

## A Basic Principles Approach for Determining Radionuclide Aerosol Releases from Accidental Explosions in Reprocessing Facilities

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### INTRODUCTION

Spent nuclear fuel reprocessing is a back-end fuel cycle option for recovering useable actinides and reducing the volume of radioactive waste. The chemical processing involves several steps that under accident situations may result in the release of radioactive respirable aerosol. An overview of the issues with modeling hypothetical accidents in reprocessing facilities is given in a companion paper [1]. A common feature in some of these accidents is that an explosive mixture is formed in a processing vessel, and the explosion not only ruptures the vessel but also aerosolizes some of the contents of the vessel. These accidents have been well documented, but data on the aerosol concentration and particle size distribution of the aerosol formed have not been found. Furthermore, we also have not found aerosol data for systems of the scale typical of reprocessing facilities. Clearly for safety analysis, determining the generation of aerosol particles as a function of the processing fluid properties, equipment dimension, and explosive energy are needed.

Previous approaches for determining the generation of aerosol particles by necessity were made using correlations from bench-scale tests for various solutions that generally did not include explosive releases from ruptured vessels. In this work, we report on a physics-based approach to model the explosion effects on the radionuclide solutions, the rupture or failure of the containing processing vessel, the forced ejection of the radionuclide solution, and the break-up of the solution to form aerosols. Thus we model the creation of aerosols from initial explosion to release.

The basic problem is that the liquid solution dimensions in reprocessing facilities are on the order of meters in scale, yet the aerosol particles of interest are on the order of micrometers. To simulate this range in scale requires resolving one part in a million. Furthermore, since the interest is in the mass of aerosolized solutions, the range is actually the cube of the linear dimension. Thus we need to model the formation of particles that are one part in  $10^{18}$  of the system by mass. The objective of the model is to determine the particle size distribution and total aerosolized mass for use as input to transport codes.

### MODELING APPROACH

Our approach is to couple structural and fluid mechanics codes, including a drop break-up model that is

stable and accurate. All these codes have been developed under a common architecture called Sierra to facilitate the multi-physics coupling [2]. We use Sandia's Presto structural mechanics code, which is a Lagrangian, three-dimensional, explicit, transient code to solve the structural problem with large deformations and short time scales. The radionuclide solutions are modeled with Smoothed Particle Hydrodynamic (SPH) elements, which are coupled to the explosive and the processing vessel walls [3]. SPH allows for radionuclide solutions to both impart momentum to solid structures and for the solutions to be dispersed upon ejection from the vessel. The solid walls and equipment in the vessel are modeled with structural finite elements because these elements may deform and separate, but they do not get atomized by the explosive. After the fluid has been ejected and drops on the order of centimeters to millimeters have separated, the system is then modeled with Sandia's Fuego fluid mechanics code. Fuego is a low Mach number control-volume finite element code that solves the Navier-Stokes equations for the flow induced by the explosion and the ejected drops. Drop break-up is modeled using the Taylor Analogy Break-up (TAB) model [4, 5] employing a Lagrangian transport framework coupled to the Eulerian gas phase solvers. The Presto/Fuego coupling is one-directional in that the structural code with SPH is run first, and then the fluids code with the TAB model is used to determine the aerosol particle size distribution and concentration. Typically the fluid is initially modeled with several hundred thousand SPH particles, and then the final aerosol has orders of magnitude more particles that result from the break-up of SPH particles.

### RESULTS

We have simulated two accidents that have been reported in the literature, the TOMSK-7 accident in Russia [6], and the A-Line facility accident at the Savannah River Plant [7]. In both cases aerosol data were not collected to compare with our model calculations. However, the processing vessel geometries and estimated explosive energies are available. As an example, Figure 1 shows the mesh and simulation results at 20 ms. We use such information to show that the structural code simulation can capture the major features of the event by comparing the simulations to the observed final state of the equipment. Then the code calculations of suspended aerosol provides the aerosol release for these events. We show what fraction of the initial radionuclide solution

mass is aerosolized, and how much of the solution either remains in the damaged processing vessel, or is released onto the floor.

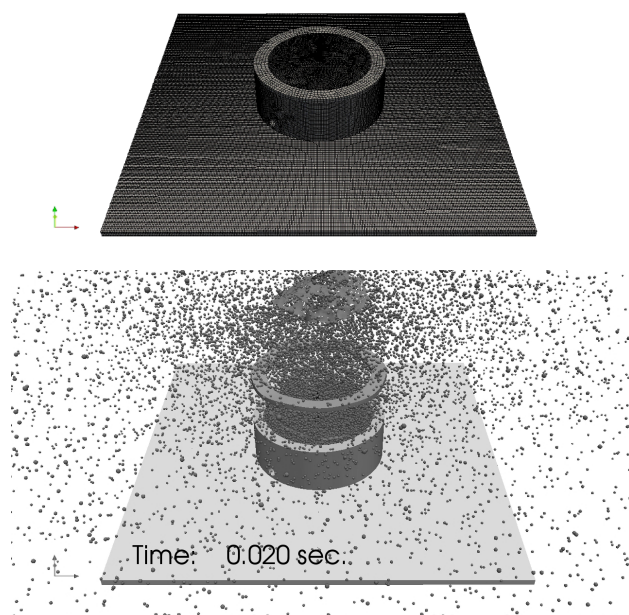


Figure 1. Test geometry with mesh at time 0 (top), and simulation results at 20 ms (bottom).

## CONCLUSIONS

Simulating the aerosol release is important for risk analysis, but only recently have models been able to capture the multi-physics aspects of the problem required for simulating coupled explosive, structural mechanics, atomization, and subsequent dispersal processes [8, 9, 10]. However, even with massively parallel computers, these calculations require several days to simulate just one event. Thus the simulations are only appropriate for extensive parameter studies in the case where significant computing resources are available. Even without significant parametric evaluation, the calculations provide insight on scenarios that form micrometer-sized aerosol particles from accidental explosive events.

## REFERENCES

1. N. E. BIXLER, D. LOUIE, F. GELBARD, and P. R. REED, "Source Term Evaluation for a Spent Fuel Reprocessing Facility," ANS-Winter, 10-14 November 2013, Washington DC, (2013).

2. H. C. EDWARDS, "SIERRA Framework Version 3: Core Services Theory and Design," SAND report SAND2002-3616, November (2002).
3. J. J. MONAGHAN, "Smoothed Particle Hydrodynamics." *Rep. Prog. Phys.* **68**, 1703-1759, (2005).
4. P. J. O'ROURKE, and A.A. AMSDEN, "The TAB Method for Numerical Calculation of Spray Droplet Break-up," SAE Technical Paper 870289, (1987).
5. P.E. DESJARDIN and L.A. GRITZO, "A Dilute Spray Model for Fire Simulations: Formulation, Usage and Benchmark Problems," Sandia National Laboratories, SAND2002-3419, October (2002).
6. E. A. RODRIGUEZ and R. F. DAVIDSON, "TOMSK-7 Radiochemical Facility Explosion: Chemical Vessel Burst Failure Analysis," Los Alamos National Laboratory, LA-UR-95-1756 (1995).
7. J. M. MCKIBBEN, "Explosion and Fire in the Uranium Trioxide Production Facilities at the Savannah River Plant on February 12, 1975," DPSPU 76-11-1, E. I. du Pont de Nemours & Company, Savannah River Plant, October (1976).
8. A.L. BROWN, "Predictive Impulse Dispersal of Liquid Employing a Code Coupling Methodology," The 2013 International Seminar on Fire and Explosion Hazards, May 2013, Providence, RI, USA (2013).
9. A.L. BROWN, "Impact and Fire Modeling Considerations Employing SPH Coupling to a Dilute Spray Fire Code," *Proceedings of the ASME 2009 Summer Heat Transfer Conference*, ASME SHTC-2009, San Francisco, CA, July 19-23, 2009, HT2009-88493, (2009).
10. A.L. BROWN, G.J. WAGNER, and K.E. METZINGER, "Impact, Fire and Fluid Spread Code Coupling for Complex Transportation Accident Environment Simulation," *Journal of Thermal Science and Engineering Applications*, **4**, 2, 021004-1 to 021004-10, June (2012).

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