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NUCLEAR FACILITY SAFETY ENHANCEMENT USING SANDIA NATIONAL LABORATORIES' COMPUTER CODES

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ABSTRACT

This paper describes the ongoing study of nuclear facility safety enhancement using Sandia National Laboratories' (SNL) computer codes, supported by U.S. Department of Energy (DOE) Nuclear Safety Research and Development (NSR&D) Program. Continued DOE NSR&D support, since 2014 has allowed the use of the SNL engineering code suite (SIERRA Mechanics) to further substantiate data in the DOE Handbook published in 1994: DOE-HDBK-3010-94, "Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities." The use of SIERRA codes allows for a better understanding of the mechanics, dynamics, chemistry and overall physics of airborne release scenarios. SIERRA codes provide insights into the contributing phenomena of source term releases from events such as liquid fires. The 1994 Handbook documents small-scaled, bench-top and limited experiments involving liquid fires, powder spills, pressurized releases, and mechanical insult-induced fragmentation scenarios. Data recorded from these scenarios has been substantiated using SIERRA solid mechanics and fluid mechanics codes.

Data passing among multi-physics SIERRA codes predicted the contaminant release from a drum rupture due to fire even though there is no experimental data available. In the anticipated revision effort of the Handbook by DOE, these computational capabilities could enhance the data in a broader usage and could provide confidence in the safety analysis SIERRA codes can provide the initial source term to be used in the leak path factor (LPF) analyses, which predicts the ST release out of the facility. Typical LPF analysis is done using the MELCOR code, developed at SNL for the U.S. Nuclear Regulatory Commission. Widely used in nuclear reactor applications, MELCOR is a toolbox safety code in the DOE's central registry for LPF applications. A recent LPF guidance study done by SNL indicated that MELCOR 2.1, along with updated guidance, should replace the obsolete MELCOR 1.8.5 guidance. This new guidance is significantly improved over the previous guidance, utilizing extensive MELCOR validation, including applicable reactor experiments and experiments described in the DOE-HDBK-3010-94 for LPF applications. The latest version of MELCOR should be included in DOE's central registry, and should be used by safety analysts for LPF analyses.

INTRODUCTION

Source term determination at the U.S. Department of Energy (DOE) utilizes the Five-Factor Formula (FFF), which is given as MAR×DR×ARF×ARF×LPF, where MAR is the material-at-risk, DR is the damage ratio for a container, ARF is the airborne release fraction, RF is the respirable fraction, and LPF is leak path factor, which measures the release out of the facility. Within the DOE complex, safety analysts reply heavily on the data provided in the DOE Handbook, DOE-HDBK-3010 [1] to determine source terms that may be incorporated into the document safety analysis (DSA). Most often, analysts simply take the bounding values due to time constraints or simply to bound calculations. This is a safe approach that helps avoid regulatory critique; however, it may not provide results that are meaningful or relevant to the conditions being evaluated. The derivation of the data, such as ARFs and RFs in the Handbook often depend on very limited table-top and bench/laboratory experiments, as well as engineering judgment which may not be well substantiated, and may not be representative of the actual situation.

In response, we have proposed research over the past three years for the inclusion of high fidelity modeling to provide a more accurate method to identify not only bounding values but also more representative ones for the Handbook and for analysts tasked with risk assessments. Advances in computing capability, such as the SIERRA engineering tools developed at SNL (see Fig. 1), enable us to use code simulation methods to provide more representative values for the source terms. If our proposed research determines that the data is too conservative, the source term calculated for the DSA may over-specify the

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implementation and design controls. This over-specification of controls often leads to substantial design/construction and/or implementation cost to DOE. If our research determines that the data is non-conservative, this means that the analysis underestimates the source term in the DSA, which could translate to a potential significant safety concern to workers and the public. In either case, the results of our investigations could enhance how the safety analysts across the DOE complex approach the selection of adequate bounding ARFs and RFs, which could improve the defensibility of the safety analyses. As mentioned earlier this research conducted over the past several years was aimed at using SIERRA tools for substantiating the Handbook data [3-5]. This research has been supported by DOE's Nuclear Safety Research and Development (NSR&D) Program.[1]

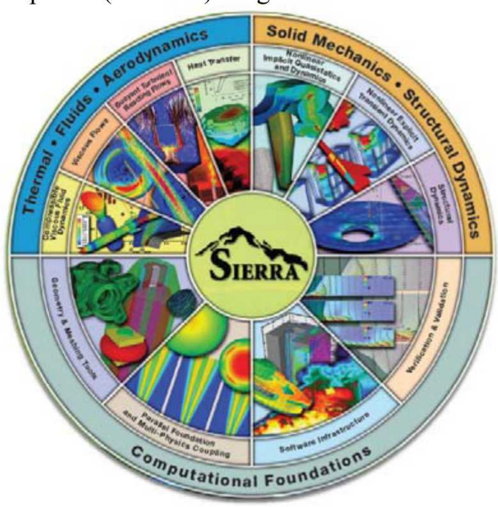

Figure 1. SIERRA Mechanics Computer Tool [2]

In addition, the DOE Central Registry contains safety codes for LPF analysis, which points to the obsolete MELCOR version (1.8.5). Only the latest version of MELCOR (2.x) is maintained and supported by SNL, which is warranted. To maintain supports and provide improved models, SNL has published a new LPF guidance report [6] using MELCOR 2.1. This guidance report includes experimental validations and best practice information which is intended to replace or substantiate the existing guidance report using obsolete MELCOR version [7].

This paper first describes the SIERRA tools and MELCOR. Then it addresses the use of SIERRA tools for substantiating ARF and RF from experiments. This paper also describes using the last version of MELCOR to provide LPF guidance. Finally, the paper provides a summary and conclusion.

NOMENCLATURE

ARF	Airborne release fraction
AMMD	Aerodynamic mass mean diameter
DOE	U.S. Department of Energy
DR	Damage ratio
DSA	Document safety analysis
EHSS	Environmental, Health, Safety and Security
FFF	Five factor formula
LPF	Leak path factor
MAR	Material-at-risk
NRC	U.S. Nuclear Regulatory Commission
NSR&D	Nuclear Safety Research and Development
PARE	Pressurized Airborne Release Equipment
PNL	Pacific Northwest Laboratory
QA	Quality assurance
RART	Radioactive Aerosol Release Tank
SD	Structural dynamics
SM	Solid mechanics
SNL	Sandia National Laboratories
SPH	Smoothed particle hydrodynamics
RF	Respirable fraction
TF	Thermal, fluids and aerodynamics
V&V	Validation and verification

SNL COMPUTER CODES

Advances in computing capability at national laboratories have enabled us to use computer simulations to better model hydrodynamic, structural dynamic, and thermal/fluid dynamic phenomena. This provides a better understanding of the insights on the fundamental physics related to potential accident scenarios that could occur or could be postulated. Today, the availability of the high-fidelity computer resources (both hardware and software) that incorporate state-of-the-art models at national laboratories allows safety and risk analysts to utilize these methods for non-weapon-related safety activities. An example of the use of these state-of-the-art models in supporting source term calculations and in ARFs for postulated scenarios is the SIERRA high fidelity codes developed at Sandia National Laboratories (SNL). The SIERRA codes are designed to solve multi-physics engineered problems, particularly for weapon applications (see Fig 1). As shown in Fig. 1, SIERRA code capabilities include thermal, fluids and aerodynamics (TF) as well as solid mechanics (SM) and structural dynamics (SD) with many interfaces, pre- and post-processing of these codes within the SIERRA framework. Within this framework, supported programs for meshing generation, data interfacing, pre-processing and post-processing are included to ease the transitioning or coupling codes.

In this research, both SM and TF codes, such as Presto/Adagio and Fuego, are used. The Presto version of SM code is capable of modeling explosions. Adagio is a standard SM code that provides both explicit and implicit solver capabilities. A smoothed particle hydrodynamics (SPH) model is included in the SM codes. Fuego has a capability to model pool and solid fires with a particle model. Although the code is a non-compressible flow code and only applicable for low Mach number (< 0.7), it performs well for many fire experiments. Note Fuego's particle model includes a

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resuspension model, but the ability to model agglomeration is not fully implemented.

Unlike SIERRA, MELCOR is a system-level code, which is developed at SNL for U.S. Nuclear Regulatory Commission (NRC). MELCOR has been developed over the span of 30 years, and is used worldwide with nearly 1000 licensed MELCOR users. Although most of these users are not using MELCOR for facility safety analyses, the large user base indicates how well the code has been exercised, and provides confidence for its use at nuclear installations. In addition, MELCOR has been designated as a DOE Toolbox safety code for the LPF application. This paper provides a description of the LPF guidance for using MELCOR. In the next two sections, we describe the ARF and RF applications of SIERRA tools for substantiating experimental data from the Handbook, and the use of MELCOR 2.1 for LPF applications, including the use of SIERRA tool results for MELCOR input.

SIERRA TOOL FOR ARF AND RF

As previously described, the SIERRA code set at SNL is a multi-physics engineering tool that has been applied to various physical problems (i.e., experiments), including impacts, liquid fire and pressurized release and free falls of the particles (or contaminants) [3-5]. In our research, we have improved the SIERRA tools for addressing particle resuspension, fragmentation and multi-component evaporation which are important for ARF and RF determinations. Table 1 describes the status of our research using SIERRA tools as computational capabilities to substantiate the Handbook data. As shown in this table, a wide range of capabilities that can be used to substantiate experimental and empirical data in the Handbook. These data include ARF and RF values as described in FFF.

Table 1. Computational Capability Using SIERRA Tool to Substantiating Data for DOE-HDBK-3010

Research Task	**Status**
Exploratory simulations of energetic impacts using Presto/Adagio (SIERRA/SM).	• A simulation model of a bullet hitting a can filled with small particles has been simulated and formulated such that we could use a non-export version of the SIERRA/SM (see [3] for more details). • Based on this simulation, we are conducting additional impact analyses of actual waste drum geometry to determine the DR.
Liquid fire experiments using Fuego (SIERRA/TF). In this research, we improved Fuego by adding a multi-component evaporation model which is important in modeling transport behavior within a contaminant [4].	• A beaker fire experiment was first simulated [8] to provide additional physics insights into the experiment. • A gasoline pool fire experiment was also simulated [9] to provide the effect of the wind on fire, and determine the importance of the physics.
Free fall and pressurized powder release using Fuego and Presto [3-4]. As previously described, Fuego is a low Mach number code. It may not be suitable for high Mach number situations in the case of high pressurized releases. Presto is used for simulating the initial release and the particle information is passed to Fuego to simulate the rest [4].	• A free-fall powder experiment was simulated [10] to provide fluid dynamics behavior, which can provide input to MELCOR code, which particles are treated as trace particles. • A pressurized powder release experiment was simulated [11] to investigate how fluid dynamic behavior and surface impact. • At high pressures (>0.34 MPa or 50 psig), the Fuego code may not give reliable results. The use of Presto/Fuego can address high pressure cases as demonstrated in [4].
Investigation of particle resuspension using Fuego – A resuspension model [12] has been added to Fuego [4].	• Particle resuspension is an important phenomenon in particle transport. Many resuspension experiments were used to simulate this phenomenon. See Ref 4. For more details.
Fragmentation of solids using SIERRA/SM –Sequential and con-current fragmentation models have been developed [4-5]. Inclusion of the micromorphic physics is being carried out, which includes the effect of temperature, porosity and grain size for ceramics.	• To simulate the fragmentation of a solid (i.e., weight dropped on a ceramic pellet) [13], SIERRA/SM needs to be improved to allow the modeling of smaller fragments, since the length scale issue may not be easily addressed. • Thus, macro- and microscopic fragmentation models are being developed to address this issue (see [4,5] for more details).
Release simulation of a waste drum from a fire using SIERRA/TF (Aria and Fuego) and SIERRA/SM (Presto). Aria contains a chemical decomposition model, which can estimate the by-product gas generation. Providing the internal pressure and temperature, Presto can be used to estimate the drum rupture conditions. Because of the particle model in Fuego, it can be used to estimate the release once the drum is ruptured (see Fig. 2).	• To simulate a fire engulfing waste drums, SIERRA/TF were used. The data from a recent SNL drum fire experiment was used to identify the ability to model the drum release [14]. • This release is due to the internal pressure build-up by the decomposition of the trash inside the drum because of the external heat flux, such as a nearby liquid fire. • Although the capability is provided (see [5] for a more detail), a refined model needs to be developed.

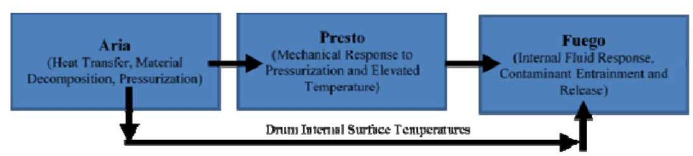


Figure 2. SIERRA Coupling Scheme to Model Drum Failure Release in an Engulfing Fire.

This section describes several of SIERRA capabilities as shown in Table 1 and how these data can be used further to estimate the LPF using MELCOR code. For LPF applications, almost all DOE sites must consider major accidents, such as seismic, fire, spill and explosion. In this section, we first describe a gasoline pool fire such as what might occur in a vehicle accident. Then we describe a spill situation, particularly a free-fall powder. Finally, we discuss the pressurized release of the powder, which can occur when a vessel or container is over-pressurized.

Gasoline Pool Fire

A simulation of a gasoline pool fire experiment conducted in a wind tunnel attached to the Radioactive Aerosol Release Tank (RART) located at the Pacific Northwest Laboratory (PNL) as documented in the experimental report, BNWL-1732 [9]. Fig. 3 shows the adapted 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. In this experiment, ~20 g of UO_2 powder was sprinkled into a steel pan and then ~4 liters (1 gallon) of gasoline was poured into the pan. This experiment was simulated using Fuego (see Fig. 4 for the computational mesh used and brief experimental data for this experiment).

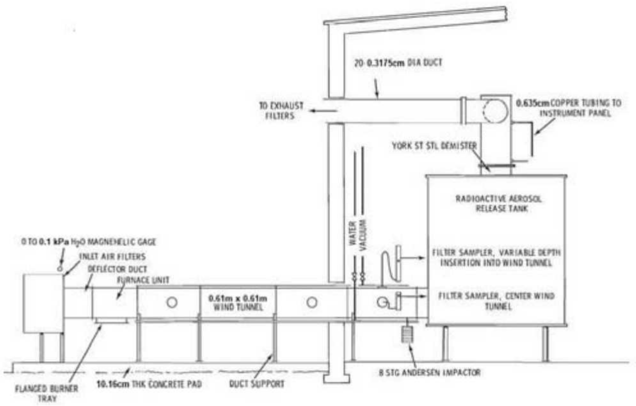
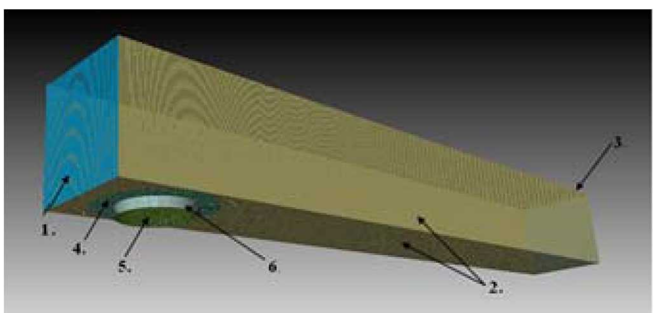


Figure 3. Gasoline Pool Fire Experiment Apparatus with a Wind Tunnel to Measure ARF from UO_2 Particles [9]



1. It is the air inflow boundary, with a fixed flow rate and temperature of 1 m/s (2.2 mph, assumed from the test report) and 298 K respectively.
2. It represents the stainless-steel tunnel walls, modelled with a 1.3 cm conducting wall boundary condition, with a backside temperature of 298 K.
3. This surface is the outflow boundary condition placed near the experimental filter location, set to collect entrained particles.
4. It represents the dirt ring in which the fuel pan is set, modelled as a 1.3 cm thick 1D conducting surface.
5. It represents the fuel pan. The circular pan measured 0.381 meters in diameter and is assumed in the model to be filled with pure heptane fuel (C_7H_{16}) as a surrogate for the gasoline used in the experiment.
6. This surface is the exposed lip of the stainless-steel pool, modelled as a conducting boundary condition

Figure 4. Fuego Model for Gasoline Pool Fire Experiment

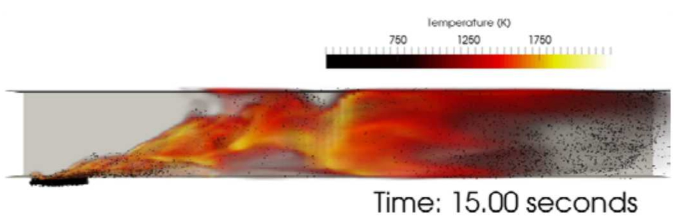


Figure 5. Fuego Simulation of the Gasoline Pool Fire Experiment

A typical computational burning result for this experiment is shown in Fig. 5. Fig. 6 displays the predicted airborne release fractions for the various scenarios alongside the reported experimentally determined release fraction. Lacking certain experimental feature information such as turbulence conditions, boiling duration and inflow velocity contributed to the discrepancy between experimental and predictive values.

As shown in this figure, most of the scenarios presented here involving multiple species particle tracking result in higher ARF values than those seen in the single component scenarios. While this deviates more from the reported ARF, the multiple species involve increased physical fidelity. The increase in ARF was expected, since the volatile fuel evaporates off from the particle surface, leaving the significantly smaller solid particle contaminant. The reduced particle diameter enables a greater percentage of contaminate to entrain into the flow and pass through the outflow boundary, while the previous work saw more particles fall back to the pool surface. In comparison with experimental data, our simulations with multi-component evaporation model predict higher ARF.

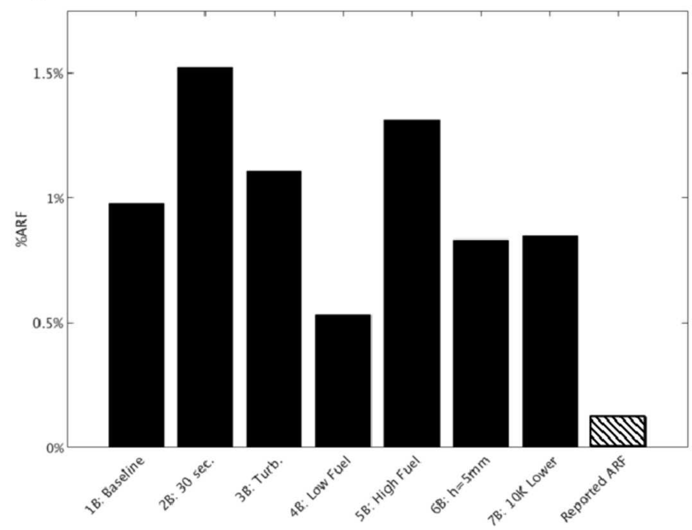


Figure 6. Fuego Results on Gasoline Pool Fire Experiment (see Table 2 for the case descriptions)

Table 2. Fuego Simulation Cases for Gasoline Pool Fire Experiment

Case	Description
1B	Baseline. 25 second simulation, 10 mm particle injection height, particle size distribution, empty pan (high lip) mesh, 370 K particle injection temperature, and gas velocity representing the fuel pool.
2B	Simulated for 35 seconds with particle injections from 3 to 30 seconds.
3B	Turbulence parameter increased to 100%
4B	Fuel pool height lowered to 1 mm.
5B	Fuel pool height increased to 3 mm.
6B	Particles injected at 5 mm above the bottom of the fuel pan.
7B	Particle injection temperature decreased to 361 K

In conclusion, including the multi-component particle capability in this study provided significant insight into the entrainment dynamics observed in the boiling scenarios. Observing that the volatile fuel component evaporates rapidly, the solid, non-volatile particle contaminant is seen to entrain through the outflow in higher volumes, as the smaller particle size is more easily suspended in the flow. If a particle escaped the pool, above the lip, the particle would likely entrain and deposit on either the tunnel walls or the outflow.

Free Fall Powder Release

Free-fall spills are important in nuclear facilities across the DOE complex since spills tend to occur during the handling of radioactive materials, such as waste drum loading and transportation. A series of spill experiments were conducted at PNL [10]. These experiments were conducted at the RART, which is the same tank as the gasoline pool fire experiment reported earlier. Fig. 7 shows the sampling for a free-fall spill apparatus inside the RART with the sampling equipment. As shown in this figure, the RART is 2.9 m in diameter and 3 m height with a total free volume of 20 m^3. The beaker (~ 1 liter in volume) containing the particulates is located at the center of the RART. The spill is simulated by overturning the beaker. The particulates include both liquid and powders (TiO_2 and depleted uranium dioxide). The spill height ranged from 1 m to 3 m. Also shown in this figure is the sampling equipment, which contains 4 high-volume filters and a cascade impactor. The locations of the sampling are shown in this figure. The sampling is done by pulling specific air flow through the sampling equipment to be measured as the airborne release amount. The experimental data is shown in Table 3.

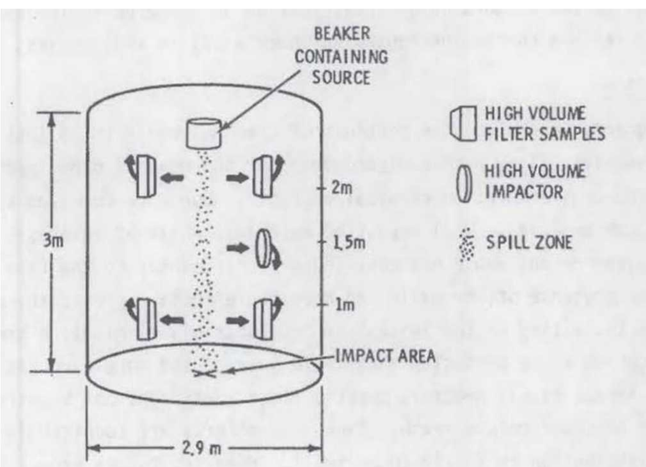


Figure 7. Free-fall Spill Experiments in RART [10]

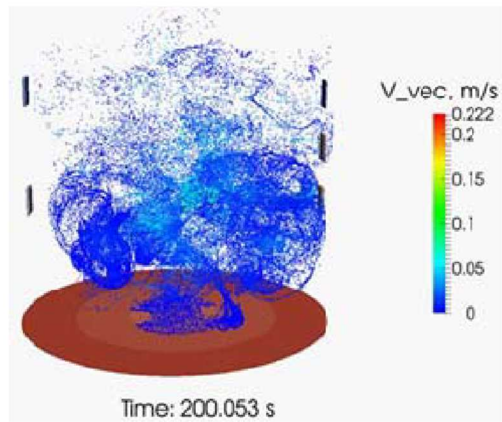
To simulate this experiment, computational mesh is formulated to capture the fluid flow induced by the free-fall powder. See details of the simulation assumptions in a recent report [4].

The powder was released vertically from the beaker, allowing gravity to force the particles in a downward direction. Fig. 8 shows the particle velocity and fluid velocity at ~200 seconds. As shown in Fig.8a, the sampling flow (toward the filter and impactor) had a high degree of influence on particle motion, particularly for the smaller particles which tend to stay airborne.

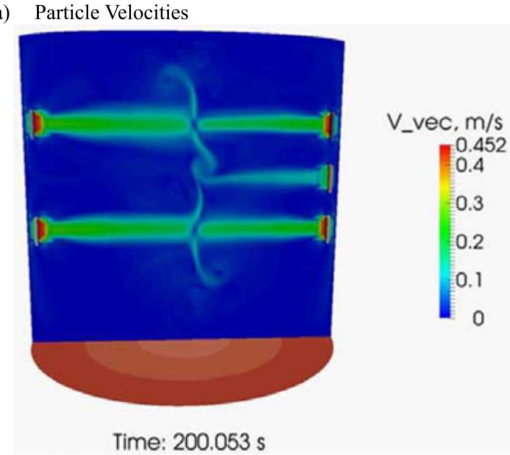
Table 3. 100 g TiO_2, 3-m Free-fall Spill Experimental Data [10]

Parameter	Value
Filters** specifications:	
Location from the bottom of RART, m	1 and 2
Filter height, width, and assumed thickness, m (inches)	0.2 (8), 0.25 (10), 0.02(1)
Designed flow rate each, m^3 per minute	1.4
Duration, minutes	30
Impactor specifications:	
Location from the bottom of RART, m	1.5
Dimension: height, width, and thickness	Assumed same as filters
Designed flow rate, m^3 per minute	
Duration, minutes	0.56
	30

*A particle distribution from [10] was used, instead of mass mean diameter (MMD) of 1.7 µm and standard deviation of 2.
**Glass fiber filters with 99.9% efficient for 0.3 µm



(a) Particle Velocities



(b) Fluid Velocities

Figure 8. Velocity Distributions from 3-m Spill Simulation at ~200 seconds

In terms of particle depositions onto the floor and onto the samples (filters and impactor), Fig. 9 shows the Fuego simulation results. As shown in this figure, the middle ring floor yields the highest value, followed by the outer ring. The least is in the inner ring. This behavior may be caused by the total cross-sectional area in each ring and the sample flow near the outer region of the RART volume so that the particles near the outer region may be pulled by the sampling flow. The middle region may not experience a larger sample flow than the outer region. The lowest deposition is in the inner region, since it was evidenced in early time that the larger particles settled at the inner and middle regions.

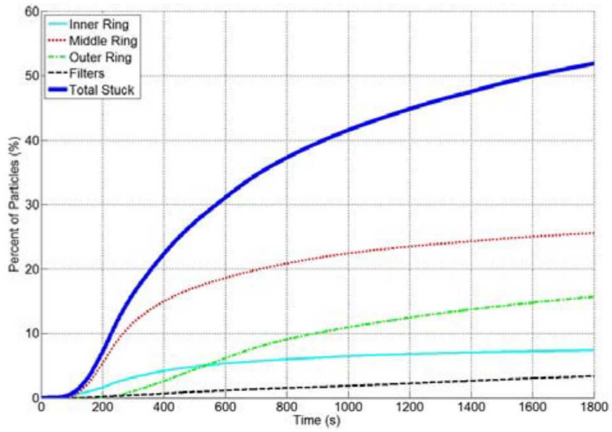


Figure 9. Fuego Simulation on the Particle Depositions at Various Locations (Ring location on the floor)

In conclusion, the aerosol result of the simulation overestimates the ARF in terms of the particles collected in the samples. This difference may be due to the following factors:

- Fuego currently does not model agglomeration, which may cause the settling to occur faster.
- The assumption of 10^8 particles (including the parcel value of 1000) in the model versus the actual number of particles of 10^{13} may overestimate the number of particles pulled through the samples.
- The turbulence flow model used may influence the mixing that causes the overestimation.
- The percent particle reported is a number percent, which may be different from the experimental data as a mass percent.

Pressurized Powder Release

Similar to the free-fall powder release simulation described in the previous section, the pressurized powder release experiment was conducted in RART. The only difference between this experiment and the spill experiment is the location of the release equipment and method. The release equipment for this experiment is a power enclosure that is called Pressurized Airborne Release Equipment (PARE). Fig. 10 shows the schematic of the RART configuration and the PARE for the pressurized release experiment. The PARE is placed on the center floor of RART. The test material is placed inside the PARE (assumed the same size of the beaker in the free-fall experiment) and pressurized with air to the test pressure. The release is due to the removal of the air between two designated rupture disks at design pressure. This section describes the simulated 50 psig (0.34 MPa) and 250 psig (1.72 MPa) tests for the release of 100 g TiO_2.

(a) RART (b) PARE

Figure 10. Schematic of RART and PARE for Pressurized Release Experiment [11]

50 psig (0.34 MPa) Case

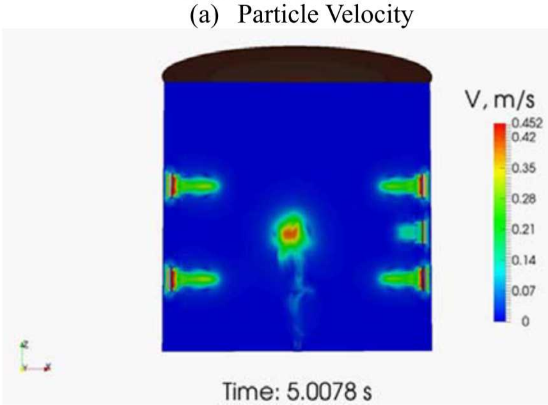
Using the same computational mesh as in the free-fall powder simulation in the previous section, the rupture disk timing is assumed to open at 0.5 millisecond. The peak fluid velocity (643.0 m/s) was based on a momentum balance at this pressure. This corresponds to a Mach number of 0.38, which is marginally in the subsonic range. Additional assumptions and calculation specifics (such as turbulence parameters) for this simulation are well documented [4]. For this simulation, we ran the model out to 30 minutes of the experiment. Fig. 11 shows the particle velocity and fluid velocity results at 5 seconds, respectively. As shown in this figure, the particles inducted by the pressure-driven flow are rising, while the sampling flow begins to pull. At the end of the 30-minute simulation, very little particulate stuck to the RART ceiling which is different from the experiment, which indicates some sticking on the ceiling as the pressure increases. At this 0.34 MPa case, some particles remained in the PARE. Therefore, the total ceiling deposition was estimated using the open boundary condition. Fig. 14 shows the ceiling deposition results.

In conclusion, these types of open boundary conditions would be corrected if they were modeling the filters, since particles are trapped onto the filter while gas can flow through. Despite this issue, the deposition values are reported for both the ceiling and filters.

250 psig (1.72 MPa) Case

For this pressure case, we used the SIERRA/SM (Presto) code to perform the initial blast of the powder and pass the particle data to Fuego for simulating the rest of the experiment condition. Initially, a coarse mesh was used to model the TiO2 powder by using the SPH model in the PARE with the prescribed pressure as the induced pressure (or stress) load. However, the size of this stress is insufficient to induce the release of the powder in the analysis. Therefore, this stress is increased by a factor of 1000. This increase in value is justified because Presto primarily model's solids, and it does not model fluid. When the PARE is pressurized, both powder and air inside the PARE are at pressure. Without modeling the gas portion, the induced stress needs to be larger to push the particles out of the PARE volume. When passing the particles to Fuego, the induced fluid flow by the injecting particles may not yield the actual fluid conditions as in the experiment. That is why the use of the multiplier is justified.

(a) Particle Velocity



(b) Fluid Velocity

Figure 11. Fuego Results on Velocities for 50 psig (0.34 MPa) Pressurized Release at 5 Seconds

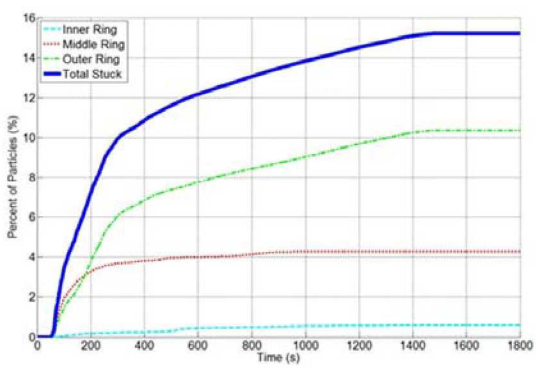
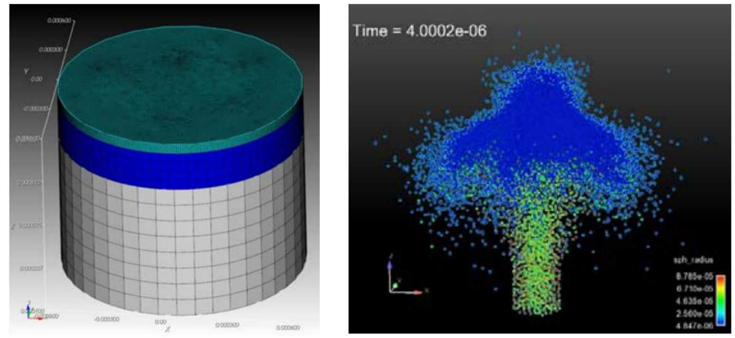


Figure 12. Fuego Results of Ceiling Deposition for 50 psig (0.34 MPa) Case

For Fuego to utilize the particle output from Presto, a translation method was used to generate a series of particle files to be read by Fuego. The particle files are generated using a series of scripts designed to extract the Presto outputs. Once this file was done, the Fuego simulations were conducted.

Many sensitivity studies were conducted to ensure that the kinetic energy of the particles from Presto simulations could induce flows in Fuego because the fine particle sizes as in the 50 psig (0.34 MPa) case lose all their kinetic energy when entering the fluid space of the Fuego domain, causing no flow. In the final simulation as reported here, multiple sizes of the particles were used in the Presto simulation to induce fluid flow in the Fuego simulation (see Ref. 4 for more details). Fig. 13 shows the multi-particle regions and particle release at 4 micro-second. Fig. 14 shows the Fuego results for the multi-particle region from Presto.



(a) 3 Particle Region Mesh (b) Particle Radii

Figure 13. Presto Final Simulation of Multi-Particle Regions and Results for the 250 psig (1.72 MPa) Case

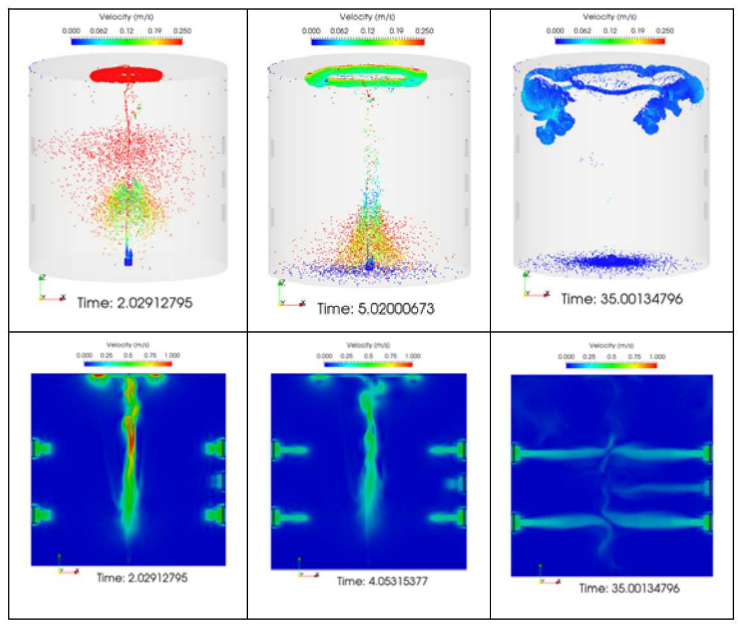


Figure 14. Fuego Results of Multi-Particle Regions from Presto for the 250 psig (1.72 Mpa) Case – Top: Particles, Bottom: Fluid Velocities

Additional runs were conducted because the same issues were encountered as reported in the 50 psig (0.34 MPa) case. See more details in the recent report [4]. The next section describes how SIERRA results can be used with MELCOR LPF calculations.

MELCOR 2.1 FOR LPF CALCULATIONS

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. As previously described, MELCOR is a DOE Toolbox Code for LPF applications. 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 reactor applications' experiment data and from DOE-HDBK-3010, can provide QA for LPF code development and applications. Thus, a guidance report using MELCOR 2.1 was written [6]. This guidance report provides many validation and verification (V&V), along with suggestions for best practices for modeling the common and major accidents encountered at the DOE complex (i.e., explosion, fire, nuclear criticality and spills). Additionally, because the MELCOR code has been applied to reactor applications over last 30 years, the specific applicable reactor validations have been included in the MELCOR 2.1 guidance report [6].

<u>Gasoline Pool Fire</u>

As reported in the SIERRA section, a MELCOR model was developed to simulate the gasoline pool fire experiment (see Fig. 17). Results from Fuego analyses were used as input to MELCOR in this section, since MELCOR does not currently have a fire entrainment model. (MELCOR is not a fire code, because it lacks the dynamic hot gas layer. However, MELCOR can model the fire chemistry and aerosols well (see the further discussions the guidance report [6] for the comparison with CFAST [15].)

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 UO_2 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. Like 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.

In terms of comparing to the experimental data, Table 4 shows the comparison of the MELCOR results. 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.

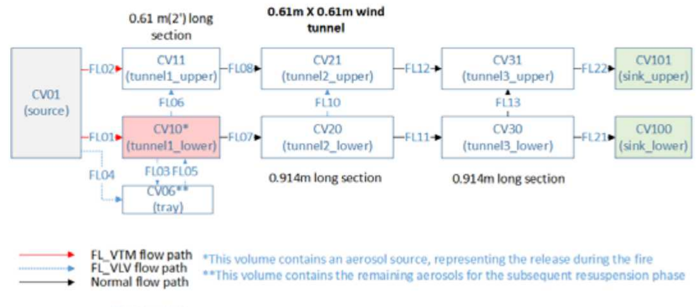


Figure 15. MELCOR 2.1 Model for Gasoline Pool Fire Case

Table 4. Aerosol Deposition and Resuspension in Tray Volume

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. However, the experimenters indicated that they had taken appropriate corrections of the samples [9]

With the aid of the SIERRA 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.

<u>Free Fall Powder Release</u>

In modeling the free fall spill experiment, three MELCOR nodalizations represented the RART volume: 1-volume, 5-volume and 15-volume (see Fig. 16 for the MELCOR nodalization models).

For the aerosol source material for the beaker volume, 1 g, 25 g, 100 g, 450 g or 1000 g of TiO_2 were sourced into the beaker using a tabular function with the assumption that the total source mass is in the atmosphere of the beaker within 0.05 seconds. MELCOR treats aerosol as a trace element, so it does not affect the problem hydrodynamically. Therefore, the fluid flow information from the Fuego result on the free-fall simulation was used.

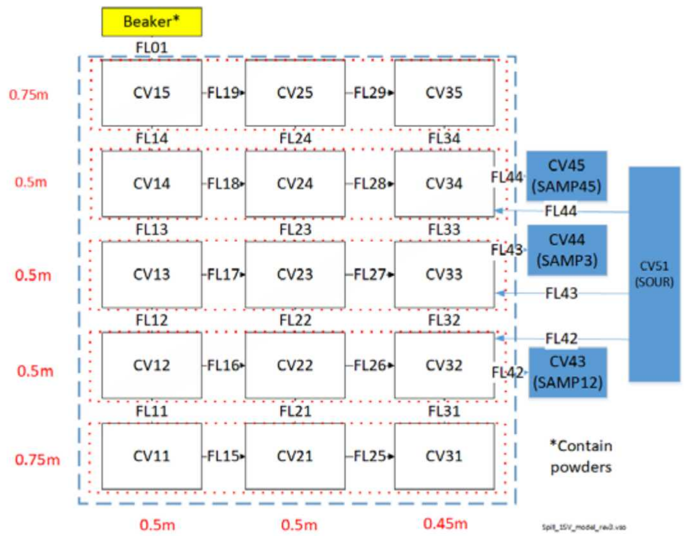


Figure 16. MELCOR 15-Volume Nodalization Diagram for Gravitational Spill. (with Model Representation for the 1V in blue dash and 5V in red dash Models).

When comparing to the experimental data as shown in Fig.17, without the addition of fluid velocity introduction from Fuego to the RART, no base case can obtain results closer to the data. 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 AMMD (aerodynamic mass mean diameter) size, the results seem to match closer to the experimental data. The experimental data in Fig. 17 shows airborne release is independent of source mass used. As shown in Fig.17, using a 1-g estimate to perform spill simulation may yield results significantly differently for larger mass cases (several MELCOR data points lay outside of the displayed y axis range). Using Fuego fluid velocities may bring the results closer to the experimental data as shown in Fig.17. 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. 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. Note the 1-g case is not originated from the experiment.

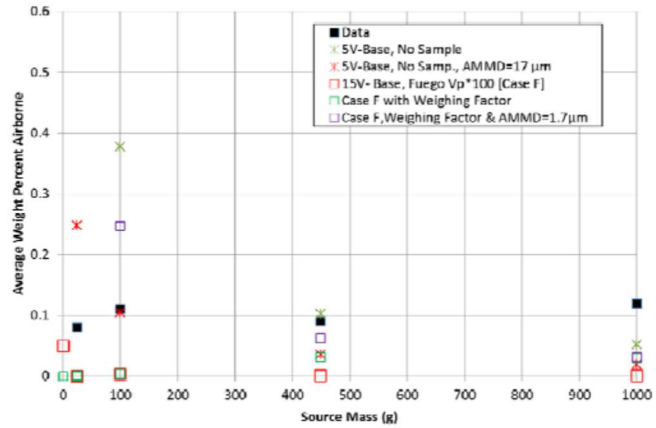


Figure. 17. MELCOR Results for Free-Fall Spill at 3 m.

<u>Pressurized Powder Release</u>

The MELCOR calculations utilized all three MELCOR nodalization models as previously described in the spill case (1V, 5V and 15V) shown in Fig. 18, except that the beaker volume is replaced with the PARE volume of the same size and connected to CV11, instead of CV15.

Fig.18 shows the MELCOR results for the pressurized release of the 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 account for the concentration of the aerosol in a volume. In addition, the stacking volume arrangement in the 5V case resulted in substantial 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.

Fig. 19 shows the turbulent deposition predicted in MELCOR. The values are much smaller as expected. Thus, the use of the results from SIERRA may be required to rescale the ARF results. Although the capability of the SIERRA for higher pressure cases, such as 250 psig (1.72 MPa) are shown in [4], additional SIERRA simulations are required to estimate the turbulent deposition onto the ceiling of RART.

SUMMARY AND CONCLUSION

In this paper, we demonstrated the SNL computational tools which can be used to estimate the airborne release of particles in the respirable size range. The SIERRA tool provides the initial particle releases from the accidents, such as fire and free-fall/pressure. The use of SIERRA tools can enhance the results of the MELCOR code, since MELCOR code is used to predict the LPF estimate. These tool can enhance the safety of nuclear facilities.

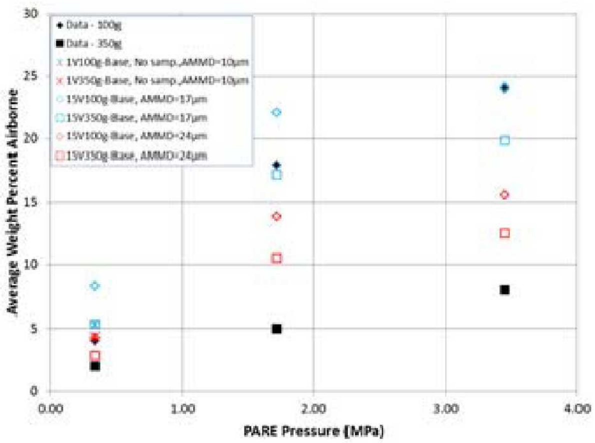


Figure 18. MELCOR Results for Pressurized Powder Release of TiO_2 in RART.

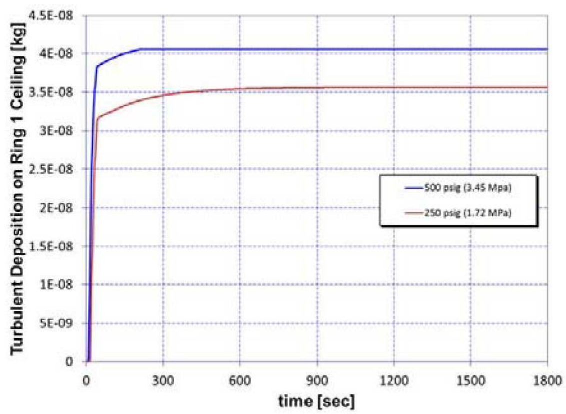


Figure 19. Turbulent Deposition Results for Higher Pressure Cases

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