based on the initial exhaust rate and pressure. To capture correctly, the radiation heat loss fraction of the combustion power is accounted for. It is consistent for methane gas (see Appendix C.2 for the hand calculation). As shown in the appendix, the hand calculation matches closely in the expected radiation loss in [NFPA 1995]. In this validation, we simulate two tests (T9 and T11), with the experimental data provided in Table 3-16 and Table 3-17, respectively. In both tests, we programmed the initial temperature and the pressure in the enclosure volume to be that of time zero experimental data from these tables. Additional atmosphere condition in the problem is obtained from CFAST simulations for these tests. For example, the relative humidity is taken to be 50%.

The thickness of the surfaces is modeled to be 0.1 m according to the CFAST. However, we assume the stainless steel for the surfaces of the enclosure. A rock burner heat structure is modeled, and assumed to be an annular cylinder having a high of 0.23 m and an inner radius of 0.25 m and outer radius of 0.57 m. It is also assumed to be made of stainless steel. In each run, we assume the end time of 4000 s with a ramp rate from 0 to 100% of the fire power for each test. To model the fire, we used a number of control functions to model the oxygen consumption as a source sink, carbon dioxide and water vapor production as sources. The fire energy rate which has subtracted the thermal radiation loss is sourced, along with the gas sources and sinks for the fire to CV100. Using the experimental pressure measurement as input, we created a control function to model this pressure drop using a “QUICK-CF” in FL 910 (see Figure 3-33).

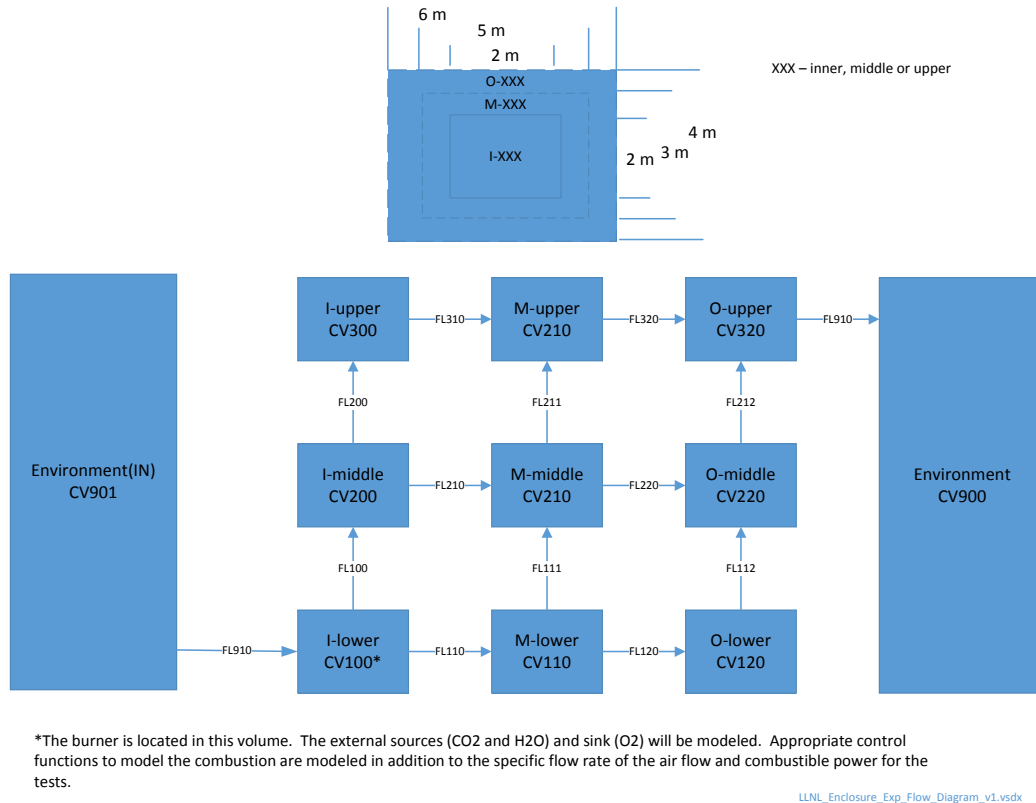


Figure 3-33. MELCOR 9-Volume Model for LLNL Enclosure Fire Experiment.

Table 3-18 CFAST Test 9 Heat Structure Data*

Structure	Thermal Conductivity	Heat Capacity	Density (kg/m ³)	Wall Thickness (m)	Emissivity
Walls	0.39	1000	1440	0.1	0.94
Ceiling/Floor	0.63	1000	1920	0.1	0.94

*obtained from https://github.com/firemodels/cfast/blob/master/Validation/LLNL_Enclosure/LLNL_09.in

3.3.1.3 Results of MELCOR Simulations

In this section, we describe the results of the simulations of T9 and T11 tests for the LLNL enclosure experiment. In the simulations, we used version 8018 of MELCOR 2.1. This version is an official release, which allows us to utilize the formula control functions. In these simulations, we assumed the thermal radiation loss of 20% of the fire energy (see the calculation sheet in Appendix C.2). In comparison with CFAST, it assumes 35% for the thermal radiation loss. A 200 s time was used for establishing the steady state, before starting the fire at time zero. In the results, efforts have been made to compare the results of the CFAST simulations as documented in the CFAST validation report [Peacock 2016].

3.3.1.3.1 T9 Test

The simulation for this test is based on the experimental data provided in Table 3-16 and using the MELCOR model described above. Figure 3-34 shows the pressure drop modeled by

MELCOR for the enclosure volumes and compared to both CFAST and Experimental data. As shown in this figure, MELCOR is within the experiment data. Figure 3-35 shows the calculated mass flow rate to the exhaust duct. As shown in the figure, there is an initial pulse and decay down slightly below the experiment measured flow rate. This corresponds to the under-prediction of the pressure drop in Figure 3-34.

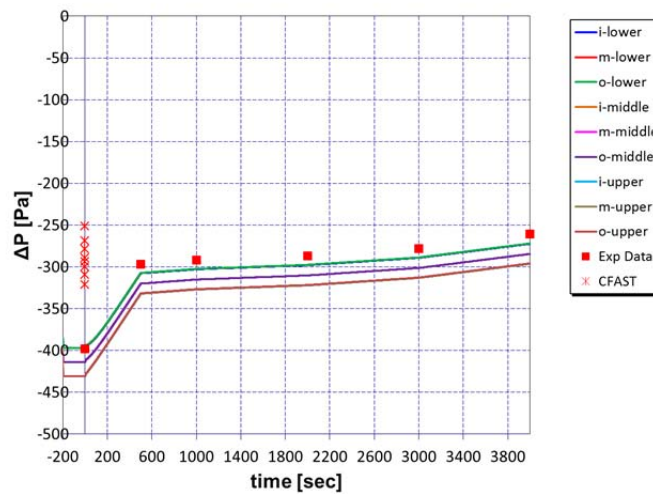


Figure 3-34. MELCOR Results on Pressures for Test 9.

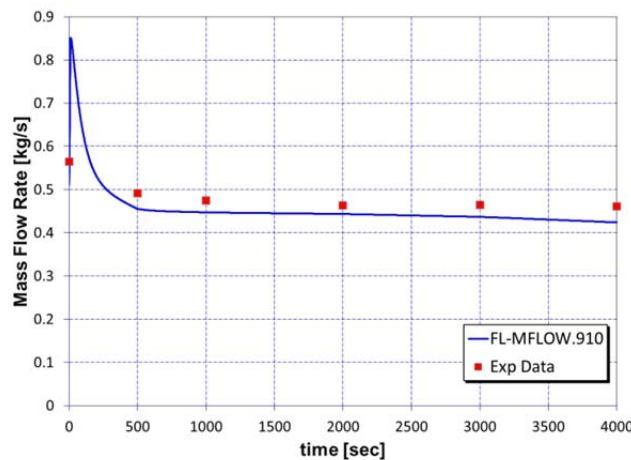


Figure 3-35. MELCOR Results on Exhausted Air Flow for Test 9.

In terms of temperatures, we compared three regions – lower, middle, and upper – where an average temperature of five thermocouples were done in the experiment. Figure 3-36 shows the lower temperature comparison. As shown in this figure, MELCOR over-predicts the temperature by $\sim 50^{\circ}\text{C}$. For the middle section as shown in Figure 3-37, MELCOR slightly over-predicts the temperature $< \sim 10^{\circ}\text{C}$. For the upper section as shown in Figure 3-38, MELCOR predicts with the experiment data while CFAST over-predicts compared to that of MELCOR and the data.

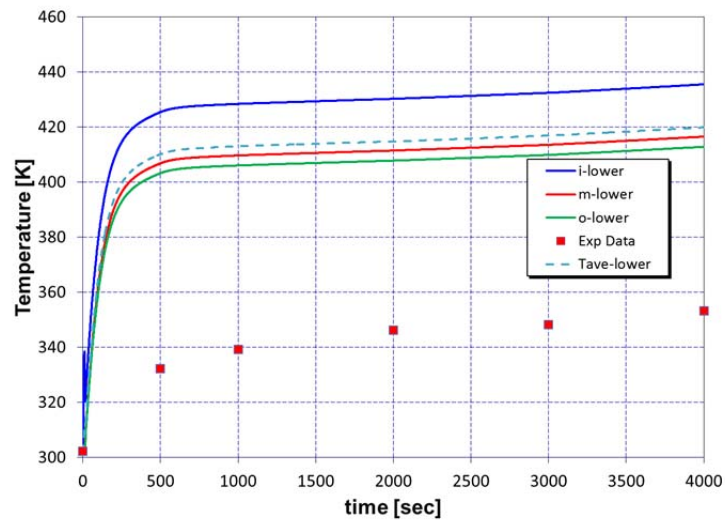


Figure 3-36. MELCOR Results on Lower Temperatures for Test 9.

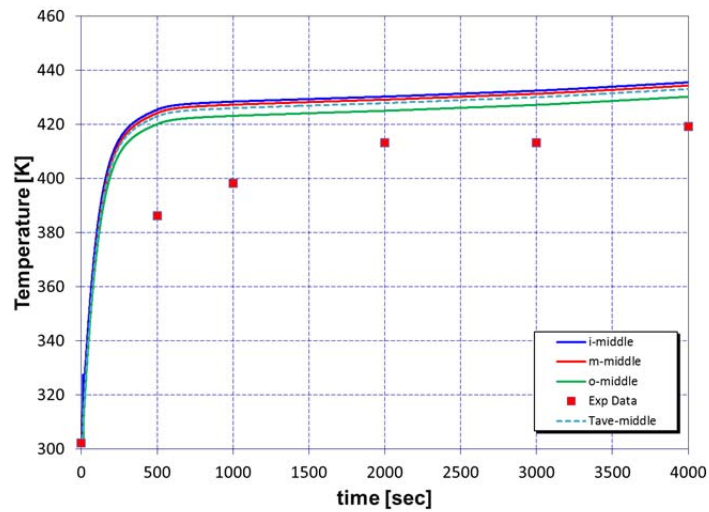


Figure 3-37. MELCOR Results on Middle Temperatures for Test 9.

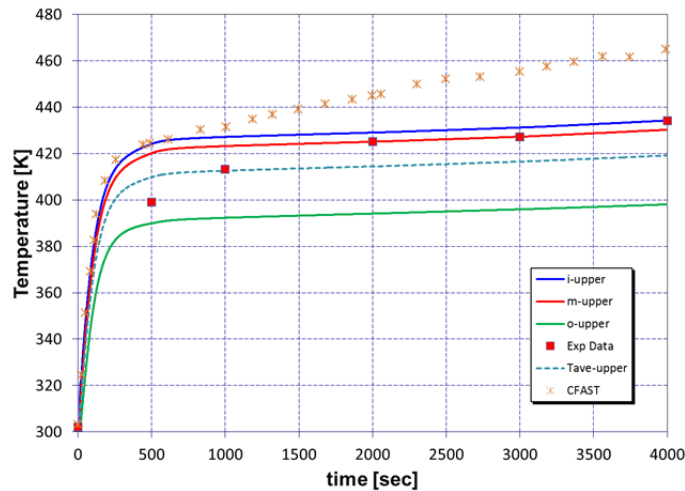


Figure 3-38. MELCOR Results on Upper Temperatures for Test 9.

In terms of the reaction species prediction, we modeled the generation based on the discussion of the methane gas reaction in the previous sections. Figure 3-39 and Figure 3-40 show the reaction product source rate and reactant sink rate for the fire volume (CV100), respectively. In comparison to the experiment data, Figure 3-41 shows the CO_2 mole fraction calculated by MELCOR. As shown in this figure, MELCOR under-predicts this mole fraction. A similar finding is true for the oxygen mole fraction (see Figure 3-42).

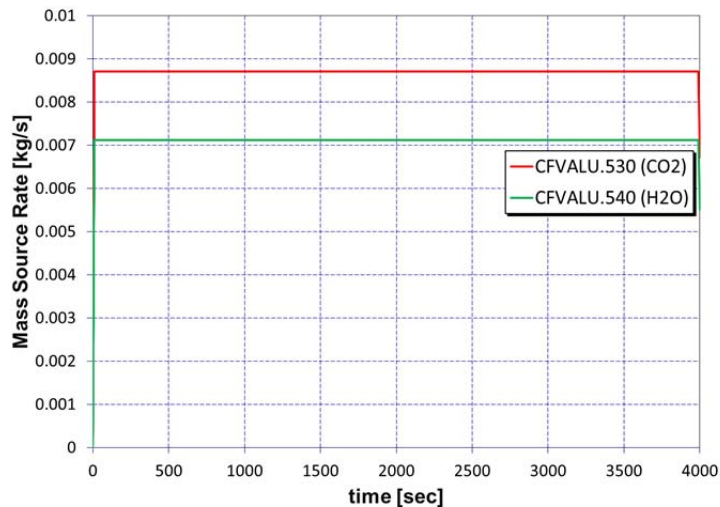


Figure 3-39. Calculated Product Mass Source Flow Rates for Test 9.

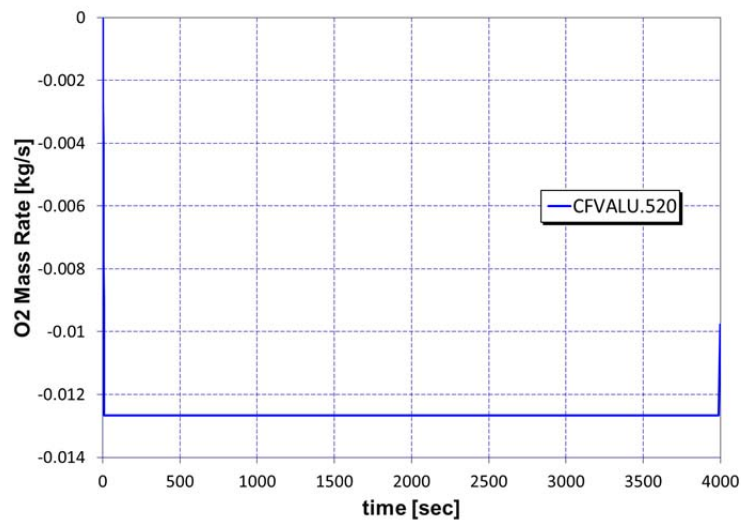


Figure 3-40. Calculated Oxygen Sink Flow Rate for Test 9.

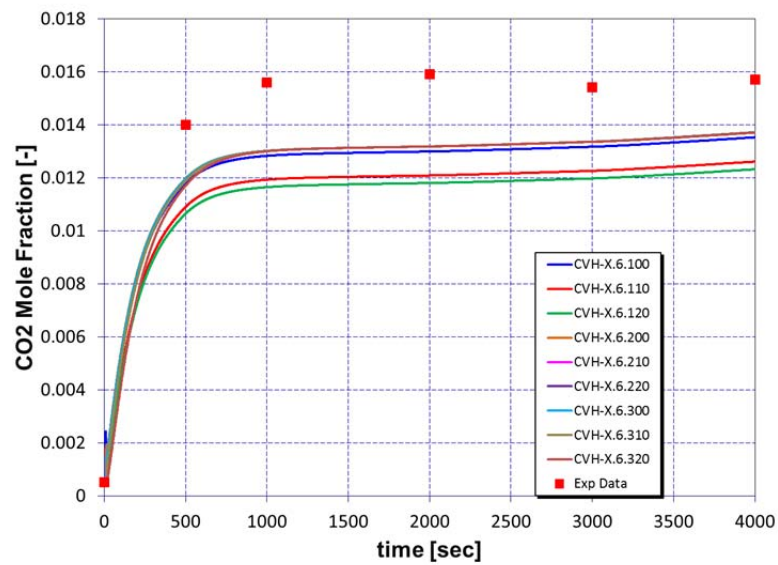


Figure 3-41. MELCOR Results on CO₂ Mole Fractions for Test 9.

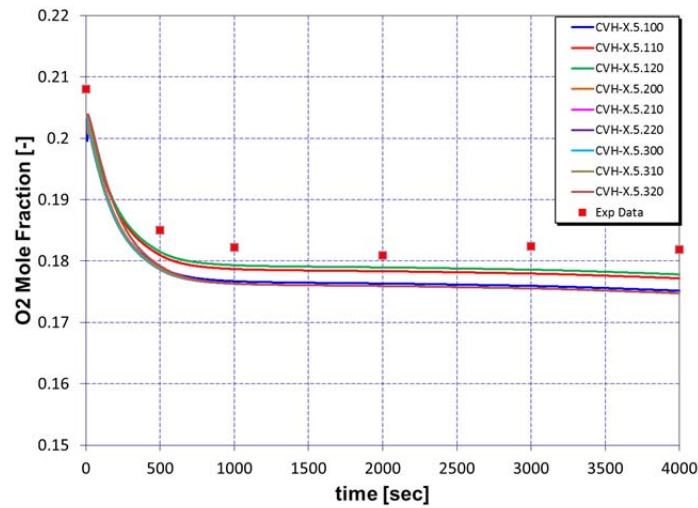


Figure 3-42. MELCOR Results on O₂ Mole Fractions for Test 9.

3.3.1.3.2 T11 Test

This test had a lower pressure drop and lower gas flow rate than the T9 test. Figure 3-43 shows the pressure drop modeled in MELCOR. As shown in this figure, MELCOR under-predicts the pressure drop while CFAST over-predicts the pressure drop during the fire. However, MELCOR agrees well with the exhaust flow from the experiment data as shown in Figure 3-44.

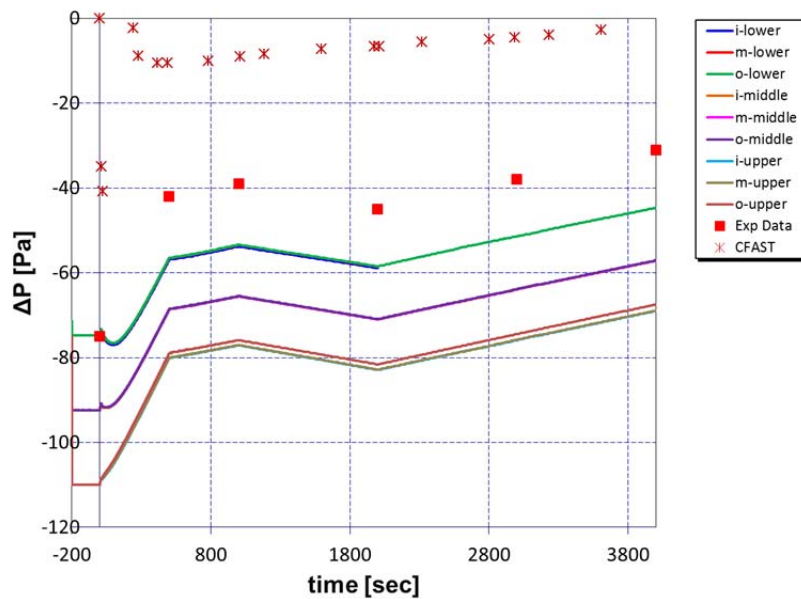


Figure 3-43. MELCOR Results on Pressures for Test 11.

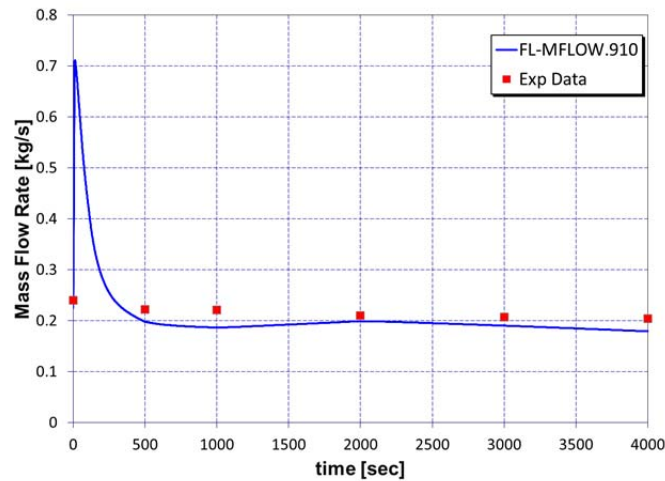


Figure 3-44. MELCOR Results on Exhausted Air Flow for Test 11.

In terms of temperature comparison as shown in Figure 3-45 for the lower sections, MELCOR over-predicts 50–70°C. For the middle section as shown in Figure 3-46, MELCOR over-predicts the temperature and the difference is smaller near the end of the fire. For the upper section as shown in Figure 3-47, MELCOR bounds the data while CFAST deviates larger as the fire goes on.

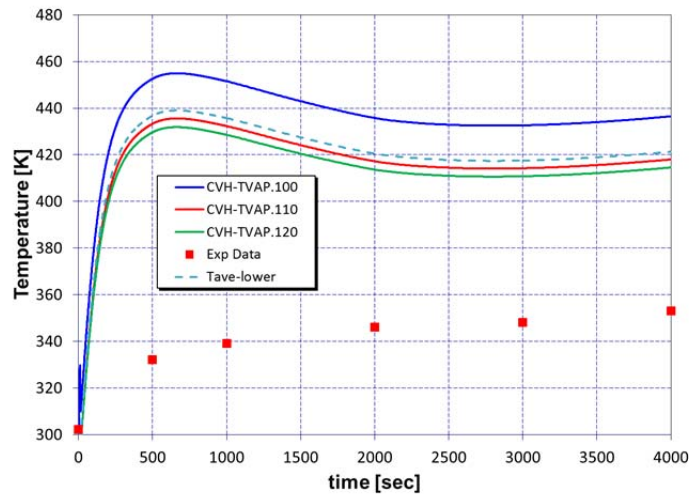


Figure 3-45. MELCOR Results on Lower Temperatures for Test 11.

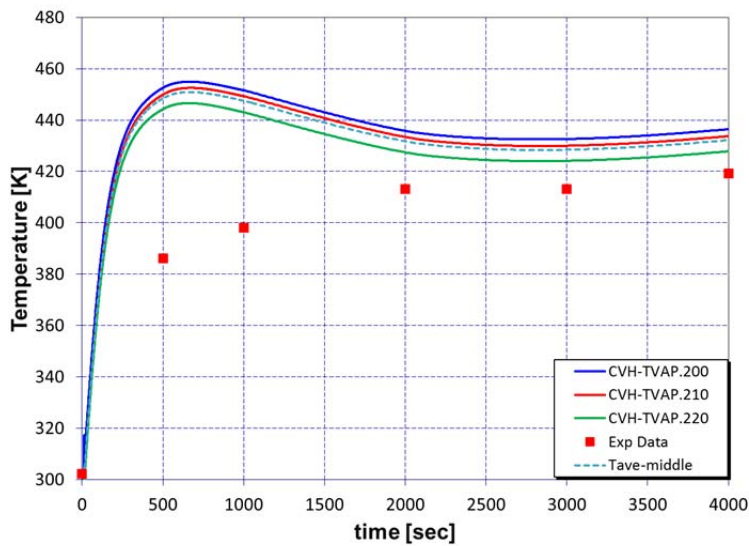


Figure 3-46. MELCOR Results on Middle Temperatures for Test 11.

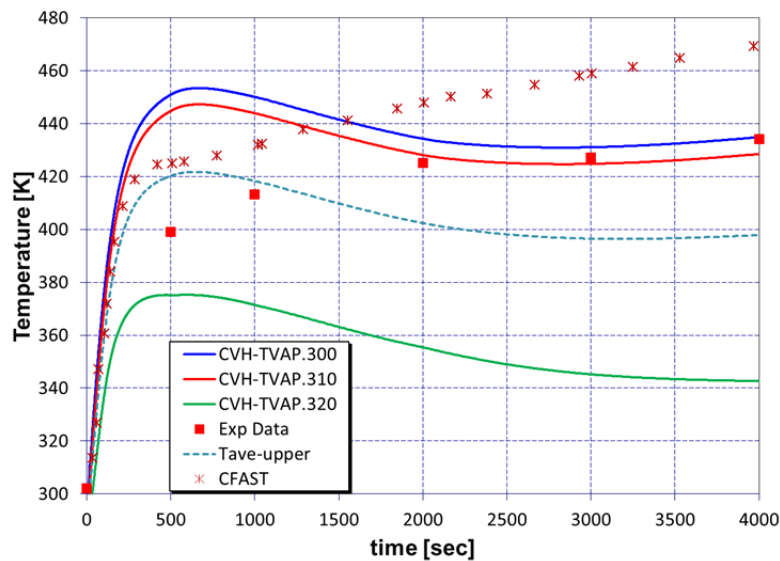


Figure 3-47. MELCOR Results on Upper Temperatures for Test 11.

In terms of the gas product predictions, Figure 3-48 and Figure 3-49 show the product source flow and reactant sink flow modeled in the fire volume (CV100), respectively. Figure 3-50 shows the O_2 mole fraction prediction of MELCOR. As shown in this figure, MELCOR predicts well with the data. Similarly, Figure 3-51 shows the CO_2 mole fraction calculated by MELCOR. As shown in this figure, the O_2 mole fraction predicted by MELCOR is within the bounds of the data in the first 1000 s, and under-predicts slightly in the remainder of the fire.

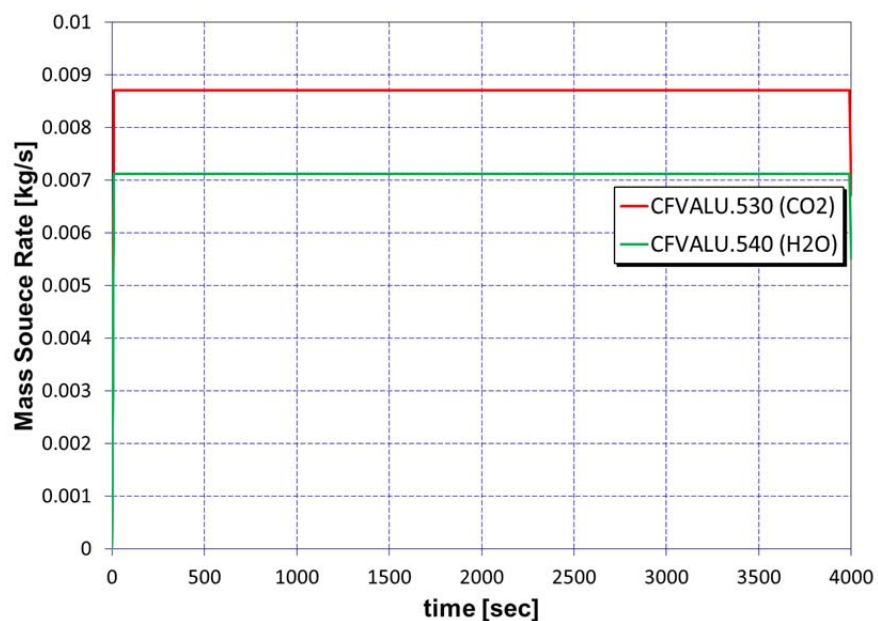


Figure 3-48. Calculated Product Mass Source Flow Rates (CO₂ and H₂O) for Test 11.

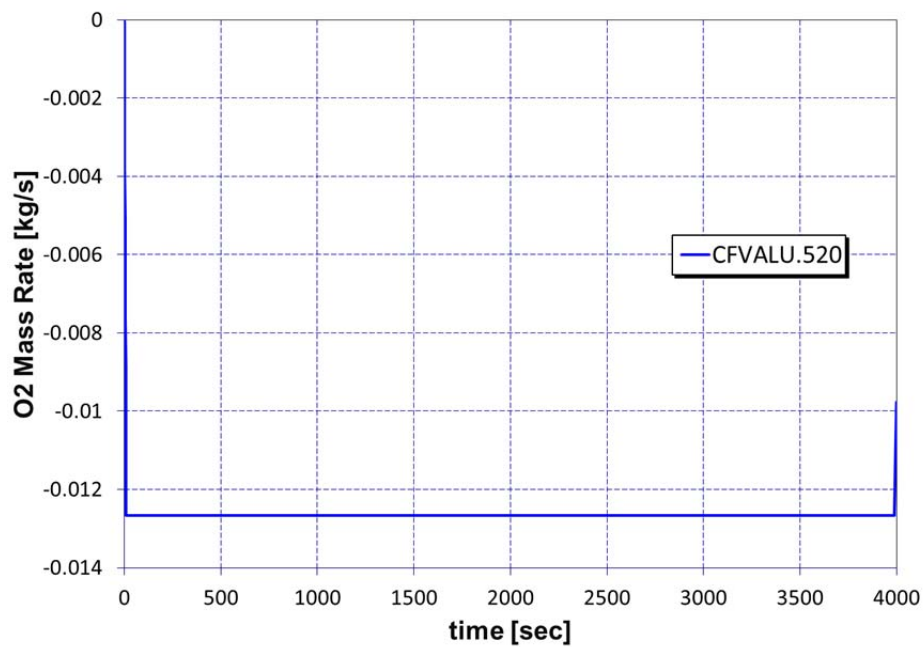


Figure 3-49. Calculated Oxygen Sink Flow Rate for Test 11.

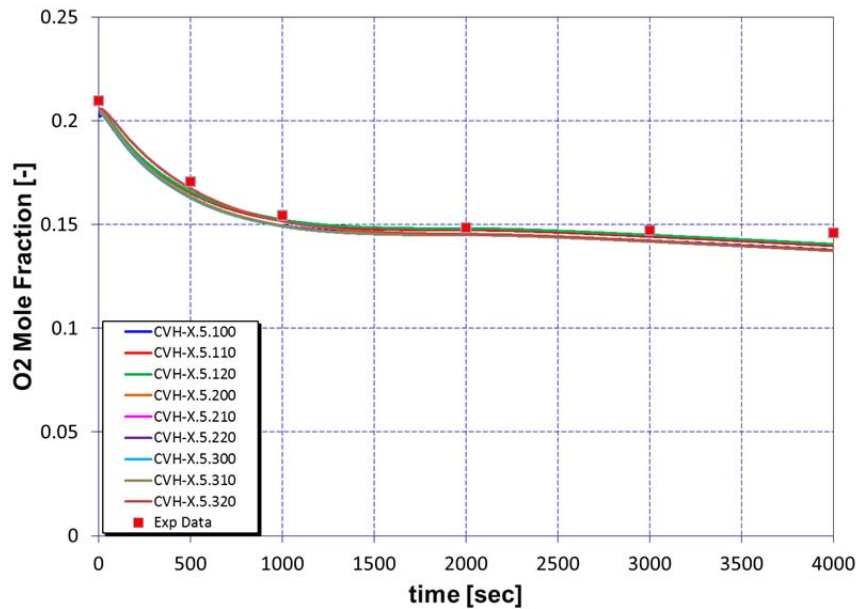


Figure 3-50. MELCOR Results on CO₂ Mole Fractions for Test 11.

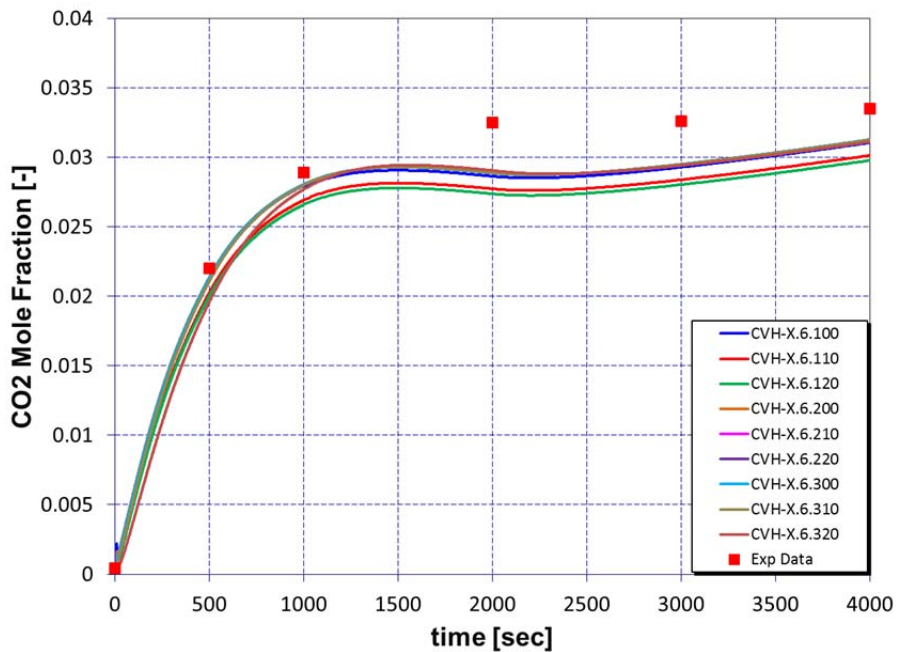


Figure 3-51. MELCOR Results on O₂ Mole Fractions for Test 11.

3.3.1.4 Summary and Conclusion

For the LLNL enclosure methane gas experiment, we have demonstrated that MELCOR can be used to model the combustion reactions of methane gas for both T9 and T11 tests. For the T9 test, MELCOR tends to under-predict the product gas mole fraction, while MELCOR predicts well with the exhaust flow rate. For the T11 test, which models a lower exhaust flow rate,

MELCOR tends to under-predict the pressure drop, even though the pressure drop curve is modeled in the input. However, the exhaust flow rate agrees well with the data. Similarly, MELCOR predicts the product gas mole fractions well. In terms of temperatures, MELCOR under predicts the hot gas layer (upper temperatures) before 1500 s and matches closely with the data at the later time. In terms of comparison with CFAST, MELCOR predicts a lower hot gas layer temperature than CFAST, even though CFAST assumes a higher thermal radiation loss.

This simulation indicates that MELCOR can be used to model fire scenarios in terms of predicting the thermal-hydraulic behavior, even though MELCOR does not have a combustible model and a dynamic hot gas layer model. With the power of control functions, we can model fire scenarios well.

3.3.2 *STORM-SR11 Experiment (Deposition and Resuspension)*

The development of the aerosol resuspension model in MELCOR primarily is for reactor applications. Therefore, we chose a reactor experiment to show the release of aerosol from resuspension, because we did not show the release in the simulations for the wind tunnel gasoline fire experiment. Although the fluid (or gas) velocity from the experiment may not be commonly found in DOE nuclear facilities, there is a potential high gas velocity that can occur during an explosion accident. In particular, in a situation when a waste treatment pipe contained previous deposits extended from the inside of the facility to the environment, an explosion can induce a high enough gas velocity through the pipe that resuspends deposited materials which leads to a source term to the environment.

In this section, we describe the STORM SR-11 experiment briefly, since the experiment contains a deposition phase and a resuspension phase. The deposition phase was well documented in the MELCOR assessment report [Humphries 2015c]. However, the assessment report did not contain the resuspension phase simulation. Therefore, this section will discuss both phases of the experiment. However, we primarily focus on the resuspension phase comparison with the experimental data, since we do not want to duplicate the deposition phase which has already been described in the MELCOR assessment report [Humphries 2015c].

3.3.2.1 Experimental Data

In this section, we will briefly describe the apparatus of this experiment. As shown in Figure 3-52, the STORM test facility consists of gas and aerosol generators, a mixing vessel, a test section, and a wash and filtering system. Carrier gas and aerosol pass through the test section, which is a straight stainless steel pipe that is 5.0055 m long with a 6.3-cm inner diameter. Because the STORM tests consist of two parts – deposition and resuspension – the sampling of the aerosols for both parts is also shown in this figure. The aerosol size distribution and concentration are measured at the upstream and downstream of the test section. To ensure resuspension, the test section is enclosed in an oven. The oven is open during the deposition phase to maximize the thermophoresis deposition and is closed and heated immediately at the beginning of the resuspension phase. The deposition phase lasts about 2.5 hours and is followed

by the resuspension phase that lasts 1.75 hours. The carrier gas flow rate for the deposition phase is shown in Table 3-19. Then the resuspension phase is followed by increasing the nitrogen gas flow rate by stages as shown in Table 3-20. There is a discrepancy between the two STORM reports on the duration of the resuspension phase. For this report, the duration of 1.75 hours was used. The aerosol material used in the experiment includes both SnO_2 and CsOH . For this report, we only examined the SnO_2 . The characteristics of the SnO_2 are given in Table 3-21. As shown in this table, the flow rate of the aerosol ($\sim 3.83 \times 10^{-4} \text{ kg/s}$) at the entrance of the test section was practically constant during the entire deposition phase of the experiment. The particle size distribution is assumed lognormal with a $0.43 \mu\text{m}$ geometric mean diameter and a 1.7 geometric standard deviation [Castelo 1999]. An aerosol material density of 4000 kg/m^3 was used [Castelo 1999].

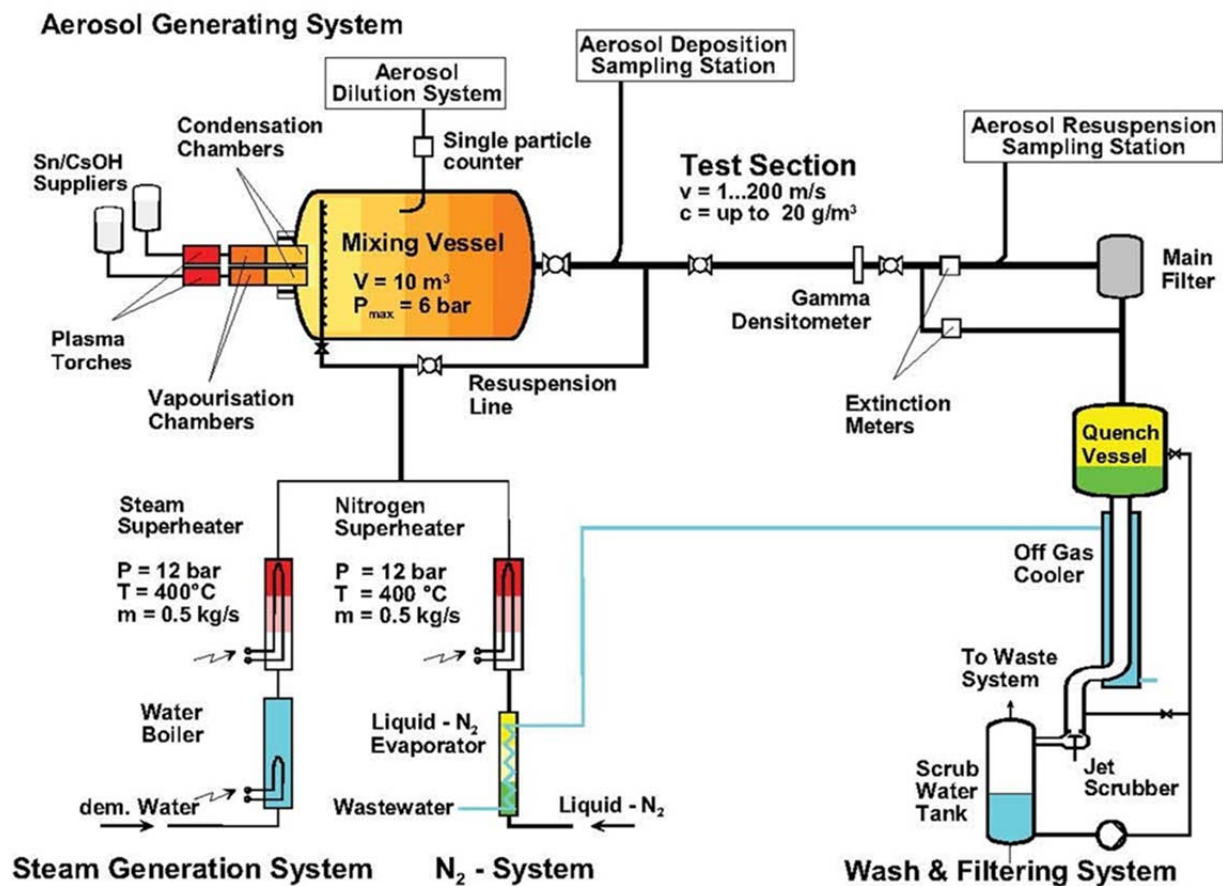


Figure 3-52. STORM Experimental Facility Setup [NEA 1999].

Table 3-19. Carrier Gas Mass Flow Rate for the Deposition Phase [NEA 1999]

Gas	Mass Flow Rate (kg/s)
Steam	1.1060×10^{-2}
Nitrogen	0.5467×10^{-2}
Air	0.5728×10^{-2}

Argon	0.7194×10^{-2}
Helium	0.0119×10^{-2}

Table 3-20. Nitrogen Gas Mass Flow Rate for the Resuspension Phase [Dilara 1998, NEA 1999]

Step	Time (minutes)	Mass Flow Rate (kg/s)	Velocity (m/s)
1	23	0.102	58
2	26	0.126	72
3	16	0.152	86
4	17	0.175	100
5	16	0.199	113
6	7	0.224	127

Table 3-21. Characteristics of Aerosol Used in Experiment – SnO₂ [NEA 1999]

Parameter	Value
Aerosol Flow Rate (kg/s)	3.83×10^{-4}
Duration (hours)	2.5
Mass mean diameter (μm)	0.43
Geometric standard deviation	1.7
Aerosol density (kg/m ³)	4000

3.3.2.2 MELCOR Calculations

The MELCOR assessment report describes the MELCOR nodalization model used in the experiment [Humphries 2015c]. In brief, the MELCOR model consists of five equal segments of the straight pipe test section as shown in Figure 3-52. Each segment is represented as a 1-meter-long pipe in the model with a single control volume. We conducted several simulations using the following assumptions.

Assumptions:

- The geometric mass diameter in Table 3-21 was entered as a negative value for the input variable of GEOMM in RN1_AS01 record. All other parameters listed in Table 3-21 are included in the MELCOR inputs. Note that this case is similar to Case 0 documented in the MELCOR assessment report (Run 1 in this section).
 - In addition, we provided three additional simulations for entering GEOMM as negative values (Run 2), used the definition of the mass mean diameter as shown in Section 4.2.7.2, and recalculated the AMMD as 0.86 μm in one case (as Run 3). Finally, we used the definition of geometric mass mean diameter (GMMD) as described in Section 4.2.7.2, GEOMM = 0.43 μm, and the aerosol density of 1000 kg/m³ (Run 4). The last simulation is modeled, because the experimental report [NEA1999] indicated that the 0.43 μm given in the table is GMMD.

- Both Table 3-19 and Table 3-20 were modeled for the carrier gas rates in the deposition and resuspension phases, respectively.
- We only examined Case 0 of the STORM cases in the MELCOR assessment manual [Humphries 2015c].
- The aerosol source and carrier gas flow rates were input to Segment 1, the first segment volume of the test section.

To better understand the expected resuspension in the experiment, Figure 3-53 shows the calculated critical diameter for the resuspension of the deposited SnO_2 . As shown in this figure, any aerosol larger than this critical diameter will be resuspended according to the gas velocity. Note that in MELCOR, the resuspension of the aerosol size is the same as they were first deposited. No agglomeration currently is modeled for deposited mass.

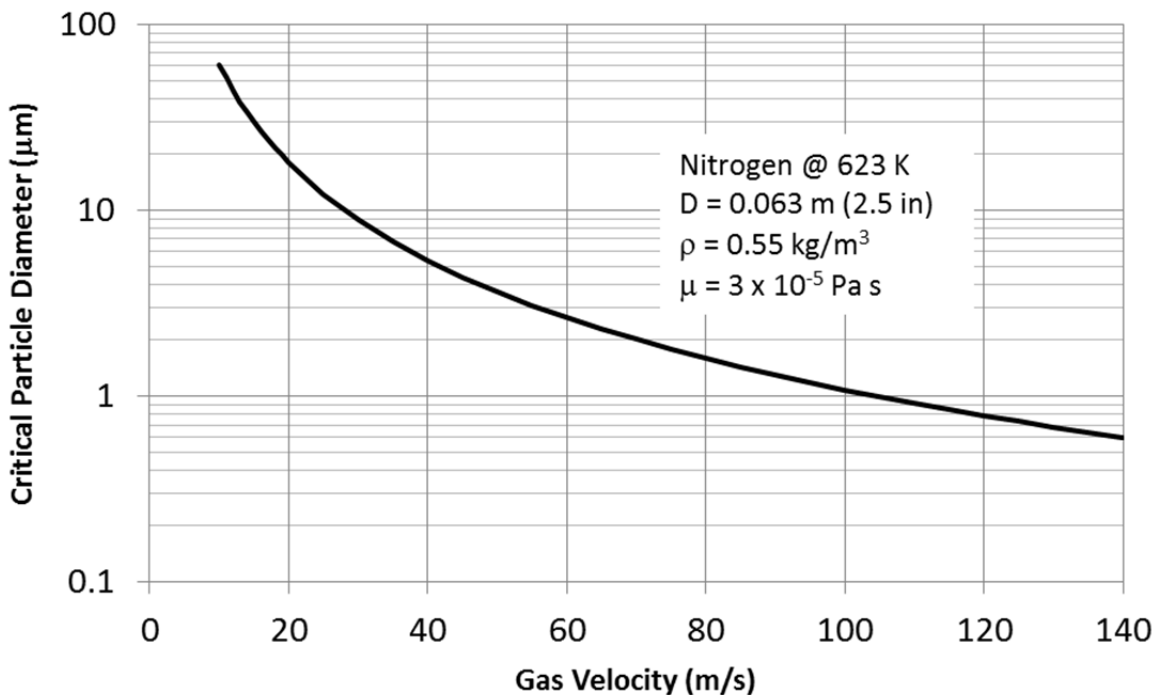


Figure 3-53. Critical Diameter versus the Gas Velocity for STORM Resuspension Phase.

3.3.2.3 Calculation Results and Discussion

Using the MELCOR nodalization and the experimental data as described in the previous section, MELCOR simulation is completed to the end time of 4.25 hours using MELCOR reversion update 8018.

Figure 3-54 and Figure 3-55 show the respective gas mass flow rates and control volume gas velocities by MELCOR. As shown in the gas velocity figure, the calculated value matches closely with the experimental data (see Table 3-20), except for the segment 1 (the meter 1 segment); the disparity is due to the introduction of the sources in the control volume that may

reduce the velocity. Future models will introduce the source in a volume before the meter 1 segment to ensure that all segments have similar gas velocities. In terms of aerosol deposition and resuspension, Figure 3-56 shows the aerosol mass deposited as a function of time for each of the five segments and overall total deposited mass. As shown in this figure, the deposition mass increases to about 2.5 hours when the deposition phase is ended. The increasing nitrogen flow as shown in this figure resuspends the deposited aerosol according to the nitrogen flow rate. Note that the meter 1 segment did not yield significant decrease in deposited mass (low resuspension mass), which may be due to the low control volume gas velocity as shown in Figure 3-55 for Run 1. Figure 3-57 shows the accumulated mass along the test section of all of five-segments for Run 1. As shown in this figure, the meter 1 segment shows a very small resuspension mass by subtracting the deposition curves at 2.5 hr from at 4.25 hr. The total accumulative mass that was resuspended during the resuspension phase of 1.75 hours is about 23.8 g, which is five times smaller than that of the experiment data of 113.3 g. If we would have input a 0.43- μm GEOMM as a negative value in the RN1_AS01 record, the calculated resuspension mass is much larger as shown in Figure 3-58 and Figure 3-59 for the accumulated mass of each segment as a function of time and the accumulated mass along the test section of all five segments (Run 2), respectively. As shown in Figure 3-59, the total resuspended mass is 88.3 g, in comparison with the experimental data of 113.3 g for the total resuspension mass. This result is closer to that of the experimental data. This difference may be due to the low gas velocity in the meter 1 segment. If we were to input the diameter as an AMMD of 0.86 μm GEOMM (Run 3), using the definition as described in Section 4.2.7.2, the resuspension amount is closer to the negative GEOMM results (see Figure 3-60). Furthermore, if we assume that the GEOMM is GMMD as described in Section 4.2.7.2 (Run 4), the resuspension amount is about the same as Run 1. Thus the modeling of GEOMM is very important. The effect of the aerosol density may not be significant, as shown by the results of Run 1 and Run 4. In this validation, if we use the definition of AMMD to model the lognormal distribution of the aerosol source in this experiment, MELCOR yields a closer agreement with the experimental data for the resuspension phase.

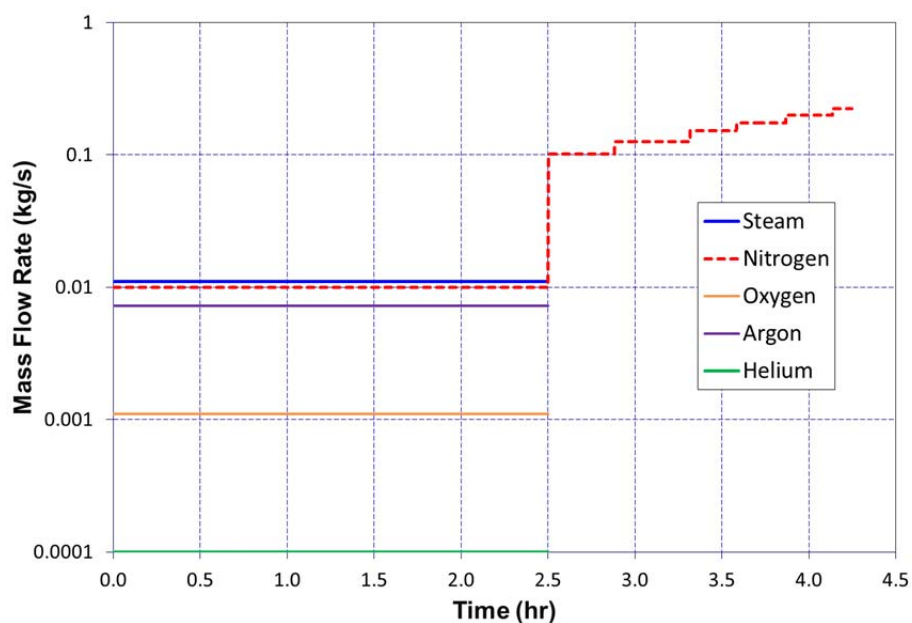


Figure 3-54. Prescribed Carrier Gas Mass Flow
(0 to 2.5 hr for Deposition Phase, 2.5 to 4.25 hrs for Resuspension Phase).

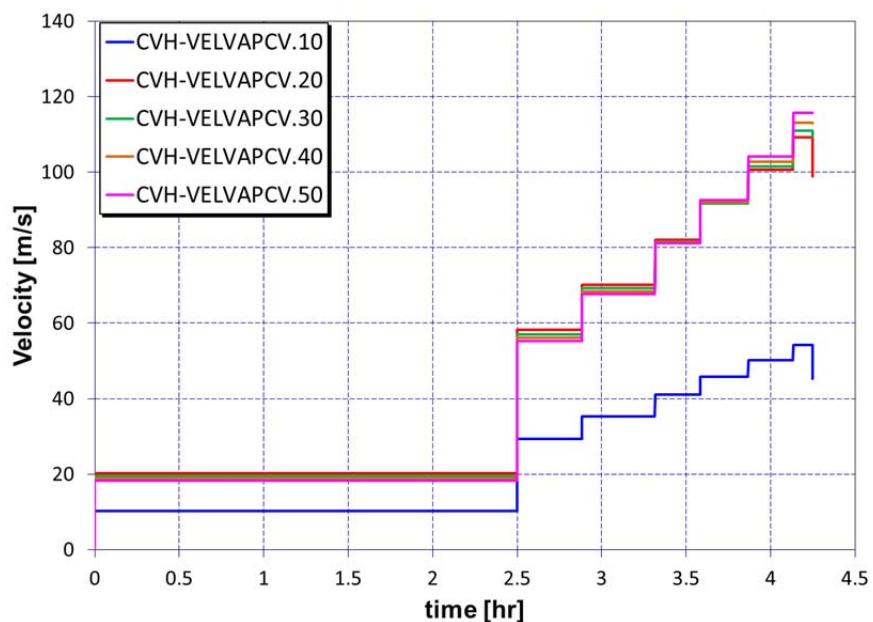


Figure 3-55. The Calculated Control Volume Gas Velocities Used in Calculating the Resuspension of Aerosol.
(10 for meter 1 segment, 20 for meter 2 segment, etc.).

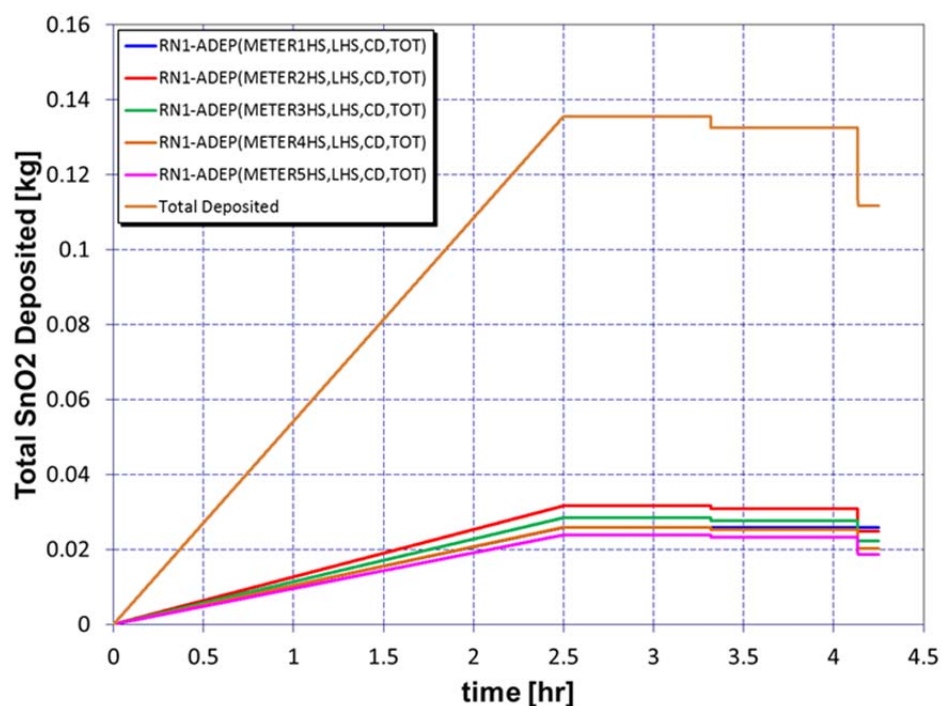


Figure 3-56. Calculated Deposition Mass as a Function of Time (Run 1).

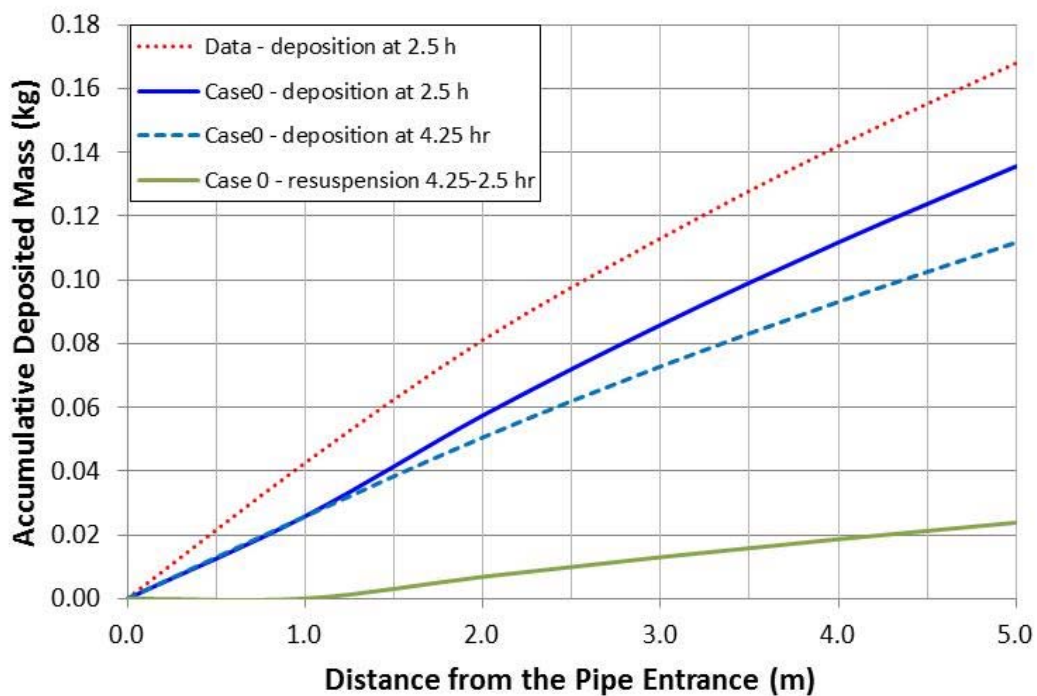


Figure 3-57. Calculated Accumulative Masses at the Deposition Phase and Resuspension Phase for GEOMM = 0.43 μm (Run 1).

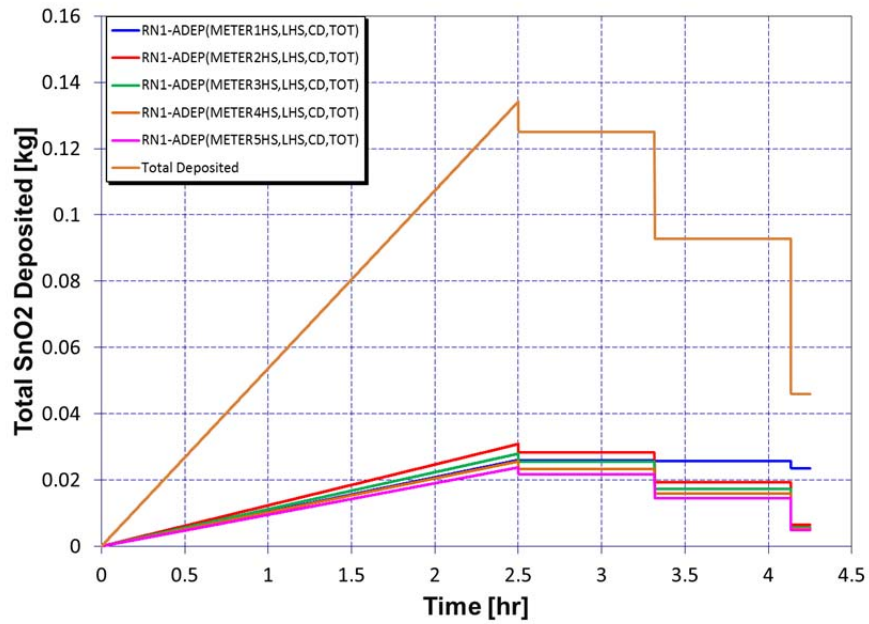


Figure 3-58. Calculated Deposition Mass as a Function of Time (Run 2).

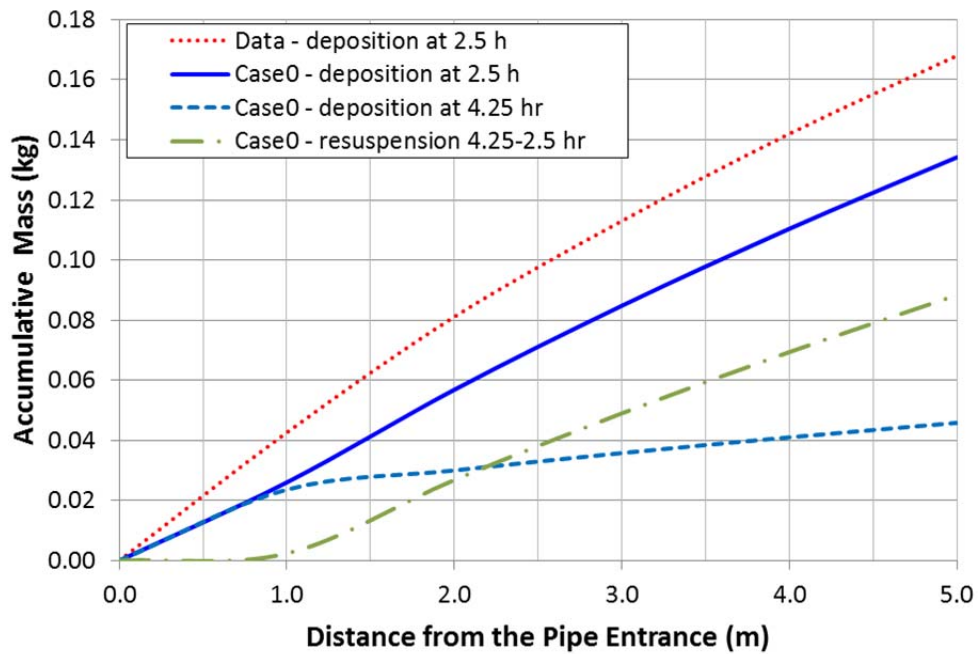


Figure 3-59. Calculated Accumulative Masses at the Deposition Phase and Resuspension Phase for GEOMM = $-0.43 \mu\text{m}$ (Run 2).

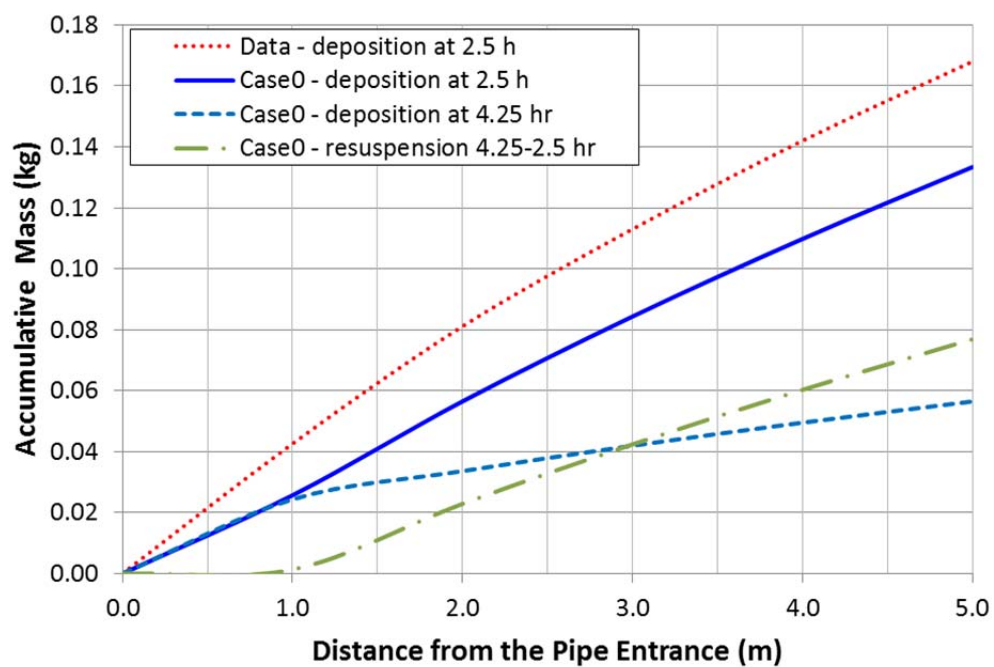


Figure 3-60. Calculated Accumulated Masses at the Deposition Phase and Resuspension Phase for GEOMM = $0.86 \mu\text{m}$ (Run 3).

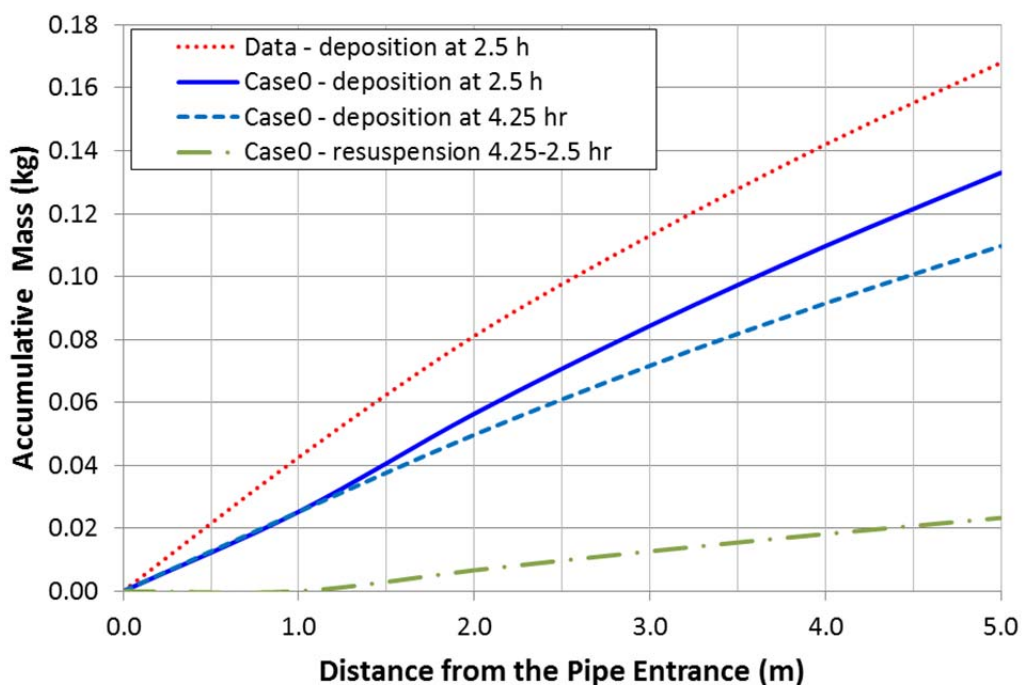


Figure 3-61. Calculated Accumulated Masses at the Deposition Phase and Resuspension Phase for GEOMM = $0.43 \mu\text{m}$ with Aerosol Density = 1000 kg/m^3 (Run 4).

3.4 Summary and Conclusions

This chapter summarizes the review of the reactor experiments and analytical validations available. The current MELCOR 2.1 assessment report provides a number of validation experiments, particularly for thermal-hydraulics and aerosol physics/transport. The applicability of many experiments validated in this assessment report was described. In most parts, the range of the applicable experiments cover the range encountered in the DOE non-reactor nuclear facilities well. The range includes thermal and pressure conditions, aerosol species, and aerosol physics, such as agglomeration, depositions, and resuspension. Other important conclusions are as follows:

- Analytical validation provides simple problems to benchmark thermal-hydraulic models and aerosol physics models in MELCOR. Although the current MELCOR 2.1 assessment report did not include any analytical aerosol validation, the addition of a simple analytical aerosol problem should address this deficiency.
- Reactor experiments presented in this letter report are mostly included in the MELCOR 2.1 assessment report with these findings:
 - Some experiments that were intended for modeling core heat-up and degradation, and modeling of the ex-vessel debris interactions, are not appropriate for DOE non-reactor nuclear facilities.
 - Many of the separate effect and some integral experiments that are designed to address thermal-hydraulics and aerosol physics are applicable for LPF determination using MELCOR 2.1.
 - Many containment thermal hydraulic experiments may be applicable for LPF determination, particularly for those experiments focusing on thermal-hydraulics in terms of heating, cooling, condensation and transport.
 - Specific experiments related to spray and hydrogen burn may be applicable for LPF determination, since spray can be used in modeling the water sprinklers, and hydrogen burn is possible at a DOE facility if hydrogen gas is used in the processes or is generated due to radiation or decomposition.
- Additional experiments and analytical validations have been recommended for the inclusion of this research, some of which are being funded under the NRC assessment project.

In this chapter, we provided the experiment validations from DOE-HDBK-3010 for the MELCOR code, in addition to experiment data from the reactor safety applications. In particular, we provided early results for validations with the pressurized and spill experiments. The results show that MELCOR can be validated with experiments. The use of a detailed MELCOR nodalization is recommended for both pressurized and spill experiment validations. However, because MELCOR is a lumped parameter code, it requires additional information from experiments, such as actual release distribution out of the PARE experimental chamber for the pressurized release. In addition, the fluid velocity profile is needed, especially in a free fall spill

case, since aerosols in MELCOR do not influence hydrodynamic materials. In this case, the results from a CFD code may help. We conducted a case using the results from NSRD-11 project [Louie 2016]. Using CFD code results seems to work well. We also conducted other experiment validations using data from the Handbook as well. We have modeled the gasoline pool fire experiment done at the wind tunnel apparatus attached to the RART facility. Because MELCOR currently does not model the entrainment of the contaminant from fire, we rely on the results from CFD code, such as Fuego. Using the NSRD-6 results [Louie 2015], we were able to model the gasoline fire combustion and source the combustion energy and by-products to MELCOR model and the contaminant (UO_2).

The computations of the combustion and by-product generation were done using the control function (CF) package. Chapter 4 describes how we model fire accidents using MELCOR. In fact, MELCOR can be used to model fire scenarios, which we have demonstrated in the LLNL enclosure fire experiment, even though MELCOR does not have a built-in combustion model and a dynamic hot gas layer. Using the control function to explicitly model the combustion of methane gas to allow the removal of oxygen and addition of the CO_2 and H_2O into the atmosphere can be done. In fact, the results compared well with the experiment data in terms of the hot gas layer temperature. It is comparable with CFAST prediction as well.

To test the recent aerosol resuspension, we modeled the resuspension phase of the STORM SR-11 experiment, in which the deposition phase was modeled in the recent published MELCOR assessment report [Humphries 2015c]. The results show that the MELCOR resuspension model agrees with the experiment data.

We believe that the validation cases discussed in this chapter are quite applicable to the DOE facility accident analyses. This should provide the confidence level for which MELCOR can be used in the LPF applications.

4 BEST PRACTICES

This chapter describes the best practices for using MELCOR 2.1 for LPF applications. Although the obsolete MELCOR 1.8.5 guidance report [DOE 2004] and other existing literatures provide some default values and recommendations for using MELCOR, we intent to provide a more detailed best practice information in using MELCOR to model a number of accident conditions, such as explosions, fires, inadvertent nuclear criticality and spills. These postulated accident conditions, except inadvertent nuclear criticality, are commonly found in most DOE facilities.

In this chapter, the best practices are provided based on the validation efforts described in the preceding chapters of this report, particularly in Chapter 3 which the MELCOR 2.1 validations are discussed. We provide the best practices per each accident condition. We will also summarize the useful information from the previous guidance report [DOE 2004] and other literatures that are useful for modeling LPF.

4.1 Accident Types

This section describes the major types of accidents that can occur across the DOE complex. Table 4-1 describes the common accidents encountered across the complex. As shown in this table, an earthquake can cause the loss of confinement to induce spills, including induced explosion and/or fire. In most cases where we discuss a seismic event, we often refer to its induced accident, such as spill, explosion or fire. A seismic-induced spill is also possible. In general, fires are the most common accidents found in the DOE complex. After fire, explosions can occur in the complex induced by a fire. Nuclear criticality or inadvertent criticality can occur when a sufficient quantity of special nuclear material (fissionable materials) is presented. Thus, the fissionable material is limited to the places in the complex that would have the potential for a nuclear criticality accident. Spills are considered to be the least in terms of source term, as shown in this table. The following subsections discuss the four major accident types associated with the use of MELCOR for LPF applications.

Table 4-1. Effects and Descriptions of Major Accident Types [Louie 2015]

Accident Type	Description	Typical Source Term Severity*	
		Worker	Public
Earthquake	Earthquakes often cause the loss of confinement and induce spills first. In addition, they can cause induced explosion and fire	significant	significant
Explosion ^A	Explosions usually occur within 10 ⁻⁴ s or longer time ranges with a large energy surge. Detonation creates shock waves and deflagration creates blast effect. Explosions can be chemically and physically induced. A chemically induced explosion tends to yield a more energetic event than a physical explosion, because of accompanying product gases. Physical explosion is due to pressure buildup.	significant	significant
Fire ^{A,B}	Duration of fire, ranging from minutes to hours, depends on the amount of combustible (flammable liquid or solids) available and other reactants that yield fires.	significant	significant
Nuclear Criticality ^C	An event that depends on the available fissile/fissionable material presence, geometry, reflection, moderation and other conditions allows nuclear excursion to occur.	significant	Minor ^D
Spill	This event includes drops (free-fall), which usually yield the least release in comparison to other accident types.	significant	extremely small

*This measures the dose consequence to both workers and public – significant means that the dose associated to this accident type generally would result in large source term, minor means that because of distance and magnitude of the accident a small source term would result, and

extremely small means that the airborne release fraction for this accident type is generally very small, and the resulting source term may not have an effect. PuO₂ is a hazardous material that could contribute most of the dose consequence.

^A In some accidents, explosion can lead to secondary fire or vice versa.

^B Although the amount of energy release per unit time for fire is much smaller than that of the explosion, the long duration could yield a total energy that could exceed the total energy release from an explosion.

^C Unlike a chemical explosion, where the explosion may be a point, a real or a segment source, nuclear criticality usually associates with a volume, because criticality requires some homogeneity in the solution and solid to permit nuclear excursion to occur, which may last from a few seconds to minutes; the nuclear excursion will not involve large product gases. Only a small portion of gases and vapors may result from fission.

^D Nuclear excursion accompanies gamma and neutron radiation, which may not have a direct exposure to the public, because of the distance rule, assuming that the facility structure and ventilation could contain most of the fission-induced airborne radionuclides.

In most cases of accident scenarios, such as explosion, nuclear criticality, and fire, the user can specify the source of mass and energy to the control volume input where the accident is occurred (using – CV_SOU record, if hydrodynamic material is involved). If using an aerosol source, such as the by-product aerosols, then the source should be input through RN1_AS record of the RN package.

4.1.1 Explosions

This section discusses the explosion accident types associated with the use of MELCOR for the LPF determination. As shown in Table 4-1, explosions can be induced by seismic events as well as induced by another explosion or fire event. Explosions that we usually encounter at a DOE complex are mainly chemical explosions such as solid (high) explosives, combustible liquid (i.e., gasoline), and combustible gases (i.e., natural gas and hydrogen). Two types of explosions can be categorized: detonation and deflagration. Detonation is usually associated with solid explosives, and the duration is much shorter compared to deflagration. Detonation is more powerful, whereas deflagration is usually associated with the flammable gases. However, gas detonation can be possible, especially when the explosion is confined [Louie 2004]. The ability to model explosion as a part of LPF determination is necessary.

In this section, we provide guidance to model explosions in MELCOR. It is important to understand the failure of the structures within the facility if an explosion has occurred. As shown in Table 4-2, the failure of many structures could be possible at about 1 to 5 psig (3.45 to 31 kPa). About 1-2 psig (3.45-13.8 kPa) can fail the ventilation ducts in a facility. Any failure of the structures within the facility would aid to add or subtract flow paths or volumes in the MELCOR model. To determine the failure of the structures within a facility, a number of methods have been done in the past for estimating overpressures and impulse of an explosion from the high explosive to flammable gas. Both an analytical approach and the aid of a computer code have been used. The following two sections will describe the analytical approach and a computer code method.

Table 4-2. Estimate of Blast Overpressure for Structural Damage [Merrifield 1989]

Pressure		Damage
(psig)	(kPa)	
0.5-1.0	3.45-6.89	Large and small windows usually shattered, window frames failure
2-3	13.8-20.7	Non-reinforced concrete or cinder brick walls failure, 8-12" (20.32-30.48 cm)
4.5	31	Severe distortion to frames of steel girder framed buildings

4.1.1.1 Analytical Approach

The analytical approach described in this section provides a method to estimate the failure of the structures or estimate an approximate overpressure due to a blast so that it can be modeled or confirmed using the MELCOR simulation. A number of reference documents can be useful for describing the analytical approach for modeling explosions as overpressures [AIChE 2010, Baker 1977, DOE 1992]. In this section, the analytical models described here are referenced in [Bixler 2016].

Blast overpressure models discussed herein are based on shock wave propagation into the surroundings once the pressure vessel breach has occurred [AIChE 2010]. Many of the analytical explosion methods, especially in the area of gas explosions in terms of detonation/deflagration (in relation to the flame speed) and confined explosions, have been examined in [Louie 2004]. While direct simulation of structural damage is possible with CFD analyses, it is unclear whether a CFD code will be available or chosen for future applications, given the limited availability of data to represent a facility. The analytical expressions presented below provide a means to estimate whether or not structural damage occurs. However, the methods are somewhat simplified and often may not be applicable for certain geometries.

In the Baker-Strehlow model, Sach's scaling (or Energy scaling) is used to estimate the overpressure and impulse as a function of the scaled distance ($\bar{R}$) for gas explosions [AIChE 2010] as,

$$\bar{R} = R \left(\frac{P_0}{E_{\text{exp}}} \right)^{1/3} \quad (4-1)$$

where P_0 = ambient pressure, E_{exp} = explosion energy, and R = standoff distance. The scaled overpressure ($\bar{P}$), is defined as,

$$\bar{P} = \frac{P_s}{P_0} \quad (4-2)$$

where P_s = side-on pressure.

A shock wave consists of positive and negative phases. Often only the positive phase is considered because it usually represents the largest change in pressure.

The scaled impulse ($\bar{i}$) is defined as:

$$\bar{i} = \frac{i a_0}{P_0^{2/3} E_{\text{exp}}^{1/3}} \quad (4-3)$$

where i = impulse, and a_0 = sound speed at the ambient condition.

To obtain the reflected overpressure (P_r) experienced by structures (e.g., walls), the following equations are needed [DOE 1992]:

$$\bar{P}_r = P_r / P_0 \quad (4-4)$$

And

$$\bar{P}_r = 2 \bar{P} + \frac{(\gamma + 1) \cdot \bar{P}^2}{(\gamma - 1) \cdot \bar{P} + 2\gamma} \quad (4-5)$$

As indicated in Equation (4-5) the scaled reflected overpressure ($\bar{P}_r$) is more than twice the scaled side-on pressure ($\bar{P}$). If $\bar{P}$ approaches to zero, then $\bar{P}_r$ approaches to $2 \bar{P}$. By substituting Equation (4-5) with Equation (4-2), it establishes the ratio of reflected overpressure and side-on overpressure. For air, $\gamma = 1.4$.

Based on the above scaled quantities and solid explosive blast data, one could obtain P_s and i graphically. Without using curves, Table 4-3 shows the fitted scaled side-on overpressure as a function of scaled standoff distance for vessel explosions.

Table 4-3. Fitted $\bar{P}$ equations* for Cylindrical Vessels [Ferradas 2006].

$\bar{R}$ Interval	Scaled Overpressure Equation	
	Cylindrical Vessel	Spherical Vessel
$0.1 \leq \bar{R} \leq 0.2$	$\bar{P} = 4.99 \bar{R}^{-1.92}$	$\bar{P} = 1.25 \bar{R}^{-1.92}$
$0.2 < \bar{R} \leq 1.5$	$\bar{P} = 0.86 \bar{R}^{-2.80}$	$\bar{P} = 0.58 \bar{R}^{-2.39}$
$1.5 < \bar{R} \leq 1000$	$\bar{P} = 0.49 \bar{R}^{-1.13}$	$\bar{P} = 0.26 \bar{R}^{-1.11}$

*The non-scaled dimensions are in the MKS (Meter-Kilogram-Second) system. For example, the pressure is in Pascals, distance is in meters, and energy is in joules. Note, $\bar{R}$ is measured from the center of the explosion, which means that this value cannot be zero because of the presence of the vessel.

As indicated previously, the information provided in this section is used to estimate the overpressure from the blast center of an explosive, either a solid explosive or flammable gas. Note that for a vessel explosion, about 50% to 80% of the remaining energy may damage

surrounding structures. Once the vessel fails, the expanded gas fills the accident room first and some energy is dissipated by this process. Any weak point in the accident room, such as unbolted equipment, ventilation ducting, windows, or doors, can be propelled by the expanding gas. A portion of the remaining energy may fail walls or ceiling, or drive the gas to adjoining rooms. Eventually, the expanding gas dissipates its remaining kinetic energy and attains equilibrium with the surrounding air. Therefore, both the shock overpressure and expanding gases from the pressure vessel breach event should be accounted for when assessing damage to the facility.

4.1.1.2 Computer Code Approach

The use of the computer code approach is often used, particularly if the facility is a high explosive facility where detonation is possible. The reason is that detonation or blast overpressure occurs very fast – in the order of milliseconds or less, as indicated in the previous section. For deflagration scenarios, MELCOR contains a deflagration model (BURN package) to model the hydrogen burn and carbon monoxide burn. See BURN package in the MELCOR 2.1 users guide for details of the input specification [Humphries 2015a]. To use this package for deflagration, the user must understand the models and their limitations. The reader is encouraged to consult the MELCOR 2.1 reference manual for the burn models in MELCOR [Humphries 2015b].

For dealing with solid explosion or blast in the order of 1 milliseconds or less, an explosion code was often used. In the past, we tended to rely on the use of an explosion code, such as BLASTX, to provide the destruction within the facility, such as failed doors, failed walls and/or damaged ventilation systems. For specific DOE facility types, particularly for the high explosive facilities such as the Device Assembly Facility at Nevada Nuclear Security Site, BLASTX code [Britt 2001] has been used to estimate the overpressure, impulse, and failure of structures. Both overpressure and impulse are output as a function of time, which can be used for MELCOR inputs. Because a blast is so quick, no feedback is needed in order to model the explosion in MELCOR. Although BLASTX code contains a number of high explosive data (including both explosive in a casing and without a casing), some conversions are of the explosive gas combustion energy into a solid explosive equivalent, such as TNT (trinitrotoluene). However, it is necessary to estimate the efficiency factor for converting the combustion gas energy to a TNT equivalent. The efficiency factor is greatly dependent on the confined condition of the gas explosion [Louie 2004, Louie 2005].

In MELCOR, both the explosion energy as a function of time and the associated by-product gases must be sourced into MELCOR using an input record CV_SOU within the CVH Package. Within the record of CV_SOU, the user can provide a mass or energy source. To model both explosion energy and by-product gas masses, both energy and mass sources can be specified in this record for the control volume where the explosion has occurred.

4.1.2 Fires

This section describes fire modeling using MELCOR. Before proceeding to model in MELCOR, it is necessary to understand the fire phenomena. A number of fire hazard analysis technique literatures are available for review. We chose to use the information from Hurley and Bukowski in the recent fire protection handbook [NFPA 2008]. In Chapter 7, Section 3, of this NFPA handbook, Hurley and Bukowski describe in detail the fire curve formation, which is necessary to create a power profile for the fire simulation. This power profile is often viewed as an isosceles trapezoid-shaped profile. Figure 3-20 shows the temperature profile of a typical fire curve, which contains an ignition phase, a growth phase, flashover, a fully developed fire region (steady burn), and a decay phase where the fire is distinguished. In general, all combustibles should have this shape; however, the magnitude of both growth and decay phases as described in this figure is greatly dependent upon the combustible involved: solid, liquid, and gas combustibles behave very differently. In this section, ignition, fire growth, steady burn and decay phases will be described briefly. A detailed explanation can be found in the NFPA handbook [NFPA 2008].

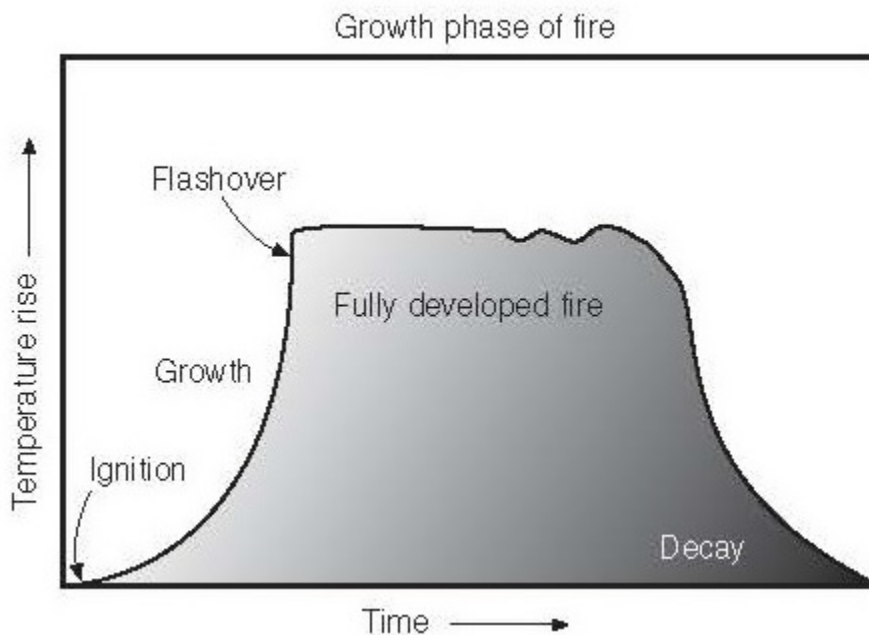


Figure 4-1. Typical Fire Curve [NFPA 2008].

4.1.2.1 Ignition

In order for the combustible to ignite, it may require an ignition source or spontaneous ignition. An ignition source, such as a spark or a flame initiates flaming, is often referred to as “piloted” ignition. The “non-pilot” ignition requires no ignition source, resulting from heating or a condition to carry out the combustion without any flame or spark. The temperature for the non-pilot ignition for the combustible is referred as its auto-ignition temperature. All materials must first be heated before ignition can take place, except for ignition sources of gases and liquid with

a temperature above their flashpoint. For gases, the oxygen concentration as well as the combustible concentration must be intermixed so that it can be ignited. The lower flammable limit of the gas combustible is required to start the combustion with an ignition source. Unless the temperature is at or above its auto-ignition temperature, then flaming is started. For solids, it is greatly dependent upon the form of the solids, which requires oxygen or other materials to ignite. For example, solid propellant may not require available oxygen to ignite. However, in order for it to ignite, the solid combustible must be heated sufficiently to release flammable vapors or gases. There are a number of ways to heat the solids besides the ignition source. Thermal radiation can be an effective way to initiate the solid for flaming. For liquids, the ignition temperatures must be at a temperature that is at or above its flashpoint. Flashpoint is defined as the minimum temperature of a liquid at which sufficient vapor is given off to form an ignitable mixture with air, near the surface of the liquid.

4.1.2.2 Fire Growth

Once ignited, the fire may grow to burn on the rest of the combustible(s), with the thermal conditions sustaining the fire, such as oxygen and other reactants completing the reaction. The slope of the growth as shown in Figure 3-20 depends on the combustible form and materials involved. In general, the fire growth has the following relation:

$$Q = \alpha t^n \quad (4-6)$$

Where Q = rate of heat release (W), α = fire intensity coefficient (W/secⁿ), and t = time (sec), and $n = 1, 2, 3$, etc.

In most case, $n = 2$ is used for flaming fires, except flammable liquids and other combustibles. When $n = 2$, it is often called the “t-squared” growth rate. As shown in Figure 4-2, the t-squared growth rate can be defined as slow, medium, fast, and ultra-fast for the ramp time of 600, 300, 150 and 75 seconds, respectively. Corresponding ramp time for each type of material/form is shown in this figure. For liquid pool fires, a short rise within ~100 seconds is possible. Solid materials such as solid wood may take a while to ramp up in the order of 1000 seconds. Thus the growth time is greatly dependent upon the material form, particularly for solids as shown in Figure 4-3. The slow curve is more for fires involving thick, solid objects. Therefore, the t-squared curves often represent fire growth starting with a reasonably large, flaming ignition source. There may be an incubation period before established flaming for small sources.

4.1.2.3 Steady Burning

Once the fire is established after the fire growth, the fire can be sustained with the continued supply of combustible materials and oxygen or reactants. Thus, the fire output is constant in this case, as shown in Figure 3-20. To predict fire temperatures, simple correlations are available for fully developed compartment fires. The Law’s method is given by [NFPA 2008]:

$$T_{\text{gas}} = T_{\text{max}}(1 - e^{-0.05\Psi}) \quad (4-7)$$

Where $T_{\max}$ = the maximum temperature of the flame, Ψ is given by:

$$\Psi = \frac{m_f}{\sqrt{A_{\text{surface}} \cdot A_v}} \quad (4-8)$$

Where m_f = mass of fuel (kg), A_{surface} = total surface area seen by the fire (m^2), and A_v = ventilation area opening (m^2).

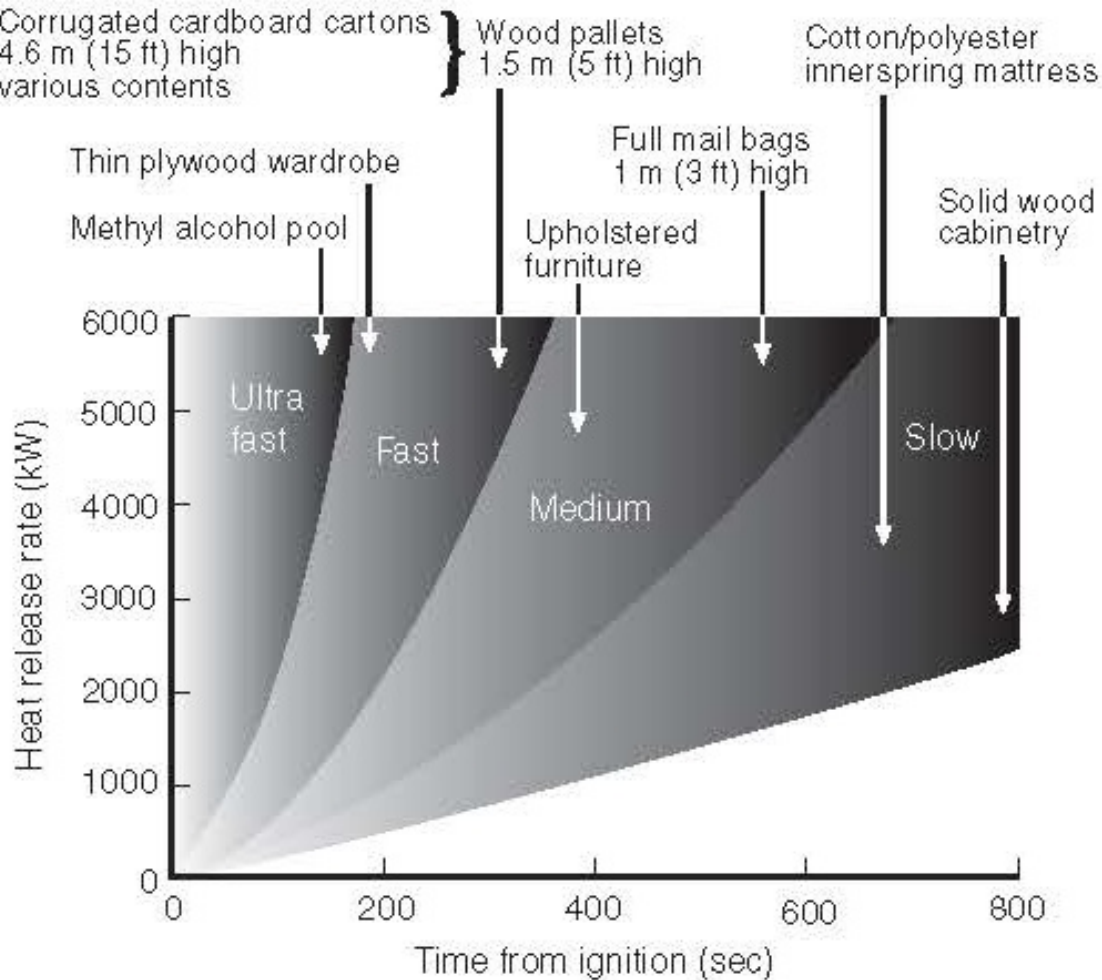


Figure 4-2 .T-Squared Growth Curves [NFPA 2008].

Table 2-9.2 of [NFPA 1995] lists a number of hydrocarbons' thermodynamic equilibrium properties, which includes the lower limit (LL), stoichiometric limit (SL) and adiabatic temperatures. Thus the adiabatic SL temperature for hydrocarbons is 1700 K, for carbon monoxide is 1450 K, and for hydrogen is 1090 K. This temperature can be used for $T_{\max}$.

In calculating the amount of thermal radiation from the fire to the surfaces, the following simple radiation model can be used:

$$q_r'' = \varepsilon_{\text{gas}} \sigma (T_{\text{gas}}^4 - T_{\text{surface}}^4) \quad (4-9)$$

Where q_r'' = radiation power flux, ε_{gas} = emissivity of gas mixture, σ = Stephan-Boltzmann constant ($5.67 \times 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$), T_{gas} = gas temperature given by Eq.(4-7), and T_{surface} = temperature corresponding to the surface area. It is assumed that all surfaces are at the same temperature, even though the surface temperature may be different because of the view angle and surface type. A complicated thermal radiation model considers the view factor and atmosphere absorptivity.

The emissivity of the gas mixture can be calculated as a sum of individual gases in the mixture. For water vapor, its emissivity can be a function of its vapor pressure and path length, the distance to the structure surface. The emissivity of carbon dioxide is based on similar parameters, except that its vapor pressure at constant is about $3 \times 10^{-4} \text{ atm}$.

To estimate the amount of combustion power loss to thermal radiation, F_{rad} , one can use Eq.(4-9) to estimate the radiative heat flux loss to the surfaces. According to Table 3-11.9 of [NFPA 1995], methane gas has a flame radiative temperature of 1289 K and an emissivity power flux at 157 kW/m^2 . In addition, Table 3-11.8 of [NFPA 1995] lists a number of F_{rad} for the methane gas and other hydrocarbons. In addition, this table lists the value of the fuel mass fraction that would produce carbon particles while the combustion occurs. For methane, it is 0.189.

4.1.2.4 Decay

Fire eventually subsides as the available combustible, oxygen, or reactants become limited or exhausted. Of course, the suppression is also a cause of the fire decay. In general, a decay rate of 10° C/min or 7° C/min can be used for fires with a predicted duration of < 60 minutes or > 60 minutes [NFPA 2008].

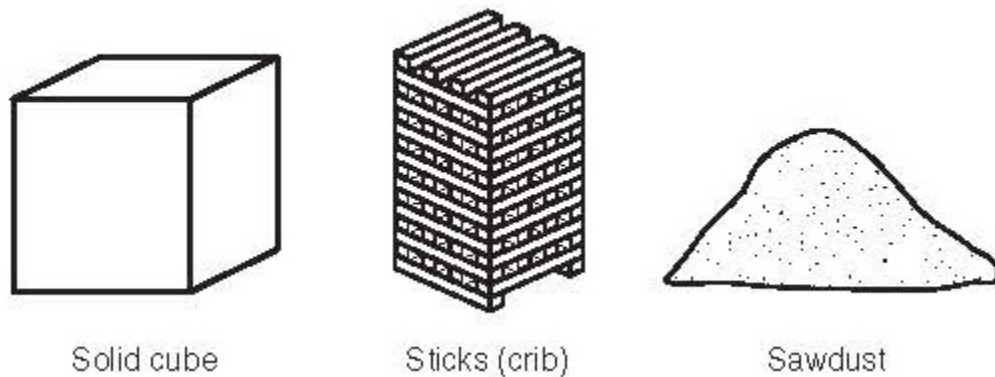


Figure 4-3. Dependence of Fire Growth on Combustible Form, Particularly for Solids [NFPA 2008].

4.1.2.5 MELCOR Modeling of Fire

In this section, we validate MELCOR for modeling fire scenarios. To do that, we examined the CFAST verification and validation guide [Peacock 2016]. In this guide, a number of experiments are described. To validate MELCOR, we are interested in one particular CFAST experiment, even though MELCOR currently does not have a hot gas layer model or combustion model besides the hydrogen and CO burn. In order to accurately model the dynamic hot gas layer in MELCOR, substantial code modifications may be required. To compensate for these inadequacies for fire modeling, the fire room must be subdivided to model the hot gas layer. MELCOR can only model a fixed hot gas layer as a volume. In reality, this layer should grow or sink depending on the state of the fire and convection surrounding the fire room. In addition, we can model the combustion using control functions in MELCOR, even though the modeling is explicit in nature. Suggestions for modeling a fire using MELCOR are as follows:

- Once the reaction of the combustion is identified, the depletion of the reactants and the production of the by-products are required to input to MELCOR appropriately to capture the internal energies as well as the mass sinks or sources.
 - *Hydrodynamic materials as reactants input to the CVH package as an external sink.* For example, the depletion of oxygen is modeled as a negative mass source and its associated heat changes. In this case, it should be modeled as the atmosphere temperature of the fire room.
 - *Hydrodynamic materials as by-products input to the CVH package as external sources.* For example, the production of CO₂ and water vapor in the combustion of methane gas is modeled as positive mass sources.
 - *The combustion power can be modeled to be sourced into the atmosphere.* This powder is the end result of subtracting the thermal radiation heat loss from the combustion power of the fire.
 - *Aerosol materials as by-products input to the RN package as atmosphere aerosol sources.* Because aerosols in MELCOR are treated as traced materials, they do not contribute to the hydrodynamics. However, it is necessary to account for the reaction energy to be added to the hydrodynamics. For example, the reaction of sodium and oxygen produces the sodium peroxide and/or monoxide, which are treated as aerosols. Thus the reaction energy needs to be included into the system. Therefore, the introduction of a very small quantity of hydrodynamic material and the associated reaction energy may be required.
- To model the reaction or burning of the combustibles effectively, the stoichiometric reaction needs to be identified. For example, the burning of methane gas requires that one mole of CH₄ reacts with 2 moles of oxygen to generate one mole of CO₂ and 2 moles of hydrogen.

- o Since MELCOR uses mass, *the conversion of mass to mole requires the molecular weight of the reactants and products for the reaction.*
- o *Burning rate must be defined as kg per second of the combustible being modeled.*
- o *Combustion energy rate is in terms of joule per unit mass of the reactant, whether the reactant is a combustible or oxygen.*
- o Because the high radiation temperature of the fire, *some fractions of the combustion energy may be lost to the surfaces of the enclosure.* Therefore, this fraction loss is estimated using Equation (3). Since methane gas is hydrocarbon, its adiabatic flame temperature is taken as 1700 K.
- As mentioned earlier, MELCOR does not contain a hot gas layer. To model a fixed hot gas layer, the fire room needs to be subdivided into several axial volumes. In most cases, each axial volume needs to be subdivided into several radial volumes to ensure recirculation occurs so that the hot temperature is at the top of the fire room.

In Chapter 3, we described the fire modeling of fire experiments using MELCOR. This section discusses the described model and captures some best practices for modeling fires. The modeling of the current flow is very important, as described in [Jordan 2003], during the fire, particularly when the hot gas layer grows and expands downward to reach an open, the hot gas escapes, while cooler air comes into the fire volume. This exchange needs to be captured. In Section 4.2, we discuss a new counter current flow model within MELCOR which can be used for this purpose.

In general, both the fire energy as a function of time and the associated by-product gases must be sourced into MELCOR using an input record CV_SOU within the CVH Package if the gases are hydrodynamic in nature. Within the record of CV_SOU, the user can provide a mass or energy source. For smoke or by-product non-gas materials, the input record, RN1_AS should be used to model the aerosol source in the control volume where the fire occurs. In addition, the user may use control functions to develop the combustion of the fire and the controls of the fire. For example, the user might include the end time of the fire or the time when the fire ceased due to water sprinkler activation or the unavailability of oxygen.

4.1.3 Inadvertent Nuclear Criticality

In modeling a nuclear criticality event, particularly for liquid criticality, the estimate of the energy to be sourced into MELCOR is based on the number of fissions occurred in a given criticality event. Typical excursion energy is about 10^{15} to 10^{18} fissions, and the excursion could last seconds or longer, depending on the number of pulses, particularly for the liquid criticality. 10^{18} fission yields about 32 MJ. Unlike in a chemical explosion, excursion does not associate with a significant amount of by-product gases. Thus the introduction of source energy input through the CV_SOU record should be used. In terms of fission product yields from a liquid criticality, DOE-HDBK-3010 [DOE 1994] shows the data for 10^{18} fissions. Note that criticality event due to flooding is not a major concern because only a few DOE nuclear facilities may

include significant amount of fissionable materials. In addition, nuclear excursion due to flooding to fissionable solids and containers with fissionable solid materials may not yield significant airborne release.

4.1.4 Spills

Spill is the least energetic event, compared to other major accident types described previously. The modeling of a spill usually involves the interaction of the gravitational force. The materials involved in spills include powders and liquids of interest. In MELCOR, we model powders and liquid droplets, other than water as aerosols which has not affected the thermodynamic materials. Thus, a gravitational spill involved with aerosols will not affect the air or gases in the atmosphere in MELCOR. Therefore, an estimate of the effect to the atmosphere must be provided to MELCOR in order to induce or introduce hydrodynamic conditions to initiate any changes. In the previous chapter on MELCOR validation, we simulated a gravitational spill experiment from the Handbook.

4.2 MELCOR Specific Models

Although MELCOR is designed for severe reactor accident applications, it is being used for non-reactor applications, such as for the spent nuclear fuel reprocessing, and LPF applications at DOE nuclear and non-nuclear facilities. We have included in Chapter 2a list of DOE facilities in which MELCOR has been applied for LPF. In general, the default values for the sensitivity coefficients described in MELCOR users guide [Humphries 2015a] should represent the best available value for generation applications. We recognize that there is uncertainty in each value and the default represents an average value analogous to the mean in a probability distribution. In each package input, there is a default value for the package – CV_DFT, HS_DFT, RN1_DFT, which may be applicable for LPF applications. Note that there is a global default for the entire problem, which is “EXEC_GLOBAL_DFT in the EXEC package. The options for the default values are “2.0” or “1.86” for MELCOR 2.1 or MELCOR 1.8.6, respectively. The second option simulates the MELCOR 1.8.5 or 1.8.6 results. Note that some of the defaults were based on MELCOR 1.8.5 experiences only. Below is a list of default values that were used in the containment analysis for design basis accidents. However, the reader is encouraged to examine the default values used for LPF applications.

Since there was specific guidance on using MELCOR for LPF applications in terms of sensitivity coefficients used in a dry volume, the adoption from the design basis accident studies done on comparing MELCOR and CONTAIN codes can benefit from applying MELCOR for LPF applications at DOE facilities [Tills 2009]. The suggestions provided here are intended to examine the thermal-hydraulic aspect of the simulations:

- Time-step: The maximum time chosen should be based on the accuracy (small time-stepping) in both the advancement of the control volume dependent variables such as pressure and temperatures, and the heat transfer from the atmosphere to heat structures.

- **Material properties:** Because MELCOR does not have an explicating modeling method for treating painted surfaces, a method must be specified. The effective, painted surface node conductivity is therefore included in the material properties (MP) package input, and it is specified for the surface node of painted structures in the HS package. The paint surface modeling may be applicable for hot cells at DOE facilities.
- **Structure heat and mass transfer:** The atmospheric natural convection between the heat structure and the atmosphere is recommended to increase from 0.1 to 0.14 for the sensitivity coefficient 4110 (natural convective correlation multiplier).
- **Heat structure node thickness:** This should be set to a fraction of thermal diffusion length. This value should prevent surface temperature oscillations that may develop for an explicit coupling of atmosphere and structure energy transfers.

This section describes the specific models to be used in LPF applications. These models include environment volume, filters, and spray.

4.2.1 *Environment Volume*

Beginning in MELCOR 1.8.6, and in MELCOR 2.0 and later, the user is no longer required to model the environment volume as a large volume (as required in MELCOR 1.8.5). Typical environment volume should be modeled at least at the same height as the facility volume being connected. Any deviation from it may result in unexpected flow from the donor volume or vice versa. In addition, the time-dependent volume is often used to model the environment, if the ambient condition is modeled.

4.2.2 *Door Gap Model*

This model is important, particularly if the facility maintains a negative pressure via forced ventilation, so that door gap is often used to allow the model to maintain this negative pressure. The ambient condition is usually higher than the facility, so that the negative pressure is maintained as in the tier confinement system as shown in Figure 2-1. The door gap specification for a steel door and frame is provided in Table 4-4. Note that the modeling of these clearances is important because of the potential release path for the aerosol out of the facility, which may enhance LPF. It is particularly important when the forced ventilation system is unavailable. The next section discusses the influence of external wind that could play a role of increasing LPF through these clearances.

Table 4-4. Clearance Dimensions for Standard Steel Doors and Frames

Data from ANSI A250.8 – 2014, Specification for Standard Steel Doors and Frames (SDI-100)	
Description	Maximum Dimension
Between door and frame	1/8" (3.2 mm)
Between door bottom to frame bottom	3/4" (19.1 mm) ± 1/16" (1.6 mm)
Between face of door and door stop	1/32" (0.8 mm) to 3/32" (2.4 mm)

4.2.3 Effect of External Wind

As mentioned in the previous section, the facility may not be sealed tight to maintain negative pressure inside. The gaps in the external doors of the facility may subject to enhancing LPF through the effect of external wind, particularly when the active ventilation system is not available or destroyed. Thus, the pressure drops (ΔP) between the pressure in the facility and the environment is greatly dependent upon the wind speed (u_{wind}), air density (ρ_{air}) and pressure coefficient (C_p) as shown in the following relation:

$$\Delta P = C_p \rho_{\text{wind}} \frac{u_{\text{wind}}^2}{2} \quad (4-10)$$

C_p in Equation (4-10) is given in Table 4-5.

Table 4-5. Typical C_p , Pressure Coefficients [DOE 2004]

Wind Direction	Value
Upwind	0.7
Downwind	-0.4
Side and top of building	-0.35

4.2.4 Countercurrent Flow Model

The countercurrent flow (CCF) model in MELCOR can be used to enhance the countercurrent flow in a fire scenario as shown in Figure 4-4. As shown in this figure, the CCF model can be used to model a doorway between the fire room and the adjacent volume (i.e., corridor). This CCF model has been used in modeling the natural recirculation gas flow in the severe reactor accident application between the hot reactor vessel (analogous to a fire room) and cooler heat exchanger (analogous to a corridor) via the hot leg (analogous to a doorway). The CCF model is placed in the hot leg or doorway as shown in this figure.

The CCF model is used to connect two flow paths: the top and bottom of the doorway, for example. The top flow path may have flow in one direction, and the bottom flow path may have flow in the opposite direction as in the top flow path. This model is located in the FL package input (FL_CCF). This model is only applied for the horizontal flow paths.

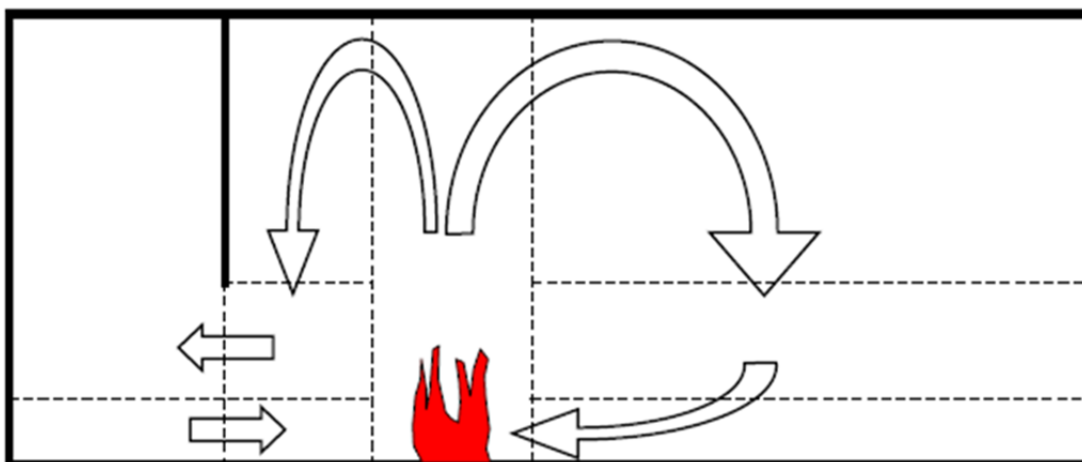


Figure 4-4. Example of a MELCOR Model of a Fire in a Room [Jordan 2003].

4.2.5 Filters

In MELCOR, there is a filter model described in the RN package, which can be used to model a filter component of the ventilation system. Because a filter component is a model for capturing aerosols, its function can be represented as an inter-volume process via a flow path. RN2_FLT is the input record for modeling a filter component. This component is associated as a flow path in MELCOR. It can be used to remove aerosols or fission product vapors. In MELCOR, the aerosol removal is done as a global decontamination factor. In addition, the model can be specified as radionuclide class, aerosol size, etc. Users can input the performance of the filter, the charcoal filter specific, etc. All these are discussed in Section 3.18 of the RN users guide.

Table 4-6. Specific Filter Input Records

Input Record	Brief Description
RN2_FLT	Specifies the associated flow path in MELCOR, and type of removal: aerosol or FP vapors. The user can specify the function of the global decontamination factor (DF) or class specific through RN2_FCL
RN2_FCL	Allows users to input MELCOR aerosol class removal specific data as DF.
RN2_FDA	Allows users to specify DF for class specific. It is only used for aerosol type filter.
RN2_FDC	Allows users to model a more complicate aerosol class specific DF than in RN2_FDA.
RN2_FIM	Provides a way to model an existing filter with contaminant on it.
RN2_FAC	Specifies the performance characteristics of aerosol filters, including minimum size can be removed via a DF, and the pressure drop across it, and failure of the filter information. This allows to model the actual filter used in a facility.
RN2_FVC	Similar to that of RN2_FAC, but for the charcoal filters for capturing fission product vapors.
RN2_FTD	Provides the thermal desorption data for charcoal filters.
RN2_FRD	Allows users to model radiolytic desorption data for charcoal filters.
RN2_FCD	Provides a way to model combustion of charcoal filters.

4.2.6 Spray

The spray model in MELCOR is intended specifically for the containment engineered safety feature of a nuclear reactor plant. This model is specifically used for cooling the containment, and reducing the pressure in the containment. At the same time, it can be used to remove aerosol in the atmosphere. As described in Chapter 4 on the reactor validation studies, there were a number of experiments used to validate the spray model in MELCOR (see Table 3-2). These tests include CSE Spray A9, JAERI Spray, and NUPEC. In general, this model can be used for creating a similar effect for modeling as a water sprinkler system in DOE facilities. However, there are a number of limitations when using this spray model for the water sprinkler system in a room.

In the MELCOR reference manual [Humphries 2015b], a detailed model description of the physics and limitations are described. The user's guide for this spray package is provided in Table 4-7. As shown in this table, the input records are intended to reduce the atmosphere's pressure and temperature. If the intent is to remove aerosols from the atmosphere, specific radionuclide input records are required (see user's guide for the input descriptions). For fighting the fire, the user may combine the use of the spray model and the control functions describing the combustion to terminate the fire. The use of the spray model for a water sprinkler model may require elevating the water sprinkler system to a safety class designation.

Table 4-7. Specific Spray Input Records.

Input Record	Brief Description
SPR_SRD	Specifies the reservoir data, such as the storage tank where the water sprinkler is located
SPR_DTFR	Specifies the spray droplet temperature and flow data.
SPR_DSD	Input the spray droplet size distribution. If aerosol removal is modeled, additional care is required (see the users guide for guidance).
SPR_JUN	Allows users to model spray droplet fall through to other volumes.
SPR_SUMP	Provides a way for the model to recirculate the spray source back to the spray system. This may not be applicable for the water sprinkler system.

4.2.7 Aerosol Modeling

One of the major reasons we use a computer code, such as MELCOR, is to estimate the respirable aerosols to be released out of the facility or enclosure (see Chapter 2 for a more detailed discussion on this topic). As described in Chapter 2, MELCOR contains MAEROS, which models the agglomeration and various deposition modes of aerosol transport. Recently, a simple resuspension model has been added to MELCOR [Young 2015]. For the detailed input and model options in MELCOR, the reader is encouraged to consult the MELCOR manuals [Humphries 2015a-c]. In this section, we provide the guidance for modeling aerosols in the context of LPF applications.

4.2.7.1 Material Density

In the RN package, the aerosol material density is defaulted to 1000 kg/m³, the density for pure water. If the aerosol contains two or more materials, their densities should be used for simulating aerosol dynamics. The following four concepts should be taken into account for the

treatment of the aerosol density until MELCOR is updated to include the actual density of materials.

1. For hygroscopic material such as water-soluble material or material in a steam environment, the use of the default aerosol density of water is appropriate since particles will absorb water from the atmosphere, and the mass of water will, in general and for our purposes, dominate the particle mass. However, this situation may not be true in most accident conditions at DOE facilities.
2. For a dried condition and insoluble aerosol, a mass-weighted density should be used. For example, if the aerosol mass is 75% SnO₂ which has a density of 6950 kg/m³, and 25% CaCO₃ which has a density of 2710 kg/m³, then the density MELCOR should use is $(0.75)(6950) + (0.25)(2710) = 5890 \text{ kg/m}^3$.
3. The intermediate case when the existence of steam or the materials in the aerosol change with time present a more difficult situation to model. Until more detailed aerosol modeling is implemented in MELCOR, applying a time-average density based on the two rules given above is recommended.

4.2.7.2 Geometric Mean Diameter

In MAEROS, the geometric mass mean diameter, GMMD (D_g), for aerosol calculations is used. This diameter is a physical diameter which can be observed in a microscope or using a light scattering instrument which refers to an optical diameter. Other aerosol instrument, such as the cascade impactor, which measures the aerosol concentration as functions of aerodynamic diameter, uses the aerosol mass mean diameter (AMMD), D_a . For an approximation, the relationship between D_a and D_g is given by:

$$D_a = D_g \sqrt{\frac{\rho_{\text{aerosol}}}{\rho_{\text{water}}}} \quad (4-11)$$

Where ρ_{aerosol} = aerosol density and $\rho_{\text{water}} = 1000 \text{ kg/m}^3$. For example, a TiO₂ with a density of 4260 kg/m³ has D_g of 1.7 μm , then $D_a = 3.51 \mu\text{m}$ according to Equation (4-11).

In practice, MELCOR allows the user to provide the aerosol sources through the use of RN1_AS input record from the RN package. In addition, the user can specify the sectional distribution parameters in which the aerosol source will be distributed according to the user input for the section (or bin) of the diameters (see RN1_AS01 input record description in the MELCOR users guide [Humphries 2015a]). In brief, the RN1_AS01 record allows three options:

- Uniform distribution (no additional input values required)
- Lognormal distribution:
 - Requiring a source mass mean diameter (MMD) and the geometric standard deviation (GSD) to be given.
- Manual distribution through the use of the section-by-section method, in which the user is required to use the fraction of the source mass for each section or bin.

In most experiments, the MMD and GSD are given. If the MMD is given as D_g according to Equation (4-11), then ρ_{aerosol} in this equation should be assumed to be that of water. These should be reflected in the MELCOR inputs. If MMD is given as D_a , then the actual aerosol density should be used.

Note that the terminology of AMMD defined is the same as in the aerosol equivalent diameter (AED) used in most DSAs and in the Handbook [DOE 1994]. Equation 1-2 in the Handbook is defined AED for a single particle with all shape and slip factors included. It has the similar form as in Equation 4-11 above which the shape and slip factors are assumed unity. MAEROS treats these factors in the overall aerosol equations (see RN package reference manual [Humphries 2015b]).

4.2.8 Radiation Enclosure Model

A new thermal radiation model is available for the HS package. This allows the heat structure surfaces to see each other as a network. This new model includes the transmissivity of gas. Following are the key important options for this new model:

- Multiple enclosure networks can be defined. Each network with multiple heat structures is defined by the user.
- User defines ALL surfaces exchanging radiant heat:
 - Matrix of view factors connecting surfaces
 - View factors are constants and cannot be changed
 - Do not account for surfaces submerged below the pool
- Gases in the atmosphere:
 - Transmissivity accounts for reduction in thermal radiation between surfaces
 - Only one control volume is allowed to associate with all surfaces
 - User supplies the beam length for thermal radiation

To activate this new model, HS_RAD input record is used. This model is very useful in modeling fire scenarios.

5 SUMMARY, CONCLUSION AND RECOMMENDATION

This report discusses an NSRD project proposing the replacement of the obsolete MELCOR 1.8.5 LPF guidance report with the MELCOR version 2.1, since older versions before version 2.0 of MELCOR are no longer supported at SNL. First, we provided a review of the literature on LPF. We also provided a review of the obsolete guidance report, which did not contain any code validation, whereas this report describes and conducts code validations for both reactor and non-reactor applications. From the reactor applications, we reviewed the MELCOR 2.1 assessment report and identified the applicable reactor experiments that could be applied to DOE facilities.

We also examined experimental data from DOE-HDBK-3010 which could be applicable for accident conditions across the DOE complex. Then, we apply MELCOR 2.1 to analyze fire scenarios. In the past, the safety analysts at DOE facilities would first perform fire calculations using fire codes, such as CFAST. In previous DOE SB efforts, the results from CFAST are input to MELCOR for determining LPF. Here, we discussed modeling the fire scenario using MELCOR 2.1 and compared the thermal hydraulic predictions of MELCOR to experiment data and CFAST.

In addition, we described a validation on the newly implemented aerosol resuspension model in MELCOR 2.1. Aerosol resuspension is an important phenomenon which has been identified in the LPF literature as well as in DOE-HDBK-3010. Although we did not yield any resuspension data from experiments for the gasoline fire discussed in Section 3.2.3, we did validate the resuspension model using the STORM SR-11 experimental data discussed in Section 3.3.2.

In this report, we included a number of experiment validations from DOE-HDBK-3010: powder release and gasoline pool fire experiments done at RART at PNL. Additionally, we included two other validations: (1) to assess if MELCOR can model fire scenarios without using a fire code to provide input data, and (2) test the newly added aerosol resuspension model to MELCOR. We believe the validation cases discussed in Chapter 3 are applicable to the DOE facility accident analyses. This should provide the confidence level for which MELCOR 2.1 can be used in the LPF applications by SB analysts. In Chapter 4, we provided a number of best practices for SB analysts to model the major accident types often encountered at DOE facilities. Attempts have been made to provide guidance on the modeling of these accident types in MELCOR 2.1. We provided a detailed discussion on the modeling of fire, since it is the most common accident analyzed at DOE facilities. We also described many specific models in MELCOR that can be useful for LPF modeling applications, such as sprays and filters. Filter models have been greatly enhanced since MELCOR 1.8.5; the new filter models allow the user to model many related situations from filter decontamination factors to filter failure and the burning of filters.

Finally, we offer the following detailed conclusions and recommendations:

Reactor Experiments

- Analytical validation provides simple problems to benchmark thermal-hydraulic models and aerosol physics models in MELCOR. Although the current MELCOR 2.1

assessment report did not include any analytical aerosol validation, the addition of a simple analytical aerosol problem should address this deficiency.

- Reactor experiments presented in this report are mostly included in the current MELCOR assessment report with these findings:
 - Some experiments that were intended for modeling core heat-up and degradation, and modeling of the ex-vessel debris interactions are not appropriate for DOE non-reactor nuclear facilities.
 - Many of the separate effects and some integral experiments that are designed to address thermal-hydraulics and aerosol physics are applicable for LPF determination using MELCOR 2.1.
 - Many containment thermal hydraulic experiments may be applicable for LPF determination, particularly for those experiments focusing on thermal-hydraulics in terms of heating, cooling, condensation, and aerosol transport within the facility.
 - Specific experiments related to spray and hydrogen burns may be applicable for LPF determination, since spray can be used in modeling the water sprinklers, and hydrogen burns are possible at a DOE facility if hydrogen gas is used in the processes or is generated due to radio-decomposition.
- Additional experiments and analytical validations have been recommended for inclusion in this research. As shown in Section 3.1, these validations are being funded under the NRC assessment project.

DOE-HDBK-3010 Experimental Data

- The powder release experiments for the RART at PNL were validated for both gravitational spill and pressure releases.
 - A number of current MELCOR models have been used for the validation (1-volume, 5-volume and 15-volume models for RART).
 - The 15-volume model or a larger number of volumes is required, since it allows recirculation and better captures the aerosol effect, since the aerosol model in current MELCOR is based on concentrations. A larger volume will yield less agglomeration and settling, while a small volume tends to agglomerate and settle faster.
 - Because MELCOR does not function well when no flow condition is imposed on the model, such as in the gravitational spill case, a steady-state condition may require to be established for the model, before the simulation can proceed.
 - This would minimize the artificial flow, and
 - Some instability may occur when doing the steady state calculation.

Aerosol Resuspension Test

- The use of the STORM SR-11 experiment to validate the aerosol resuspension model in the current MELCOR is appropriate. Even though the gas velocity used in the experiment may not be commonly found in DOE facilities, it can occur in explosions or high pressure conditions.
 - The resuspension model in MELCOR yields results similar to that of the experiment.
 - In the validation tests, the treatment of the aerosol source diameter for the experiment may influence the resuspension results.

Best Practices Recommendations

- A number of suggestions for modeling accident scenarios, such as explosions, fires, nuclear criticality, and spills are described in Chapter 4:
 - The timing of the source with respect to explosion energy is important and on the order of microseconds to milliseconds. The time-step size needs to be comparable to the source table time values.
 - The modeling of the fire curve in fire scenarios requires a ramp up and decay as parts of the curve. The system time-step must be smaller than these two parts of the fire curve.
 - Based on the validation cases examined in Chapter 3, the current MELCOR (version 2.1) default values are adequate. Any deviation from the default values of sensitivity coefficients in CVH, HS and RN need to be carefully considered, selected, and documented.
- Using MELCOR 2.1 for LPF analysis is required, since this version has many thermal-hydraulic and aerosol physics improvements over MELCOR 1.8.5. Additionally, version 2.1 is supported by SNL, and version 1.8.5 and version 1.8.6 are not supported by SNL.
- Using the initial suspended material with agglomeration and/or deposition disabled for the simulation (instead of using “1” g mass) is recommended.
- Beginning with MELCOR 2.0, it is not recommended to model a large environmental volume on the order of 10^{10} m^3 . The use of the time-independent volume feature in MELCOR eliminates the need for such a large environment volume.
- Using the counter-current flow (CCF) model in the FL package better represents a counter-current situation in a fire scenario. This new model is an improvement over MELCOR 1.8.5.
- Use the new filter models in MELCOR version 2.1 for modeling the HEPA filter conditions experienced in accident situations (see Chapter 4 for more details).
- Use the SPR package to model the fire water sprinkler system (see Chapter 4 for more details).
- Use control functions to model a solid combustible burn for a fire scenario, since advanced features for the CF models are available in MELCOR 2.1. This is an

alternative method to using a fire code such as CFAST for generating the heat energy data (see Chapter 3 for a MELCOR simulation of fire scenarios).

- Important aerosol physics models have been validated through the use of experimental data and analytical models:
 - Agglomeration (see Section 2.1, Section 3.1, and Section 3.2),
 - Deposition (see Section 2.1, Section 3.1, and Section 3.2), and
 - Resuspension (see Section 3.3.2 for the validation).

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APPENDIX A

MELCOR Verifications

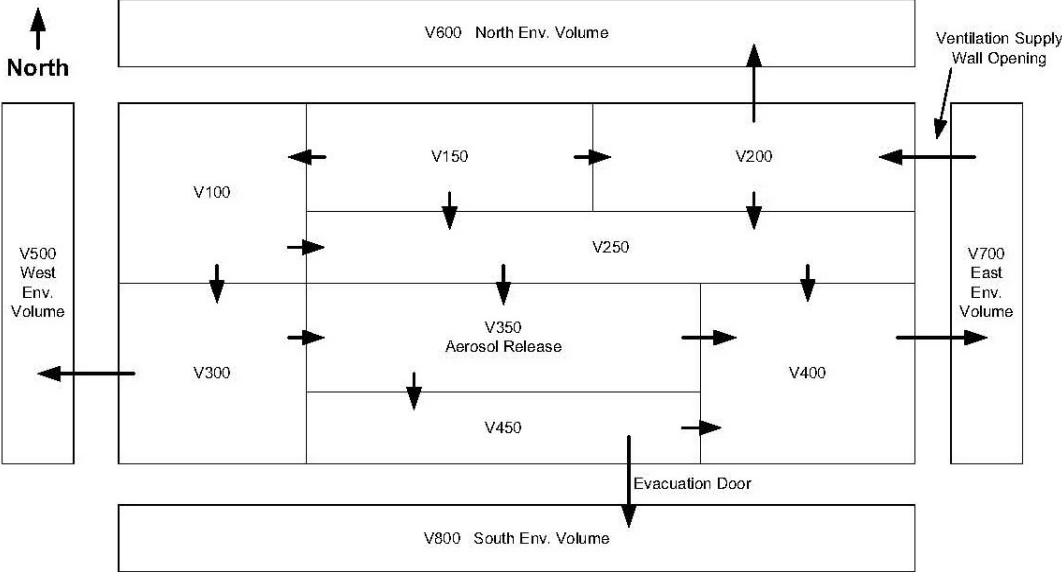
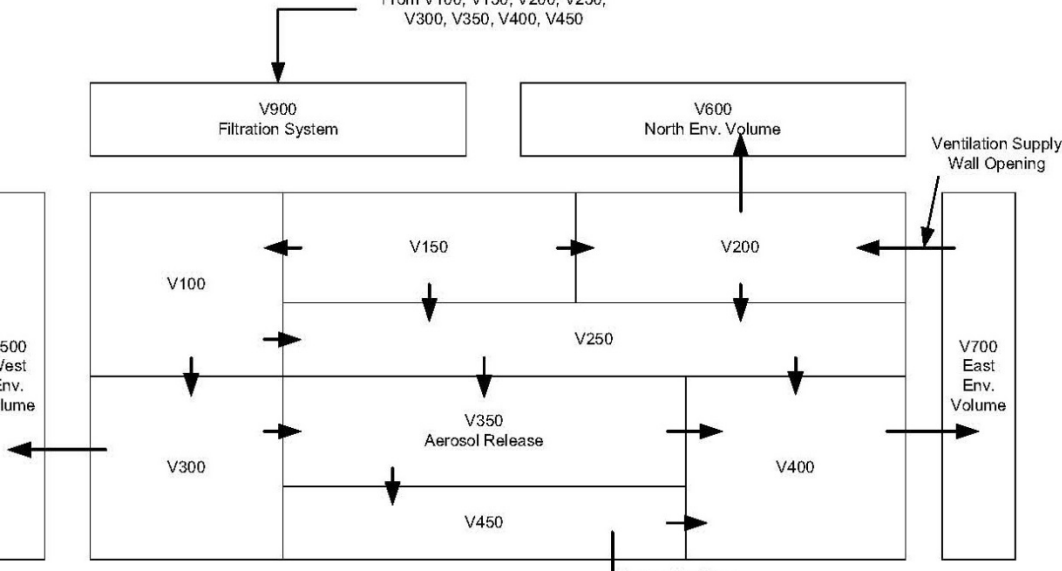
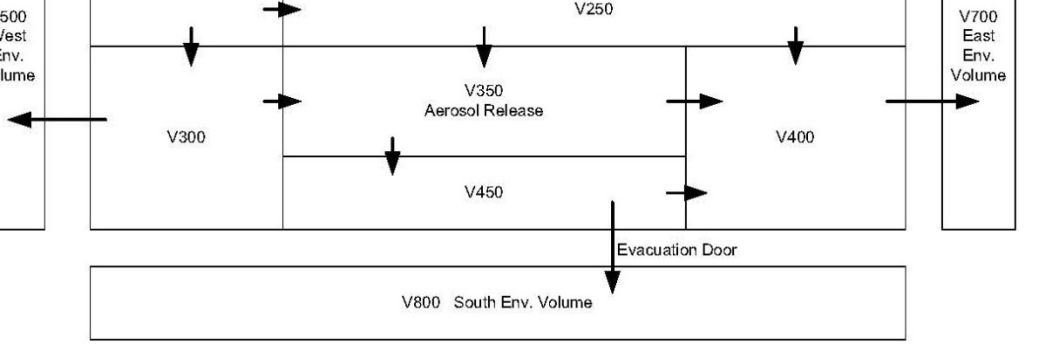
This appendix details verification problem sets that were described in the MELCOR 1.8.5 guidance report [DOE 2004]. The inclusion of these verification problem sets is done primarily to document the results generated from version differences, if any. The validation of the MELCOR code has been described in Chapter 3 of this document. Note that the intent of these verification problems is to demonstrate the code's applicability to many accident scenarios, which includes seismic events, spills, and fires. In this appendix, we document the verification problems from the 2004 guidance report using the obsolete MELCOR 1.8.5 [DOE 2004]. In addition, we are documenting the verification problems reported in LA-UR-03-7945 [Jordan 2003]. Note that this appendix was done as a part of the on-going assessment report for MELCOR 2.1 funded by U.S. Nuclear Regulatory Commission (NRC).

A.1 MELCOR 1.8.5 Guidance Report Problems

As described in Chapter 2 of this report, we reviewed the MELCOR 1.8.5 guidance report [DOE 2004]. In that report, a number of sample problems were conducted. In the past, safety basis analysts used these verification problems as the way to assure the quality of MELCOR 1.8.5 and MELCOR 1.8.6 without using any experiment validation. The analysts also documented any difference between code versions. In this section, we briefly describe the verification problems which include fire, seismic, and spill events from that report. Figure A-1 briefly describes each sample and shows its corresponding MELCOR nodalization.

Since the version of the MELCOR code used in the guidance report was MELCOR 1.8.5, it is necessary to run MELCOR 1.8.5, MELCOR 1.8.6 and MELCOR 2.1 to verify that code changes have not changed the acceptability of the results. Prior to conducting this comparison, it was reported in [Sanchez 2007] that there was an issue relating the assignment of the PuO_2 in Class 1 with the original input decks listed in the guidance report and the result discrepancy in the Appendix G sample problem from the guidance report. With that in mind, the input decks used herein have re-assigned PuO_2 in Class 8 instead, which is identical to those used in [Sanchez 2007]. Table A-1 shows the comparison of the major MELCOR versions and the results from the guidance report. As shown in this table, all sample problems except Appendix G of the guidance report show close agreement with different versions of MELCOR. The discrepancy in results of Appendix G of the guidance report is consistent with those reported in [Sanchez 2007].

Figure A-1. Sample Problem Descriptions in MELCOR 1.8.5 Guidance Report [DOE 2004].

Sample	Description
Appendix C – Building seismic event with powder spill	
Appendix D – Building seismic event with powder spill and exhaust ventilation operating	
Appendix F – Building seismic event with powder spill and post seismic fire and exhaust ventilation	

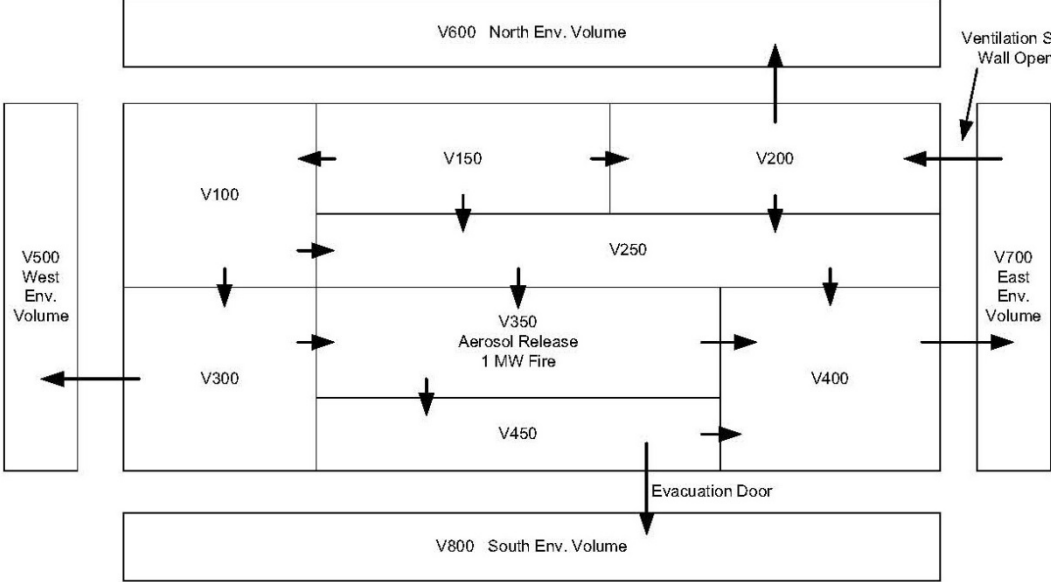
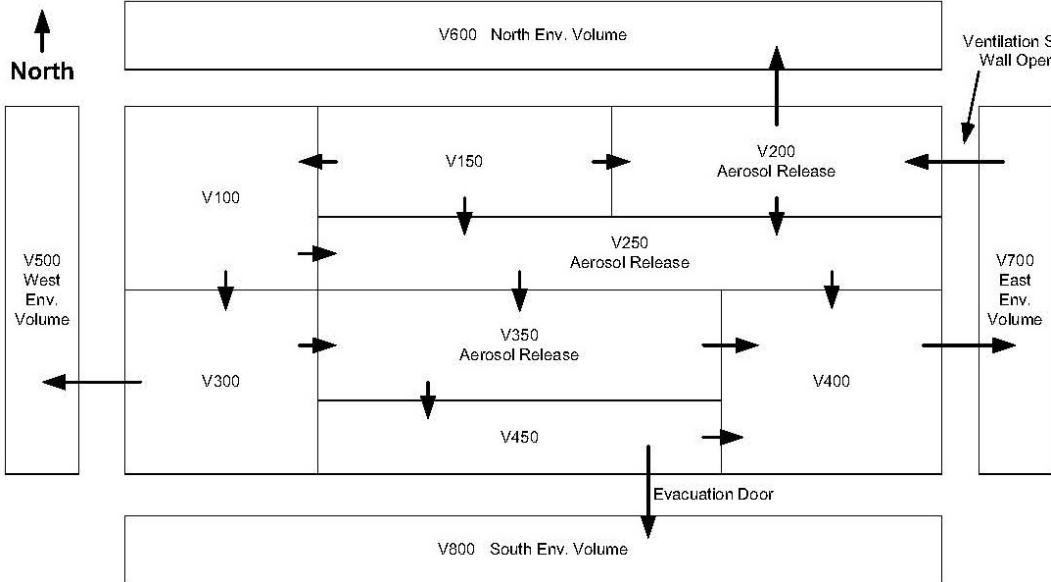
Sample	Description
Appendix E – Building seismic event with powder spill and 1 MW fire	
Appendix G – Seismic problem with multiple spills. Sensitivity cases were performed based on the total suspended material of 1 kg, 0.1 kg, 0.01 kg and 0.001 kg.	

Table A-1. MELCOR LPF Results (%)* from Test Problems in MELCOR Guidance

Test Problem	Reference Value interpolated from (figures) in the MELCOR 1.8.5 Guidance Report [DOE 2004]	1.8.5	1.8.6	2.1
Appendix C	~8.1 (7-6)	8.13	8.10	8.14
Appendix D	~0.39 (7-12)	0.39	0.39	0.39
Appendix E	~26.3 (7-18)	26.66	26.64	26.69
Appendix F	~0.43 (7-21)	0.43	0.43	0.43
Appendix G				
1 kg	~11.58 (7-26)	10.42	10.39	10.44
01 kg	~12.03 (7-26)	10.79	10.75	10.80
0.01 kg	~12.09 (7-26)	10.83	10.79	10.84
0.001 kg	~12.09 (7-26)	10.83	10.79	10.84

*1.8.5 is calculated using the official release version RL, 1.8.6 is calculated using the official release version Revision 3964, and 2.1 is calculated using Revision 6110.

A.2 LA-UR-03-7945 Verification Problems

This sample problem (Example 3 from LA-UR-03-7945 [Jordan 2003]) is based on an accidental release and transport of plutonium aerosol within a nuclear material storage facility [Shaffer 1999]. The facility stores nuclear materials (metal and oxide) in air-cooled arrays located in a subterranean vault below the main floor of the facility. The main floor of the facility (which is the subject of this example) contains shipping/receiving docks, shipping container packing/unpacking areas, container inspection facilities, and office space. Each area is accessed through a serpentine corridor that winds through the center of the facility. Building emergency exit doors for the facility are located at each end of the corridor. Personnel entrance doors are located at the front of the facility and in the shipping/receiving area.

A MELCOR model was developed for this facility and was used to calculate the LPF under a wide variety of postulated accident conditions [DOE 2006]. The MELCOR model consists of a network of control volumes, flow pathways, and structural surfaces modeled as heat structures. Each room of the facility is treated as a distinct control volume, and each doorway separating adjacent rooms is treated as a distinct flow path. The normal position of doors between adjacent rooms is reflected in the flow area specified for the associated flow path. Corridors with long characteristic transport lengths are subdivided into a series of connected control volumes to represent the gradual migration of suspended material along their length (see [Jordan 2003]). Major building structures, such as walls, floors, and ceilings, are defined and linked to appropriate control volumes to account for heat transfer being modeled as heat structures. The position of individual doors (or more properly, size of flow path areas) can be adjusted to investigate the importance of door position to the LPF.

In addition to the control volumes simulating the movement of air and contaminants among various rooms in the facility, heat and ventilation air conditioning (HVAC) systems are represented in the MELCOR model. Key features of the HVAC model include exhaust and recirculation fans, inline high efficiency particulate air (HEPA) filters, flow control dampers, and flow distribution ductwork. The HVAC ductwork and intake/exhaust registers are defined in a manner that preserves their actual elevation, thus allowing natural circulation flow through the system to be represented during postulated accident scenarios in which the ventilation fans do not operate. The accident scenario examined here involves a fire in a container-inspection-laboratory near the center of the main floor of the facility (see Figure A-2). The fire is assumed to be a quantity of ordinary combustibles based on an average loading of 4.887 kg/m^2 (1 lb/ft^2). The entire fuel load was assumed to burn at a steady rate 0.145 kg/sec (0.32 lb/sec) for the first 2,700 seconds of the accident, with a subsequent ramp to zero (i.e., the fire is completely extinguished) at 1 hour. The doorway connecting the laboratory to the facility's main corridor is assumed to be fully open. A sealed canister of plutonium oxide powder is assumed to be engulfed by the fire, causing the internal pressure to rise above the canister's burst point. Failure of the canister is assumed to occur 20 minutes after the onset of the fire, instantaneously releasing a fixed quantity of respirable plutonium oxide aerosol.

One of the limitations in MELCOR is analyzing a fire-type scenario, because currently MELCOR does not contain models for calculating details of the fire behavior. Another improvement of MELCOR has been identified in Section A.1.

A number of sensitivity cases were conducted for this example:

- Gap width (crack width) for the exit door frames
- Wind speed
- Smoke density, modeled as aerosol
- Collection efficiency of the HEPA filter

Table A-0-2 shows the results of the example problem simulated with several major versions of MELCOR, namely MELCOR 1.8.5, MELCOR 1.8.6 and MELCOR 2.1. The reason for the use of MELCOR 1.8.5 for this example was that the original calculation and reported results for this example was in MELCOR 1.8.5. As shown in this table, the referenced MELCOR results uses MELCOR 1.8.5, which yields slightly higher results than the results from other versions of MELCOR used for this assessment, except in those cases when smoke aerosols were modeled. In these smoke cases, unlike the referenced results, all code versions predict that LPF decreases as the amount of smoke aerosols increases due to the agglomeration. These differences with the referenced results are unexplained. In comparing results amongst different versions of MELCOR, all versions predict similar results as shown in Table A-0-2, except Case 5 for MELCOR 1.8.5.

One interesting point in this exercise is that Case 10 shows the smoke generation of 50 kg, which is enough to threaten a large filter bank (see Table A-0-2). If a single filter bank were to capture this much material, filter loading might be excessive to the point where the associated air handlers shut down or where the filters blow out. MELCOR can model these phenomena with the use of control function capability (see Chapter 1 of this report).

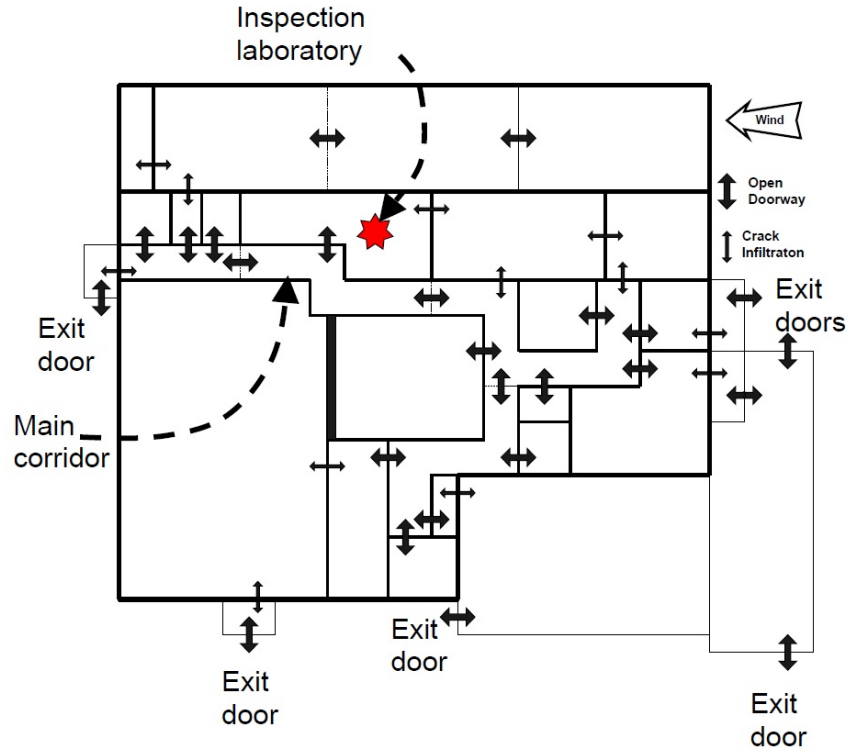


Figure A-2. Floor Plan for the Main Floor of Example 3 [Jordan 2003].

Table A-0-2. MELCOR Results on Example 3

Case	Crack Width (mm)	Wind Speed (mph)	Smoke Generated by Fire (kg)	HEPA Collect Efficiency (%)	MELCOR LPF Results (fraction)*			
					1.8.5 Reference**	1.8.5	1.8.6	2.1
1	0.5	30	None	99.98	3.9×10^{-3}	3.0×10^{-3}	3.0×10^{-3}	3.0×10^{-3}
2	1	30	None	99.98	9.3×10^{-3}	7.5×10^{-3}	7.5×10^{-3}	7.4×10^{-3}
3	2	30	None	99.98	2.0×10^{-2}	1.7×10^{-2}	1.7×10^{-2}	1.7×10^{-2}
4	5	30	None	99.98	5.1×10^{-2}	4.5×10^{-2}	4.4×10^{-2}	4.4×10^{-2}
5	0.5	1	None	99.98	2.8×10^{-7}	1.2×10^{-7}	2.3×10^{-7}	2.3×10^{-7}
6	0.5	10	None	99.98	1.1×10^{-4}	7.2×10^{-5}	7.6×10^{-5}	7.3×10^{-5}
7	0.5	20	None	99.98	1.0×10^{-3}	9.6×10^{-4}	9.6×10^{-4}	9.3×10^{-4}
8	0.5	30	10	99.98	2.6×10^{-5}	2.8×10^{-3}	2.8×10^{-3}	2.7×10^{-3}
9	0.5	30	25	99.98	1.1×10^{-5}	2.5×10^{-3}	2.5×10^{-3}	2.4×10^{-3}
10	0.5	30	50	99.98	3.9×10^{-3}	2.1×10^{-3}	2.1×10^{-3}	2.0×10^{-3}
11	0.5	30	None	99.95	3.9×10^{-3}	3.0×10^{-3}	3.0×10^{-3}	3.0×10^{-3}

*1.8.5 values are using the official release version RL, 186 values are calculated using the official release. 186 values are calculated using the official release version 3964, and 2.1 values are calculated using official release version RL NL 6110.

**1.8.5 reported values from Table 4-2 of LA-UR-03-7945 [Jordan 2003].

A.3 Summary and Conclusions

In this appendix, we have conducted the verification tests on the example problems as described in the MELCOR 1.8.5 guidance report and in LA-UR-03-7945. We reported the comparison results of version differences among MELCOR 1.8.5, 1.8.6 and 2.1. MELCOR 2.1 is the latest version of MELCOR that is currently used. The results show that there are not significant differences among code versions. Thus, MELCOR 2.1 should be used for future safety basis analyses for leak path factor applications. Note that the verification test alone is insufficient; the

experiment validation is necessary (see Chapter 3 of this report on MELCOR validation). In Chapter 3, we provided a number of experimental data comparisons, including some from DOE-HDBK-3010 [DOE 1994].

APPENDIX B

Selected Inputs

This appendix documents a number of MELCOR input decks described in Chapter 3 of this report.

B.1 Gasoline Pool Fire

```
!
! cvh / fl / hs inputs for wind tunnel
! controls for variable wind speed (in mph)
!
! 2 ft x 2 ft wind tunnel
! 1/5" walls assumed; stainless steel
!
! tunnel centerline are z=0
! hydro bottom surface of tunnel = -0.3048 m
! hydro top surface of tunnel   =  0.3048 m
!
! main tunnel volumes only active after t=0
! burner tray volume active before t=0 for settled source
!
!
meg_diagf      'gastunnel.gdia'
meg_outputf    'gastunnel.gout'
meg_restartf   'gastunnel.rst'
plotfile       'gastunnel.ptf'
messagef       'gastunnel.mes'
extdiagf       'gastunnel.ext'
mel_diagf      'gastunnel.dia'
mel_outputf    'gastunnel.out'
stopfile       'gastunnel.stp'
mel_restartf   'gastunnel.rst' ncycle -1
RN1VISUALFILE  'aerosolfile'
!
! *****
program melgen
! *****
!
! Executive package input
!
EXEC_INPUT
!
EXEC_TITLE     'gastunnel'
EXEC_DTTIME    0.05
EXEC_JOBID     'gastunnel'
EXEC_TSTART    -2000.0
EXEC_GLOBAL_DFT 2.0
!
! add plots
!
EXEC_PLOT      24
1 RN1-DEPHS('trayfloor',LHS,U02,GRAV)
2 RN1-DEPHS('trayfloor',LHS,U02,THERM)
3 RN1-DEPHS('trayfloor',LHS,U02,DIFF)
4 RN1-DEPHS('trayfloor',LHS,U02,FALL)
5 RN1-ADEP('trayfloor',LHS,U02,TOT)
6 RN1-TOTRES('trayfloor',LHS)
7 RN1-ADEP('floor01',LHS,U02,TOT)
8 RN1-ADEP('floor02',LHS,U02,TOT)
9 RN1-ADEP('floor03',LHS,U02,TOT)
10 RN1-ADEP('wall01_lower',LHS,U02,TOT)
11 RN1-ADEP('wall02_lower',LHS,U02,TOT)
12 RN1-ADEP('wall03_lower',LHS,U02,TOT)
13 RN1-ADEP('wall01_upper',LHS,U02,TOT)
14 RN1-ADEP('wall02_upper',LHS,U02,TOT)
15 RN1-ADEP('wall03_upper',LHS,U02,TOT)
16 RN1-TOTRES('floor01',LHS)
```

```

17 RN1-TOTRES('floor02',LHS)
18 RN1-TOTRES('floor03',LHS)
19 RN1-TOTRES('wall01_lower',LHS)
20 RN1-TOTRES('wall02_lower',LHS)
21 RN1-TOTRES('wall03_lower',LHS)
22 RN1-TOTRES('wall01_upper',LHS)
23 RN1-TOTRES('wall02_upper',LHS)
24 RN1-TOTRES('wall03_upper',LHS)

! ----- control volumes
cvh_input
!
CV_TENDINI 0.0
!
cv_id   'source' 1
cv_typ  'source'
cv_thr  EQUIL FOG TIME-INDEP
cv_pas  SEPARATE ONLYATM SUPERHEATED
cv_ptd  PVOL 1.016000e5
cv_aad  TATM 289.26
cv_are  NOCF 0.3716
cv_ncg  2 RHUM 0.37
        1 'O2' 0.21
        2 'N2' 0.79
cv_vat  2
        1 -0.3048 0.0
        2 0.3048 1.0
!
! -- Aerosol Tray
cv_id   'tray' 6
cv_typ  'tray'
cv_thr  NONEQUIL FOG ACTIVE
cv_pas  SEPARATE ONLYATM SUPERHEATED
cv_ptd  PVOL 1.016000e5
cv_aad  TATM 289.26
cv_are  NOCF 0.015
cv_ncg  2 RHUM 0.37
        1 'O2' 0.21
        2 'N2' 0.79
cv_vat  2
        1 -0.3548 0.0 ! 0.05 m below bottom of duct surface
        2 -0.3048 0.05 ! arbitrary small volume
!
! main air duct - split between lower / upper volumes
! - first (01) volume(s) receive aerosol source, burn energy source
cv_id   'tunnel1_lower' 10
cv_typ  'tunnel'
cv_thr  NONEQUIL FOG ACTIVE
cv_pas  SEPARATE ONLYATM SUPERHEATED
cv_ptd  PVOL 1.016000e5
cv_aad  TATM 289.26
cv_are  NOCF 0.1858
cv_ncg  2 RHUM 0.37
        1 'O2' 0.21
        2 'N2' 0.79
cv_vat  2
        1 -0.3048 0.0 ! middle of tunnel --> z=0
        2 0.0 0.1133 ! half of 2 ft x 2 ft x 2 ft
!
! add energy and burn product (hydro materials)
!
CV_SOU  5 ! two by-product gases will be generated, but one reactant gas consumed
!
      n  CTYP  INTERP  IESSRC  CF/TFNAME  IDMAT  ESSCAL
      1  MASS  RATE    CF      O2MASS      02      1.0      ! consumed
      2  TE    RATE    CF      O2TEMP      -1
      3  MASS  RATE    CF      H2OMASS      3        1.0      ! produced
      4  MASS  RATE    CF      CO2MASS      CO2       1.0      ! produced
      5  AE    RATE    CF      'qatm'      1.0
!
cv_id   'tunnel1_upper' 11
cv_typ  'tunnel'

```

```

cv_thr  NONEQUIL  FOG  ACTIVE
cv_pas  SEPARATE  ONLYATM  SUPERHEATED
cv_ptd  PVOL  1.016000e5
cv_aad  TATM  289.26
cv_are  NOCF  0.1858
cv_ncg  2  RHUM  0.37
        1  'O2'  0.21
        2  'N2'  0.79
cv_vat  2
        1      0.0      0.0 ! middle of tunnel --> z=0
        2  0.3048  0.1133 ! half of 2 ft x 2 ft x 2 ft
!
cv_id   'tunnel2_lower' 20
cv_typ  'tunnel'
cv_thr  NONEQUIL  FOG  ACTIVE
cv_pas  SEPARATE  ONLYATM  SUPERHEATED
cv_ptd  PVOL  1.016000e5
cv_aad  TATM  289.26
cv_are  NOCF  0.1858
cv_ncg  2  RHUM  0.37
        1  'O2'  0.21
        2  'N2'  0.79
cv_vat  2
        1 -0.3048      0.0 ! middle of tunnel --> z=0
        2      0.0  0.1699 ! half of 2 ft x 2 ft x 3 ft
!
cv_id   'tunnel2_upper' 21
cv_typ  'tunnel'
cv_thr  NONEQUIL  FOG  ACTIVE
cv_pas  SEPARATE  ONLYATM  SUPERHEATED
cv_ptd  PVOL  1.016000e5
cv_aad  TATM  289.26
cv_are  NOCF  0.1858
cv_ncg  2  RHUM  0.37
        1  'O2'  0.21
        2  'N2'  0.79
cv_vat  2
        1      0.0      0.0 ! middle of tunnel --> z=0
        2  0.3048  0.1699 ! half of 2 ft x 2 ft x 3 ft
!
cv_id   'tunnel3_lower' 30
cv_typ  'tunnel'
cv_thr  NONEQUIL  FOG  ACTIVE
cv_pas  SEPARATE  ONLYATM  SUPERHEATED
cv_ptd  PVOL  1.016000e5
cv_aad  TATM  289.26
cv_are  NOCF  0.1858
cv_ncg  2  RHUM  0.37
        1  'O2'  0.21
        2  'N2'  0.79
cv_vat  2
        1 -0.3048      0.0 ! middle of tunnel --> z=0
        2      0.0  0.1699 ! half of 2 ft x 2 ft x 3 ft
!
cv_id   'tunnel3_upper' 31
cv_typ  'tunnel'
cv_thr  NONEQUIL  FOG  ACTIVE
cv_pas  SEPARATE  ONLYATM  SUPERHEATED
cv_ptd  PVOL  1.016000e5
cv_aad  TATM  289.26
cv_are  NOCF  0.1858
cv_ncg  2  RHUM  0.37
        1  'O2'  0.21
        2  'N2'  0.79
cv_vat  2
        1      0.0      0.0 ! middle of tunnel --> z=0
        2  0.3048  0.1699 ! half of 2 ft x 2 ft x 3 ft
!
cv_id   'sink_lower' 100
cv_typ  'sink_lower'
cv_thr  EQUIL  FOG  TIME-INDEP

```

```

cv_pas SEPARATE ONLYATM SUPERHEATED
cv_ptd PVOL 1.016000e5
cv_aad TATM 289.26
cv_are NOCF 0.1858
cv_ncg 2 RHUM 0.37
      1 'O2' 0.21
      2 'N2' 0.79
cv_vat 2
      1 -0.3048 0.0
      ! 0.0 1.0
      2 0.3048 1.0 ! kwr
!
cv_id 'sink_upper' 101
cv_tpy 'sink_upper'
cv_thr EQUIL FOG TIME-INDEP
cv_pas SEPARATE ONLYATM SUPERHEATED
cv_ptd PVOL 1.016000e5
cv_aad TATM 289.26
cv_are NOCF 0.1858
cv_ncg 2 RHUM 0.37
      1 'O2' 0.21
      2 'N2' 0.79
cv_vat 2
      ! 0.0 0.0
      1 -0.3048 0.0 ! kwr
      2 0.3048 1.0
!
! -- environment, around duct
cv_id 'environment' 999
cv_tpy 'environment'
cv_thr EQUIL FOG TIME-INDEP
cv_pas SEPARATE ONLYATM SUPERHEATED
cv_ptd PVOL 1.016000e5
cv_aad TATM 289.26
cv_ncg 2 RHUM 0.37
      1 'O2' 0.21
      2 'N2' 0.79
cv_vat 2
      1 -1.0 0.0
      2 1.0 1.0
!
! ----- flow paths
fl_input
!
! duct area = 2 ft x 2 ft = (0.3048*2)**2 = 0.3716 m**2
! half area for upper / lower split = 0.1858 m**2
!
! lower FL elevation = (-0.3048 + 0) / 2 = -0.1524 m
! upper FL elevation = 0.1524 m
!
fl_id 'inlet_lower' 1
fl_ft 'source' 'tunnel1_lower' -0.1524 -0.1524
fl_geo 0.1858 0.6096 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf -0.3048 0.0
fl_jlt -0.3048 0.0
fl_seg 1
      1 0.1858 0.6096 0.3048 5.0e-6 CONST 16.0
!
fl_id 'inlet_upper' 2
fl_ft 'source' 'tunnel1_upper' 0.1524 0.1524
fl_geo 0.1858 0.6096 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf 0.0 0.3048
fl_jlt 0.0 0.3048
fl_seg 1
      1 0.1858 0.6096 0.3048 5.0e-6 CONST 16.0
!

```

```

! burn tray open to fan source to get correct velocity
fl_input
fl_id 'FLtrayopen1' 4
fl_ft 'source' 'tray' -0.3048 -0.3048
fl_geo 0.015 0.05 0.0 0.01 0.01 ! closed initially
fl_jsw 0 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_seg 1
1 0.015 0.05 0.3 5.0e-6 CONST 16.0
!
fl_id 'FLtrayopen2' 5
fl_ft 'tray' 'tunnel1_lower' -0.3048 -0.3048
fl_geo 0.015 0.05 0.0 0.01 0.01 ! closed initially
fl_jsw 0 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_seg 1
1 0.015 0.05 0.3 5.0e-6 CONST 16.0
!
! main duct vertical FLs
fl_id 'tunnel_v' 6
fl_ft 'tunnel1_lower' 'tunnel1_upper' 0.0 0.0
fl_geo 0.3716 0.1 1.0 0.01 0.01 ! area = 2ft x 2ft
fl_jsw 0 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_seg 1
1 0.3716 0.1 0.6096 5.0e-6 CONST 16.0

fl_id 'tunnel1-2_low' 7 ! 10
fl_ft 'tunnel1_lower' 'tunnel2_lower' -0.1524 -0.1524
fl_geo 0.1858 0.9144 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf -0.3048 0.0
fl_jlt -0.3048 0.0
fl_seg 1
1 0.1858 0.9144 0.3048 5.0e-6 CONST 16.0

fl_id 'tunnel1-2_up' 8 ! 20
fl_ft 'tunnel1_upper' 'tunnel2_upper' 0.1524 0.1524
fl_geo 0.1858 0.9144 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf 0.0 0.3048
fl_jlt 0.0 0.3048
fl_seg 1
1 0.1858 0.9144 0.3048 5.0e-6 CONST 16.0
!
fl_id 'tunnel2_v' 10 ! 7
fl_ft 'tunnel2_lower' 'tunnel2_upper' 0.0 0.0
fl_geo 0.5574 0.1 1.0 0.01 0.01 ! area = 2ft x 3ft
fl_jsw 0 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_seg 1
1 0.5574 0.1 0.6096 5.0e-6 CONST 16.0
!
fl_id 'tunnel2-3_low' 11
fl_ft 'tunnel2_lower' 'tunnel3_lower' -0.1524 -0.1524
fl_geo 0.1858 0.9144 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf -0.3048 0.0
fl_jlt -0.3048 0.0
fl_seg 1
1 0.1858 0.9144 0.3048 5.0e-6 CONST 16.0
!
fl_id 'tunnel2-3_up' 12 ! 21
fl_ft 'tunnel2_upper' 'tunnel3_upper' 0.1524 0.1524
fl_geo 0.1858 0.9144 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf 0.0 0.3048

```

```

fl_jlt 0.0 0.3048
fl_seg 1
      1 0.1858 0.9144 0.3048 5.0e-6 CONST 16.0
!
fl_id 'tunnel3_v' 13 ! 8
fl_ft 'tunnel3_lower' 'tunnel3_upper' 0.0 0.0
fl_geo 0.5574 0.1 1.0 0.01 0.01 ! area = 2ft x 3ft
fl_jsw 0 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_seg 1
      1 0.5574 0.1 0.6096 5.0e-6 CONST 16.0
!
fl_id 'tunnelout_low' 21 ! 12
fl_ft 'tunnel3_lower' 'sink_lower' -0.1524 -0.1524
fl_geo 0.1858 0.9144 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf -0.3048 0.0
fl_jlt -0.3048 0.0
fl_seg 1
      1 0.1858 0.9144 0.3048 5.0e-6 CONST 16.0
!
fl_id 'tunnelout_up' 22
fl_ft 'tunnel3_upper' 'sink_upper' 0.1524 0.1524
fl_geo 0.1858 0.9144 1.0
fl_jsw 3 NoBubbleRise NoBubbleRise
fl_vel 0.0 0.0
fl_jlf 0.0 0.3048
fl_jlt 0.0 0.3048
fl_seg 1
      1 0.1858 0.9144 0.3048 5.0e-6 CONST 16.0
!
! Special Flow path controls
! flow control boundary condition - hardwired velocity flow paths
fl_vtm 3
      1 'inlet_lower' cf 'flowvel' ! fans
      2 'inlet_upper' cf 'flowvel'
      3 'FLtrayopen1' cf 'flowvel' ! open tray to fan
!
! valves - needed to open tray at specified time
fl_vlv 3
      1 tunnel2tray 'FLtrayload' NoTRIP 'cftrayclosevlv' ! open while fire burns ->
forward only flowpath
      2 source2tray 'FLtrayopen1' NoTRIP 'cftrayopenvlv' ! open after fire ends
      3 tray2tunnel 'FLtrayopen2' NoTRIP 'cftrayopenvlv' ! open after fire ends
!
! To get pressurized by tunnel
fl_id 'FLtrayload' 3
fl_ft 'tunnel1_lower' 'tray' -0.3048 -0.3048
fl_geo 0.015 0.05 1.0 0.01 0.01
!l_jsw 10 NoBubbleRise NoBubbleRise ! forward only
fl_jsw 0 NoBubbleRise NoBubbleRise ! forward only ! kwr
fl_vel 0.0 0.0
fl_seg 1
      1 0.015 0.05 0.3 5.0e-6 CONST 16.0
!
cf_input
cf_id 'cftrayclosevlv' 1030 formula
cf_sai 1.0 0.0 1.0
cf_formula 4 1-a-ifte(t<start,open,closed)
      1 t exec-time
      2 start cf-valu('openTray')
      3 open cf-valu('trayOpenFrac')
      4 closed 0.0
!
cf_input
cf_id 'cftrayopenvlv' 1031 formula
cf_sai 1.0 0.0 0.0

```

```

cf_formula 4 1-a-ifte(t>start,open,closed)
      1 t      exec-time
      2 start   cf-valu('openTray')
      3 open    cf-valu('trayOpenFrac')
      4 closed  0.0

!
! ----- heat structures
hs_input
!
! all duct walls 1/5" thick, 0.2" = 0.508 cm = 0.00508 m
!
! radiation heat source of Rad_Q. this source is divided by the total surface area
! in the duct.
!


| HS# | Area       | Fract  |
|-----|------------|--------|
| 5   | 0.1858x0.5 | 0.0347 |
| 6   | 0.1858x0.5 | 0.0347 |
| 10  | 0.3716x0.1 | 0.0693 |
| 11  | 0.3398     | 0.0634 |
| 12  | 0.3398     | 0.0634 |
| 20  | 0.1858x2   | 0.0347 |
| 21  | 0.2787x2   | 0.0520 |
| 22  | 0.2787x2   | 0.0520 |
| 30  | 0.1858x4   | 0.0347 |
| 31  | 0.2787x4   | 0.0520 |
| 32  | 0.2787x4   | 0.0520 |


!
! bottom of tray
hs_id 'trayfloor'
hs_gd RECTANGULAR ss
hs_eod -0.35988 -1.0e-7 ! bottom = -0.3548 - 0.00508 ; left = top, right = bottom
hs_mlt 1.0
hs_src cf 'qhs' 0.0 ! jp removed to prevent pressurization
hs_nd 5 3 ! n n xi tini matnam
      1 1 0.0 - 'STAINLESS-STEEL' 1.0
      2 2 0.00127 - 'STAINLESS-STEEL' 0.0
      3 5 0.00508 -
hs_lb CalcCoefHS 'tray' NO
hs_lbp INT 0.5 0.5
hs_lbs 0.114 0.3810 0.3810 ! area taken as pan area
! jp not sure why this is limited to one half
!hs_lbar 0.5 !!! fraction that can resuspend, crit diam unspecified = let melcor determine
hs_lbar 0.5 4.0e-5 ! assume anything over 30 micron will suspend
hs_rb CalcCoefHS 'environment' YES
hs_rbp EXT 0.5 0.5
hs_rbs 0.114 0.3810 0.3810 ! area taken as pan area
hs_ft OFF
!
! floor of duct
hs_id 'floor01' 10
hs_gd RECTANGULAR ss
hs_eod -0.30988 -1.0e-7 ! bottom = -0.3048 - 0.00508 ; left = top, right = bottom
hs_mlt 0.1 ! 1.0 ! assume this floor small (tray also has settling area)
hs_src cf 'qhs' 0.0693
hs_nd 5 3 ! n n xi tini matnam
      1 1 0.0 - 'STAINLESS-STEEL' 1.0
      2 2 0.00127 - 'STAINLESS-STEEL' 0.0
      3 5 0.00508 -
hs_lb CalcCoefHS 'tunnel1_lower' YES
hs_lbp INT 0.5 0.5
hs_lbs 0.3716 0.6096 0.6096 ! area = 2 ft x 2 ft
hs_lbar 0.5 !!! fraction that can resuspend, crit diam unspecified = let melcor determine
hs_rb CalcCoefHS 'environment' YES
hs_rbp EXT 0.5 0.5
hs_rbs 0.3716 0.6096 0.6096
hs_ft OFF
!
hs_id 'floor02' 11
hs_gd RECTANGULAR ss
hs_eod -0.30988 -1.0e-7 ! bottom = -0.3048 - 0.00508 ; left = top, right = bottom
hs_mlt 1.0

```

```

hs_src  cf  'qhs'  0.0634
hs_nd    5 3 ! n n      xi tini      matnam
          1 1      0.0 - 'STAINLESS-STEEL'  1.0
          2 2 0.00127 - 'STAINLESS-STEEL'  0.0
          3 5 0.00508 -
hs_lb    CalcCoefHS 'tunnel2_lower' YES
hs_lbp   INT 0.5 0.5
hs_lbs   0.3398 0.6096 0.9144 ! area = 2 ft x 3 ft
hs_lbar  0.5 !!! fraction that can resuspend, crit diam unspecified = let melcor determine
hs_rb    CalcCoefHS 'environment' YES
hs_rbp   EXT 0.5 0.5
hs_rbs   0.3398 0.6096 0.9144
hs_ft    OFF
!
hs_id    'floor03' 12
hs_gd    RECTANGULAR ss
hs_eod   -0.30988 -1.0e-7 ! bottom = -0.3048 - 0.00508 ; left = top, right = bottom
hs_mlt   1.0
hs_src   cf  'qhs'  0.0634
hs_nd    5 3 ! n n      xi tini      matnam
          1 1      0.0 - 'STAINLESS-STEEL'  1.0
          2 2 0.00127 - 'STAINLESS-STEEL'  0.0
          3 5 0.00508 -
hs_lb    CalcCoefHS 'tunnel3_lower' YES
hs_lbp   INT 0.5 0.5
hs_lbs   0.3398 0.6096 0.9144 ! area = 2 ft x 3 ft
hs_lbar  0.5 !!! fraction that can resuspend, crit diam unspecified = let melcor determine
hs_rb    CalcCoefHS 'environment' YES
hs_rbp   EXT 0.5 0.5
hs_rbs   0.3398 0.6096 0.9144
hs_ft    OFF
!
! walls of duct - lower volumes
hs_id    'wall01_lower' 20
hs_gd    RECTANGULAR ss
hs_eod   -0.3048 1.0 ! bottom = -0.3048; vertical HS
hs_mlt   2.0 ! 2 walls
hs_src   cf  'qhs'  0.0347
hs_nd    5 3 ! n n      xi tini      matnam
          1 1      0.0 - 'STAINLESS-STEEL'  1.0
          2 2 0.00127 - 'STAINLESS-STEEL'  0.0
          3 5 0.00508 -
hs_lb    CalcCoefHS 'tunnel1_lower' YES
hs_lbp   INT 0.5 0.5
hs_lbs   0.1858 0.6096 0.3048 ! area = 1 ft x 2 ft
hs_rb    CalcCoefHS 'environment' YES
hs_rbp   EXT 0.5 0.5
hs_rbs   0.1858 0.6096 0.3048
hs_ft    OFF
!
hs_id    'wall02_lower' 21
hs_gd    RECTANGULAR ss
hs_eod   -0.3048 1.0 ! bottom = -0.3048; vertical HS
hs_mlt   2.0 ! 2 walls
hs_src   cf  'qhs'  0.0520
hs_nd    5 3 ! n n      xi tini      matnam
          1 1      0.0 - 'STAINLESS-STEEL'  1.0
          2 2 0.00127 - 'STAINLESS-STEEL'  0.0
          3 5 0.00508 -
hs_lb    CalcCoefHS 'tunnel2_lower' YES
hs_lbp   INT 0.5 0.5
hs_lbs   0.2787 0.9144 0.3048 ! area = 1 ft x 3 ft
hs_rb    CalcCoefHS 'environment' YES
hs_rbp   EXT 0.5 0.5
hs_rbs   0.2787 0.9144 0.3048
hs_ft    OFF
!
hs_id    'wall03_lower' 22
hs_gd    RECTANGULAR ss
hs_eod   -0.3048 1.0 ! bottom = -0.3048; vertical HS
hs_mlt   2.0 ! 2 walls

```

```

hs_src cf 'qhs' 0.0520
hs_nd 5 3 ! n n xi tini matnam
      1 1 0.0 - 'STAINLESS-STEEL' 1.0
      2 2 0.00127 - 'STAINLESS-STEEL' 0.0
      3 5 0.00508 -
hs_lb CalcCoefHS 'tunnel3_lower' YES
hs_lbp INT 0.5 0.5
hs_lbs 0.2787 0.9144 0.3048 ! area = 1 ft x 3 ft
hs_rb CalcCoefHS 'environment' YES
hs_rbp EXT 0.5 0.5
hs_rbs 0.2787 0.9144 0.3048
hs_ft OFF
!
! walls of duct - upper volumes
hs_id 'wall01_upper' 30
hs_gd RECTANGULAR ss
hs_eod 0.0 1.0 ! bottom = 0.0; vertical HS
hs_mlt 4.0 ! 2 walls + ceiling (ceiling is 2x large as wall segment)
hs_src cf 'qhs' 0.0347
hs_nd 5 3 ! n n xi tini matnam
      1 1 0.0 - 'STAINLESS-STEEL' 1.0
      2 2 0.00127 - 'STAINLESS-STEEL' 0.0
      3 5 0.00508 -
hs_lb CalcCoefHS 'tunnel1_upper' YES
hs_lbp INT 0.5 0.5
hs_lbs 0.1858 0.6096 0.3048 ! area = 1 ft x 2 ft
hs_rb CalcCoefHS 'environment' YES
hs_rbp EXT 0.5 0.5
hs_rbs 0.1858 0.6096 0.3048
hs_ft OFF
!
hs_id 'wall02_upper' 31
hs_gd RECTANGULAR ss
hs_eod 0.0 1.0 ! bottom = 0.0; vertical HS
hs_mlt 4.0 ! 2 walls + ceiling (ceiling is 2x large as wall segment)
hs_src cf 'qhs' 0.0520
hs_nd 5 3 ! n n xi tini matnam
      1 1 0.0 - 'STAINLESS-STEEL' 1.0
      2 2 0.00127 - 'STAINLESS-STEEL' 0.0
      3 5 0.00508 -
hs_lb CalcCoefHS 'tunnel2_upper' YES
hs_lbp INT 0.5 0.5
hs_lbs 0.2787 0.9144 0.3048 ! area = 1 ft x 3 ft
hs_rb CalcCoefHS 'environment' YES
hs_rbp EXT 0.5 0.5
hs_rbs 0.2787 0.9144 0.3048
hs_ft OFF
!
hs_id 'wall03_upper' 32
hs_gd RECTANGULAR ss
hs_eod 0.0 1.0 ! bottom = 0.0; vertical HS
hs_mlt 4.0 ! 2 walls + ceiling (ceiling is 2x large as wall segment)
hs_src cf 'qhs' 0.0520
hs_nd 5 3 ! n n xi tini matnam
      1 1 0.0 - 'STAINLESS-STEEL' 1.0
      2 2 0.00127 - 'STAINLESS-STEEL' 0.0
      3 5 0.00508 -
hs_lb CalcCoefHS 'tunnel3_upper' YES
hs_lbp INT 0.5 0.5
hs_lbs 0.2787 0.9144 0.3048 ! area = 1 ft x 3 ft
hs_rb CalcCoefHS 'environment' YES
hs_rbp EXT 0.5 0.5
hs_rbs 0.2787 0.9144 0.3048
hs_ft OFF
!
!
! ----- cf/tf controls
cf_input
!
cf_id 'mphinlet' 1 read ! wind speed of wind tunnel
cf_sai 1.0 0.0 4.0 ! speed of inlet flow (mph); flow starts at t=0

```

```

!
cf_id 'endFlowin' 2 read
cf_sai 1.0 0.0 1.0e10 ! time to end inlet flow (s), if any
!
cf_id 'openTray' 5 read
cf_sai 1.0 0.0 540.0 ! open tray time (s) Assumed fire end time open the trays
!
cf_id 'trayOpenFrac' 6 read
cf_sai 1.0 0.0 1.0 ! full open frac of tray FL
!
cf_id 'flowcheck' 10 formula
cf_liv false
cf_msg full-output 'flow B.C. starts/stops'
cf_formula 3 (t>=tstart).and.(t<tstop)
              1 t          exec-time
              2 tstart      -400.0 ! jp may consider letting the fan run before the fire
starts to drive a SS problem for CV/HS/FL
              3 tstop  cf-valu('endFlowin')
!
cf_id 'tripflow' 11 trip
cf_sai 1.0 0.0 0.0
cf_arg 1
      1 cf-valu('flowcheck')
!
cf_id 'flowmult1' 12 tab-fun ! jp should always be 1.0
cf_sai 1.0 0.0 0.0
cf_msc 'tf_flow1'
cf_arg 1
      1 cf-valu('tripflow') 1.0 0.0
!
cf_id 'flowmult2' 13 tab-fun ! jp should always be 1.0 (turns off over 5 seconds) ! though it is
not used
cf_sai 1.0 0.0 0.0
cf_msc 'tf_flow2'
cf_arg 1
      1 cf-valu('tripflow') 1.0 0.0
!
cf_id 'flowvel' 15 formula
cf_sai 1.0 0.0 0.0
cf_formula 8 1-a-ifte(chk, (fr1*mph*mpm)/sperhr, zero ) ! ((fr2*mph*mpm)/sperhr)+small)
              1 chk  cf-valu('flowcheck') ! no flow until time zero see cf10 tstart
              2 fr1  cf-valu('flowmult1') ! gradual start
              3 fr2  cf-valu('flowmult2') ! gradual stop
              4 mph   cf-valu('mphinlet')
              5 mpm           1609.34 ! meters per mile
              6 sperhr        3600.0 ! sec per hour
              7 small         1.0e-5 ! residual small amount of flow
              8 zero          0.0
!
cf_id 'flowveltray' 17 formula
cf_sai 1.0 0.0 0.0
cf_formula 7 1-a-ifte(t>=topen, (fr*mph*mpm)/sperhr, zero )
              1 t          exec-time
              2 topen  cf-valu('openTray')
              3 fr     cf-valu('frtrayopen')
              4 mph     cf-valu('mphinlet')
              5 mpm           1609.34 ! meters per mile
              6 sperhr        3600.0 ! sec per hour
              7 zero          0.0
!
cf_id 'openTrayCheck' 20 1-ge
cf_liv false
cf_cls LATCH
cf_msg full-output 'tray opens at user time'
cf_arg 2
      1          exec-time 1.0 0.0
      2 cf-valu('openTray') 1.0 0.0
!
cf_id 'triptray' 22 trip
cf_sai 1.0 0.0 0.0
cf_arg 1

```

```

1 cf-valu('openTrayCheck')
!
cf_id 'frtrayopen' 24 tab-fun
cf_sai 1.0 0.0 0.0
cf_msc 'TfopenTray'
cf_arg 1
1 cf-valu('triptray') 1.0 0.0
!
CF_ID 'fdensity' 406 equals
CF_SAI 0.0 870.0 ! gasoline density page 3-213 of NFPA 1995
CF_ARG 1 !n
1 exec-time 1.0 0.
!
CF_ID 'ce_oct' 411 equals
Cf_SAI 0.0 4.443E+7 ! combustion energy (J/kg) of Octane
CF_ARG 1 !n
1 exec-time 1.0 0.
!
CF_ID 'f_rad' 412 equals
Cf_SAI 0.0 0.35 ! assume 35% of the combustion energy to deposit to structure ! jp doesn't
match the 25 specified in write-up
CF_ARG 1 !n
1 exec-time 1.0 0.
!
CF_ID 'fcurve' 413 TAB-FUN
CF_SAI 1.0 0.0 0.0
CF_MSC 'FIRECURVE'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 0.10000000E+01 0.00000000E+00
!
CF_ID 'f_rem' 414 equals
Cf_SAI 1.0 0.0 0.0
CF_ARG 1 !n
1 cf-valu('f_rad') -1.0 1.0 ! remaining from subtracting the radiation fraction
!
!!!!!!!!!!!!!!!!!!!!
! gasoline burn rate (kg/s)
!
! burnrate = / 0 to 1.0 in 21s \
! velocity of fire front (m/min) * (a ramp up and down timer) * (1min/60s) =>gives m/s
! * pan area = 0.114m2=> m3/s
! * fdensity = 870kg/m3 => gives kg/s
!
cf_id gasburnrate 1000 formula
cf_sai 1.0 0.0 0.0
cf_formula 5 velo*fcurve*panare*fden/sixty
1 velo 0.004 !burn downward velocity m/min
2 fcurve cf-valu('fcurve') !21s linear ramp to full burn and 21s ramp back to
0 after Xsecs
3 panare 0.114 !surface area of the burn pan
4 fden cf-valu('fdensity') !assumed density of gasoline
5 sixty 60.0 !1min/60sec
!
!!!!!!!!!!!!!!!!!!!!
! Remaining fuel mass Implemented for error checking
!
! remaining mass = initial mass then:
! remaining mass = remaining mass - burnrate*dt
! (note1 if it doesn't all burn and this doesn't go to zero there is something wrong)
! (note2 after first run the fuel burns away prematurely versus the time of the experiment)
exhaust around 500s rather than 520ish
cf_id RemainFuel 1001 formula
cf_sai 1.0 0.0 3.2933 !
cf_ulb LW 0.0
cf_formula 3 fuel-brate*dt
1 fuel cf-valu(RemainFuel)
2 brate cf-valu(gasburnrate)
3 dt exec-dt
!
!!!!!!!!!!!!!!!!!!!!
! This ignores originating enthalpies (enthalpy of gas and o2)

```

```

cf_id 'q' 1002 formula
CF_SAI 1.0 0.0 0.0
CF_FORMULA 2 mdot*qoct !dr.watts
            1 mdot      cf-valu(gasburnrate) ! kg/s
            2 qoct      cf-valu('ce_oct')     ! J/kg
!
!!!!!!!!!!!!!!!!!!!!!!
! Sources of Reactant removal and Product generation
! 2C8H18 + 25O2 -> 18H2O + 16CO2 + 444.3*10^5J/kg ! jp note the report is missing the 2 before
octane
! convert to grams
! 2mol*114g/mol + 25mol*32g/mol -> 18*18 + 16*44 + DELformation
! 228g Gas + 25*32 g O2....
! 1000/228* (228g Gas + 25*32 g O2 .... >
! 1kg of Gasoline gives
! 25*32/228 kg of O2
! 18*18/228 kg of H2O
! 16*44/228 kg of CO2
! + 444.3*10^5 J
!
cf_id o2mass 1003 formula
cf_sai -1.0 0.0 0.0
cf_formula 4 BalM*MW/MWGas*Brate
            1 BalM      25. !Balancing Moles (mol)
            2 MW        32. !Molecular Weight of X (mol/g)
            3 MWGas     228. !
            4 Brate      cf-valu(gasburnrate)
!
cf_id co2mass 1004 formula
cf_sai 1.0 0.0 0.0
cf_formula 4 BalM*MW/MWGas*Brate
            1 BalM      16. !Balancing Moles (mol)
            2 MW        44. !Molecular Weight of X (mol/g)
            3 MWGas     228. !
            4 Brate      cf-valu(gasburnrate)
!
cf_id h2omass 1005 formula
cf_sai 1.0 0.0 0.0
cf_formula 4 BalM*MW/MWGas*Brate
            1 BalM      18. !Balancing Moles (mol)
            2 MW        18. !Molecular Weight of X (mol/g)
            3 MWGas     228. !
            4 Brate      cf-valu(gasburnrate)
!
cf_id 'qatm' 1010 formula
cf_sai 1.0 0.0 0.0
cf_formula 2 q*(f_rem)
            1 q cf-valu('q')
            2 f_rem cf-valu('f_rem')
!
cf_id 'qhs' 1011 formula
cf_sai 1.0 0.0 0.0
cf_formula 2 q*(f_rad)
            1 q cf-valu('q')
            2 f_rad cf-valu('f_rad')
!
CF_ID 'burnfr' 2001 equals
CF_SAI 1.0 0.0
CF_ARG 1 !n
        1 cf-valu('fcurve') 1.0 0.

CF_ID 'O2TEMP' 521 equals
CF_SAI 1.0 0.0
CF_ARG 1 !n
        1 CVH-TVAP('tunnel1_lower') 1.0 0.0
! ----- tf
tf_input
! start / stop flow over 1 sec ! 5 sec
tf_id 'tf_flow1' 1.0 0.0
tf_tab 2

```

```

1 -10.0 1.0
2 1000.0 1.0 ! 5.0 1.0
!
tf_id 'tf_flow2' 1.0 0.0
tf_tab 2
1 -5.0 0.0
2 0.0 1.0
!
! rate of tray open
tf_id 'TFopenTray' 1.0 0.0
tf_tab 2
1 0.0 0.0
2 2.0 1.0
!
! based on the measured burn time of 540 s, and calculated burn time of
! 498 s, then the ramp time is 21 s and 21 s for decay
TF_ID 'FIRECURVE' 1.0
TF_TAB 4 !n x y
1 0.0 0.0
2 21.0 1.0
3 519.0 1.0
4 540.0 0.0
!
! ----- ncg
NCG_INPUT
ncg_id 'O2' ! hydro mat 4
ncg_id 'N2' ! hydro mat 5
ncg_id 'H2' ! hydro mat 6
ncg_id 'CO' ! hydro mat 7
ncg_id 'CO2' ! hydro mat 8
ncg_id 'CH4' ! hydro mat 9
ncg_id 'HE' ! hydro mat 10
!
! ----- mp
MP_INPUT
MP_ID URANIUM-DIOXIDE
MP_ID ZIRCALOY
MP_ID ZIRCONIUM-OXIDE
MP_ID STAINLESS-STEEL
MP_ID STAINLESS-STEEL-OXIDE
MP_ID ALUMINUM
MP_ID ALUMINUM-OXIDE
MP_ID GRAPHITE
MP_ID BORON-CARBIDE
MP_ID SILVER-INDIUM-CADMIUM
MP_ID STAINLESS-STEEL-304
MP_ID 'CARBON-STEEL'
MP_ID 'CONCRETE'
!
! ----- rn / dch for aerosol calcs
DCH_INPUT
DCH_OPW 1.0
DCH_CL 'XE' DEFAULT
DCH_CL 'CS' DEFAULT
DCH_CL 'BA' DEFAULT
DCH_CL 'I2' DEFAULT
DCH_CL 'TE' DEFAULT
DCH_CL 'RU' DEFAULT
DCH_CL 'MO' DEFAULT
DCH_CL 'CE' DEFAULT
DCH_CL 'LA' DEFAULT
DCH_CL 'UO2' DEFAULT
DCH_CL 'CD' DEFAULT
DCH_CL 'AG' DEFAULT
DCH_CL 'B02' DEFAULT
DCH_CL 'H2O' DEFAULT
DCH_CL 'CON' DEFAULT
DCH_CL 'CSI' DEFAULT
DCH_CL 'CSM' DEFAULT
!
! assume 10 sections (default), min dia=0.2 and max dia=23, GSD=2

```

```

!
RN1_INPUT
RN1_DCHNORM none ! ignore the fact there's no uo2 in cor (no cor package here)
! numsec numcmp numcls numca
RN1_DIM 10 3 17 6
RN1_CC
! nstr clsnam cmpnm
  1 'XE' 1
  2 'CS' 3 ! volatile
  3 'BA' 1
  4 'I2' 3 ! volatile
  5 'TE' 1
  6 'RU' 1
  7 'MO' 1
  8 'CE' 1
  9 'LA' 1
 10 'UO2' 1
 11 'CD' 3 ! volatile
 12 'AG' 1
 13 'B02' 1
 14 'H2O' 2
 15 'CON' 1
 16 'CSI' 3 ! volatile
 17 'CSM' 3 ! volatile
!
RN1_ACOEF CALANDWR
RN1_ASP 0.1E-6 50.E-6 10900.0 ! UO2 density, with default diameters
RN1_CAF ON
RN1_SET 7 ! n ivolf ivolt elev area
  1 'source' 'source' -0.3048 1.0
  2 'sink_lower' 'sink_lower' -0.3048 1.0
  3 'sink_upper' 'sink_upper' 0.0 1.0
  4 'environment' 'environment' 0.0 1.0
  5 'tunnel1_upper' 'tunnel1_lower' 0.0 0.3716
  6 'tunnel2_upper' 'tunnel2_lower' 0.0 0.5574
  7 'tunnel3_upper' 'tunnel3_lower' 0.0 0.5574
!
! model the UO2 contaminant in the pan.
!
! using information from NSRD-06 report: Fuego simulation
! the amount of the UO2 release rate during the fire
! this rate is last to about 9 min or so, when the boiling
! release dominated. After the fire is gone, the continuation
! of the wind may resuspend the remaining UO2 still in the pan.
! Total initial UO2 aerosol is about 19.5 g (0.0195 kg)
!
! source as_burn: follows the fire at certain release rate
! assume a fraction of the UO2 release in 500 s after transient
! at a rate: 0.0195 kg * 0.06/500 = 0.0000234 kg/s
! inventory as_pan - allows the remaining UO2 settled onto the
! pan, so 1-0.06 is the fraction to be remained
! after the fire.
!
!
! name CVH IPHS iclass RFRS xm ITAB CFTFNAME
RN1_AS as_burn 'tunnel1_lower' VAPOR UO2 0.0 2.34e-6 CF 'burnfr'
! IDIST
RN1_AS01 SECTIONBYSECTION ! n fraction
  1 0.008086
  2 0.051213
  3 0.09973
  4 0.107817
  5 0.161725
  6 0.161725
  7 0.107817
  8 0.107817
  9 0.086253
 10 0.107817
!
RN1_AG as_pan 'tray' UO2 0.0
! N XMASS
  1 1.482e-4

```

```

2 9.387e-4
3 1.828e-3
4 1.976e-3
5 2.964e-3
6 2.964e-3
7 1.976e-3
8 1.976e-3
9 1.581e-3
10 1.976e-3

!
!
!
END PROGRAM MELGEN
!
!*****
PROGRAM MELCOR

!RN1_INPUT
!RN1_EDTFLG 1 1 1 1 0

!CVH_INPUT
!CVH_SC 8
! 1 4401 50.0 3 ! cvh/FL velocity iteration parameter : Maximum number of iterations
permitted before solution is repeated with a decreased (subcycle) timestep
! 2 4413 0.05 5 ! Flow Blockage Friction Parameters: Minimum porosity to be used in
evaluating the correlation
! 3 4414 0.01 1 ! Minimum Hydrodynamic Volume Fraction: Minimum fraction of the
initial volume in each segment of the volume/altitude table of a control volume that will always
be available to hydrodynamic materials
! 4 4415 1.0 1 ! Criteria for Solving the Flow Equations in Sparse Form: The maximum
fraction of nonzero coefficients for use of the sparse form.
! 5 4408 1000000.0 1 ! disable revised treatment of non-equilibrium thermo
! 6 4422 0.0 1 ! FLs in order of appearance
! 7 4407 0.9 15 ! MAX_FRAC, max fraction of QDVAP to be used for direct vaporization
(default 0.9)
! 8 4411 1.0e-6 5 ! VPHEQL, vol frac below which equil therm will be used (default of
1.0e-6)

!cvh_ccmod 0 ! courant condition based on (1) volume without mass sources or (0) default, volume
w/ mass sources
!cvh_paim 1 1 1 ! activate new pool atm model (1=on);
! boiling below surf w/ solid struct is partitioned between direct vap and pool heatup (linear
function of pool subcooling) 1=on
!

!HS_INPUT
!HS_SC 1
1 4055 0.0005 2 ! HS convergence- relative error tolerance for transient conduction
calculations.
!

EXEC_INPUT

!exec_autots 1 5.0 1.0e-10 ! auto calc of temporal relaxation = max ( 5.0*dtmax, 1.0e-10 )
!exec_tsmult 1.0e-9 1.0e-9 1.0 1.0e-9 ! time scale multipliers for heat trans, oxidation, quench
velocity, flow path opening (valves)

EXEC_TITLE 'gastunnel'
EXEC_JOBID 'gastunnel'
EXEC_TEND 2000.0 ! 10 minute, which is sufficient for the fuel burn out ! 3600.0

exec_time 5 ! n time dtmax dtmin dtedt dtplt dtrst
! -3600.0 0.1 1.0e-6 1.0e10 5.0 1.0e10 ! allow for reaching s.s.
! -3600.0 0.1 1.0e-6 300. 5.0 1.0e10 ! allow for reaching s.s. ! kwr
2 -1.0 0.1 1.0e-6 1.0e10 1.0 1.0e10
3 0.0 0.1 1.0e-6 20.0 1.0 1.0e10
4 200.0 0.2 1.0e-6 100.0 10.0 1.0e10
5 3600.0 0.5 1.0e-6 1000.0 100.0 1.0e10 ! 1 hr

!

```

```
! name of interactive CF data file
EXEC_CFEFILE 'dynamicInp'
```

```
!EXEC_PLOTCF 'Trig-Mes'
EXEC_CPULEFT      10.0
EXEC_CPULIM       1.0e10
EXEC_SOFDTDMIN 1.0e-6 100
EXEC_CYMESF       500 500
EXEC_COMTC        3
```

```
RN1_INPUT
RN1_VISUAL 4
1 'tray'
2 'tunnel1_lower'
3 'sink_lower'
4 'sink_upper'
```

```
END PROGRAM MELCOR
```

B.2 LLNL Enclosure Fire

```
! $Id: $
!
! References:
! NIST Technical Note 1889v3
! LLNL Enclosure tests uses a test enclosure with a dimension of 6 m long, 4 m wide and 4.5 m
high.
! In most tests, a methane rock burner with 0.57 m in diameter and 0.23 m height is used, with
! various fire sizes from 50 kW to 400 kW. A door (2.06 m high by 0.76 m wide) was closed and
sealed for
! most tests, and air was pulled through the space at rates from 100 to 500 g/s. In the
experiments,
! 15 thermocouples were evenly spaced from floor to ceiling on either side of the burner. The
reported
! temperatures are taken as the averages of the lower, middle and upper 5 TCs. There are two
inlet ducts
! : 1 in lower and 1 in upper part. In all cases, only one inlet duct is used. An powered
exhaust duct
! measuring 0.65 m x 0.65 m near the upper part of the enclosure.
!
! llnl_t9 simulates the test 9 as described in Table 4.3
! Room configuration: TL
! ho (m) = 0
! Qdot (kW) = 200
! mdot (g/s) = 500
! ambient T (C) = 33
!
! other assumptions from CFAST: RH% of 50, P=101325 Pa, walls: k=0.39, Cp=1000, rho=1440,
TH=0.1, Emiss=0.94
!
! Fl/Ce: k=0.63, Cp=1000, rho=1920,
TH=0.1, Emiss=0.94
!
! Time(s): 0 10 4000 4001
! HRR(W) : 0 2E5 2E5 0
!
! total combustion energy fraction lost to thermal radiation is 0.35 (default)
!
!
!
! MELCOR model: CV100(LOWER), CV200(MIDDLE), CV300(UPPER), CV900(ENV)
! Lower divides into 3 volumes, so does Middle and Upper.
! so that inner - 9 m3, mid - 13.5 m3, outer - 13.5 m3
!
! heat structures: walls, ceiling and floor, assumed emissivity of 0.94, and thickness of
0.1 m according to
! CFAST
! Rock burner: inner dia:0.25, outer dia: 0.57, height 0.23 m
!
! CF logic to model METHANE gas reaction: CH4 + 2 O2 -> CO2 + 2 H2O
```

```

!
!           it is assumed that CH4 is unlimited, so only limited quantity is O2 in the
volume
!           O2 consumed needs to be checked. If below 15% mass fraction,
!   Using Fire Handbook, 2nd Edit: Table 1-5.3, 1.26E07 J/kg O2 generated
!           MW CH4: 0.016 kg/mole
!           O2: 0.032 kg/mole
!           CO2: 0.044 kg/mole
!           H2O: 0.018 kg/mole
!
!   This input deck is created by David Louie, Sandia National Laboratories for NSRD-10 Project
!   July 2016
!
!GlobalData
! (
! t9 test
VariableValue {{{pres=100927.0}}} {{{temp=302.15}}} {{{envt=306.15}}} {{{o2m=0.208}}}
{{{co2m=0.0005}}}

! t11 test
!VariableValue {{{pres=101250.0}}} {{{temp=292.15}}} {{{envt=293.15}}} {{{o2m=0.2081}}}
{{{co2m=0.0004}}}

CommentBlock t9expf1
!CommentBlock t11expf1

(((t9expf1
MEG_DIAGFILE 'llnl_t9v9G.DIA'
MEG_OUTPUTFILE 'llnl_t9v9G.OUT'
MEG_RESTARTFILE 'llnl_t9v9.RST'
MEL_DIAGFILE 'llnl_t9v9.DIA'
MEL_OUTPUTFILE 'llnl_t9v9.OUT'
MEL_RESTARTFILE 'llnl_t9v9.RST' ncycle 0
PLOTFILE 'llnl_t9v9.PTF'
MESSAGEFILE 'llnl_t9v9.MES'
)))
(((t11expf1
MEG_DIAGFILE 'llnl_t11v9G.DIA'
MEG_OUTPUTFILE 'llnl_t11v9G.OUT'
MEG_RESTARTFILE 'llnl_t11v9.RST'
MEL_DIAGFILE 'llnl_t11v9.DIA'
MEL_OUTPUTFILE 'llnl_t11v9.OUT'
MEL_RESTARTFILE 'llnl_t11v9.RST'
PLOTFILE 'llnl_t11v9.PTF'
MESSAGEFILE 'llnl_t11v9.MES'
)))
NOTEPAD++ ON
!)
!
PROGRAM MELGEN ! (
EXEC_INPUT ! (
!
(((t9expf1
EXEC_TITLE 'LLNL Enclosure Experiment_Test 9(9-vol)'
)))
(((t11expf1
EXEC_TITLE 'LLNL Enclosure Experiment_Test 11(9-vol)'
)))
!
EXEC_DTTIME 1.0E-3
EXEC_TSTART -200.0
!
!EXEC_PLOT    21  !n

!
!
(((t9expf1
EXEC_JOBID 'llnl_t9v9'
)))
(((t11expf1

```

```

EXEC_JOBID 'llnl_t11v9'
)))
!)
!)
MP_INPUT !(
!
! matnam
MP_ID STAINLESS-STEEL
MP_ID CONCRETE
!)
! *****
CF_INPUT !(
! *****
!
! exhaust flow control functions
!
cf_id 'endFlowin' 2 read
cf_sai 1.0 0.0 1.0e10 ! time to end inlet flow (s), if any
!
cf_id 'flowcheck' 10 formula
cf_liv false
cf_msg full-output 'flow B.C. starts/stops'
cf_formula 3 (t>=tstart).and.(t<tstop)
!
! 1 t exec-time
! 2 tstart 0.0
! 3 tstop cf-valu('endFlowin')

cf_id 'tripflow' 11 trip
cf_sai 1.0 0.0 0.0
cf_arg 1
! 1 cf-valu('flowcheck')
!
cf_id 'flowmult1' 12 tab-fun
cf_sai 1.0 0.0 0.0
cf_msc 'tf_flow1'
cf_arg 1
! 1 cf-valu('tripflow') 1.0 0.0
!
cf_id 'flowmult2' 13 tab-fun
cf_sai 1.0 0.0 0.0
cf_msc 'tf_flow2'
cf_arg 1
! 1 cf-valu('tripflow') 1.0 0.0

!(((t9conf1
!cf_id 'fl-mdot' 101 equals
!cf_sai 0.0 0.5 ! 500 g/s
!)))
(((t9expfl+t11expfl
cf_id 'fl-mdot' 101 tab-fun
cf_sai 1.0 0.0
cf_msc 'mass-fl'
!)))
cf_arg 1 !n
! 1 exec-time 1.0 0.0

cf_id 'flow' 102 divide
cf_sai 1.0 0.0
cf_arg 2 !n
! 1 cvh-rho('o-upper',atm) 0.4225 0.0
! 2 cf-valu(fl-mdot) 1.0 0.0

cf_id 'fl-vel' 103 multiply
cf_sai 1.0 0.0
cf_arg 2 !n
! 1 cf-valu('flow') 1.0 0.0
! 2 cf-valu('flowmult1') 1.0 0.0
!
! exhaust delta-p calculations
!
cf_id 'delta-p' 201 tab-fun

```

```

cf_sai 1.0 0.0
cf_msc 'delta-pr'
cf_arg 1 !n
      1 exec-time 1.0 0.0
!
cf_id 'fire_cr' 299 tab-fun
cf_sai 1.0 0.0 0.0
cf_msc 'firecurve'
cf_arg 1 ! narg charg arscal aradcn
      1 exec-time 0.10000000e+01 0.00000000e+00
!
cf_id 'fire_qt' 300 equals
cf_sai 0.0 200000.0 ! 200 kw
cf_arg 1 !n
      1 exec-time 1.0 0.0 ! 1.0 0.

cf_id 'fire_q' 301 formula
cf_sai 1.0 0.0 0.0
cf_formula 3 c*qdot*fcurve ! ! assume 20% lost to thermal radiation
      1 c 0.8
      2 qdot cf-valu('fire_qt')
      3 fcurve cf-valu('fire_cr')

cf_id 'o2_exist' 302 equals ! amount of o2 mass
cf_sai 1.0
cf_arg 1 !n
      1 cvh-mass('i-lower',o2) 1.0 0.0 ! point to fire volume
!
cf_id 'Rad_Q' 303 formula
cf_sai 1.0 0.0 0.0
cf_formula 3 c*qdot*fcurve ! ! assume 20% lost to thermal radiation
      1 c 0.2
      2 qdot cf-valu('fire_qt')
      3 fcurve cf-valu('fire_cr')
!
!
! molecular weight for reactant and products
!
cf_id 'mw_ch4' 401 equals
cf_sai 0.0 1.600e-02
cf_arg 1 !n
      1 exec-time 1.0 0.

cf_id 'mw_o2' 402 equals
cf_sai 0.0 3.200e-02
cf_arg 1 !n
      1 exec-time 1.0 0.

cf_id 'mw_co2' 403 equals
cf_sai 0.0 4.400e-02
cf_arg 1 !n
      1 exec-time 1.0 0.

cf_id 'mw_h2o' 404 equals
cf_sai 0.0 1.800e-02
cf_arg 1 !n
      1 exec-time 1.0 0.
!

cf_id 'ce_o2 ' 411 equals
cf_sai 0.0 1.264e+7 ! combustion energy (j/kg) of o2
cf_arg 1 !n
      1 exec-time 1.0 0.

!
! source and sink (1)ch4+(2)o2-> (1)co2 + (2)h2o
!
cf_id 'o2mdotc' 501 divide ! o2 kg/s
cf_sai 1.0 0.0
cf_arg 2 !n
      1 cf-valu(ce_o2) 1.0 0.0

```

```

2 cf-valu(fire_q) 1.0 0.0

cf_id 'co2mdotc' 504 formula ! co2 kg/s -> o2 mole/s*0.5*mw_co2
cf_sai 1.0 0.0 0.0
cf_formula 4 omdt*c*mwco2/mwo2
1 omdt cf-valu('o2mdotc')
2 c 0.5
3 mwo2 cf-valu('mw_o2')
4 mwco2 cf-valu('mw_co2')

cf_id 'h2omdotc' 506 formula ! h2o kg/s -> o2 mole/s*1.0*mw_h2o
cf_sai 1.0 0.0 0.0
cf_formula 4 omdt*c*mwh2o/mwo2
1 omdt cf-valu('o2mdotc')
2 c 1.0
3 mwo2 cf-valu('mw_o2')
4 mwh2o cf-valu('mw_h2o')

cf_id 'ch4mdotc' 508 formula ! ch4 kg/s -> o2 mole/s*2.0*mw_ch4
cf_sai 1.0 0.0 0.0
cf_formula 4 omdt*c*mwch4/mwo2
1 omdt cf-valu('o2mdotc')
2 c 1.0
3 mwo2 cf-valu('mw_o2')
4 mwch4 cf-valu('mw_ch4')

cf_id 'o2_consumed' 511 formula ! o2 mdot*dt
cf_sai 1.0 0.0 0.0
cf_formula 2 omdt*dt
1 omdt cf-valu('o2mdotc')
2 dt exec-dt

cf_id 'o2_m_check' 512 l-gt ! if true, reaction possible
cf_arg 2 !n
1 cf-valu(o2_exist) 1.0 0.0
2 cf-valu(o2_consumed) 1.0 0.0

cf_id 'o2mass' 520 l-a-ifte ! o2 sink
cf_sai 1.0 0.0
cf_arg 3 !n
1 cf-valu(o2_m_check)
2 cf-valu(o2mdotc) -1.0 0.0 ! model as a sink
3 exec-time 0.0 ! zero

cf_id 'o2temp' 521 equals
cf_sai 1.0 0.0
cf_arg 1 !n
1 cvh-tvap('i-lower') 1.0 0.0

cf_id 'co2mass' 530 l-a-ifte ! co2 source
cf_sai 1.0 0.0
cf_arg 3 !n
1 cf-valu(o2_m_check)
2 cf-valu(co2mdotc) 1.0 0.0 ! model as a source
3 exec-time 0.0 ! zero

cf_id 'h2omass' 540 l-a-ifte ! h2o source
cf_sai 1.0 0.0
cf_arg 3 !n
1 cf-valu(o2_m_check)
2 cf-valu(h2omdotc) 1.0 0.0 ! model as a source
3 exec-time 0.0 ! zero

!
! for plotting use
!
cf_id 'tave_lower' 701 add
cf_sai 0.0278 0.0 ! divide the result by 36 m3

```

```

cf_arg 3 !n
1 cvh-tvap('i-lower') 9.0 0.0 ! t i-lower*9m3
2 cvh-tvap('m-lower') 13.5 0.0 ! t m-lower*13.5m3
3 cvh-tvap('o-lower') 13.5 0.0 ! t o-lower*13.5m3

!
cf_id 'tave_middle' 711 add
cf_sai 0.0278 0.0 ! divide the result by 36 m3
cf_arg 3 !n
1 cvh-tvap('i-middle') 9.0 0.0 ! t i-lower*9m3
2 cvh-tvap('m-middle') 13.5 0.0 ! t m-lower*13.5m3
3 cvh-tvap('o-middle') 13.5 0.0 ! t o-lower*13.5m3

!
cf_id 'tave_upper' 721 add
cf_sai 0.0278 0.0 ! divide the result by 36 m3
cf_arg 3 !n
1 cvh-tvap('i-upper') 9.0 0.0 ! t i-lower*9m3
2 cvh-tvap('m-upper') 13.5 0.0 ! t m-lower*13.5m3
3 cvh-tvap('o-upper') 13.5 0.0 ! t o-lower*13.5m3

!*****
tf_input !(
!*****
tf_id 'firecurve' 1.0
tf_tab 4 !n x y
1 0.0 0.0
2 10.0 1.0
3 4000.0 1.0
4 4001.0 0.0

!
(((t9expf1+t11expf1
tf_id 'mass-fl' 1.0
)))
(((t9expf1
tf_tab 7 !n x y
1 -200.0 0.565
2 0.0 0.565
3 500.0 0.491
4 1000.0 0.474
5 2000.0 0.463
6 3000.0 0.464
7 4000.0 0.461
)))
(((t11expf1
tf_tab 7 !n x y
1 -200.0 0.240
2 0.0 0.240
3 500.0 0.222
4 1000.0 0.221
5 2000.0 0.210
6 3000.0 0.207
7 4000.0 0.204
)))
tf_id 'delta-pr' 1.0
(((t9expf1
tf_tab 8 !n x y
1 -200.0 0.0
2 -199.0 398.0
3 0.0 398.0
4 500.0 297.0
5 1000.0 292.0
6 2000.0 287.0
7 3000.0 278.0
8 4000.0 261.0
)))
(((t11expf1
tf_tab 8 !n x y
1 -200.0 0.0

```

```

2    -199.0    75.0
3      0.0    75.0
4     500.0    42.0
5    1000.0    39.0
6    2000.0    45.0
7    3000.0    38.0
8    4000.0    31.0
)))
tf_input
! start / stop flow over 5 sec
tf_id 'tf_flow1' 1.0 0.0
tf_tab 2
1 0.0 0.0
2 5.0 1.0
!
tf_id 'tf_flow2' 1.0 0.0
tf_tab 2
1 -5.0 0.0
2 0.0 1.0

NCG_INPUT !(
!      mname
NCG_ID      'N2'
NCG_ID      'O2'
NCG_ID      'CO2'
!)
!)
CVH_INPUT !(
CV_TENDINI 0.0    ! end initial condition
!
!   enclosure: 4 m depth, 6 m length, 4.5 m high
!
!   lower: 4m X 6m X 1.5m=36 m3
!
!
! i-lower: 2m X 3m X 1.5m= 9m3
!
!       the burner is located at the center of this volume, so it needs to provide
!       the source and sink
!
!       sources: CO2 and H2O
!       sinks:   O2
!
!
!      cvname      icvnum
CV_ID      'i-lower'      100 !(
!      icvtyp
CV_TYP      'lower'
!      icvthr      ipfsw      icvact
CV_THR      NONEQUIL      FOG      ACTIVE
!      itypth      ipora      vapor
CV_PAS      SEPARATE      ONLYATM      SUPERHEATED
!      ptdit      pvol
CV_PTD      PVOL      {{{pres=}}}
!      atmid      tatm
CV_AAD      TATM      {{{temp=}}}
!      nmmat
CV_NCG      3      RHUM      0.5
!      n      namgas      mass
1      'N2'      0.7915
2      'O2'      {{{o2m=}}}
3      'CO2'      {{{co2m=}}}

!      size
CV_VAT      2 !n      cvz      cvvol
1      0.0      0.0
2      1.5      9.0
!
!
CV_SOU      5 ! two by-product gases will be generated, but one reactant gas consumed
!      n      ctyp      interp      iessrc      cf/tfname      idmat      esscal
1      mass      rate      cf      'o2mass'      02      1.0      ! consumed
2      te      rate      cf      'o2temp'      -1

```

```

3 mass rate cf 'co2mass' C02 1.0 ! produced
4 mass rate cf 'h2omass' 3 1.0 ! produced
5 AE rate cf 'fire_q'

!
! m-lower: (3m X 5m - 2m X 3m) X 1.5m= 13.5m3
!
!
! cvname icvnum
CV_ID 'm-lower' 110 !
! icvtyp
CV_TYP 'lower'
! icvthr ipfsw icvact
CV_THR NONEQUIL FOG ACTIVE
! itypth ipora vapor
CV_PAS SEPARATE ONLYATM SUPERHEATED
! ptdit pvol
CV_PTD PVOL {{{pres=}}}
! atmid tatm
CV_AAD TATM {{{temp=}}}
! nmmat
CV_NCG 3 RHUM 0.5
! n namgas mass
1 'N2' 0.7915
2 'O2' {{{o2m=}}}
3 'CO2' {{{co2m=}}}

! size
! size
CV_VAT 2 !n cvz cvvol
1 0.0 0.0
2 1.5 13.5

!
! o-lower: (4m X 6m - 3m X 5m) X 1.5m= 13.5m3
!
!
! cvname icvnum
CV_ID 'o-lower' 120 !
! icvtyp
CV_TYP 'lower'
! icvthr ipfsw icvact
CV_THR NONEQUIL FOG ACTIVE
! itypth ipora vapor
CV_PAS SEPARATE ONLYATM SUPERHEATED
! ptdit pvol
CV_PTD PVOL {{{pres=}}}
! atmid tatm
CV_AAD TATM {{{temp=}}}
! nmmat
CV_NCG 3 RHUM 0.5
! n namgas mass
1 'N2' 0.7915
2 'O2' {{{o2m=}}}
3 'CO2' {{{co2m=}}}

! size
! size
CV_VAT 2 !n cvz cvvol
1 0.0 0.0
2 1.5 13.5

!
!
! middle: 4m X 6m X 1.5m=36 m3
!
!
! i-middle: 2m X 3m X 1.5m= 9m3
!
!
! cvname icvnum
CV_ID 'i-middle' 200 !
! icvtyp
CV_TYP 'middle'
! icvthr ipfsw icvact
CV_THR NONEQUIL FOG ACTIVE

```

```

!               itypth      ipora      vapor
CV_PAS          SEPARATE    ONLYATM    SUPERHEATED
!               ptdit      pvol
CV_PTD          PVOL        {{{pres=}}}
!               atmid      tatm
CV_AAD          TATM        {{{temp=}}}
!               nmmat
CV_NCG          3          RHUM      0.5
!               n          namgas      mass
!               1          'N2'        0.7915
!               2          'O2'        {{{o2m=}}}
!               3          'CO2'       {{{co2m=}}}

!       size
!       size
CV_VAT          2 !n          cvz          cvvol
!               1          1.5          0.0
!               2          3.0          9.0

```

```

!
! m-middle: (3m X 5m - 2m X 3m) X 1.5m= 13.5m3
!
!               cvname      icvnum
CV_ID           'm-middle'    210 ! (
!               icvtyp
CV_TYP          'middle'
!               icvthr      ipfsw      icvact
CV_THR          NONEQUIL      FOG      ACTIVE
!               itypth      ipora      vapor
CV_PAS          SEPARATE    ONLYATM    SUPERHEATED
!               ptdit      pvol
CV_PTD          PVOL        {{{pres=}}}
!               atmid      tatm
CV_AAD          TATM        {{{temp=}}}
!               nmmat
CV_NCG          3          RHUM      0.5
!               n          namgas      mass
!               1          'N2'        0.7915
!               2          'O2'        {{{o2m=}}}
!               3          'CO2'       {{{co2m=}}}

!       size
!       size
CV_VAT          2 !n          cvz          cvvol
!               1          1.5          0.0
!               2          3.0          13.5

```

```

!
! o-middle: (4m X 6m - 3m X 5m) X 1.5m= 13.5m3
!
!               cvname      icvnum
CV_ID           'o-middle'    220 ! (
!               icvtyp
CV_TYP          'middle'
!               icvthr      ipfsw      icvact
CV_THR          NONEQUIL      FOG      ACTIVE
!               itypth      ipora      vapor
CV_PAS          SEPARATE    ONLYATM    SUPERHEATED
!               ptdit      pvol
CV_PTD          PVOL        {{{pres=}}}
!               atmid      tatm
CV_AAD          TATM        {{{temp=}}}
!               nmmat
CV_NCG          3          RHUM      0.5
!               n          namgas      mass
!               1          'N2'        0.7915
!               2          'O2'        {{{o2m=}}}
!               3          'CO2'       {{{co2m=}}}

!       size
!       size
CV_VAT          2 !n          cvz          cvvol
!               1          1.5          0.0
!               2          3.0          13.5

```

```

! )
!
! upper: 4m X 6m X 1.5m=36 m3
!
!
! i-upper: 2m X 3m X 1.5m= 9m3
!
!
!          cvname          icvnum
CV_ID      'i-upper'      300 ! (
!          icvtyp
CV_TYP      'upper'
!          icvthr          ipfsw          icvact
CV_THR      NONEQUIL      FOG          ACTIVE
!          itypth          ipora          vapor
CV_PAS      SEPARATE      ONLYATM      SUPERHEATED
!          ptdit          pvol
CV_PTD      PVOL          {{{pres=}}}
!          atmid          tatm
CV_AAD      TATM          {{{temp=}}}
!          nmmat
CV_NCG      3            RHUM      0.5
!          n            namgas      mass
!          1            'N2'        0.7915
!          2            'O2'        {{{o2m=}}}
!          3            'CO2'       {{{co2m=}}}

!          size
!          size
CV_VAT      2 !n          cvz          cvvol
!          1            3.0          0.0
!          2            4.5          9.0

!
! m-upper: (3m X 5m - 2m X 3m) X 1.5m= 13.5m3
!
!
!          cvname          icvnum
CV_ID      'm-upper'      310 ! (
!          icvtyp
CV_TYP      'upper'
!          icvthr          ipfsw          icvact
CV_THR      NONEQUIL      FOG          ACTIVE
!          itypth          ipora          vapor
CV_PAS      SEPARATE      ONLYATM      SUPERHEATED
!          ptdit          pvol
CV_PTD      PVOL          {{{pres=}}}
!          atmid          tatm
CV_AAD      TATM          {{{temp=}}}
!          nmmat
CV_NCG      3            RHUM      0.5
!          n            namgas      mass
!          1            'N2'        0.7915
!          2            'O2'        {{{o2m=}}}
!          3            'CO2'       {{{co2m=}}}

!          size
!          size
CV_VAT      2 !n          cvz          cvvol
!          1            3.0          0.0
!          2            4.5          13.5

!
! o-upper: (4m X 6m - 3m X 5m) X 1.5m= 13.5m3
!
!
!          cvname          icvnum
CV_ID      'o-upper'      320 ! (
!          icvtyp
CV_TYP      'upper'
!          icvthr          ipfsw          icvact
CV_THR      NONEQUIL      FOG          ACTIVE
!          itypth          ipora          vapor
CV_PAS      SEPARATE      ONLYATM      SUPERHEATED
!          ptdit          pvol
CV_PTD      PVOL          {{{pres=}}}

```

```

!          atmid          tatm
CV_AAD          TATM          {{{temp=}}}
!          nmmat
CV_NCG          3          RHUM          0.5
!          n          namgas          mass
          1          'N2'          0.7915
          2          'O2'          {{{o2m=}}}
          3          'CO2'          {{{co2m=}}}

!          size
!          size
CV_VAT          2 !n          cvz          cvvol
          1          3.0          0.0
          2          4.5          13.5

!)
!
! this is a sink environment volume
!
!          cvname          icvnum
CV_ID          'ENV'          900 ! (
!          icvtyp
CV_TYP          'ENV'
!          icvthr          ipfsw          icvact
CV_THR          NONEQUIL          FOG          time-indep
!          itypth          ipora          vapor
CV_PAS          SEPARATE          ONLYATM          SUPERHEATED
!          ptdit          pvol
CV_PTD          PVOL          101325.0
!          atmid          tatm
CV_AAD          TATM          {{{envt=}}}
!          nmmat
CV_NCG          3          RHUM          0.5
!          n          namgas          mass
          1          'N2'          0.7915
          2          'O2'          {{{o2m=}}}
          3          'CO2'          {{{co2m=}}}

!          size
!          size
CV_VAT          2 !n          cvz          cvvol
          1          0.0          0.0
          2          4.5          108.0

!
! this is a source environment volume
!
!          cvname          icvnum
CV_ID          'ENV-IN'          901 ! (
!          icvtyp
CV_TYP          'ENV-IN'
!          icvthr          ipfsw          icvact
CV_THR          NONEQUIL          FOG          time-indep
!          itypth          ipora          vapor
CV_PAS          SEPARATE          ONLYATM          SUPERHEATED
!          ptdit          pvol
CV_PTD          PVOL          101325.0
!          atmid          tatm
CV_AAD          TATM          {{{temp=}}}
!          nmmat
CV_NCG          3          RHUM          0.5
!          n          namgas          mass
          1          'N2'          0.7915
          2          'O2'          {{{o2m=}}}
          3          'CO2'          {{{co2m=}}}

!          size
!          size
CV_VAT          2 !n          cvz          cvvol
          1          0.0          0.0
          2          4.5          108.0

!)
!)
! Flowpaths section
!
!
```

```

FL_INPUT !(
!      fpname          ifpnum
FL_ID   'ilow-imid'      100
!      kcvfm          kcvto          zfm          zto
FL_FT   'i-lower'      'i-middle'  1.5          1.5
!      flara          flen          flopo          flhgtf          flhggt
FL_GEO  6.0            1.5          1.0
!      kflgfl          ibubf          ibubt
FL_JSW  0              NoBubbleRise NoBubbleRise ! vertical flow
!      fricfo          fricro          cdchkf          cdchkr
!FL_USL  0.0            0.0            1.0            1.0
!
FL_SEG  1
!      #   sarea          slen          shyd          srgh
!      1   6.0            1.5            1.5
!
! radial flow in the lower elevation
!
!      fpname          ifpnum
FL_ID   'ilow-mlow'      110
!      kcvfm          kcvto          zfm          zto
FL_FT   'i-lower'      'm-lower'  0.75          0.75
!      flara          flen          flopo          flhgtf          flhggt
FL_GEO  15.0           1.5            1.
!      kflgfl          ibubf          ibubt
FL_JSW  3              NoBubbleRise NoBubbleRise ! horizontal flow
!      fricfo          fricro          cdchkf          cdchkr
!FL_USL  0.0            0.0            1.0            1.0
!      size
FL_SEG  1 !n          sarea slen          shyd srgh lamflg slam
!      1   15.0        1.5            6.0 ! 4xArea/perimeter

!
FL_INPUT !(
!      fpname          ifpnum
FL_ID   'mlow-mmid'      111
!      kcvfm          kcvto          zfm          zto
FL_FT   'm-lower'      'm-middle'  1.5          1.5
!      flara          flen          flopo          flhgtf          flhggt
FL_GEO  9.0            1.5          1.0
!      kflgfl          ibubf          ibubt
FL_JSW  0              NoBubbleRise NoBubbleRise ! vertical flow
!      fricfo          fricro          cdchkf          cdchkr
!FL_USL  0.0            0.0            1.0            1.0
!
FL_SEG  1
!      #   sarea          slen          shyd          srgh
!      1   9.0            1.5            3.0

!
FL_INPUT !(
!      fpname          ifpnum
FL_ID   'olow-omid'      112
!      kcvfm          kcvto          zfm          zto
FL_FT   'o-lower'      'o-middle'  1.5          1.5
!      flara          flen          flopo          flhgtf          flhggt
FL_GEO  9.0            1.5          1.0
!      kflgfl          ibubf          ibubt
FL_JSW  0              NoBubbleRise NoBubbleRise ! vertical flow
!      fricfo          fricro          cdchkf          cdchkr
!FL_USL  0.0            0.0            1.0            1.0
!
FL_SEG  1
!      #   sarea          slen          shyd          srgh
!      1   9.0            1.5            1.5

!
!      fpname          ifpnum
FL_ID   'mlow-olow'      120
!      kcvfm          kcvto          zfm          zto
FL_FT   'm-lower'      'o-lower'  0.75          0.75
!      flara          flen          flopo          flhgtf          flhggt

```

```

FL_GEO 24.0 1.0 1.
! kflgfl ibubf ibubt
FL_JSW 3 NoBubbleRise NoBubbleRise ! horizontal flow
! fricfo fricro cdchkf cdchkr
!FL_USL 0.0 0.0 1.0 1.0
! size
FL_SEG 1 !n sarea slen shyd srgh lamflg slam
! 1 24.0 1.0 6.0 ! 4xArea/perimeter

! fpname ifpnum
FL_ID 'imid-iupp' 200
! kcvfm kcvto zfm zto
FL_FT 'i-middle' 'i-upper' 3.0 3.0
! flara flen flopo flhgtf flhggt
FL_GEO 6.0 1.5 1.0
! kflgfl ibubf ibubt
FL_JSW 0 NoBubbleRise NoBubbleRise ! vertical flow
! fricfo fricro cdchkf cdchkr
!FL_USL 0.0 0.0 1.0 1.0
! size
FL_SEG 1
! # sarea slen shyd srgh
! 1 6.0 1.5 1.5

!
! radial flow in the middle elevation
!
! fpname ifpnum
FL_ID 'imid-mmld' 210
! kcvfm kcvto zfm zto
FL_FT 'i-middle' 'm-middle' 2.25 2.25
! flara flen flopo flhgtf flhggt
FL_GEO 15.0 1.5 1.0
! kflgfl ibubf ibubt
FL_JSW 3 NoBubbleRise NoBubbleRise ! horizontal flow
! fricfo fricro cdchkf cdchkr
!FL_USL 0.0 0.0 1.0 1.0
! size
FL_SEG 1 !n sarea slen shyd srgh lamflg slam
! 1 15.0 1.5 6.0 ! 4xArea/perimeter

!
FL_INPUT !(
! fpname ifpnum
FL_ID 'mmld-mupp' 211
! kcvfm kcvto zfm zto
FL_FT 'm-middle' 'm-upper' 3.0 3.0
! flara flen flopo flhgtf flhggt
FL_GEO 9.0 1.5 1.0
! kflgfl ibubf ibubt
FL_JSW 0 NoBubbleRise NoBubbleRise ! vertical flow
! fricfo fricro cdchkf cdchkr
!FL_USL 0.0 0.0 1.0 1.0
! size
FL_SEG 1
! # sarea slen shyd srgh
! 1 9.0 1.5 3.0

!
FL_INPUT !(
! fpname ifpnum
FL_ID 'omid-oupp' 212
! kcvfm kcvto zfm zto
FL_FT 'o-middle' 'i-upper' 3.0 3.0
! flara flen flopo flhgtf flhggt
FL_GEO 9.0 1.5 1.0
! kflgfl ibubf ibubt
FL_JSW 0 NoBubbleRise NoBubbleRise ! vertical flow
! fricfo fricro cdchkf cdchkr
!FL_USL 0.0 0.0 1.0 1.0
! size
FL_SEG 1
! # sarea slen shyd srgh
! 1 9.0 1.5 3.0

```

```

FL_SEG 1
!      #   sarea   slen   shyd   srgh
!      1   9.0    1.5    1.5

!
!      fpname      ifpnum
FL_ID 'mmid-omid' 220
!      kcvfm      kcvto      zfm      zto
FL_FT 'm-middle' 'o-middle' 2.25 2.25
!      flara      flen      flopo      flhgtf      flhgtt
FL_GEO 24.0      1.0      1.
!      kflgfl      ibubf      ibubt
FL_JSW 3      NoBubbleRise NoBubbleRise ! horizontal flow
!      fricfo fricro cdchkf cdchkr
!FL_USL 0.0      0.0      1.0      1.0
!      size
FL_SEG 1 !n      sarea slen      shyd srgh lamflg slam
!      1      24.0 1.0      6.0 ! 4xArea/perimeter

!
! radial flow in the upper elevation
!
!      fpname      ifpnum
FL_ID 'iupp-mupp' 310
!      kcvfm      kcvto      zfm      zto
FL_FT 'i-upper' 'm-upper' 3.75 3.75
!      flara      flen      flopo      flhgtf      flhgtt
FL_GEO 15.0      1.5      1.
!      kflgfl      ibubf      ibubt
FL_JSW 3      NoBubbleRise NoBubbleRise ! horizontal flow
!      fricfo fricro cdchkf cdchkr
!FL_USL 0.0      0.0      1.0      1.0
!      size
FL_SEG 1 !n      sarea slen      shyd srgh lamflg slam
!      1      15.0 1.5      6.0 ! 4xArea/perimeter

!
!      fpname      ifpnum
FL_ID 'mupp-oupp' 320
!      kcvfm      kcvto      zfm      zto
FL_FT 'm-upper' 'o-upper' 3.75 3.75
!      flara      flen      flopo      flhgtf      flhgtt
FL_GEO 24.0      1.0      1.
!      kflgfl      ibubf      ibubt
FL_JSW 3      NoBubbleRise NoBubbleRise ! horizontal flow
!      fricfo fricro cdchkf cdchkr
!FL_USL 0.0      0.0      1.0      1.0
!      size
FL_SEG 1 !n      sarea slen      shyd srgh lamflg slam
!      1      24.0 1.0      6.0 ! 4xArea/perimeter

!
!
! ***next 2 flow paths for the ventilation
! ENV-IN to lower
! upper to ENV
!
!      fpname      ifpnum
FL_ID 'ENVIN-lower' 901
!      kcvfm      kcvto      zfm      zto
FL_FT 'ENV-IN' 'o-lower' 0.75 0.75
!      flara      flen      flopo      flhgtf      flhgtt
FL_GEO 0.018      1.5      1.
!      kflgfl      ibubf      ibubt
FL_JSW 13 NoBubbleRise NoBubbleRise ! forward horizontal flow only
!      fricfo fricro cdchkf cdchkr
!FL_USL 0.5      1.
!      size
FL_SEG 2 !n      sarea slen      shyd srgh lamflg slam
!      1      0.018 1.0      0.13 ! 4xArea/perimeter
!      2      9.0 0.5      2.40

```

```

!
!      fname      ifpnum
FL_ID 'upper-ENV' 910
!      kcvfm      kcvto      zfm      zto
FL_FT 'o-upper'   'ENV'     3.75    3.75
!      flara      flen      flopo      flhgtf      flhgtt
FL_GEO 0.4225    3.0      1.
!      kflgfl      ibubf      ibubt
FL_JSW 13 NoBubbleRise NoBubbleRise ! forward horizontal flow only
!      fricfo      fricro      cdchkf      cdchkr
!FL_USL 0.5      1.
!      size
FL_SEG 2 !n      sarea      slen      shyd      srgh      lamflg      slam
!      1      9.0      2.0      2.40
!      2      0.4225 1.0      0.65 ! 4xArea/perimeter
!
!
!FL_VTM 1 !n      FLNAME      NTFLAG      NFUN
!      1      'upper-ENV'      CF      'FL-VEL'
!
!FL_PMP 1 ! pname      flname      ptype      cfname
!      1      ''      'upper-ENV' QUICK-CF      'delta-p'
!
HS_INPUT !(
!
! Only HS models, are the enclosure walls, floor and ceiling
!
! The test does not provide any information of HS materials. However, CFAST input deck:
! provide:      k      Cp      rho      thick      emissivity
!      WALLS      0.39      1000      1440      0.1      0.94
!      Ceil/Floor 0.63      1000      1920      0.1      0.94
!
! Add heat source to represent the thermal radiation loss from combustion to the surface.
! Q combustion is 200 kW, and use 0.2 of it to distribute to all surfaces of HS, except the
! burner. Total surface area is 138 m2
!      area      fraction
! CEILING 6      0.0435
!      9      0.0652
!      9      0.0652
! FLOOR 6      0.0435
!      9      0.0652
!      9      0.0652
! S. WALL 6      0.0435
!      6      0.0435
!      6      0.0435
! L. WALL 9      0.0652
!      9      0.0652
!      9      0.0652
!
! Ceiling: 4 m X 6 m X 0.1 m
! i-upper: 6m2, m-upper: 9m2, o-upper: 9m2
!
!      hsname      ishnum
HS_ID 'iCeiling' 10 !(
!      igeom      iss
HS_GD RECTANGULAR      ss
!      hsalt      alpha
HS_EOD 4.49      0.0 ! ceiling LHS bottom
!      isrc      nameips      vsmult
HS_SRC CF 'Rad_Q' 0.0435
!      size
HS_ND 3 !n n      xi      tempin      matnam      qfrcin
!      1 1      0.0      -      STAINLESS-STEEL      1.0
!      2 2      0.05     -      STAINLESS-STEEL      0.0
!      3 3      0.1      -
!
!      ibcl      ibvl      mteval
HS_LB CalcCoefHS      'i-upper'      YES
!      emiswl      rmodl      pathl
HS_LBR 0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal

```

```

HS_LBP          EXT          1.0          1.024
!              asurfl        c1n1        bndz1
HS_LBS          6.0          2.45
!              ibcr          table
HS_RB           Symmetry
!              iflowr        cpfpr        cpfar
HS_RBP          EXT          0.0          0.0
!              iftnum
HS_FT           OFF

!
!              hsname        ishnum
HS_ID           'mCeiling'    11 ! (
!              igeom        iss
HS_GD           RECTANGULAR    ss
!              hsalt        alpha
HS_EOD          4.49          0.0 ! ceiling LHS bottom
!              isrc        nameips    vsmult
HS_SRC          CF 'Rad_Q'    0.0652
!
! size
HS_ND           3 !n n        xi tempin        matnam        qfrcin
!              1 1          0.0 -          STAINLESS-STEEL    1.0
!              2 2          0.05 -         STAINLESS-STEEL    0.0
!              3 3          0.1 -
!
!              ibcl          ibvl          mteval
HS_LB           CalcCofHs    'm-upper'    YES
!              emiswl        rmodl        pathl
HS_LBR          0.94          GRAY-GAS-A    0.0
!              iflowl        cpfpl        cpfal
HS_LBP          EXT          1.0          1.0
!              asurfl        c1n1        bndz1
HS_LBS          9.0          3.0
!              ibcr          table
HS_RB           Symmetry
!              iflowr        cpfpr        cpfar
HS_RBP          EXT          0.0          0.0
!              iftnum
HS_FT           OFF

!
!              hsname        ishnum
HS_ID           'oCeiling'    12 ! (
!              igeom        iss
HS_GD           RECTANGULAR    ss
!              hsalt        alpha
HS_EOD          4.49          0.0 ! ceiling LHS bottom
!              isrc        nameips    vsmult
HS_SRC          CF 'Rad_Q'    0.0652
!
! size
HS_ND           3 !n n        xi tempin        matnam        qfrcin
!              1 1          0.0 -          STAINLESS-STEEL    1.0
!              2 2          0.05 -         STAINLESS-STEEL    0.0
!              3 3          0.1 -
!
!              ibcl          ibvl          mteval
HS_LB           CalcCofHs    'o-upper'    YES
!              emiswl        rmodl        pathl
HS_LBR          0.94          GRAY-GAS-A    0.0
!              iflowl        cpfpl        cpfal
HS_LBP          EXT          1.0          1.0
!              asurfl        c1n1        bndz1
HS_LBS          9.0          3.0
!              ibcr          table
HS_RB           Symmetry
!              iflowr        cpfpr        cpfar
HS_RBP          EXT          0.0          0.0
!              iftnum
HS_FT           OFF

!
! floor similar to ceiling
! i-lower: 6m2, m-lower: 9m2, o-lower: 9m2

```

```

!
!      hsname      ishnum
HS_ID      'ifloor'      20 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      0.1      -1.0E-7 ! floor RHS bottom
!      isrc      nameips      vsmult
HS_SRC      CF      'Rad_Q'      0.0435
!
!      size
HS_ND      3 !n n      xi tempin      matnam      qfrcin
!      1 1      0.0      -      STAINLESS-STEEL      1.0
!      2 2      0.05      -      STAINLESS-STEEL      0.0
!      3 3      0.1      -
!
!      ibcl      ibvl      mteval
HS_LB      CalcCofHS      'i-lower'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0
!      asurfl      clnl      bndzl
HS_LBS      6.0      2.45      2.45
!      ibcr      table
HS_RB      Symmetry
!      iflowr      cpfpr      cpfar
HS_RBP      EXT      0.0      0.0
!      iftnum
HS_FT      OFF

!
!      hsname      ishnum
HS_ID      'mfloor'      21 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      0.1      -1.0E-7 ! floor RHS bottom
!      isrc      nameips      vsmult
HS_SRC      CF      'Rad_Q'      0.0652
!
!      size
HS_ND      3 !n n      xi tempin      matnam      qfrcin
!      1 1      0.0      -      STAINLESS-STEEL      1.0
!      2 2      0.05      -      STAINLESS-STEEL      0.0
!      3 3      0.1      -
!
!      ibcl      ibvl      mteval
HS_LB      CalcCofHS      'm-lower'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0
!      asurfl      clnl      bndzl
HS_LBS      9.0      3.0      3.0
!      ibcr      table
HS_RB      Symmetry
!      iflowr      cpfpr      cpfar
HS_RBP      EXT      0.0      0.0
!      iftnum
HS_FT      OFF

!
!      hsname      ishnum
HS_ID      'ofloor'      22 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      0.1      -1.0E-7 ! floor RHS bottom
!      isrc      nameips      vsmult
HS_SRC      CF      'Rad_Q'      0.0652
!
!      size
HS_ND      3 !n n      xi tempin      matnam      qfrcin
!      1 1      0.0      -      STAINLESS-STEEL      1.0
!      2 2      0.05      -      STAINLESS-STEEL      0.0

```

```

3 3 0.1 -
!
!      ibcl      ibvl      mteval
HS_LB      CalcCoefHS      'o-lower'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0
!      asurfl      clnl      bndzl
HS_LBS      9.0      3.0      3.0
!      ibcr      table
HS_RB      Symmetry
!      iflowr      cpfpr      cpfar
HS_RBP      EXT      0.0      0.0
!      iftnum
HS_FT      OFF
!
! short walls: 4 m X 4.5 m X 0.1 m in 3 equals walls in lower, middle and upper volumes
!      area1: 6 m2
!
!      hsname      ishnum
HS_ID 'short_wall_low'      41 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      0.0      1.0
!      hsmult
HS_MLT      2.0      ! 2 walls
!      isrc      nameips      vsmult
HS_SRC      CF 'Rad_Q' 0.0435
!
!      size
HS_ND      3 !n n      xi tempin      matnam      qfrcin
!      1 1      0.0 -      STAINLESS-STEEL      1.0
!      2 2      0.05 -      STAINLESS-STEEL      0.0
!      3 3      0.1 -
!
!      ibcl      ibvl      mteval
HS_LB      CalcCoefHS      'o-lower'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0
!      asurfl      clnl      bndzl
HS_LBS      6.0      1.5      1.5      ! axial height
!      ibcr      table
HS_RB      Symmetry
!      iflowr      cpfpr      cpfar
HS_RBP      EXT      0.0      0.0
!      iftnum
HS_FT      OFF
!
!
!      hsname      ishnum
HS_ID 'short_wall_mid'      42 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      1.5      1.0
!      hsmult
HS_MLT      2.0      ! 2 walls
!      isrc      nameips      vsmult
HS_SRC      CF 'Rad_Q' 0.0435
!
!      size
HS_ND      3 !n n      xi tempin      matnam      qfrcin
!      1 1      0.0 -      STAINLESS-STEEL      1.0
!      2 2      0.05 -      STAINLESS-STEEL      0.0
!      3 3      0.1 -
!
!      ibcl      ibvl      mteval
HS_LB      CalcCoefHS      'o-middle'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0

```

```

!          asurfl          clnl          bndzl
HS_LBS      6.0          1.5          1.5  ! axial height
!          ibcr          table
HS_RB      Symmetry
!          iflowr          cpfpr          cpfar
HS_RBP      EXT          0.0          0.0
!          iftnum
HS_FT      OFF
!
!          hsname          ishnum
HS_ID 'short_wall_upp'          43 !(
!          igeom          iss
HS_GD      RECTANGULAR          ss
!          hsalt          alpha
HS_EOD      3.0          1.0
!          hsmult
HS_MLT      2.0          ! 2 walls
!          isrc          nameips          vsmult
HS_SRC      CF 'Rad_Q' 0.0435
!
! size
HS_ND      3 !n n          xi tempin          matnam          qfrcin
          1 1          0.0 -          STAINLESS-STEEL          1.0
          2 2          0.05 -          STAINLESS-STEEL          0.0
          3 3          0.1 -
!
!          ibcl          ibvl          mteval
HS_LB      CalcCoefHS          'o-upper'          YES
!          emiswl          rmodl          pathl
HS_LBR      0.94          GRAY-GAS-A          0.0
!          iflowl          cpfpl          cpfal
HS_LBP      EXT          1.0          1.0
!          asurfl          clnl          bndzl
HS_LBS      6.0          1.5          1.5  ! axial height
!          ibcr          table
HS_RB      Symmetry
!          iflowr          cpfpr          cpfar
HS_RBP      EXT          0.0          0.0
!          iftnum
HS_FT      OFF
!
! long walls: 6 m X 4.5 m X 0.1 m in 3 equals walls in lower, middle and upper volumes
!          area1: 9 m2
!
!          hsname          ishnum
HS_ID 'long_wall_low'          51 !(
!          igeom          iss
HS_GD      RECTANGULAR          ss
!          hsalt          alpha
HS_EOD      0.0          1.0
!          hsmult
HS_MLT      2.0          ! 2 walls
!          isrc          nameips          vsmult
HS_SRC      CF 'Rad_Q' 0.0652
!
! size
HS_ND      3 !n n          xi tempin          matnam          qfrcin
          1 1          0.0 -          STAINLESS-STEEL          1.0
          2 2          0.05 -          STAINLESS-STEEL          0.0
          3 3          0.1 -
!
!          ibcl          ibvl          mteval
HS_LB      CalcCoefHS          'o-lower'          YES
!          emiswl          rmodl          pathl
HS_LBR      0.94          GRAY-GAS-A          0.0
!          iflowl          cpfpl          cpfal
HS_LBP      EXT          1.0          1.0
!          asurfl          clnl          bndzl
HS_LBS      9.0          1.5          1.5  ! axial height
!          ibcr          table
HS_RB      Symmetry
!          iflowr          cpfpr          cpfar
HS_RBP      EXT          0.0          0.0
!          iftnum

```

```

HS_FT          OFF
!
!
!      hsname      ishnum
HS_ID 'long_wall_mid'      52 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      1.5      1.0
!      hsmult
HS_MLT      2.0      ! 2 walls
!      isrc      nameips      vsmult
HS_SRC      CF      'Rad_Q'      0.0652
!      size
HS_ND      3      !n n      xi tempin      matnam      qfrcin
!      1 1      0.0      -      STAINLESS-STEEL      1.0
!      2 2      0.05      -      STAINLESS-STEEL      0.0
!      3 3      0.1      -
!      ibcl      ibvl      mteval
HS_LB      CalcCoefHS      'o-middle'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0
!      asurfl      clnl      bndzl
HS_LBS      9.0      1.5      1.5      ! axial height
!      ibcr      table
HS_RB      Symmetry
!      iflowr      cpfpr      cpfar
HS_RBP      EXT      0.0      0.0
!      iftnum
HS_FT      OFF
!
!
!      hsname      ishnum
HS_ID 'long_wall_upp'      53 !(
!      igeom      iss
HS_GD      RECTANGULAR      ss
!      hsalt      alpha
HS_EOD      3.0      1.0
!      hsmult
HS_MLT      2.0      ! 2 walls
!      isrc      nameips      vsmult
HS_SRC      CF      'Rad_Q'      0.0652
!      size
HS_ND      3      !n n      xi tempin      matnam      qfrcin
!      1 1      0.0      -      STAINLESS-STEEL      1.0
!      2 2      0.05      -      STAINLESS-STEEL      0.0
!      3 3      0.1      -
!      ibcl      ibvl      mteval
HS_LB      CalcCoefHS      'o-upper'      YES
!      emiswl      rmodl      pathl
HS_LBR      0.94      GRAY-GAS-A      0.0
!      iflowl      cpfpl      cpfal
HS_LBP      EXT      1.0      1.0
!      asurfl      clnl      bndzl
HS_LBS      9.0      1.5      1.5      ! axial height
!      ibcr      table
HS_RB      Symmetry
!      iflowr      cpfpr      cpfar
HS_RBP      EXT      0.0      0.0
!      iftnum
HS_FT      OFF
!
! Rock burner
!
!      hsname      ishnum
HS_ID 'rock_burner'      60
!      igeom      iss
HS_GD      CYLINDRICAL      NO
!      hsalt      alpha

```

```

HS_EOD          0.0          1.0
!
HS_MLT          hsmult
HS_MLT          1.0
!
HS_SRC          isrc
HS_SRC          NO
!
size
HS_ND           4 !n n      xi tempin      matnam
                1 1      0.25 {{{temp=}}}} STAINLESS-STEEL ! CONCRETE
                2 2      0.35 {{{temp=}}}} STAINLESS-STEEL ! CONCRETE
                3 3      0.45 {{{temp=}}}} STAINLESS-STEEL ! CONCRETE
                4 4      0.57 {{{temp=}}}}
!
!          ibcl          ibvl          mteval
HS_LB          CalcCoefHS          'i-lower'          YES
!          emiswl          rmodl          pathl
HS_LBR          0.99          GRAY-GAS-A          0.0
!          iflowl          cpfpl          cpfal
HS_LBP          ext          1.0          1.0
!          asurfl          c1n1          bndz1
HS_LBS          0.181          0.23          ! axial height
!          ibcl          ibvl          mteval
HS_RB          CalcCoefHS          'i-lower'          YES
!          emiswl          rmodl          pathl
HS_RBR          0.99          GRAY-GAS-A          0.0
!          iflowl          cpfpl          cpfal
HS_RBP          EXT          1.0          1.0
!          asurfl          c1n1          bndz1
HS_RBS          0.412          0.23          0.23 ! axial height
!          iftnum
HS_FT          OFF
!)
END PROGRAM MELGEN
!)
PROGRAM MELCOR !(
EXEC_INPUT !(
!
exec_autots 1 5.0 1.0e-10 ! auto calc of temporal relaxation = max ( 5.0*dtmax, 1.0e-10 )
exec_tsmult 1.0e-9 1.0e-9 1.0 1.0e-9 ! time scale multipliers for heat trans, oxidation, quench
velocity, flow path opening (valves)

EXEC_TITLE 'LLNL Enclosure Experiment_Test 9v9(9vol)'
!
EXEC_CPULEFT 10.0
!
EXEC_CPULIM 2.0E6
EXEC_CYMESF 500 500
EXEC_SOFDTMIN 1.0E-6 100
!
EXEC_JOBID 'REF'
!
size
EXEC_TIME      5 !n      time dtmax dtmin      dedt dtplot dtrest dcrest
                1 -200.0 0.10 1.0E-2 100.0      1.0 50000.0 1.0E10
                2 -1.0 0.10 1.0E-2 100.0      1.0 50000.0 1.0E10
                3 0.0 0.25 1.0E-2 100.0      1.0 50000.0 1.0E10
                4 1000.0 0.25 1.0E-2 100.0      10.0 50000.0 1.0E10
                5 4000.0 0.25 1.0E-2 100.0      10.0 50000.0 1.0E10
!
EXEC_TEND 4000.0 ! 0

! name of interactive CF data file
EXEC_CFEFILE 'dynamicInp'

CVH_INPUT
CVH_SC 1 ! n scnumber      value index
                1 4408 1000000.      1 ! disable revised treatment of non-equilibrium thermo

!
!)
END PROGRAM MELCOR

```

B.3 STORM SR-11

```

!*****
!* STORM ISP - Deposition Phase with correct steam flow and temperatures. *
!*****
!
! https://svn-melcor.sandia.gov/svn/melcor-II/documentation/trunk/Assessments/STORM
!
! Sensitivity analysis is provided in this input deck
!
! case0 - default
! case1 - same as case0, add HTC on HS inside is 30.0
! case2 - same as case1, add turbulent deposition 0 2 0 & roughness 5e-5m
! case3 - same as case1, except HTC on HS inside is 50.0
! case4 - same as case1, except HTC on HS inside is gradually increased
! case5 - same as case1, except HTC on HS inside is 60.0
!
!GlobalData !(
MEG_DIAGFILE      'storm0.gdia'
MEL_DIAGFILE      'storm0.dia'
MEG_RESTARTFILE   'storm0.rst'
MEL_RESTARTFILE   'storm0.rst' NCYCLE 0
MESSAGEFILE       'storm0.mes'
extdiagf          'storm0.ext'
CommentBlock case0 !comment this line to run all the cases
(((case0
MEG_OUTPUTFILE 'storm0.gout'
MEL_OUTPUTFILE 'storm0.out'
PLOTFILE 'storm0.ptf'
)))
(((case1
MEG_OUTPUTFILE 'storm1.gout'
MEL_OUTPUTFILE 'storm1.out'
PLOTFILE 'storm1.ptf'
)))
(((case2
MEG_OUTPUTFILE 'storm2.gout'
MEL_OUTPUTFILE 'storm2.out'
PLOTFILE 'storm2.ptf'
)))
(((case3
MEG_OUTPUTFILE 'storm3.gout'
MEL_OUTPUTFILE 'storm3.out'
PLOTFILE 'storm3.ptf'
)))
(((case4
MEG_OUTPUTFILE 'storm4.gout'
MEL_OUTPUTFILE 'storm4.out'
PLOTFILE 'storm4.ptf'
)))
(((case5
MEG_OUTPUTFILE 'storm5.gout'
MEL_OUTPUTFILE 'storm5.out'
PLOTFILE 'storm5.ptf'
)))
RN1VISUALFILE 'aerosolFile'

!VariableValue {{{MFR_N2=0.6}}} {{{MFR_O2=0.05}}} {{{MFR_AR=0.3}}} {{{MFR_HE=0.05}}}
{{{TATM_0=633.0}}}
!)
!
PROGRAM MELGEN !(
EXEC_INPUT !(
EXEC_TITLE 'STORM - Correct TH'
EXEC_GLOBAL_DFT 2.0
! add global default 2.0 (dll 4-10-12)
!
! add deposition plots
!
(((case0+case1+case3+case4+case5
EXEC_PLOT 30

```

```

! gravitational
1  RN1-DEPHS(METER1HS, LHS, CD, GRAV)
2  RN1-DEPHS(METER2HS, LHS, CD, GRAV)
3  RN1-DEPHS(METER3HS, LHS, CD, GRAV)
4  RN1-DEPHS(METER4HS, LHS, CD, GRAV)
5  RN1-DEPHS(METER5HS, LHS, CD, GRAV)
! thermophoresis
6  RN1-DEPHS(METER1HS, LHS, CD, THERM)
7  RN1-DEPHS(METER2HS, LHS, CD, THERM)
8  RN1-DEPHS(METER3HS, LHS, CD, THERM)
9  RN1-DEPHS(METER4HS, LHS, CD, THERM)
10 RN1-DEPHS(METER5HS, LHS, CD, THERM)
! diffusive
11 RN1-DEPHS(METER1HS, LHS, CD, DIFF)
12 RN1-DEPHS(METER2HS, LHS, CD, DIFF)
13 RN1-DEPHS(METER3HS, LHS, CD, DIFF)
14 RN1-DEPHS(METER4HS, LHS, CD, DIFF)
15 RN1-DEPHS(METER5HS, LHS, CD, DIFF)
! fall
16 RN1-DEPHS(METER1HS, LHS, CD, FALL)
17 RN1-DEPHS(METER2HS, LHS, CD, FALL)
18 RN1-DEPHS(METER3HS, LHS, CD, FALL)
19 RN1-DEPHS(METER4HS, LHS, CD, FALL)
20 RN1-DEPHS(METER5HS, LHS, CD, FALL)
! deposition Gelbard
21 RN1-ADEP(METER1HS, LHS, CD, TOT)
22 RN1-ADEP(METER2HS, LHS, CD, TOT)
23 RN1-ADEP(METER3HS, LHS, CD, TOT)
24 RN1-ADEP(METER4HS, LHS, CD, TOT)
25 RN1-ADEP(METER5HS, LHS, CD, TOT)
! resuspension plot variables
26 RN1-TOTRES(METER1HS, LHS)
27 RN1-TOTRES(METER2HS, LHS)
28 RN1-TOTRES(METER3HS, LHS)
29 RN1-TOTRES(METER4HS, LHS)
30 RN1-TOTRES(METER5HS, LHS)
)))
(((case2
EXEC_PLOT 25
! gravitational
1  RN1-DEPHS(METER1HS, LHS, CD, GRAV)
2  RN1-DEPHS(METER2HS, LHS, CD, GRAV)
3  RN1-DEPHS(METER3HS, LHS, CD, GRAV)
4  RN1-DEPHS(METER4HS, LHS, CD, GRAV)
5  RN1-DEPHS(METER5HS, LHS, CD, GRAV)
! thermophoresis
6  RN1-DEPHS(METER1HS, LHS, CD, THERM)
7  RN1-DEPHS(METER2HS, LHS, CD, THERM)
8  RN1-DEPHS(METER3HS, LHS, CD, THERM)
9  RN1-DEPHS(METER4HS, LHS, CD, THERM)
10 RN1-DEPHS(METER5HS, LHS, CD, THERM)
! diffusive
11 RN1-DEPHS(METER1HS, LHS, CD, DIFF)
12 RN1-DEPHS(METER2HS, LHS, CD, DIFF)
13 RN1-DEPHS(METER3HS, LHS, CD, DIFF)
14 RN1-DEPHS(METER4HS, LHS, CD, DIFF)
15 RN1-DEPHS(METER5HS, LHS, CD, DIFF)
! turbulent
16 RN1-DEPHS(METER1HS, LHS, CD, TURB)
17 RN1-DEPHS(METER2HS, LHS, CD, TURB)
18 RN1-DEPHS(METER3HS, LHS, CD, TURB)
19 RN1-DEPHS(METER4HS, LHS, CD, TURB)
20 RN1-DEPHS(METER5HS, LHS, CD, TURB)
!
! fall
21 RN1-DEPHS(METER1HS, LHS, CD, FALL)
22 RN1-DEPHS(METER2HS, LHS, CD, FALL)
23 RN1-DEPHS(METER3HS, LHS, CD, FALL)
24 RN1-DEPHS(METER4HS, LHS, CD, FALL)
25 RN1-DEPHS(METER5HS, LHS, CD, FALL)
)))

```

```

!)
!! *** sources ***
TF_INPUT !(
TF_ID      'H2O source'          1.0 !(
!          size
TF_TAB      3 !n                x                y
              1                0.0                0.011 ! 40 kg/hr
              2                9000.0             0.011 !   for 2.5 h
              3                9000.0             0.0   ! steam off
!)
TF_ID      'N2 source'          1.0 !(
!          size
TF_TAB      15 !n               x                y
              1                0.0                0.01 !
              2                9000.0             0.01 !   for 2.5 h
              3                9000.0             0.10194 ! 367 kg/hr
              4                10380.0            0.10194 !   for 23 min
              5                10380.0            0.12583 ! 453 kg/hr
              6                11940.0            0.12583 !   for 26 min
              7                11940.0            0.15194 ! 547 kg/hr
              8                12900.0            0.15194 !   for 16 min
              9                12900.0            0.17500 ! 630 kg/hr
             10                13920.0            0.17500 !   for 17 min
             11                13920.0            0.19889 ! 716 kg/hr
             12                14880.0            0.19889 !   for 16 min
             13                14880.0            0.22389 ! 806 kg/hr
             14                15300.0            0.22389 !   for 7 min
             15                15300.0             0.0   ! off
!)
TF_ID      'O2 source'          1.0 !(
!          size
TF_TAB      3 !n                x                y
              1                0.0                1.1E-3
              2                9000.0             1.1E-3 ! 266 NL/min air
              3                9000.0             0.0
!)
TF_ID      'AR source'          1.0 !(
!          size
TF_TAB      3 !n                x                y
              1                0.0                7.2E-3
              2                9000.0             7.2E-3 !
              3                9000.0             0.0
!)
TF_ID      'HE source'          1.0 !(
!          size
TF_TAB      3 !n                x                y
              1                0.0                1.0E-4
              2                9000.0             1.0E-4
              3                9000.0             0.0
!)
TF_ID      'temp of sourc'      1.0 !(
!          size
TF_TAB      3 !n                x                y
              1                0.0                653.0 ! 380 C
              2                9000.0             653.0 !
              3                1.0e10             653.0
!)
!! *** mole fraction for environment input ***
TF_ID      'mole fract N2'      1.0 !(
!          size
TF_TAB      1 !n                x                y
              1                0.0                0.6
!)
TF_ID      'mole fract O2'      1.0 !(
!          size
TF_TAB      1 !n                x                y
              1                0.0                0.05
!)
TF_ID      'mole fract AR'      1.0 !(
!          size
TF_TAB      1 !n                x                y

```

```

1          0.0          0.3
!)
TF_ID      'mole fract HE'          1.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.05
!)
TF_ID      'Env gas T(K)'          1.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          603.0
!)
TF_ID      'pressure'          1.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          1.0E5
!)
(((case0
TF_ID      'METER1 wall T'          1.0          523.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER2 wall T'          1.0          513.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER3 wall T'          1.0          503.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER4 wall T'          1.0          493.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER5 wall T'          1.0          483.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'ENV wall T(K)'          1.0          485.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
)))
(((case1+case2
!! *** HS HTC and temperatures ***
TF_ID      'METER1 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          3.0E1
!)
TF_ID      'METER1 wall T'          1.0          523.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER2 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          3.0E1
!)
TF_ID      'METER2 wall T'          1.0          513.0 ! (
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)

```

```

TF_ID      'METER3 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          3.0E1
!)
TF_ID      'METER3 wall T'      1.0          503.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
TF_ID      'METER4 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          3.0E1
!)
TF_ID      'METER4 wall T'      1.0          493.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
TF_ID      'METER5 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          3.0E1
!)
TF_ID      'METER5 wall T'      1.0          483.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
TF_ID      'ENV wall T(K)'      1.0          485.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
)))
(((case3
!! *** HS HTC and temperatures ***
TF_ID      'METER1 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          5.0E1
!)
TF_ID      'METER1 wall T'      1.0          523.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
TF_ID      'METER2 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          5.0E1
!)
TF_ID      'METER2 wall T'      1.0          513.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
TF_ID      'METER3 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          5.0E1
!)
TF_ID      'METER3 wall T'      1.0          503.0 ! (
! size
TF_TAB      1 !n                x              y
              1              0.0          0.0
!)
TF_ID      'METER4 HTC'          1.0          0.0 ! (
! size
TF_TAB      1 !n                x              y

```

```

1          0.0          5.0E1
!)
TF_ID      'METER4 wall T'          1.0          493.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER5 HTC'          1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          5.0E1
!)
TF_ID      'METER5 wall T'          1.0          483.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'ENV wall T(K)'          1.0          485.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
)))
(((case4
!! *** HS HTC and temperatures ***
!! Same case1, except apply gradual increases of HTC from the entrance of the test section from
!!
TF_ID      'METER1 HTC'          1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          3.0E1
!)
TF_ID      'METER1 wall T'          1.0          523.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER2 HTC'          1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          3.4E1
!)
TF_ID      'METER2 wall T'          1.0          513.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER3 HTC'          1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          3.8E1
!)
TF_ID      'METER3 wall T'          1.0          503.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER4 HTC'          1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          4.0E1
!)
TF_ID      'METER4 wall T'          1.0          493.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          0.0
!)
TF_ID      'METER5 HTC'          1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
1          0.0          4.4E1

```

```

!)
TF_ID      'METER5 wall T'          1.0          483.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
TF_ID      'ENV wall T(K)'          1.0          485.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
)))
(((case5
!! *** HS HTC and temperatures ***
TF_ID      'METER1 HTC'            1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          6.0E1
!)
TF_ID      'METER1 wall T'          1.0          523.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
TF_ID      'METER2 HTC'            1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          6.0E1
!)
TF_ID      'METER2 wall T'          1.0          513.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
TF_ID      'METER3 HTC'            1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          6.0E1
!)
TF_ID      'METER3 wall T'          1.0          503.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
TF_ID      'METER4 HTC'            1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          6.0E1
!)
TF_ID      'METER4 wall T'          1.0          493.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
TF_ID      'METER5 HTC'            1.0          0.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          6.0E1
!)
TF_ID      'METER5 wall T'          1.0          483.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
TF_ID      'ENV wall T(K)'          1.0          485.0 !(
! size
TF_TAB      1 !n          x          y
              1          0.0          0.0
!)
)))
!
```

```

!
!! *** aerosol source ***
TF_ID      'SnO2 source'          1.0 ! (
!      size
TF_TAB      3 ! n              x              y
              1              0.0              3.8E-4
              2              9000.0             3.8E-4
              3              9000.0              0.0

!)
!)
MP_INPUT ! (
MP_ID      'CARBON-STEEL'
!)
NCG_INPUT ! (
NCG_ID      'N2'
NCG_ID      'O2'
NCG_ID      'AR'
NCG_ID      'HE'
!)
CVH_INPUT ! (
CV_ID      'METER1'              10 ! (
!      icvtyp
CV_TYP      'CTYP-1'
!      icvthr      ipfsw      icvact
CV_THR      NONEQUIL      FOG      ACTIVE
!      icfvel      cvara
CV_ARE      NOCF      3.1E-3
!
CV_THERM      2
              1      PVOL      1.0E5      TATM      648.      PH20      0.0
              2      N2      0.60      O2      0.05      AR      0.30      HE      0.05
!      size
CV_VAT      2 ! n              cvz              cvvol
              1              0.0              0.0
              2              0.063             3.1E-3
!      size
CV_SOU      10 ! n ctyp      interp      iessrc      srcname      idmat
              1      MASS      RATE      TF      'H2O source' 'H2O-VAP'
              2      TE      RATE      TF      'temp of sourc' 'H2O-VAP'
              3      MASS      RATE      TF      'N2 source'      'N2'
              4      TE      RATE      TF      'temp of sourc'      'N2'
              5      MASS      RATE      TF      'O2 source'      'O2'
              6      TE      RATE      TF      'temp of sourc'      'O2'
              7      MASS      RATE      TF      'AR source'      'AR'
              8      TE      RATE      TF      'temp of sourc'      'AR'
              9      MASS      RATE      TF      'HE source'      'HE'
              10     TE      RATE      TF      'temp of sourc'      'HE'
!)
CV_ID      'METER2'              20 ! (
!      icvtyp
CV_TYP      'CTYP-2'
!      icvthr      ipfsw      icvact
CV_THR      NONEQUIL      FOG      ACTIVE
!      icfvel      cvara
CV_ARE      NOCF      3.1E-3
!
CV_THERM      2
              1      PVOL      1.0E5      TATM      639.      PH20      0.0
              2      N2      0.60      O2      0.05      AR      0.30      HE      0.05
!      size
CV_VAT      2 ! n              cvz              cvvol
              1              0.0              0.0
              2              0.063             3.1E-3
!)
CV_ID      'METER3'              30 ! (
!      icvtyp
CV_TYP      'CTYP-3'
!      icvthr      ipfsw      icvact
CV_THR      NONEQUIL      FOG      ACTIVE
!      icfvel      cvara
CV_ARE      NOCF      3.1E-3

```

```

CV_THERM 2
1 PVOL 1.0E5 TATM 630. PH20 0.0
2 N2 0.60 02 0.05 AR 0.30 HE 0.05
CV_VAT 2 !n cvz cvvol
1 0.0 0.0
2 0.063 3.1E-3
!)
CV_ID 'METER4' 40 !
! icvtyp
CV_TYP 'CTYP-4'
! icvthr ipfsw icvact
CV_THR NONEQUIL FOG ACTIVE
! icfvel cvara
CV_ARE NOCF 3.1E-3
CV_THERM 2
1 PVOL 1.0E5 TATM 623. PH20 0.0
2 N2 0.60 02 0.05 AR 0.30 HE 0.05
CV_VAT 2 !n cvz cvvol
1 0.0 0.0
2 0.063 3.1E-3
!)
CV_ID 'METER5' 50 !
! icvtyp
CV_TYP 'CTYP-5'
! icvthr ipfsw icvact
CV_THR NONEQUIL FOG ACTIVE
! icfvel cvara
CV_ARE NOCF 3.1E-3
CV_THERM 2
1 PVOL 1.0E5 TATM 612. PH20 0.0
2 N2 0.60 02 0.05 AR 0.30 HE 0.05
! size
CV_VAT 2 !n cvz cvvol
1 0.0 0.0
2 0.063 3.1E-3
!)
CV_ID 'ENVIRONMENT' 60 !
! icvtyp
CV_TYP 'CTYP-99'
! icvthr ipfsw icvact
CV_THR NONEQUIL FOG PROP-SPECIFIED
! icfvel cvara
CV_ARE NOCF 10000.0
CV_THERM 6
1 TATM 'TF' 'Env gas T(K)'
2 N2 'TF' 'mole fract N2'
3 O2 'TF' 'mole fract O2'
4 AR 'TF' 'mole fract AR'
5 HE 'TF' 'mole fract HE'
6 PVOL 'TF' 'pressure'
! size
CV_VAT 2 !n cvz cvvol
1 0.0 0.0
2 1.0E6 1000.0
!)
!)
! Test section is measured 5 meter long straight pipe
! with 6.3 cm inner diameter (see reference: NEA/CSNI/R(99)4)
! This test section is divided into 5 equal length pipes which
! are modeled into 5 flow paths.
!
FL_INPUT !
!FL_VTM 5 !
! flname ntflag nfun
! 1 METER1-METER2 TF 'Flow Rate'
! 2 METER2-METER3 TF 'Flow Rate'
! 3 METER3-METER4 TF 'Flow Rate'
! 4 METER4-METER5 TF 'Flow Rate'
! 5 METER5-ENVIRO TF 'Flow Rate'
FL_ID METER1-METER2 12 !
! kcvfm kcvto zfm zto
FL_FT 'METER1' 'METER2' 0.0315 0.0315

```

```

!          flara          fllen          flopo
FL_GEO      3.1E-3          1.0          1.0
!
! size
FL_SEG      1 !n  sarea slen  shyd srgh lamflg slam
              1 3.1E-3  1.0 0.063
!)
FL_ID      METER2-METER3      23 ! (
!          kcvfm          kcvto          zfm          zto
FL_FT      'METER2'          'METER3'          0.0315      0.0315
!          flara          fllen          flopo
FL_GEO      3.1E-3          1.0          1.0
!
! size
FL_SEG      1 !n  sarea slen  shyd srgh lamflg slam
              1 3.1E-3  1.0 0.063
!)
FL_ID      METER3-METER4      34 ! (
!          kcvfm          kcvto          zfm          zto
FL_FT      'METER3'          'METER4'          0.0315      0.0315
!          flara          fllen          flopo
FL_GEO      3.1E-3          1.0          1.0
!
! size
FL_SEG      1 !n  sarea slen  shyd srgh lamflg slam
              1 3.1E-3  1.0 0.063
!)
FL_ID      METER4-METER5      45 ! (
!          kcvfm          kcvto          zfm          zto
FL_FT      'METER4'          'METER5'          0.0315      0.0315
!          flara          fllen          flopo
FL_GEO      3.1E-3          1.0          1.0
!
! size
FL_SEG      1 !n  sarea slen  shyd srgh lamflg slam
              1 3.1E-3  1.0 0.063
!)
FL_ID      METER5-ENVIRO      56 ! (
!          kcvfm          kcvto          zfm          zto
FL_FT      'METER5' 'ENVIRONMENT' 0.0315 0.0315
!          flara          fllen          flopo
FL_GEO      3.1E-3          1.0          1.0
!
! size
FL_SEG      1 !n  sarea slen  shyd srgh lamflg slam
              1 3.1E-3  1.0 0.063
!)
!)
HS_INPUT ! (
HS_ID      'METER1HS'          10 ! (
!          FractResuspend CriticalDiameter  Gelbard
HS_LBAR      0.5
!          igeom          iss
HS_GD      CYLINDRICAL          SS
!          hsalt          alpha
HS_EOD      -0.01          0.0
!          isrc
HS_SRC      NO
!
! size
HS_ND      2 !n n          xi tempin          matnam
              1 1 0.0315      - 'CARBON-STEEL'
              2 2 0.0415      -
(((case0
!          ibcl          ibvl          mteval
HS_LB      CalcCoefHS          'METER1'          YES
)))
(((case1+case2+case3+case4+case5
!          ibcl          table          ibval
HS_LB      CoefTimeTF 'METER1 HTC'          'METER1'
)))
!          iflowl          cpfpl          cpfal
HS_LBP      INT          0.0          1.0
!          ctdpl          ctdal          xhtfc1          xmtfc1
HS_LBT      100.0          100.0          1.0          1.0
!          asurfl          c1n1          bndz1
HS_LBS      0.215          0.063          1.0

```

```

!          ibcr          table
HS_RB      TempTimeTF 'METER1 wall T'
!          iflowr          cpfpr          cpfar
HS_RBP      INT          0.0          0.0
!          iftnum
HS_FT      OFF
!)
HS_ID      'METER2HS'          20 !(
!          FractResuspend CriticalDiameter Gelbard
HS_LBAR      0.5
!          igeom          iss
HS_GD      CYLINDRICAL          SS
!          hsalt          alpha
HS_EOD      -0.01          0.0
!          isrc
HS_SRC      NO
!          size
HS_ND      2 !n n          xi tempin          matnam
          1 1 0.0315          - 'CARBON-STEEL'
          2 2 0.0415          -

(((case0
!          ibcl          ibvl          mteval
HS_LB      CalcCoefHS          'METER2'          YES
)))
(((case1+case2+case3+case4+case5
!          ibcl          table          ibval
HS_LB      CoefTimeTF 'METER2 HTC'          'METER2'
)))
!          iflowl          cpfpl          cpfal
HS_LBP      INT          0.0          1.0
!          ctdpl          ctdal          xhtfc1          xmtfc1
HS_LBT      100.0          100.0          1.0          1.0
!          asurfl          c1n1          bndz1
HS_LBS      0.215          0.063          1.0
!          ibcr          table
HS_RB      TempTimeTF 'METER2 wall T'
!          iflowr          cpfpr          cpfar
HS_RBP      INT          0.0          0.0
!          iftnum
HS_FT      OFF
!)
HS_ID      'METER3HS'          30 !(
!          FractResuspend CriticalDiameter Gelbard
HS_LBAR      0.5
!          igeom          iss
HS_GD      CYLINDRICAL          SS
!          hsalt          alpha
HS_EOD      -0.01          0.0
!          isrc
HS_SRC      NO
!          size
HS_ND      2 !n n          xi tempin          matnam
          1 1 0.0315          - 'CARBON-STEEL'
          2 2 0.0415          -

(((case0
!          ibcl          ibvl          mteval
HS_LB      CalcCoefHS          'METER3'          YES
)))
(((case1+case2+case3+case4+case5
!          ibcl          table          ibval
HS_LB      CoefTimeTF 'METER3 HTC'          'METER3'
)))
!          iflowl          cpfpl          cpfal
HS_LBP      INT          0.0          1.0
!          ctdpl          ctdal          xhtfc1          xmtfc1
HS_LBT      100.0          100.0          1.0          1.0
!          asurfl          c1n1          bndz1
HS_LBS      0.215          0.063          1.0
!          ibcr          table
HS_RB      TempTimeTF 'METER3 wall T'
!          iflowr          cpfpr          cpfar

```

```

HS_RBP          INT          0.0          0.0
!
HS_FT           iftnum
!           OFF
!)
HS_ID           'METER4HS'          40 !(
!           FractResuspend CriticalDiameter Gelbard
HS_LBAR         0.5          ! 1.e-9
!           igeom          iss
HS_GD           CYLINDRICAL          SS
!           hsalt          alpha
HS_EOD          -0.01          0.0
!           isrc
HS_SRC          NO
!
! size
HS_ND           2 !n n          xi tempin          matnam
!           1 1 0.0315          - 'CARBON-STEEL'
!           2 2 0.0415          -

(((case0
!           ibcl          ibvl          mteval
HS_LB           CalcCoefHS          'METER4'          YES
)))
(((case1+case2+case3+case4+case5
!           ibcl          table          ibval
HS_LB           CoefTimeTF 'METER4 HTC'          'METER4'
)))
!           iflowl          cpfp1          cpfal
HS_LBP          INT          0.0          1.0
!           ctdpl          ctdal          xhtfc1          xmtfc1
HS_LBT          100.0          100.0          1.0          1.0
!           asurfl          cln1          bndz1
HS_LBS          0.215          0.063          1.0
!           ibcr          table
HS_RB           TempTimeTF 'METER4 wall T'
!           iflowr          cpfpr          cpfar
HS_RBP          INT          0.0          0.0
!           iftnum
HS_FT           OFF
!)
HS_ID           'METER5HS'          50 !(
!           FractResuspend CriticalDiameter Gelbard
HS_LBAR         0.5          ! 'CritDia'
!           igeom          iss
HS_GD           CYLINDRICAL          SS
!           hsalt          alpha
HS_EOD          -0.01          0.0
!           isrc
HS_SRC          NO
!
! size
HS_ND           2 !n n          xi tempin          matnam
!           1 1 0.0315          - 'CARBON-STEEL'
!           2 2 0.0415          -

(((case0
!           ibcl          ibvl          mteval
HS_LB           CalcCoefHS          'METER5'          YES
)))
(((case1+case2+case3+case4+case5
!           ibcl          table          ibval
HS_LB           CoefTimeTF 'METER5 HTC'          'METER5'
)))
!           iflowl          cpfp1          cpfal
HS_LBP          INT          0.0          1.0
!           ctdpl          ctdal          xhtfc1          xmtfc1
HS_LBT          100.0          100.0          1.0          1.0
!           asurfl          cln1          bndz1
HS_LBS          0.215          0.063          1.0
!           ibcr          table
HS_RB           TempTimeTF 'METER5 wall T'
!           iflowr          cpfpr          cpfar
HS_RBP          INT          0.0          0.0
!           iftnum
HS_FT           OFF

```

```

! )
HS_ID      'ENV-HS'          60 ! (
!          igeom             iss
HS_GD      CYLINDRICAL      SS
!          hsalt             alpha
HS_EOD      -0.01           0.0
!          isrc
HS_SRC      NO
! size
HS_ND      2 ! n n          xi tempin          matnam
          1 1 0.0315        - 'CARBON-STEEL'
          2 2 0.0415        -
!          ibcl             ibvl mteval
HS_LB      CalcCoefHS 'ENVIRONMENT' YES
!          iflowl          cpfp1          cpfal
HS_LBP      INT            0.0           1.0
!          ctdpl          ctdal          xhtfc1          xmtfc1
HS_LBT      100.0          100.0          1.0           1.0
!          asurfl          cln1          bndz1
HS_LBS      1.0            1.0            1.0
!          ibcr            table
HS_RB      TempTimeTF 'ENV wall T(K)'
!          iflowr          cpfpr          cpfar
HS_RBP      INT            0.0            0.0
!          iftnum
HS_FT      OFF
! )
CF_INPUT
cf_id 'CritDia' 3 read
cf_sai 1.0 0.0 1.0e-9
!
RN1_INPUT      0 ! (
!          dft
! RN1_DFT      1.86
!          numsec          numcmp          numcls          numca
RN1_DIM      10           1           17           6
!          dmin          dmax          rhonom
RN1_ASP      1.0E-7       5.0E-5       4000.0
!          icoeff
RN1_ACOEF      CALANDWR
!          name          ivol          iphs          iclss          rfrs          xm          itab          cfnam
RN1_AS      'AS000' 'METER1' VAPOR 'CD' 0.0 1.0 TF 'SnO2 source'
!          idist          geommm          gsd
RN1_AS01      LOGNORMAL      -4.3E-7          1.7
!
! turbulent deposition model
(((case2
RN1_TURB 0 2 0
!
RN1_TDS 5
      1 'METER1HS' LHS 0.063 0 0.0 0.0 5.e-5
      2 'METER2HS' LHS 0.063 0 0.0 0.0 5.e-5
      3 'METER3HS' LHS 0.063 0 0.0 0.0 5.e-5
      4 'METER4HS' LHS 0.063 0 0.0 0.0 5.e-5
      5 'METER5HS' LHS 0.063 0 0.0 0.0 5.e-5
)))
!
! )
RN2_INPUT
! )
END PROGRAM MELGEN

PROGRAM MELCOR ! (
EXEC_INPUT ! (
EXEC_CFEFILE 'dynamicInp'
EXEC_TITLE 'STORM - Correct TH'
EXEC_CPULEFT 20.0
EXEC_CPULIM 1.0e10
EXEC_DTTIME 1.0E-3
EXEC_CYMESF 500 500 ! preclude screen-induced seizure

```

```

EXEC_TIME      2 !n      time dtmax  dtmin  dedit  dtplot  dtrest  dcrest
                1      0.0    1.0 1.0E-3 100.0    2.0 2000.0 1.0E10
                2 9000.0    1.0 1.0E-3 200.0    5.0 4000.0 1.0E10
EXEC_TEND 15300.0 ! 18000.0 ! 9000.0
!)
RN1_INPUT
RN1_VISUAL 5
1  'METER1'
2  'METER2'
3  'METER3'
4  'METER4'
5  'METER5'
!)
END PROGRAM MELCOR

```

APPENDIX C

Calculation Sheets

This appendix documents the calculation sheets for the gasoline pool fire validation and LLNL enclosure fire validation as described in Chapter 3 of this report.

C.1 Gasoline Pool Fire

This worksheet is for the Gasoline Pool Fire modeling for BNWL-1732 report. Case SA-17a from Table II of the report. UO2 powder: 19.5 g, Wind speed < 4 mph, Temperature of 1000 C. Burn time of 9 minutes. Sampling time of 0.15 hr (or 9 min). The pan is made of stainless steel. Dimension is 15 inches and 2 inch in depth. Gasoline used 1 gallon

$$m_{\text{UO2}} := 0.0195 \text{ kg} \quad V_{\text{wMPH}} := 4 \text{ mph} \quad T_{\text{exp}} := 1000 \text{ C}$$

$$V_{\text{wind}} := V_{\text{wMPH}} \cdot 0.44704 \quad V_{\text{wind}} = 1.788 \text{ m/s}$$

$$D_{\text{pan}} := 0.381 \text{ m} \quad H_{\text{pan}} := 0.0508 \text{ m} \quad A_{\text{pan}} := \frac{\pi \cdot D_{\text{pan}}^2}{4} \quad A_{\text{pan}} = 0.114 \text{ m}^2$$

$$1 \text{ gallon} = 3.78541 \text{E-3 m}^3$$

According to Figure 3-11.2 of [NFPA 1995], gasoline burn velocity is about 4 mm/min. On page 3-213 of the same reference, the gasoline molecular weight is 100 g/mole, and liquid density of 870 kg/m³.

$$\rho_{\text{fuel}} := 870 \frac{\text{kg}}{\text{m}^3} \quad \text{VOL}_{\text{fuel}} := 3.78541 \cdot 10^{-3} \text{ m}^3 \quad \rho_{\text{air}} := 1.2 \text{ kg/m}^3$$

$$p_{\text{vap}} := 3.49 \text{ kg/m}^3 \text{ for gasoline} \quad g := 9.8 \text{ m/s}^2$$

$$\text{MASS}_{\text{fuel}} := \rho_{\text{fuel}} \cdot \text{VOL}_{\text{fuel}} \quad \text{MASS}_{\text{fuel}} = 3.293 \text{ kg}$$

$$\text{Mass burn rate:} \quad \text{MASS}_{\text{dotflux}} := \frac{0.004 \cdot \rho_{\text{fuel}}}{60} \quad \text{MASS}_{\text{dotflux}} = 0.058 \text{ kg / m}^2\text{-s}$$

$$\text{MASS}_{\text{dot}} := \text{MASS}_{\text{dotflux}} \cdot A_{\text{pan}} \quad \text{MASS}_{\text{dot}} = 6.613 \times 10^{-3} \text{ kg/s}$$

$$\text{For Octane, the specific combustion energy, } Q_{\text{oct}} \text{ is given: } Q_{\text{oct}} := 44.3 \cdot 10^5 \text{ J/kg}$$

$$q_{\text{comb}} := \text{MASS}_{\text{dot}} \cdot Q_{\text{oct}} \quad q_{\text{comb}} = 2.938 \times 10^5 \text{ W}$$

$$\text{TIME}_{\text{burn}} := \frac{\text{MASS}_{\text{fuel}}}{\text{MASS}_{\text{dot}}} \quad \text{TIME}_{\text{burn}} = 498.04 \text{ s, compared to 540 s measured burn time}$$

To calculate the flame height, using Eq (14) on page 3-204 of [NFPA 1995] for height to dia ratio (H/D), including the effect of wind.

$$U_{\text{star}} := \frac{V_{\text{wind}}}{\left(\frac{1}{g \cdot \text{MASS}_{\text{dotflux}} \cdot \frac{D_{\text{pan}}}{\rho_{\text{vap}}}} \right)^{\frac{1}{3}}} \quad U_{\text{star}} = 4.517$$

$$H_{flame} := \frac{55 \cdot \left(\frac{MASSdotflux}{\rho_{air} \cdot \sqrt{g \cdot D_{pan}}} \right)^{0.67} \cdot U_{star}^{-0.21}}{D_{pan}} \quad H_{flame} = 8.886 \quad m$$

with the absence of wind, then Eq(13) on page 3-204 of [NFPA 1995] is used

$$H_{flame1} := \frac{42 \cdot \left(\frac{MASSdotflux}{\rho_{air} \cdot \sqrt{g \cdot D_{pan}}} \right)^{0.61}}{D_{pan}} \quad H_{flame1} = 11.62 \quad m$$

From Table 3-11.3 of [NFPA 1995], for gasoline pool size:

Size (m)	η (radiation fraction of combustion),%
1.22-3.05	40-13
1.0-10.0	60-10.0

In addition, this table lists its radiation temperature of 1240 K

Based on this, we can assume

$$\eta := 0.35 \quad \text{percent/100}$$

Chemical reaction for gasoline: both butane and octane can be used for simulating gasoline.
 Butane: C_4H_{10} , Octane: C_8H_{18} .
 Consider Octane: $2 C_8H_{18} + 25 O_2 \rightarrow 18 H_2O + 16 CO_2$ as complete reaction. S in fuel products $\rightarrow SO_2$ (g) generated. Beside SO_2 , carbon particles can be produced when rich-fuel environment exists. Thus the fuel mass fraction for the carbon particle started to form, is given by Equation 80 on page 3-223 of [NFPA 1995].

$$FracC(n,m) := \frac{12 \cdot n + m}{12 \cdot n + m + \frac{n \cdot 137.3}{2}}$$

For CH_4 , $FracC(1,4) = 0.189$ Same as in Table 3-11.8 of [NFPA 1995]

For Butane, C_4H_{10} , $FracC(4,10) = 0.174$

For Octane, C_8H_{18} , $FracC(8,18) = 0.172$

Note that a gas with higher value of FracC has less tendency to form solid particles than a gas with a lower value of FracC. Therefore, higher values of FracC corresponds to lower radiation level.

During a fire, smoke often creates when the reaction is incomplete as carbon particles may be generated. In some cases, the smoke production rate is nearly equal to the rate of air entrained into the rising fire plume.

Estimate the CO2 and H2O generated from the MASSdot given:

$$MW_{\text{oct}} := 114 \quad \text{kg/kmole} \quad MW_{\text{oxygen}} := 32 \quad \text{kg/kmole} \quad MW_{\text{H}_2\text{O}} := 18 \quad \text{kg/kmole}$$

$$MW_{\text{CO}_2} := 44 \quad \text{kg/kmole}$$

$$MDOT_{\text{oxy}} := \frac{\text{MASSdot} \cdot MW_{\text{oxygen}} \cdot 25}{2MW_{\text{oct}}} \quad MDOT_{\text{oxy}} = 0.023 \quad \text{kg/s}$$

$$MDOT_{\text{H}_2\text{O}} := \frac{\text{MASSdot} \cdot MW_{\text{H}_2\text{O}} \cdot 18}{2MW_{\text{oct}}} \quad MDOT_{\text{H}_2\text{O}} = 9.397 \times 10^{-3} \quad \text{kg/s}$$

$$MDOT_{\text{CO}_2} := \frac{\text{MASSdot} \cdot MW_{\text{CO}_2} \cdot 16}{2MW_{\text{oct}}} \quad MDOT_{\text{CO}_2} = 0.02 \quad \text{kg/s}$$

Calculate the critical diameter for resuspension of aerosol:

$$\text{width} := 0.6096 \quad \text{m} \quad \text{height} := 0.6096 \quad \text{m} \quad H_d := 4 \cdot \text{width} \cdot \frac{\text{height}}{2 \cdot (\text{width} + \text{height})} \quad H_d = 0.61 \quad \text{m}$$

$$\rho := 1.2 \quad \text{kg/m}^3$$

$$Re(v) := \frac{H_d \cdot v \cdot \rho}{2 \cdot 10^{-5}} \quad Re(2) = 7.315 \times 10^4$$

$$f(v) := \frac{0.0791}{Re(v)^{0.25}} \quad f(2) = 4.81 \times 10^{-3}$$

$$\tau_w(v) := 0.5 \cdot f(v) \cdot \rho \cdot v^2 \quad \tau_w(2) = 0.012$$

$$D_{\text{crit}}(v) := \frac{4 \cdot 10^{-5}}{\pi \cdot \tau_w(v)} \quad D_{\text{crit}}(2) = 1.103 \times 10^{-3} \quad \text{m}$$

$$D_{\text{crit}}(1.78) = 1.353 \times 10^{-3} \quad \text{m}$$

C.2 LLNL Enclosure Fire

This worksheet intends to fire temperature and radiation heat loss.

$$A_i := 138 \quad \text{surface area of interior enclosure (m}^2\text{)}$$

$$A_v := 0.65 \cdot 0.65 \quad A_v = 0.423 \quad \text{ventilation area (m}^2\text{)}$$

$$H_v := 4.5 - 0.57 - 0.325 \quad H_v = 3.605 \quad \text{ventilation opening (m)}$$

$$\text{Dimension of enclosure: } D_i := 4 \quad D_j := 6 \quad D_k := 4.5 \quad \text{m}$$

$$\text{vol} := D_i \cdot D_j \cdot D_k \quad \text{vol} = 108 \quad \text{m}^3 \quad \text{area} := D_i \cdot D_j \quad \text{area} = 24 \quad \text{m}^2$$

$$\text{radius} := \sqrt{\frac{\text{area}}{\pi}} \quad \text{radius} = 2.764 \quad \text{m}$$

According to Table 2-9.2 in [NFPA 1995], it lists a number of hydrocarbons' thermodynamic equilibrium properties, which includes lower limit, stoichiometric limits, and adiabatic temperatures. Thus the adiabatic SL temperature for hydrocarbons is 1700 K, for carbon monoxide is 1450 K and for hydrogen is 1080 K.

$$T_{ad} := 1700 - 273.15 \quad \text{C, for adiabatic SL temperature}$$

For T9 test, the following flow rate is for methane:

$$\text{mf}_{\text{dot}} := 0.004 \quad \frac{\text{kg}}{\text{s}} \quad \text{time} := 4000 \quad \text{s} \quad T_{\text{amb}} := 302.15 \text{ K}$$

$$\text{mf} := \text{mf}_{\text{dot}} \cdot \text{time} \quad \text{kgs} \quad \text{mf} = 16$$

$$\psi := \frac{\text{mf}}{\sqrt{A_i \cdot A_v}} \quad \psi = 2.095 \quad \text{The computation of } T_{\text{gas}} \text{ is based on the correlation from [NFPA 2008].}$$

$$T_{\text{gas}} := T_{ad} \cdot (1 - \exp(-0.05 \cdot \psi)) \quad T_{\text{gas}} = 141.927 \quad \text{C} \quad T_{\text{gask}} := T_{\text{gas}} + 273.15 \quad \text{K}$$

$$T_{\text{gask}} = 415.077 \quad \text{K}$$

$$\sigma := 5.67 \cdot 10^{-8} \quad \frac{\text{W}}{\text{m}^2 \cdot \text{K}^4} \quad T_{\text{adk}} := T_{ad} + 273.15 \quad \text{K} \quad T_{\text{adk}} = 1.7 \times 10^3 \quad \text{K}$$

Estimate the water vapor partial pressure in atmosphere is given: $RH := 0.5$

$$P_w := RH \cdot \exp\left(14.4114 - \frac{5328}{T_{\text{amb}}}\right) \quad P_w = 0.02 \quad L1 := \text{radius} \quad L2 := H_v$$

$$PwL(\text{path}, \text{temp}) := P_w \cdot \text{path} \cdot \left(\frac{\text{temp}}{T_{\text{amb}}}\right)$$

$$PwL(L1, T_{\text{adk}}) = 0.31 \quad PwL(L1, T_{\text{gask}}) = 0.076$$

$$PwL(L2, T_{\text{adk}}) = 0.404 \quad PwL(L2, T_{\text{gask}}) = 0.099$$

Emissivity is a function of its partial pressure and path length (PwL), and the value is a lookup through Figure 3-11.18 of [NFPA 1995] - 0.1 to 0.2

$$\epsilon_{h2o} := 0.2$$

$$P_{co2L}(\text{path}, \text{temp}) := 0.0003 \cdot \text{path} \left(\frac{\text{temp}}{T_{amb}} \right)$$

$$P_{co2L}(L1, T_{adk}) = 4.665 \times 10^{-3} \quad P_{co2L}(L1, T_{gask}) = 1.139 \times 10^{-3}$$

$$P_{co2L}(L2, T_{adk}) = 6.085 \times 10^{-3} \quad P_{co2L}(L2, T_{gask}) = 1.486 \times 10^{-3}$$

It is a function of its partial pressure and path length. For CO₂, its partial pressure is constant at 3E-4 atm. Figure 3-11.19 of [NFPA 1995] is used. It can be ranged from 0.017 to 0.04.

$$\epsilon_{co2} := 0.04$$

$$\epsilon_g := \epsilon_{h2o} + \epsilon_{co2}$$

$$\epsilon_g = 0.24$$

$$T_{avg} := T_{adk} \cdot 0.5 + T_{gask} \cdot 0.5$$

$$T_{avg} = 1.058 \times 10^3$$

$$Q_{dotr}(\text{temp}) := \epsilon_g \cdot \sigma \cdot (\text{temp}^4 - T_{amb}^4)$$

$$Q_{dotr}(T_{adk}) = 1.135 \times 10^5 \quad \text{W/m}^2$$

$$Q_{dotr}(T_{avg}) = 1.691 \times 10^4 \quad \text{W/m}^2$$

$$Q_{dotr}(T_{gask}) = 290.512 \quad \text{W/m}^2$$

$$Q_{dot} := Q_{dotr}(T_{avg}) \cdot A_i$$

$$Q_{dot} = 2.333 \times 10^6 \quad \text{W}$$

$$Q_{comb} := 200000 \quad \text{W, given by both Test 9 and Test 11 of the LLNL Enclosure test for fire}$$

$$F_{rad} := \frac{Q_{dot}}{Q_{comb}}$$

$$F_{rad} = 11.666$$

$$Q_{dot} := Q_{dotr}(T_{gask}) \cdot A_i$$

$$Q_{dot} = 4.009 \times 10^4 \quad \text{W}$$

$$Q_{comb} := 200000 \quad \text{W}$$

$$F_{rad} := \frac{Q_{dot}}{Q_{comb}}$$

$$F_{rad} = 0.2$$

Fraction of thermal radiation to combustion

check:

$$W_w := 4 \quad \text{m}$$

$$D := 6 \quad \text{m}$$

$$\text{criteria} := \left(\frac{D}{W_w} \right)^{0.5} \cdot \frac{\dot{m}}{A_v \sqrt{H_v}} \quad \text{criteria} = 6.107 \times 10^{-3}$$

According to Table 3-11.9 of [NFPA 1995], the flame radiative temperature is 1289 K and the emissivity power flux is 157 kW/m²

Using the 200 kW above for the combustion power, and divided it by the burner cross sectional area, using diameter of 0.57 m

$$A_{\text{burner}} := \pi \cdot \frac{0.57^2}{4} \quad A_{\text{burner}} = 0.255 \quad \text{m}^2$$

Fraction of radiation to combustion power is:

$$F := \frac{157000}{\frac{Q_{\text{comb}}}{A_{\text{burner}}}}$$

$$F = 0.2$$

Same as Frad calculated above and in the range discussed in Table 3-11.8 of [NFPA 1995]. The effect of cross winds and jet velocity may alter this fraction up and down but within 0.1 to 0.3 (see Figure 3-11.26 and Figure 3-11.27 of [NFPA 1995]).

Thus the default value used for the fraction of radiation loss from combustion of 0.35 may be overestimated for methane gas.

In reality, the amount of carbon particles produced from a methane gas fire is significant. According to Table 3-11.8 of [NFPA 1995], this fraction is 0.189 for methane. In this simulation, we will ignore it, since we are interested to investigate the thermal aspect of the experiment.

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