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Evaluating a Historical Airborne Release Test with Modern Modeling Methods

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INTRODUCTION

Safety analysts throughout the U.S. Department of Energy (DOE) complex rely 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. 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 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.

One historical dataset included a test where a solid contaminant was sprinkled over a liquid gasoline pool and set on fire (also referred to as Mishima and Schwendiman's test [2] later in this paper). The airborne release was measured over the duration of the burn, but then collected separately for a time after the burning was completed [2]. It can be assumed that the collected contaminant in the latter period corresponds to re-suspended particles, whereas the earlier period collected contaminant includes a combination of directly released as well as early released re-suspended particles. This scenario was recently modeled using SIERRA/Fuego [3] as part of a parametric sensitivity study [4], however there were some shortcomings of the analysis methods. First, the code at the time lacked a multi-component particle evaporation model, which is necessary to capture the particle size effect of liquid/solid particles that can dynamically evaporate the liquid component. Second, a particle sticking and re-suspension model did not exist at the time of the study. Recent model implementation now permits the study be repeated with the improved physical models.

In the earlier work [4], four potential mechanisms were considered to potentially contribute to the release of the particles. These were:

1. Evaporation Induced Entrainment (EIE)
2. Surface Agitation by Wind
3. Surface Agitation by Boiling
4. Residue Entrainment (Resuspension)

The sensitivity study evaluated mechanism 1 and 3 in the above list. Parameters varied were selected to be a reflection of a practical range of test conditions. The varied parameters included the boiling duration, fuel height, injected mass, particle size, turbulence intensity, and initial particle height. The boiling duration was the most significant parameter. The most significant mechanism was #3, Surface Agitation by Boiling.

This paper reports the implementation of the new multi-component evaporation model and its effect on the findings from the previous effort. The Mishima and Schwendiman [2] test was re-modeled with the new evaporation model, and the results of the re-evaulation are presented [4].

MODELING APPROACH

Multi-component evaporation is a phenomenology that is driven primarily by temperature, species properties, and gas conditions. Since evaporation occurs at an interface, the surface area is also important. Considering a two-component system, the surface area for each component will depend on how the components are distributed within the drop. If they are miscible, the best assumption may be that each has a volume proportional surface representation within a drop. If they are immiscible, one component may be more heavily represented at the surface compared to another on a volume proportional basis. For our particular problem we have a UO_2 particle and gasoline (which we are modeling as pure heptane, C_7H_{16}). Our initial model implementation assumes a volume proportional exposure of each component at the surface of the particle. This is a simple approximation made at this point. Considerations will be made in the future to better represent this feature of the drops. We also assume spherical, homogeneous, well-mixed drops in thermal equilibrium. More can be found on higher detail modeling of multi-component fuels in some recent literature [5-8].

As with the previous work, we assume that the particles are primarily released from the fuel surface as drops formed in the boiling liquid rupture at the surface between the liquid and gas. To model this phenomenon, we employ the near-surface correlation of Kataoka and Ishii [9]. The size distribution is assumed based on the data of Borkowski et al. [10]. In the previous work [4], we found the boiling time to be a very significant parameter. As we have no way presently to determine this feature from any model or correlations we are aware of, we treat this as a free parameter in the models.

We have assumed a wind speed of 1 m/s (this feature was under-reported in the tests), and we assume the flow is in a channel 0.66 m square. Fuel is modeled with a 1-D pool model, which predicts the evaporation from the

surface as a function of the incident convective and radiative flux to the surface from the gas. Figure 1 illustrates the model mesh.

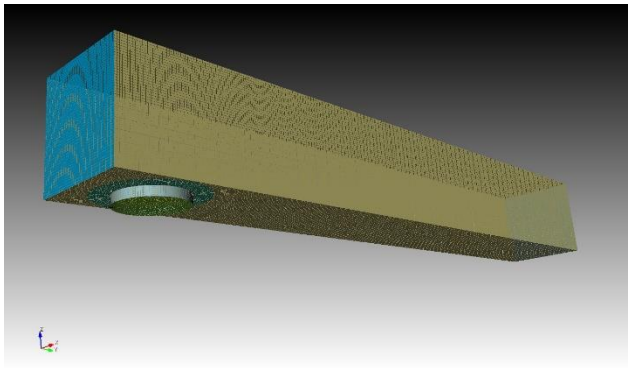

Fig. 1. Mesh and boundary conditions for the scenario.

RESULTS AND SUMMARY

In the prior work without a multi-component drop model, the ARF results for the nominal (baseline) scenario are shown in Table 1. The EIE mechanism was not a significant source of release, although we understand that this mechanism can be significant enough to cause warning detectors to activate. The boiling mechanism was the driving mechanism.

Table 1. Baseline ARF for Evaporation and Boiling

Mechanism	ARF (%)
Evaporation (EIE)	1.3×10^{-7}
Boiling	0.40

The boiling scenarios are being re-run with a multi-component drop model. A parametric study is in progress, which is in part due to the numerical requirements of the multi-component model. As a particle species approaches burn-out, it is typically characterized by a small particle at or near the boiling temperature of the species. Flames are typically much hotter than the boiling temperature. Small particles can respond quite rapidly to temperature changes. A comparatively large time-step for integrating the particle dynamics results in unstable or unrealistic results because the dynamics are resolved at smaller time scales. Our implementation accommodates small particle integration time steps, however this results in long computation times. We are in the process of implementing robust solutions to these problems. Such a solution may involve adaptive particle time stepping, solution projection near the evaporation limits, or solving non-linear scaled variables.

We anticipate involving the resuspension model work also presented at this conference [11] and attempting to simulate mechanism 4 in our above list to evaluate the ability of our models to predict this important phenomenology.

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REFERENCES

1. Department of Energy, DOE HANDBOOK: Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities, DOE-HDBK-3010-94, Reaffirmed 2013 (2013).
2. MISHIMA, J., SCHWENDIMAN, L.C., "Some Experimental Measurements of Airborne Uranium (Representing Plutonium) in Transportation Accidents," BNWL-1732, August, 1973.
3. Sierra Thermal/Fluid Development Team, SIERRA Low Mach Module: Fuego User Manual – Version 4.40, SAND2016-4157.
4. BROWN, A.L., ZEPPER, E., LOUIE, D. L. Y., AND RESTREPO, L., "Contaminant Entrainment from a Gasoline Fuel Fire," the Fall 2015 meeting of the Western States Section of the Combustion Institute in Provo, UT, USA, SAND2015-7185C. Paper 134IE-0033.
5. ZHANG, L., AND KONG, S-C. "High-pressure vaporization modeling of multi-component petroleum-biofuel mixtures under engine conditions," Combustion and Flame, 158, 9, 1705-1717, 2011.
6. ZHANG, L., AND KONG, S-C. "Vaporization modeling of petroleum-biofuel drops using a hybrid multi-component approach," Combustion and Flame, 157, 11, 2165-2174, 2010.
7. ZHANG, L., AND KONG, S-C. "Modeling of multi-component fuel vaporization and combustion for gasoline and diesel spray," Chemical Engineering Science, 64, 16, 3688-3696, 2009.
8. YASIN, M.F.M., CANT, R.S., CHONG, C.T., HOCHGREB, S., "Discrete multicomponent model for biodiesel spray combustion simulation," Fuel, 126, 44-54, 2014.
9. KATAOKA, I., AND ISHII, M., "Mechanistic Modeling and Correlations for Pool-Entrainment Phenomenon," NUREG/CR-3304, April 1983.
10. BORKOWSKI, R., BUNZ, H., AND SCHOECK, W., "Resuspension of Fission Products during Severe Accidents in Light-Water Reactors, KfK3987, EUR 10391, May 1986.
11. VOSKUILEN, T.G., PIERCE, F., BROWN, A.L., GELBARD, F., AND LOUIE, D.L.Y., "Particle Resuspension Simulation Capability to Substantiate DOE-HDBK-30010 Data," ANS Winter Meeting, Las Vegas, NV, USA, 2016.