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Computational Capability to Substantiate DOE-HDBK-3010 Data

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Background:

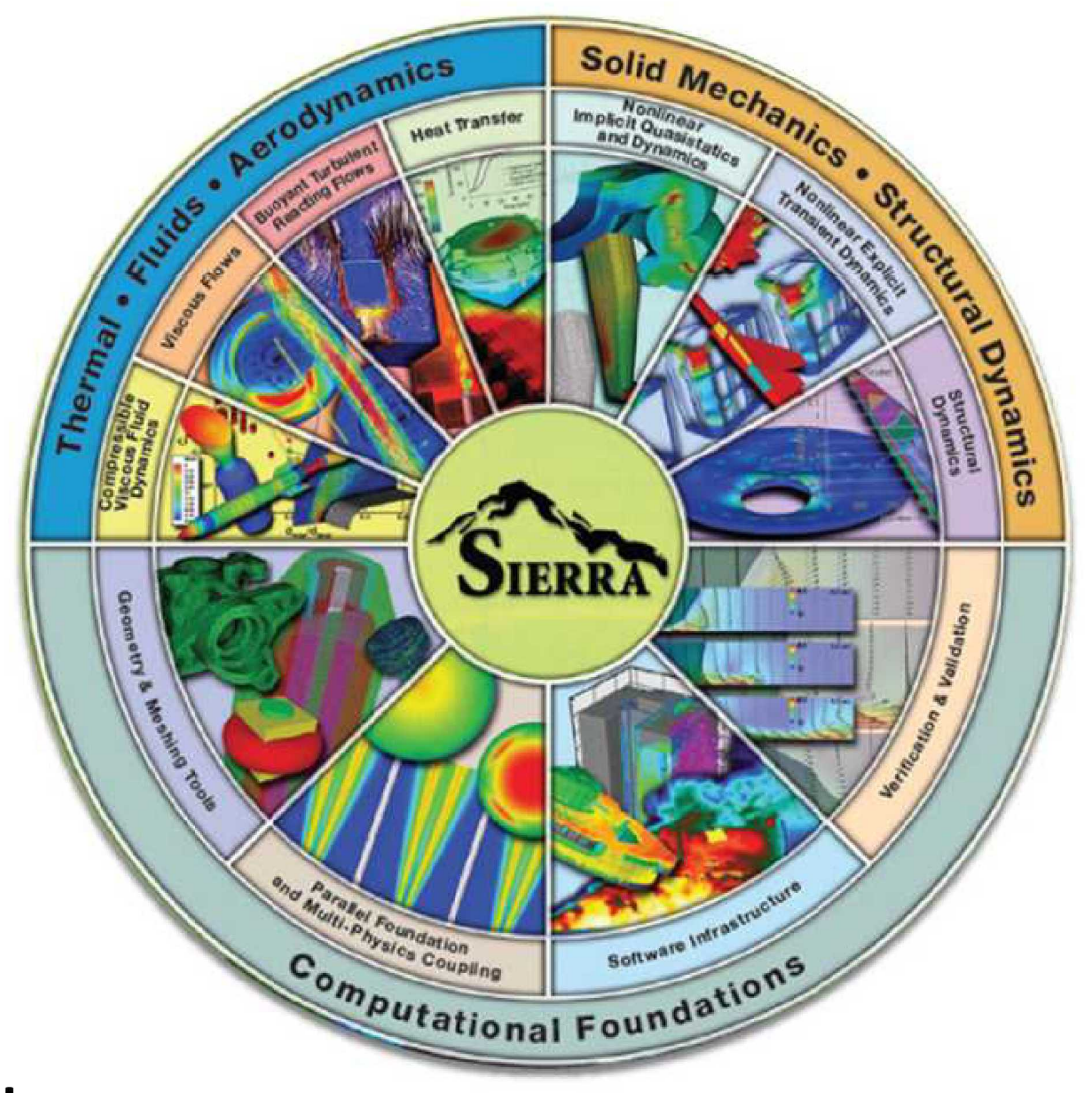
Safety basis analysts throughout the complex rely heavily on the information provided in the DOE Handbook, DOE-HDBK-3010, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities to determine source terms*. Most often, the analysts simply take the bounding values due to time constraint and avoiding regulatory critique. Although the Handbook is very comprehensive in terms of data to derive airborne release fractions and respirable fractions to bound the main types of accidents that could be encountered in the complex, the derivation of the data often depended on table-top and bench/laboratory experiments, as well as engineered judgment which may not be substantiated, and may not be representative to the actual situation.

Approach:

This research should provide insights about the fundamental physics and phenomena associated with the types of accidents based on the maturity of the simulation tools developed for the weapon complex. Although these tools require intense computational power, the availability of these tools and computing power allows safety analysts to utilize these tools for non-weapon related safety activities. These simulation tools would be used to assess whether the data used to derive the airborne release fractions and respirable fractions in the Handbook are reasonably accurate and bounding, or not.

Sandia's SIERRA Code Suites

SIERRA Framework
Thermal/Fluid Dynamics (TF)
  Fuego– low Mach, fire & reacting flow capabilities, particles
  Aria – multi-physics, chemistry, fluid, free surface (no particle)
Solid Mechanics (SM)
  Adagio –Quasi-static (implicit)
  Presto – Transient (explicit), can handle explosions (ITAR)
  Both codes have SPH to model particles
Applications: ARF/RF and DR
  Fire release
  Release due to mechanical insults
  Impact/fragmentation
  Container breach



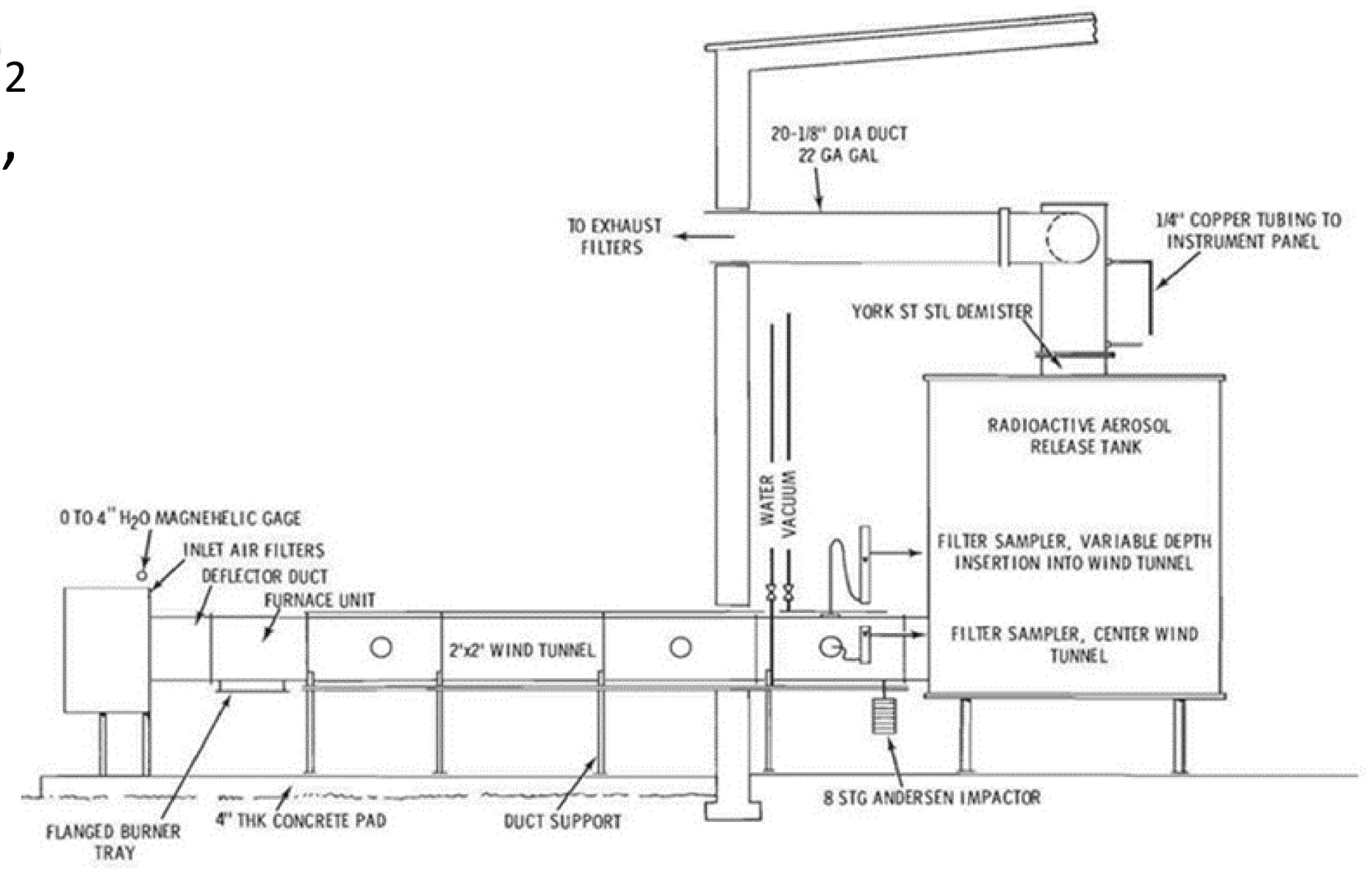
Code improvement: Fuego – multicomponent evaporation, particle resuspension

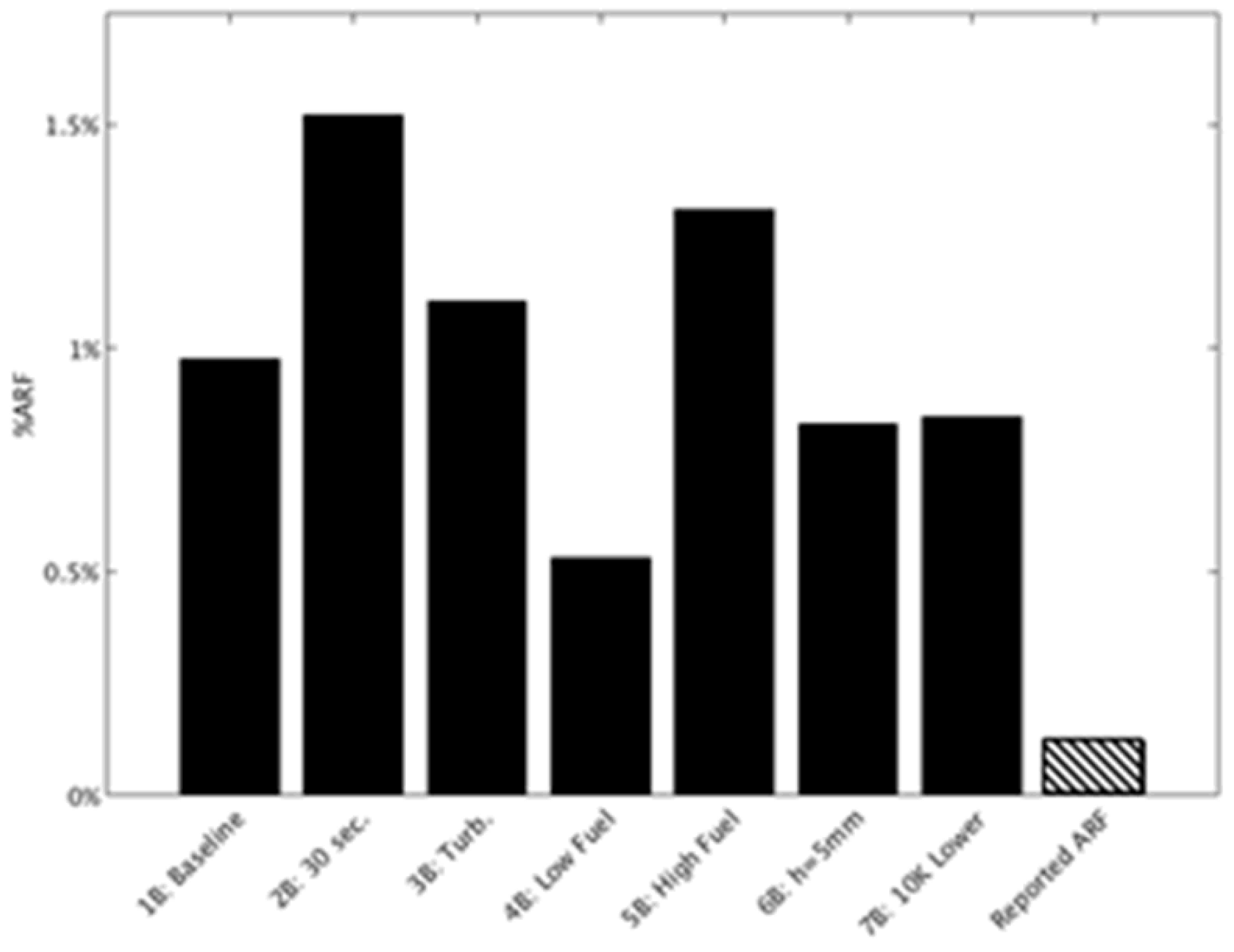
Research Task	Status
Exploratory simulations of energetic impacts using Presto/Adagio (SIERRA/SM).	• A simulation model of a bullet hitting a can filled with small particles has been simulated and formulated such that we could use a non-export version of the SIERRA/SM (see SAND2015-10496 for more details). • 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 [SAND2016-12167].	• A beaker fire experiment was first simulated [BNWL-B274] to provide additional physics insights into the experiment. • A gasoline pool fire experiment was also simulated [BNWL-1732] 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 [SAND2015-10496, SAND2016-12167]. 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 [SAND2016-12167.	• A free-fall powder experiment was simulated [PNL-3786] 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 [PNL-4566] 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 [SAND2016-12167].
Investigation of particle resuspension using Fuego – A resuspension model [SAND2015-6119 has been added to Fuego [SAND2016-12167].	• Particle resuspension is an important phenomenon in particle transport. Many resuspension experiments were used to simulate this phenomenon. See SAND2016-12167. For more details.
Fragmentation of solids using SIERRA/SM –Sequential and con-current fragmentation models have been developed [SAND2016-12167, SAND2018-0436]. 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) [ANL-82-39], SIERRA/SM needs 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 [SAND2016-12167] 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.	• 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 [SAND2017-5684]. • 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 [SAND2018-0436] for a more detail), a refined

Result Example:

Gasoline Pool Experiment (BNWL-1732)

- Experiment distributed UO_2 in a stainless steel fuel pan, added one gallon of gasoline, and performed the test in a wind tunnel
- Air drawn in at ~1 m/s for the duration of the fire
- Filters downstream collected entrained contaminants
- Filters replaced at 9 minutes and air flow continued for 4.8 hours to collect resuspended particles
- Four natural entrainment mechanisms
  - Evaporation induced
  - Surface agitation by wind
  - Surface agitation by boiling
  - Residue entrainment





Summary and Conclusion:

Since FY14, we have substantiated a number of benchtop and small scaled experiments documented in the DOE-HDBK-3010. We have employed Sandia's SIERRA code suite to simulate and analyze these experiments, and added improvement in SIERRA codes for better simulations. In this final year, we try to finish up the fragmentation model for Equation 4-1, and generate DR values for waste containers (SWB and 7A).

In conclusions, SIERRA code suites do provide a way for researchers to better understand the physics in the experiments. Also SIERRA allows us to simulate the accident scenarios that may not yet have experiment data, and allow us to conduct sensitivity studies for a wide range of the parameters that may affect the results.

Acknowledgements:

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