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Computer Capability to Substantiate DOE-HDBK-3010 Data

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INTRODUCTION

Safety analysts throughout the U.S. Department of Energy (DOE) complex rely 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 analyses (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 airborne release fractions (ARFs) and respirable fractions (RFs) in the Handbook often depend on very limited able-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 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 enable us to use code simulation methods, such as the hydro codes, structural dynamics (SD) and fluid dynamics codes (FD), to provide more representative values for the source terms. If our proposed research determines that the data is too conservative, the source term used for the DSA may over-specify the 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 DSA underestimates the source term, which could translate to a potential significant safety concern to the workers and public. In either case, the results of our investigation could enhance how the safety analysts across DOE complex approach the selection of adequate bounding ARFs and RFs, which could result in improving the defensibility of the safety analyses.

This paper describes the initial progress of this research funded by DOE Nuclear Safety Research and Development (NSRD) Program for Fiscal Year 2015. In this year, we are addressing the impact of fires (or thermal insults) on the liquid material form as presented in Chapter 3 of the Handbook. Based on the recent study done for a spent fuel processing source term for the Nuclear Regulatory Commission, we have already shown that both SD and FD codes can be used to provide ARF and RF of a red oil explosion accident [2]. We are presently examining the use of a FD code to address the source term from a contaminated pool fire. If this work is proven successful, we believe that we could have capabilities to address releases for explosion/criticality[a] and fire for liquid materials in the Handbook. In addition, we are providing the computer code capability and exploratory simulations to address the Handbook data for other materials besides liquid such as solids, powders and contaminated surfaces.

MODELING APPROACH

We are using SNL computer codes (see Table 1 for the codes being considered for this work) to substantiate the Handbook data to develop insights and provide predictions regarding the fundamental physics and phenomena associated with the types of accidents outlined in the Handbook (e.g., explosion, nuclear criticality and fire).

Table 1. Relevant Computer Codes at SNL

Code Name	Capability	Applications
CTH	A multi- material, Eulerian, large deformation, strong shock physics and solid mechanics code	Shock physics, penetration, fragmentation and impact
SIERRA/ Fluid Mechanics (FUEGO)[A]	A low-Mach number fluid mechanics computational fluid dynamic fire code	Fuel fire, droplet dynamic, and gas/particle transport
SIERRA/ Solid Mechanics (PRESTO)[A]	A finite element Lagranigan structural dynamics code	Impacts and explosion for solid and liquid

[A] These are part of the Sierra code suite [3]. It has been used to simulate a denitrator explosion accident [2].

In what follows the model and approach for pool fire simulation is described first. For this, we utilize the lab-scaled experimental data in the Handbook to validate the mechanistic FD capability in FUEGO. Additionally, we provide verification and validation (e.g., FUEGO validation), before actually performing up-scaled predictions for detailed analysis of the Handbook's release fractions. We report preliminary results for the mechanistic FUEGO capability, and the plan for upscaling simulations to address the more practical scale pool fire. To address the non-liquid form of materials in the Handbook, we report our progress by summarizing the code capability and the plan to provide exploratory simulations.

Pool Fire Simulations Using FUEGO

The evolution of airborne contaminants from a burning liquid is not a well-established phenomenon. While much work exists on the basic phenomenology, it has yet to be consolidated and verified in a way that provides confident predictions of fuel fire ARF and RF for a variety of scenarios. The physical mechanism for entrainment is believed to primarily relate to the drops formed as boiling bubbles are ruptured at the surface of the liquid/gas interface. Two regimes exist. In the first regime, the drops are formed as the bubble dome collapses. This is commonly referred to as the film breakup regime. For fluids commonly studied (water and salt water), this results in drops in the 1-100 μm range. The other rupture entrainment mechanism is called the jet regime, and results from the elevation and pinch-off of a tendril of liquid as the liquid collapses around the bubble void after the film ruptures. This results in much larger drops, usually in the range of 100-300 μm. According to the Handbook, the film breakup regime is active for bubbles greater than 0.2 mm in diameter. The bubble mechanism is illustrated in Figure 1 on the left. On the right, the potential for wave action to create entrainment from stretching and collapsing waves is illustrated. This entrainment mechanism is highly dependent on the wind speed for outdoor fires and on ventilation rates for indoor fires. Entrainment is also possible in the residual layer after the fuel has burned off, or from deposits on the surrounding surfaces.

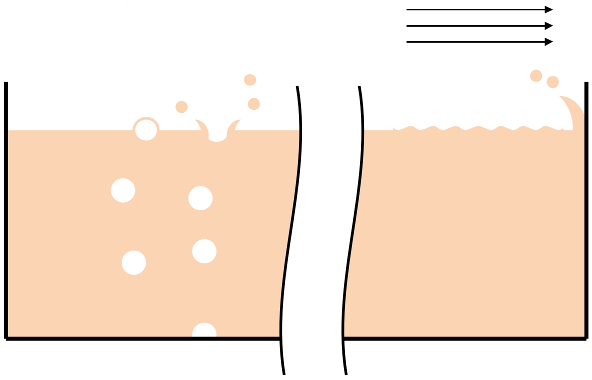

Figure 1. An illustration of boiling entrainment (left) and surface wave entrainment for liquid in air.

The Handbook recommends the model from Kataoka and Ishii [4]. They reviewed an extensive quantity of literature from previous work and developed an analytical model for entrainment using an entrainment factor that is defined as the upward liquid mass flux divided by the upward gas mass flux. They provide separate models for the entrainment in three distinct regions that are separated by a characteristic height. The near surface region entrains the most, but the drops are mostly expected to fall back to the surface.

Boiling data from Borkowski, Bunz and Schoeck [5] comprise a component of the drop size data presented and recommended by the Handbook.

As a test scenario, the liquid entrainment experiments of Mishima and Schwendiman [6] are replicated using FUEGO. The entrainment factor is taken from Kataoka and Ishii [4] assuming near-surface regime data are applicable. The particle size distribution is taken from the 1.4 mm bursting bubble data for a 0.1 NaCl water solution as presented in Borkowski, Bunz and Schoeck [5]. Mishima and Schwendiman [6] report ARF data from a kerosene/30% TBP mixture involving various contaminants. They pre-heated the liquid to the boiling point, and then ignited the fuel in a 250 mL beaker.

Figure 2 shows predicted flame temperatures and particles (exaggerated in scale for visibility) based on modeling performed with the SIERRA/Fluid Mechanics code. Significant deposition is predicted on the sides of the beaker, as was speculated in the data report. For this scenario, the distribution from boiling at the surface resulted in number mean particle size of around 4 μm, and a mass mean of around 130 μm.

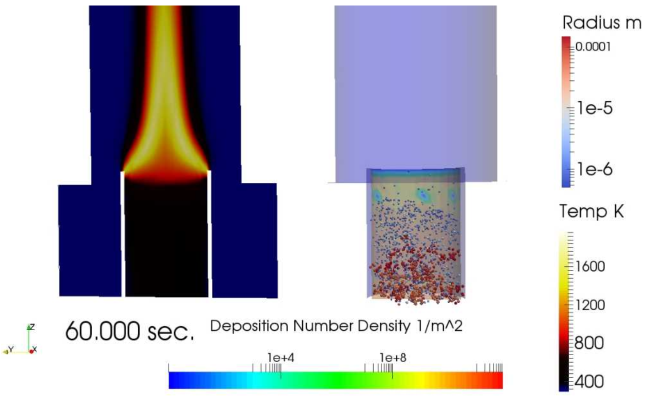

Figure 2. An illustration of the predicted liquid entrainment from the tests of Mishima and Schwendiman [6] with particle parcel sizes exaggerated for visibility.

A curious finding from the simulations of this scenario is that the mass release occurs mostly during the initial transient as the fire is ignited. At this point in time, the flames are close to the surface, and the high velocities and buoyancy associated with the flames help induce the release. Subsequent release continues, but at a much slower rate. Figure 3 shows escaped mass and particle count from the simulation of the first 10 minutes of the test (for tests that ran for 42-56 minutes). The majority of mass escapes in the 1-2 second range, and although particles continue to escape, their contribution to the escaped mass is negligible.

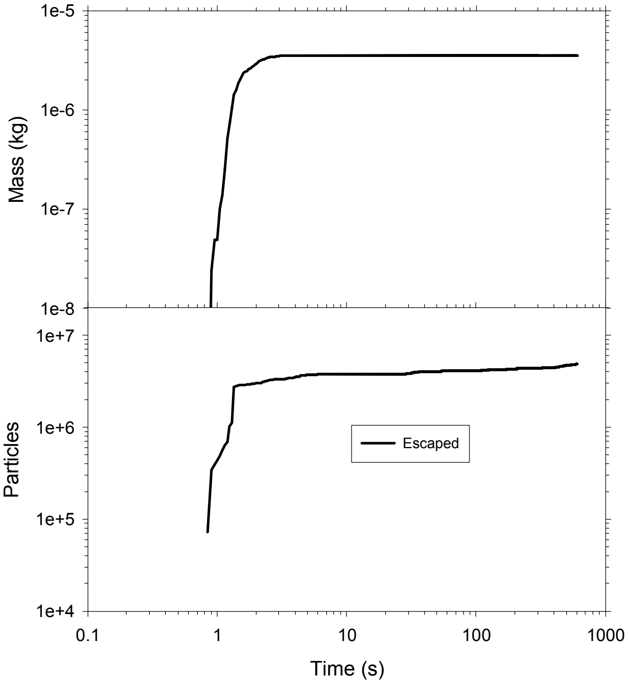

Figure 3. Predicted escaped (entrained) mass and particles as a function of time for the tests of Mishima and Schwendiman [6]

The method for forming particles employed a random function that fit the prescribed distribution functions from the previously described references [4-5]. The particle formation model was used to form six input files, and each was tested in the CFD transport model for the first 6 seconds to obtain the release from the early transient. The average ARF from this exercise was 0.018%, with a fairly large standard deviation of 0.013. The data from Mishima and Schwendiman [6] suggest that ARF for an inert contaminant (uranium) was 0.023-0.027% based on two tests. The model predicts an average release that is below this, but still within one standard deviation of the model predictions. Work is underway to characterize the final transient to quantify how much this increases the predicted ARF.

The reason the mass was mostly released during the initial transient in the simulations is because the burning liquid was well below the top of the beaker. Once ignited, the flames migrated to the top of the beaker where the oxygen was available, and then could no longer effectively entrain significant quantities of particles. This suggests that the use of these data for globally conservative ARF estimates may not be as conservative as it would be, had the liquid level been maintained close to the top lip of the beaker in the experiments.

It would be helpful to replicate these tests with higher experimental fidelity to verify the simulation results. If the bulk of the release is indeed found to be during the initial transient, it would suggest that these tests should be repeated with a higher liquid level to better capture the conservative case.

Code Capability and Exploratory Simulation for Non-Liquid Materials

Solid material releases of particulates is typically involved with an energetic accident that causes a solid (such as PuO_2, which is important to the public dose consequence) to fragment or vaporize, resulting in airborne particles. Most likely the types of accidents that can cause solids to fragment and vaporize would be an explosion and a nuclear criticality. Thus the types of the codes that can be used to simulate these kinds of accidents could be CTH [7] and/or PRESTO [3] (see Table 1). The powder material form can be easily made airborne with air disturbance (such as winds) if it is not inside a container. If the powder is inside a container, the container can be damaged due to impact resulting from explosion or other energetic event. Both CTH and PRESTO can be used to address the impact scenario. Once the container is breached, depending on the nature of the impact that yields particle airborne, a FD code such as FUEGO may be used to simulate the subsequent movement or entrainment of airborne particles employing a code-coupling methodology described previously [8]. For a release not involving a container, such as entrainment of particles from a contaminated surface, a FD code such as FUEGO may be used to model the release from such surfaces.

Plans are underway to examine the entrainment of both solids and powders using the SNL codes described. A simulation of the powders inside a container using CTH/PRESTO is in the development stage. Predictions of particle suspension due to a cross flow is also in the development stage. This simulation should characterize the adequacy of these codes to address these phenomena. The need for code improvements will also be identified from these simulations.

RESULTS AND SUMMARY

This paper describes the first steps in an effort to substantiate airborne contamination data in the Handbook. The use of the modern computation tools, such as SNL codes described in Table 1, can provide additional confidence for using the existing data in the Handbook for safety analysis. Since this work is on-going, only the preliminary results for the FUEGO code capability are provided. Additional results will be provided once the work for this year is completed. The contaminated pool fire simulations using the FUEGO code has demonstrated that the beaker fire experiment of Mishima and Schewndiman [6] can be simulated. The simulation tools predict that entrainment occurs almost entirely during the early transient, and suggests that the lip height for these tests was higher than might be considered conservative. Predicted and measured ARFs are within the uncertainty of the computational model. FUEGO can be used to simulate the release from the small pool fire, and is expected to retain accuracy when applied to the large pool fire such as gasoline fire during a transportation accident. For the large pool fire, particularly those with shallow pools, the wall effect is expected to be less significant. It is expected that similar entrainment mechanisms will exist regardless of the scale of the fire, but the relative contribution of the mechanisms may change.

ENDNOTES

[a] This is based on the work reported in Reference [2]. Since both explosion and nuclear criticality accidents are considered highly energetic events, except that criticality produces fission product gases rather than chemical reaction by-product gases, both accident types can be treated similarly in the simulation.

ACKNOWLEDGEMENT

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