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DOE-HDBK-3010-94
December 1994
Reaffirmed 2013

DOE HANDBOOK

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Volume I - Analysis of Experimental Data

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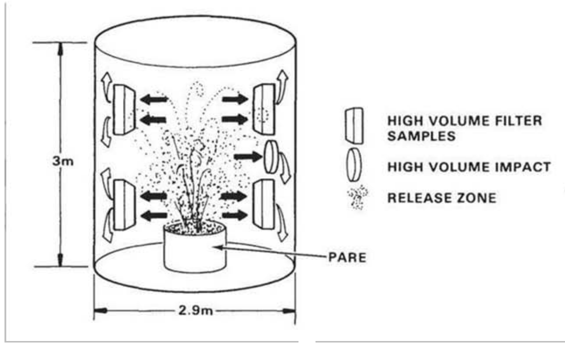

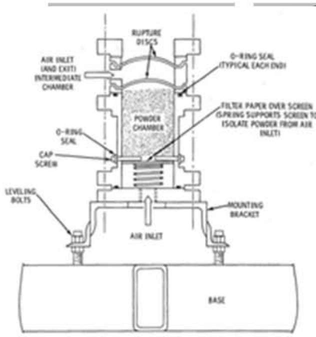

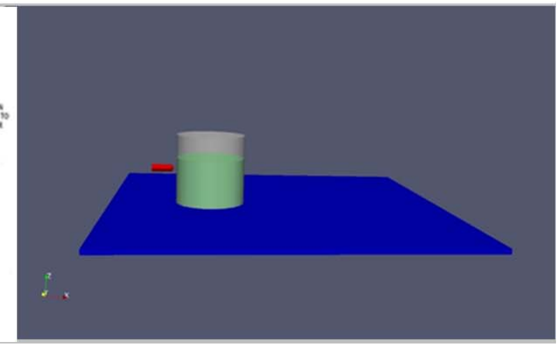

NSRD-11/15: Computational Capability to Substantiate DOE-HDBK-3010 Data

Presented by David Louie , Ph.D.

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We are gratefully that DOE consistently fund Sandia to work on Nuclear Safety Research & Development (NSR&D) Program at DOE Office of Nuclear Safety under Dr. Alan Levin and Mr. Patrick Frias. This work is funded under WAS Project#2016HS201601210

2017 EFCOG NFS Workshop – NSR&D Subgroup

March 14, 2017

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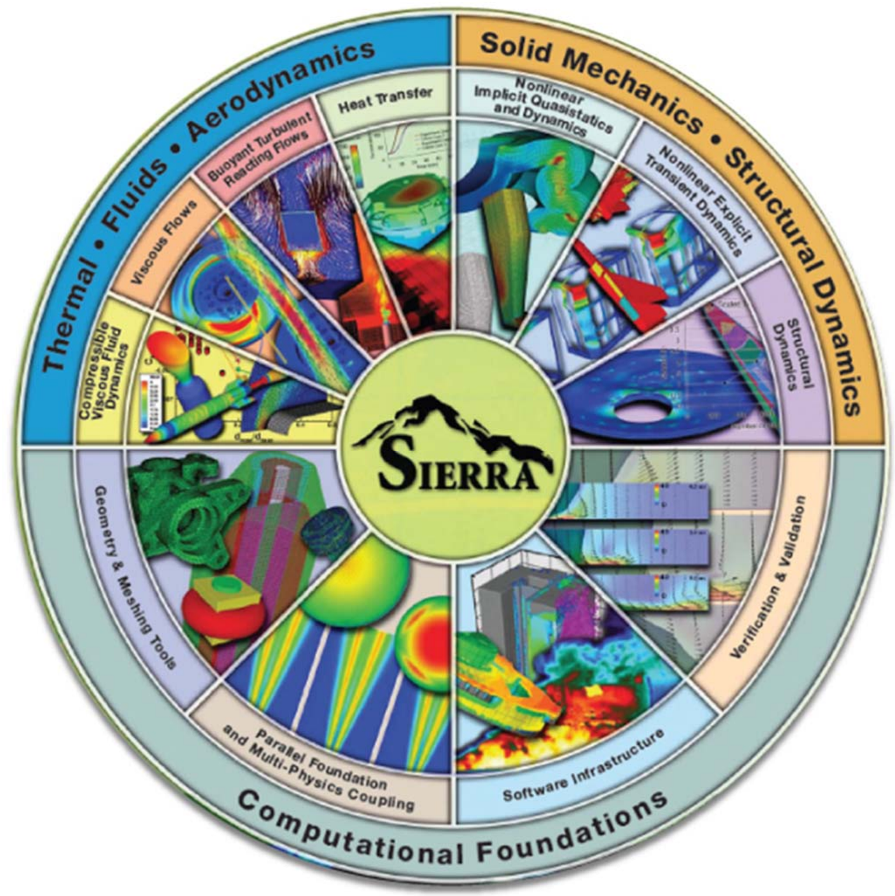
U.S. DEPARTMENT OF ENERGY

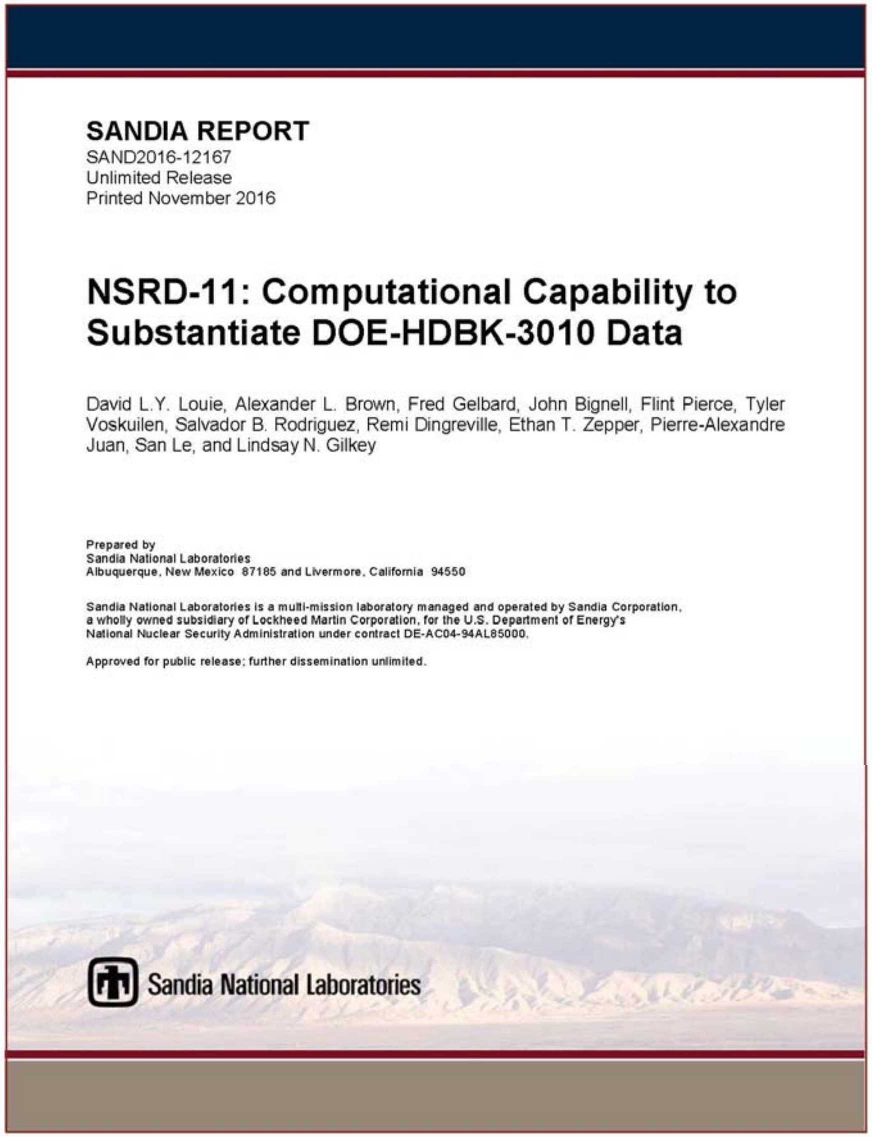
NNSA National Nuclear Security Administration

Sandia's Codes for 3010 Data Substantiation

- SIERRA High Fidelity Code Suites
  - SIERRA Framework
  - Fluid Dynamics
    - Fuego – low Mach, fire/reacting flow capabilities
    - Aria – multi-physics, fluid, free surface
  - Solid Mechanics
    - Adagio –Quasi-static (implicit)
    - Presto – Transient (explicit), can handle explosions (ITAR)
    - Both codes have SPH to model particles
- MELCOR



NSRD-11 Project Accomplishment



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NSRD-11: Computational Capability to Substantiate DOE-HDBK-3010 Data

David L.Y. Louie, Alexander L. Brown, Fred Gelbard, John Bignell, Flint Pierce, Tyler Voskuilen, Salvador B. Rodriguez, Remi Dingreville, Ethan T. Zepper, Pierre-Alexandre Juan, San Le, and Lindsay N. Gilkey

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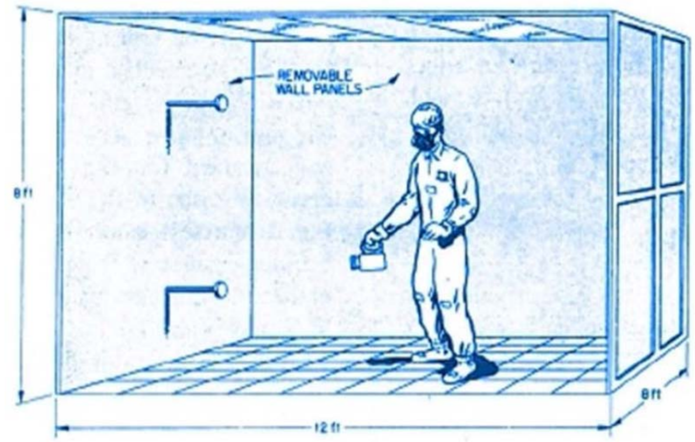
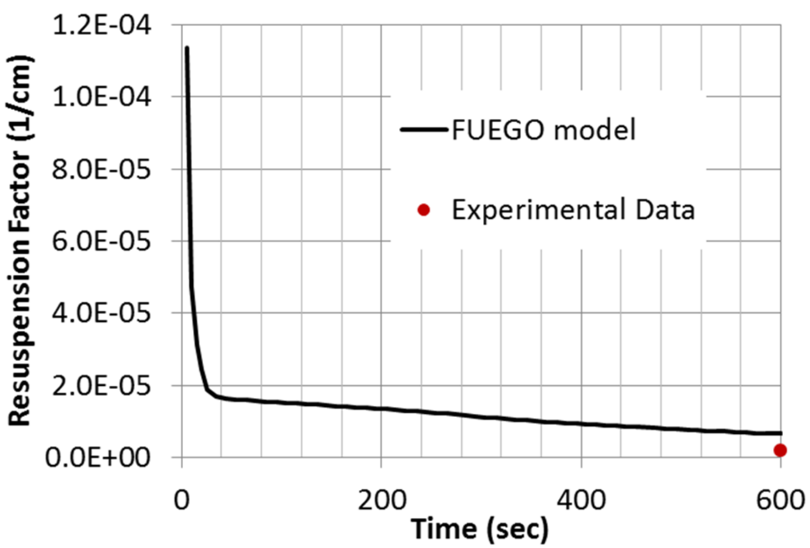
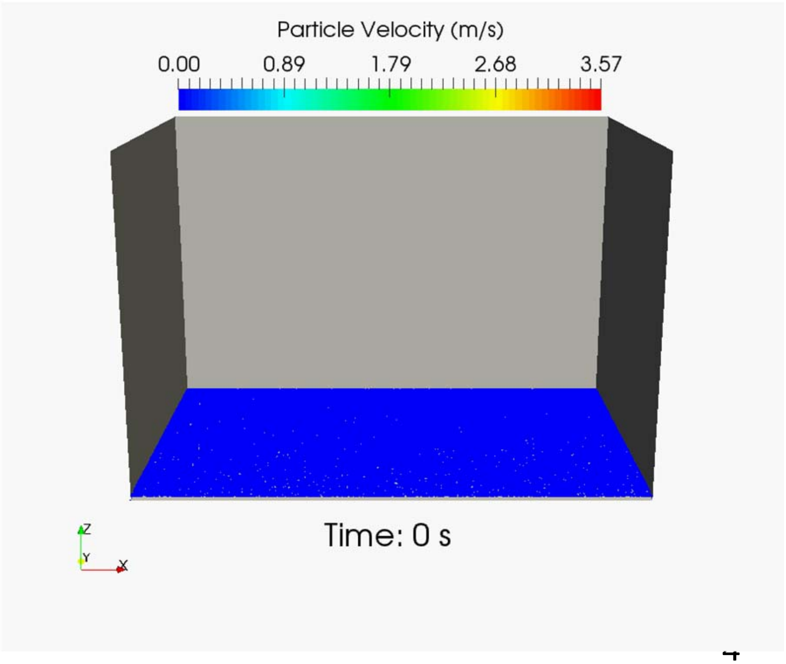
- Fuego Code Improvement
  - Multi-component capability
  - Particle resuspension capability
- Substantiating 3010 Data
  - Resuspension experiment using Fuego
  - Fire experiments using Fuego
    - Beaker fire
    - Gasoline pool fire
  - Powder release experiments (using Fuego and Adagio)
    - Pressurized release (50/250 psi)
  - Fragmentation experiment
    - Micro and Macroscopic approach

Resuspension Exp (Fish 1967)

- 8’x8’x12’ room
- ZnS particles dispersed on floor using $2.44x10^{-6}$ particles/cm2, 3.1 µm, 4.1 g/cc
- Simulation
  - Floor was divided into 24 BCs of equal surface area (mimic person walking and sweeping)
  - 100,000 particles modeled
  - Various boundary conditions are used
  - Simulated time of 24 s for vigorous human activity, 600 s time simulation

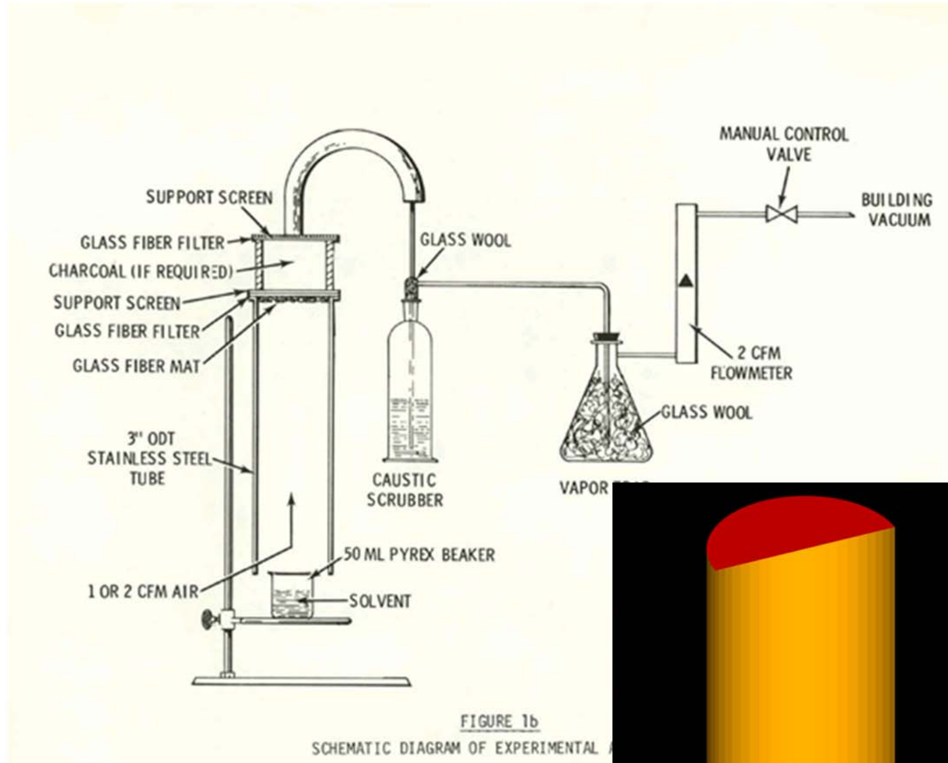


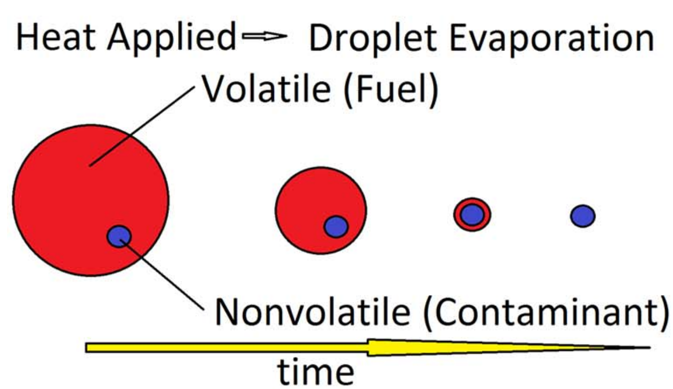


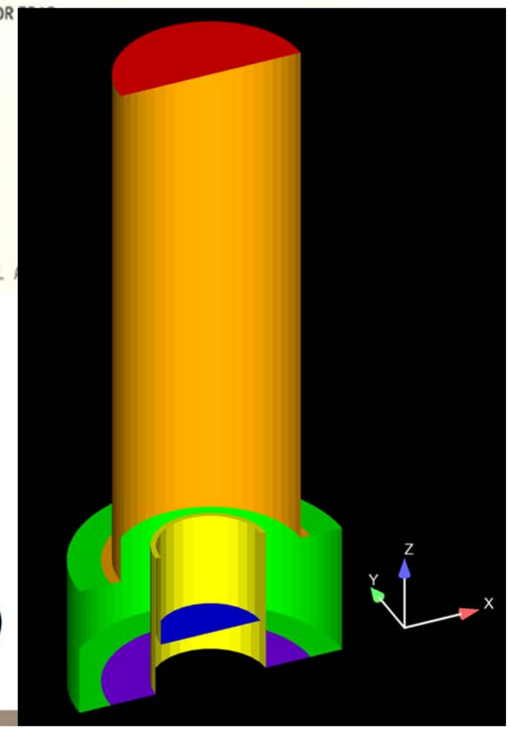


Beaker Exp. (Mishima/Schwendiman 1973)

- Burning of beaker filled with kerosene and 30% tributyl phosphate (TBP) w/ contaminant materials
- UO_2 in our case
- Liquid fuel pre-heated to boiling point, ignited in 50 mL beaker
- Fuego code simulation
  - Multi-component evaporation model

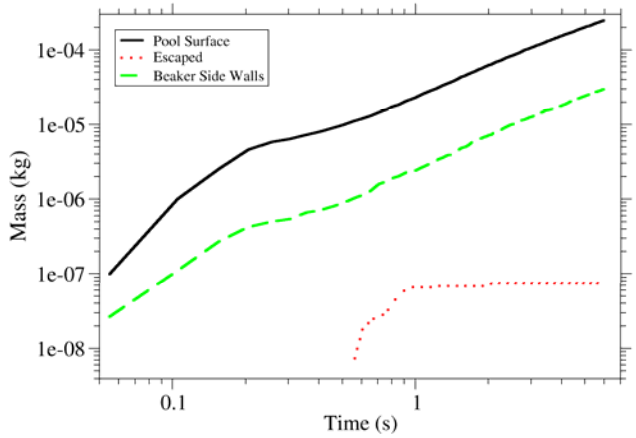


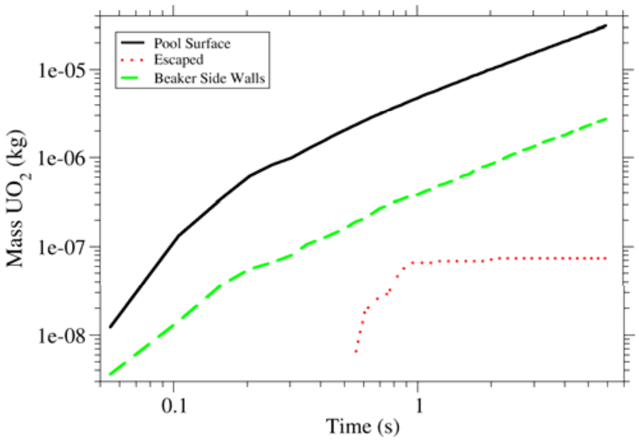




Base 1

- 20 mm Height
- Baseline parameters





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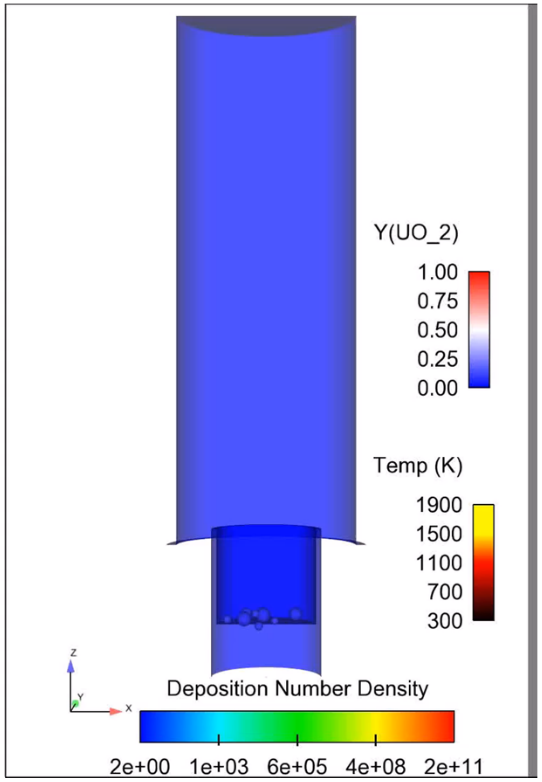
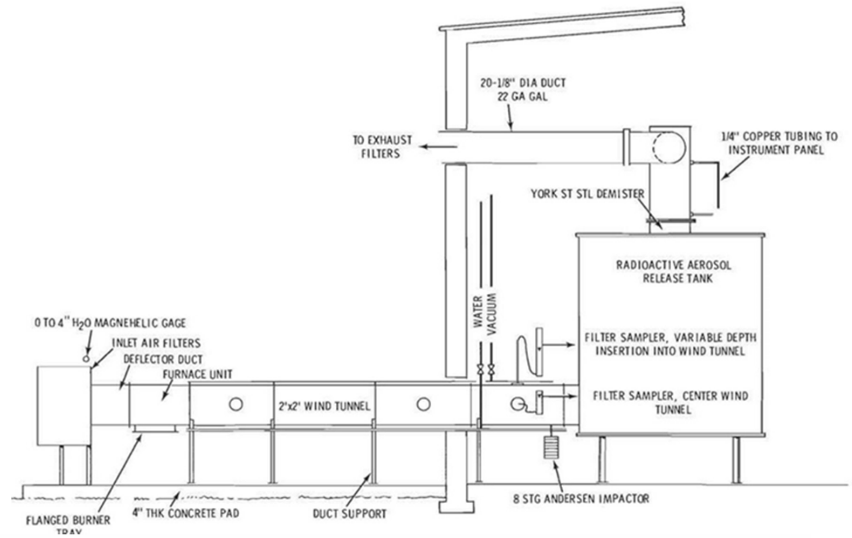
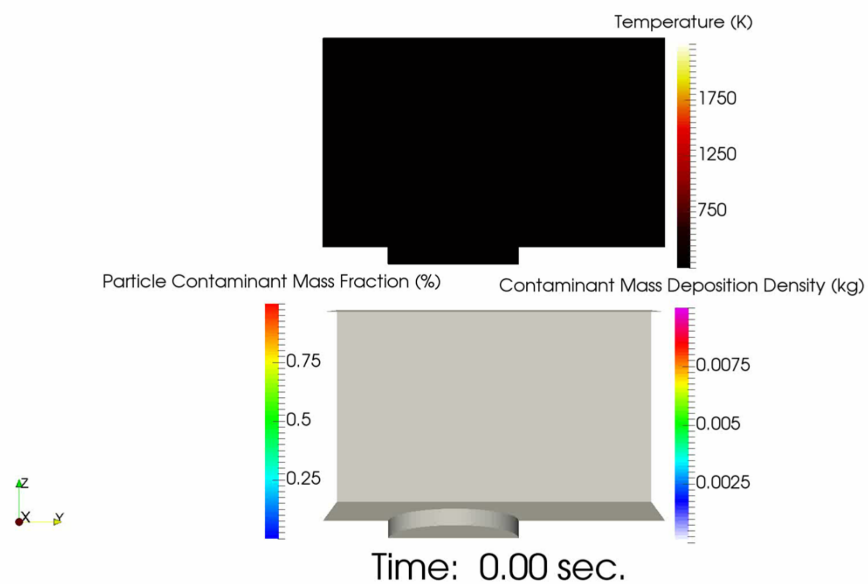


Gasoline Pool Exp (Mishima/Schwendiman 1973)

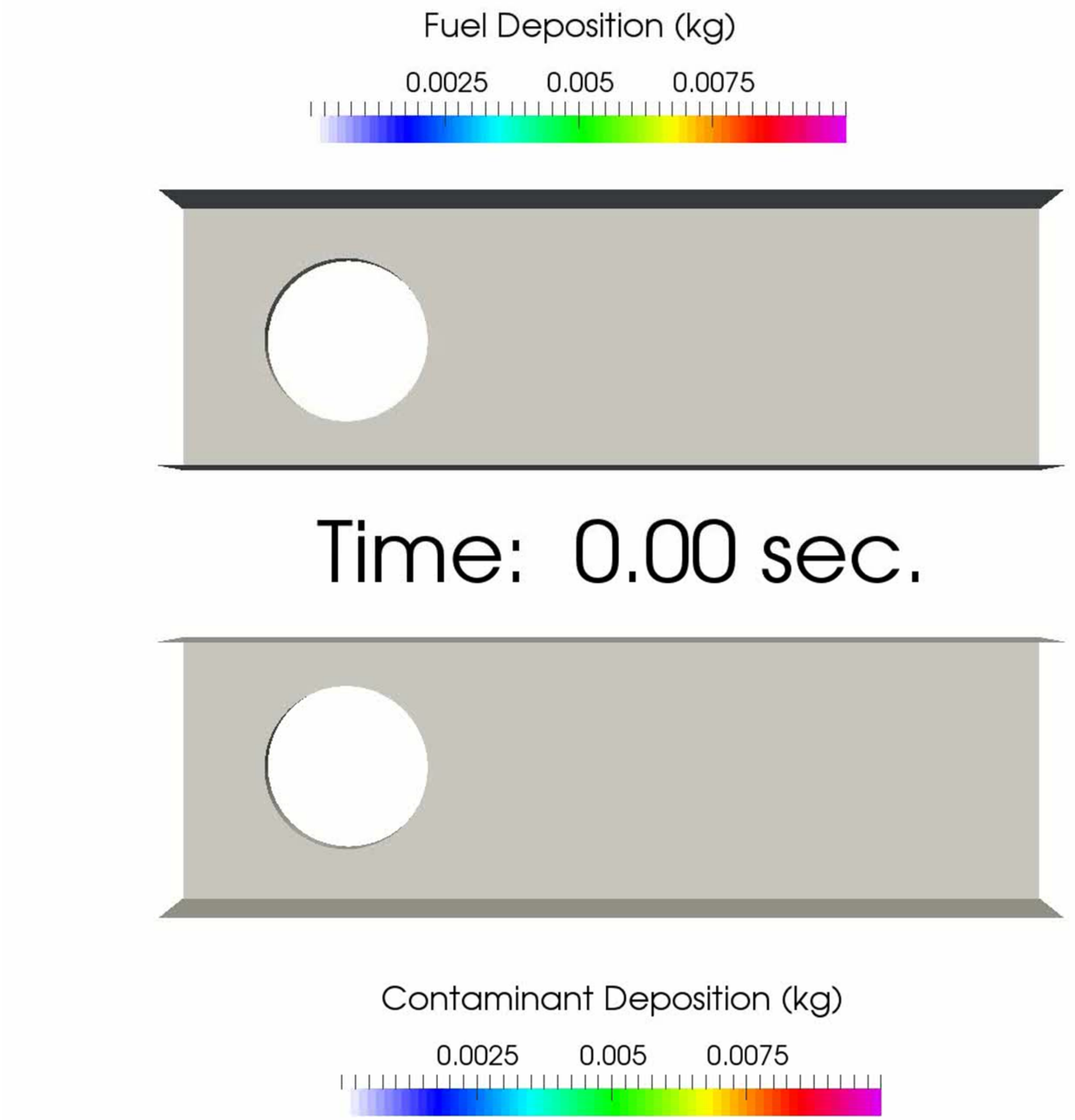
- Experiment distributed UO_2 in a stainless steel fuel pan, added one gallon of gasoline, and performed the test in a wind tunnel
- Air drawn in at 1 m/s for the duration of the fire
- Filters downstream collected entrained contaminants
- Filters replaced at 9 minutes and air flow continued for 4.8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





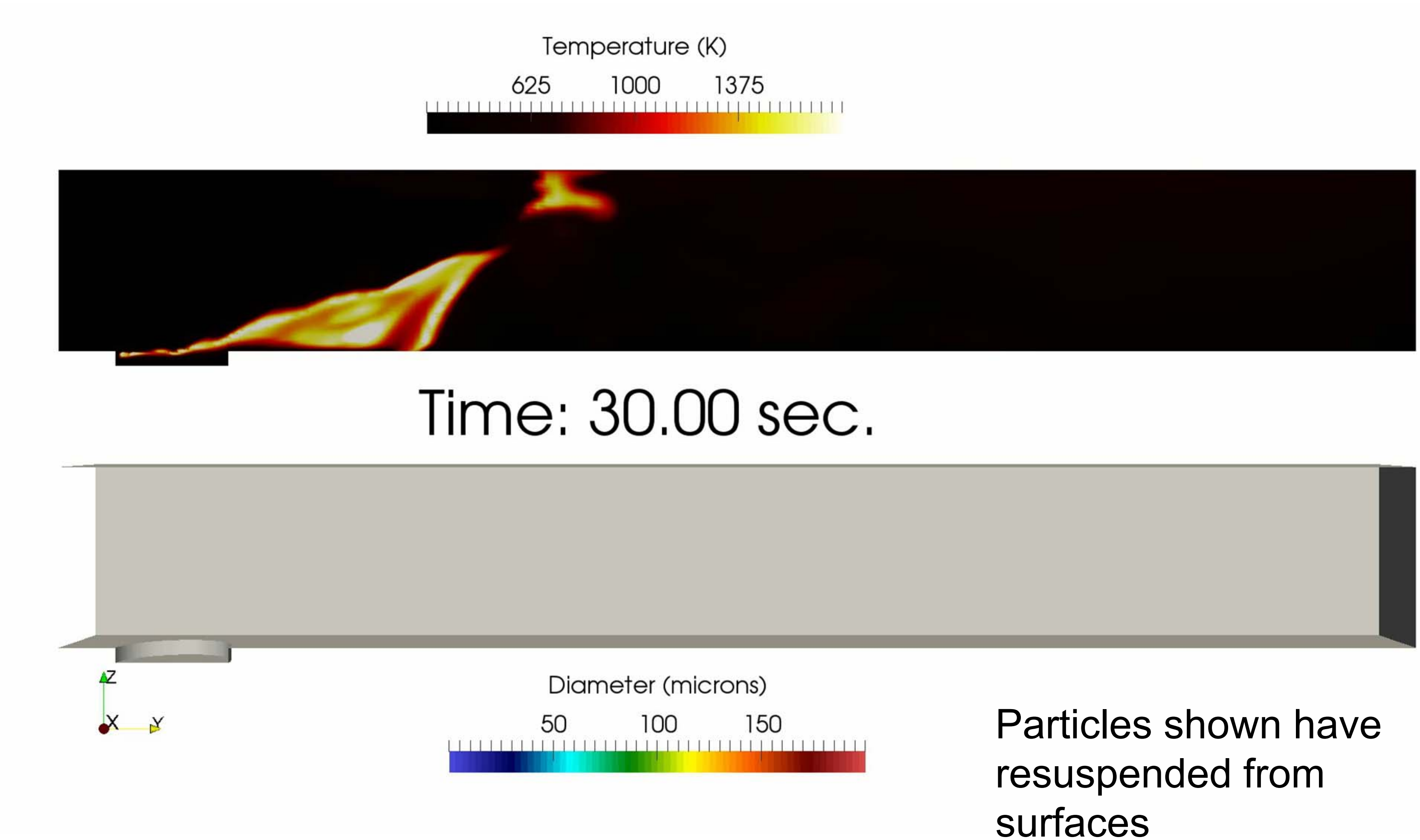
Particles with a higher fuel mass fraction (blue) stay low in the fuel pan, either falling to the pool surface or evaporating until the particle lofts into the flow as mostly contaminant (red)

Simulation Visualization: Boiling Entrainment Multi-component Evaporation(1B)



The fuel deposits closer to the pool, while the lighter contaminant particles carry further downstream

Simulation Visualization: Resuspension Entrainment (1R)



Particles shown have resuspended from surfaces

Powder Release Exp (Sutter 1981)

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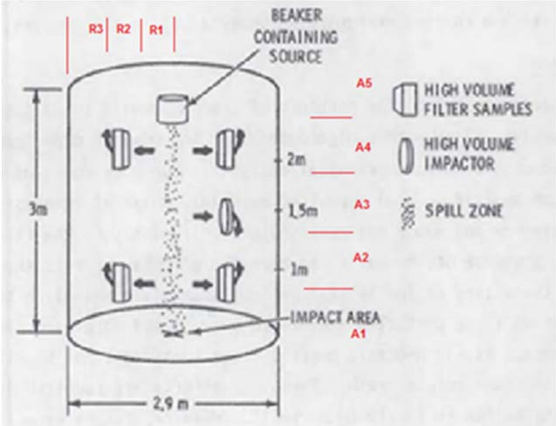
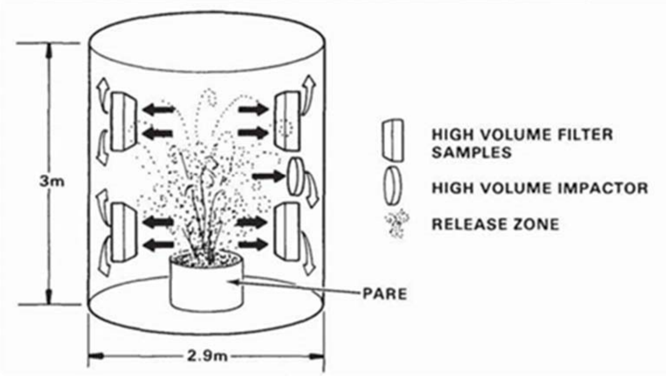
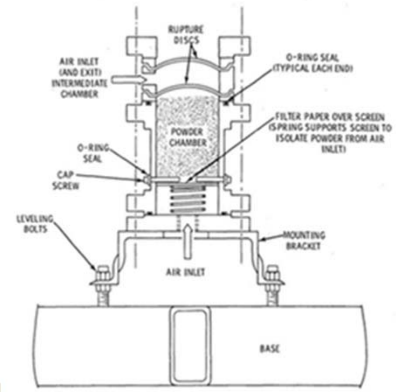
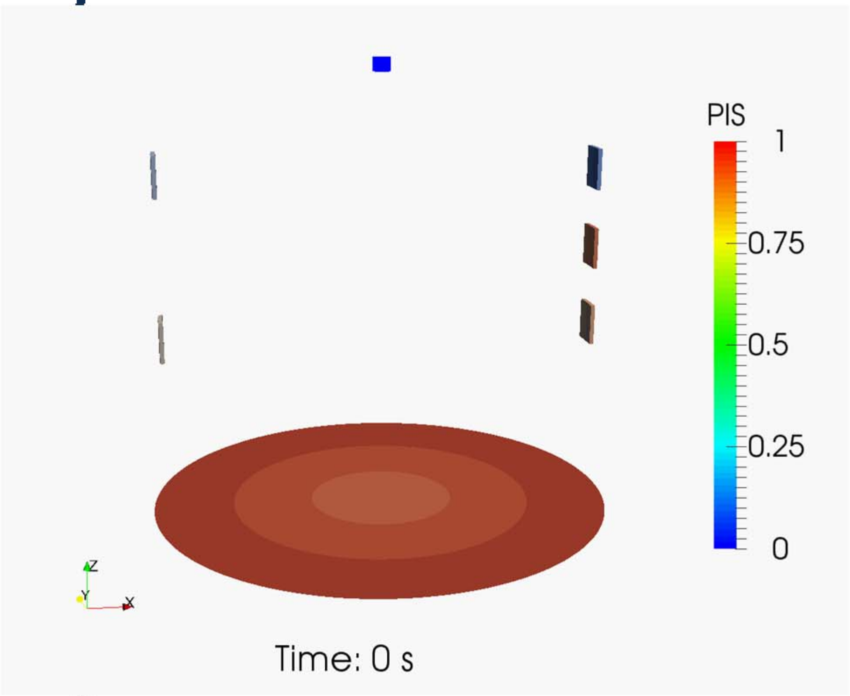
- Cylindrical chamber: 3 m tall by 2.9 m in diameter.
- Four filters and 1 impactor collected the particles and recorded the concentrations.
    - Active for 30 minutes
- Powder was released vertically from the beaker, i.e., gravity spill.
- Initial pressure = 1 atm at T = 300 K
- 100,000 particles modeled for both spill and pressurized release cases
- TiO_2 particles with 1.7 µm, using a distribution as described from experiment
- Only 50 psig pressurized release can be modeled using Fuego.

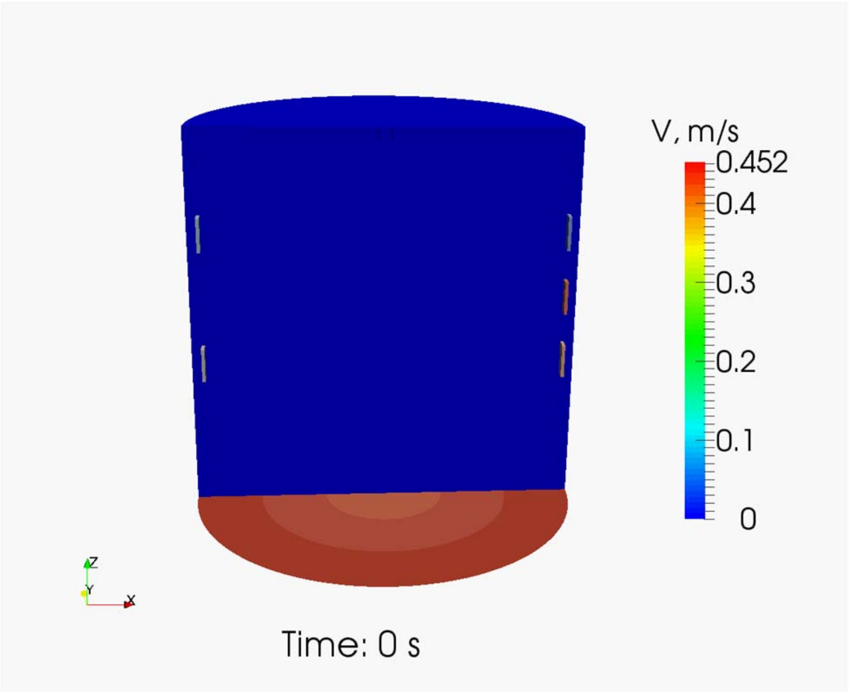


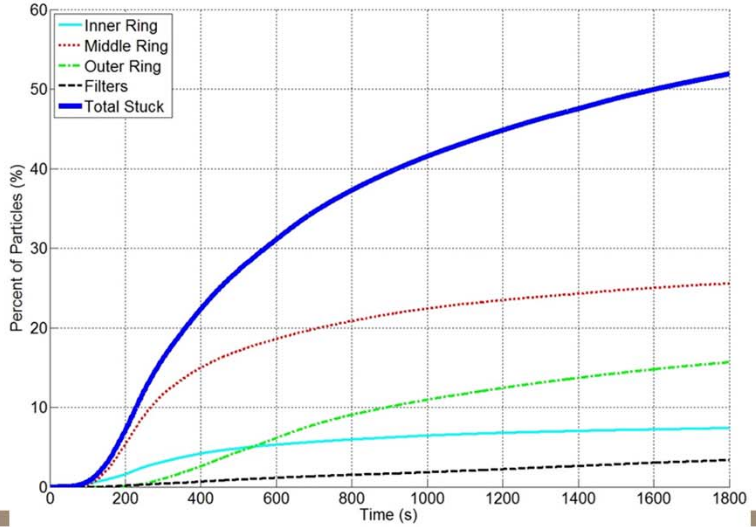




Spill Simulation



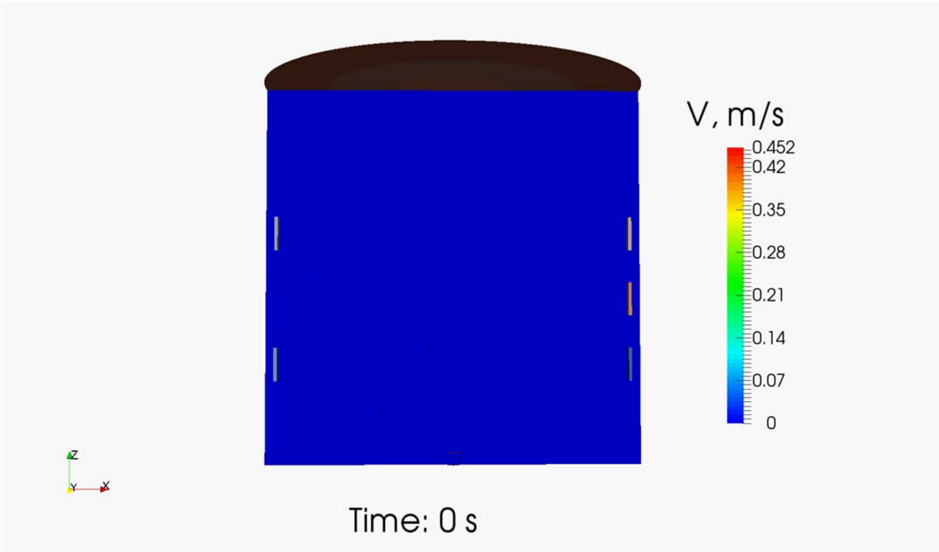


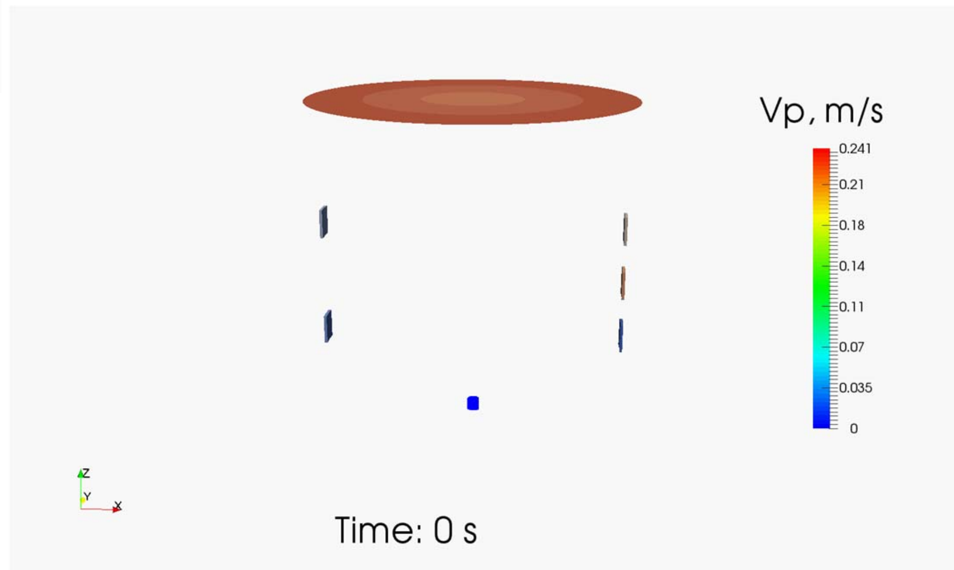


Particle “clusters” comprised of the larger particles first reached the bottom of the chamber at around 50 s.

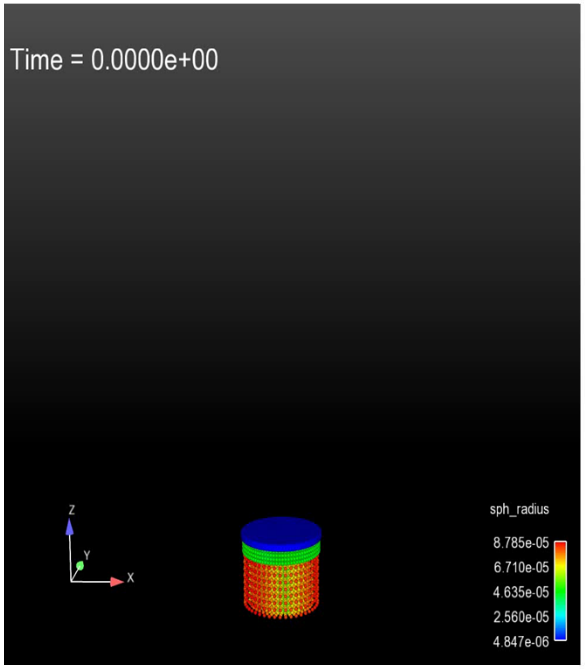
The lighter particles first reached the floor at 200 s and continued settling on the floor for the duration of the transient.

Pressurized Release Simulation (50 psig)





250 psig Adagio/Fuego Simulation

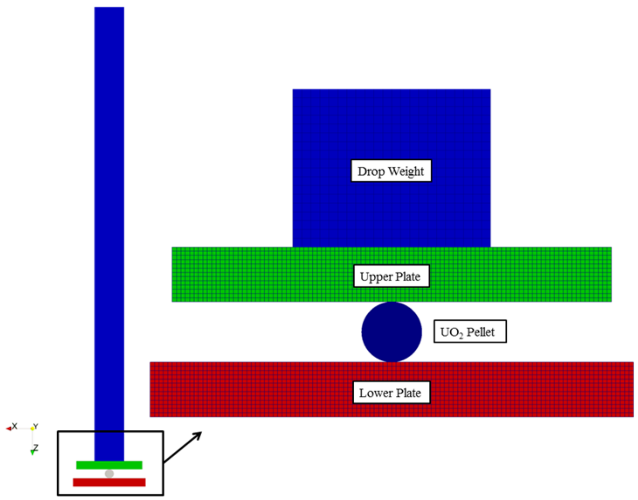


- Multi-SPH models used for Adagio to create sufficient particle flows
- One way couple method use: Adagio results translate into Fuego inputs
- This capability is demonstrated so that particles lose kinetic energy to induce fluid flow

NSRD-15 Progress

- Task 1: Implement microscopic fragmentation model into SIERRA/SM
  - A new material model has been created (John Bignell, Remi Dingreville, Chris O'Brien and Pierre-Alexandre Juan)
- Task 2: Update and revise Chapter 6 "Inadvertent Nuclear Criticality"
  - This work supports a master student for a master thesis (University of New Mexico) – Dr. Robert Busch, Corey Skinner
- Task 3: Simulate a 55-gallon drum fire release (Alex Brown, John Bignell and Ethan Zepper)
  - Using Sandia's FLAME experiment on POC
  - This experiment provides initial information for the simulation to drum failure

Modeling Fragmentation of Ceramic Fuel Material (Task 1)



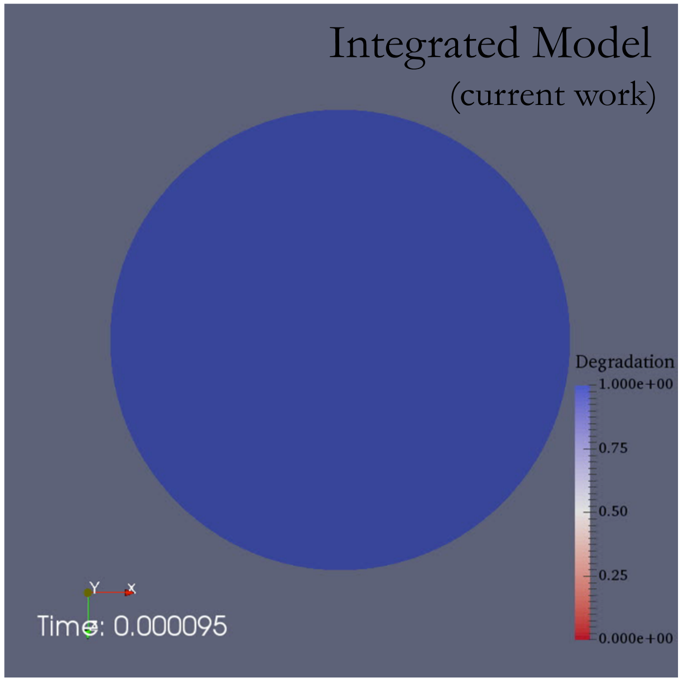
- Primary interest is in the generation of fragments small enough to become airborne
- Sierra finite element model (FEM) system includes ceramic pellet, support plates, and drop-weight.

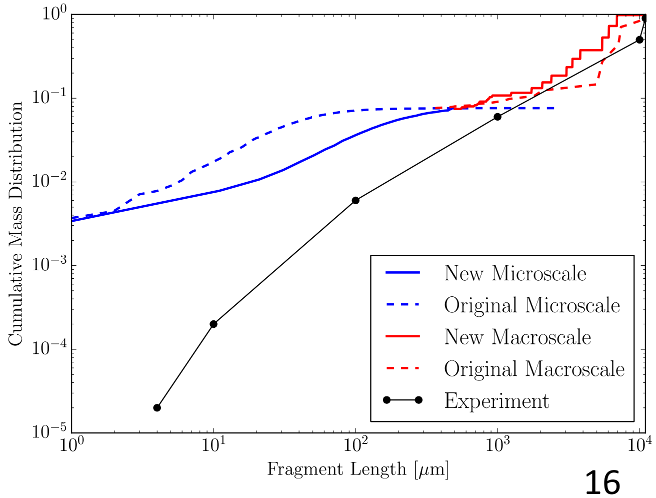
- Macroscale fragments (≥200 μm) are calculated using gradient damage model
- Microfragmentation calculated using a 1D fragmentation model for each fully damaged element
- Resulting particle size distribution based on both the macro and microscale fragments

Current Status & Comparison

- **Current Status:**
  - Separate 1D fragmentation model integrated into Sierra as part of a new material model
  - Methodology for output of fragmentation data developed
  - Advanced two-way coupled model under development

- **Comparison to Sequential Model (Prior year)**
  - Total mass of fragmented material agrees with prior model within 0.19%
  - Macroscale fragmentation pattern compares favorably
  - Small differences necessary to enable the integration of the 1D model directly in Sierra result in the differences observed in the microscale (those determined by the 1D model) fragment distribution





Advanced Integrated Fragmentation Model

- **Current Integrated Model Limitations:**
  - One-way coupled. Micro-scale fragmentation does not affect macro-scale response.
  - 1D model boundary conditions based on single strain rate obtained from macro-scale model at one point in time. No evolution of 1D model boundary conditions with time.
  - Micro-fragmentation only calculated for fully damaged elements.

- **Advanced Model Improvements**
  - Two-way coupled (energy based): Macro-scale model provides displacement (strain rate) boundary conditions to micro-scale model, which in turn provides damage (energy dissipation and reduction in stiffness) information to the macro-scale model.
  - Continuously updated boundary and state conditions at both length scales.
  - Incorporate microstructure effects via a micromorphic model

Task 2 Progress from UNM

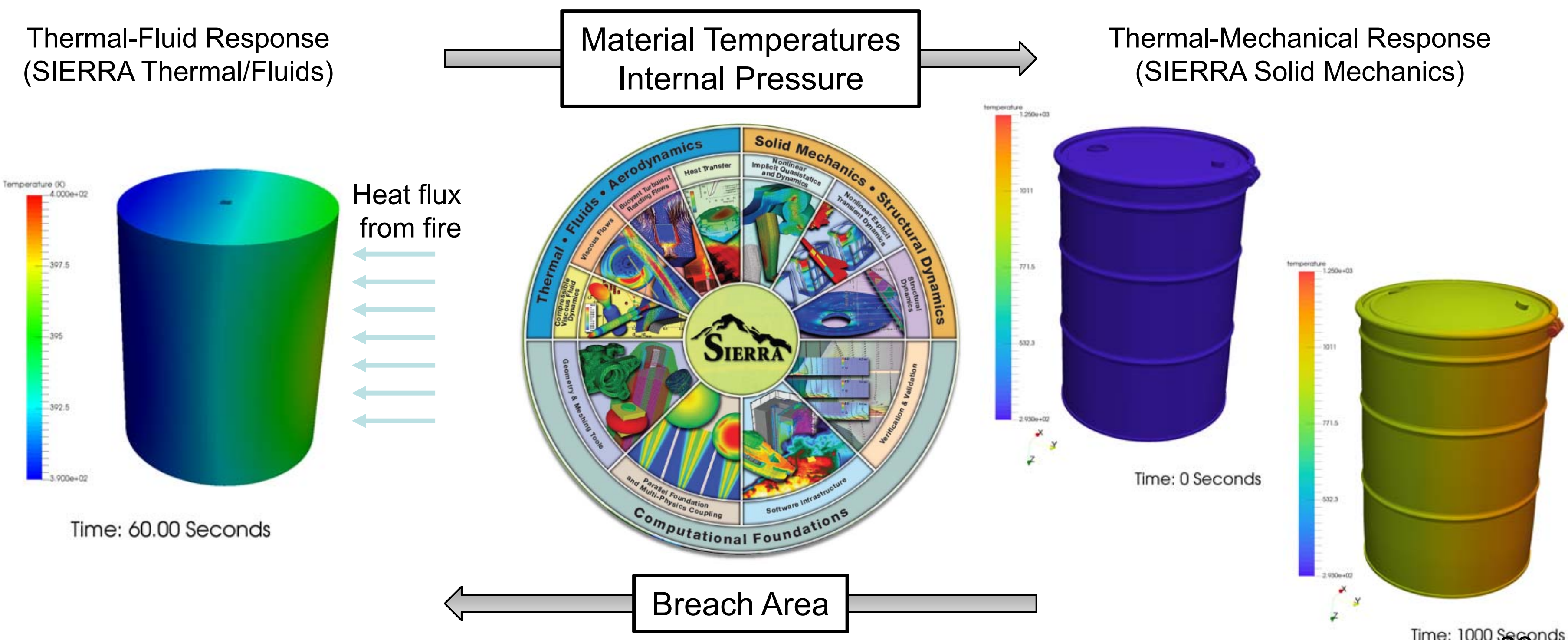
- Literature review of recent data for criticality accidents and fission yields thereof
  - Short report with found information: Complete
  - Updated pertinent information in Chapter 6: Complete
- Revision of structure of Chapter 6
  - Characterizing systems as open or closed, general rewording: Partially Complete
- Code simulations of criticality accidents:
  - Source term and depletion calculations using TRITON and ORIGEN-S: In Progress
  - Solutions criticality modeling and feedback in representative systems: In Progress
- Release fraction determination; information to be gleaned from solutions and metal accidents
  - Revise assumptions about radioactive release: In Progress

Task 2: Literature Review and Proposed Changes/Updates

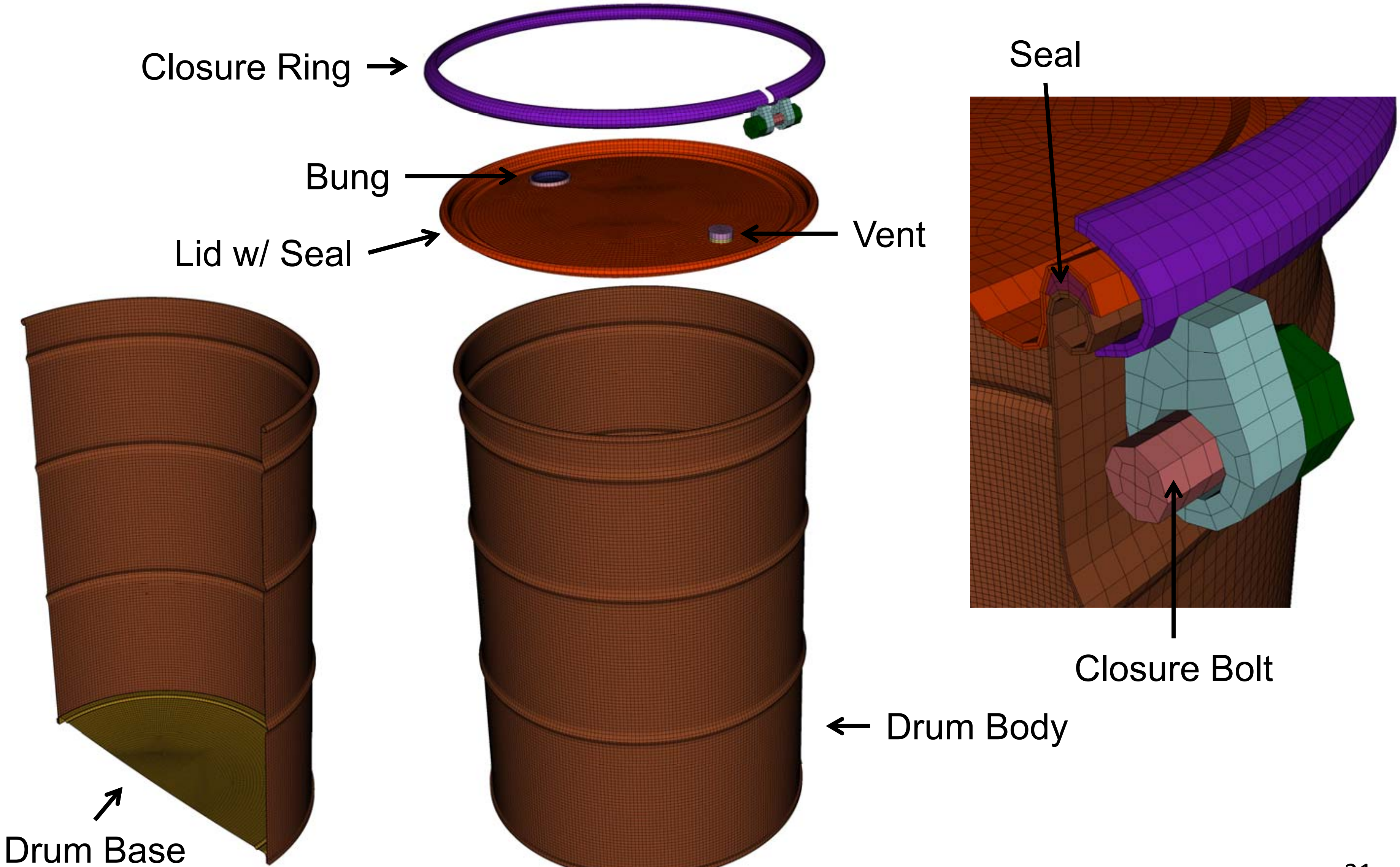
- Tables and data in Chapter 6 have been updated for consistency as presented in LA-13638 “A Review of Criticality Accidents”, 2000 Revision
  - This includes updates to Tables 6-1, 6-2, 6-3, and 6-4
    - Fission yields
    - Critical geometry
    - Accident cause/damage/contamination and date of occurrence
  - Additional tables:
    - Summary of accidents by duration
    - Acceptable fission yield correlations: solutions & metals
- Primary differentiation between known accidents:
  - Metal vs. Solution
  - Open vs. Closed
    - Open → larger effective release
    - Closed → longer duration of criticality (in solution systems)

Task 3: Drum Fire Failure Simulation

- Estimate airborne release fraction (ARF) and respirable fraction (RF) using SIERRA analysis tools for a type 7A waste drum exposed to a fire accident scenario.



Thermal-Mechanical Model Components

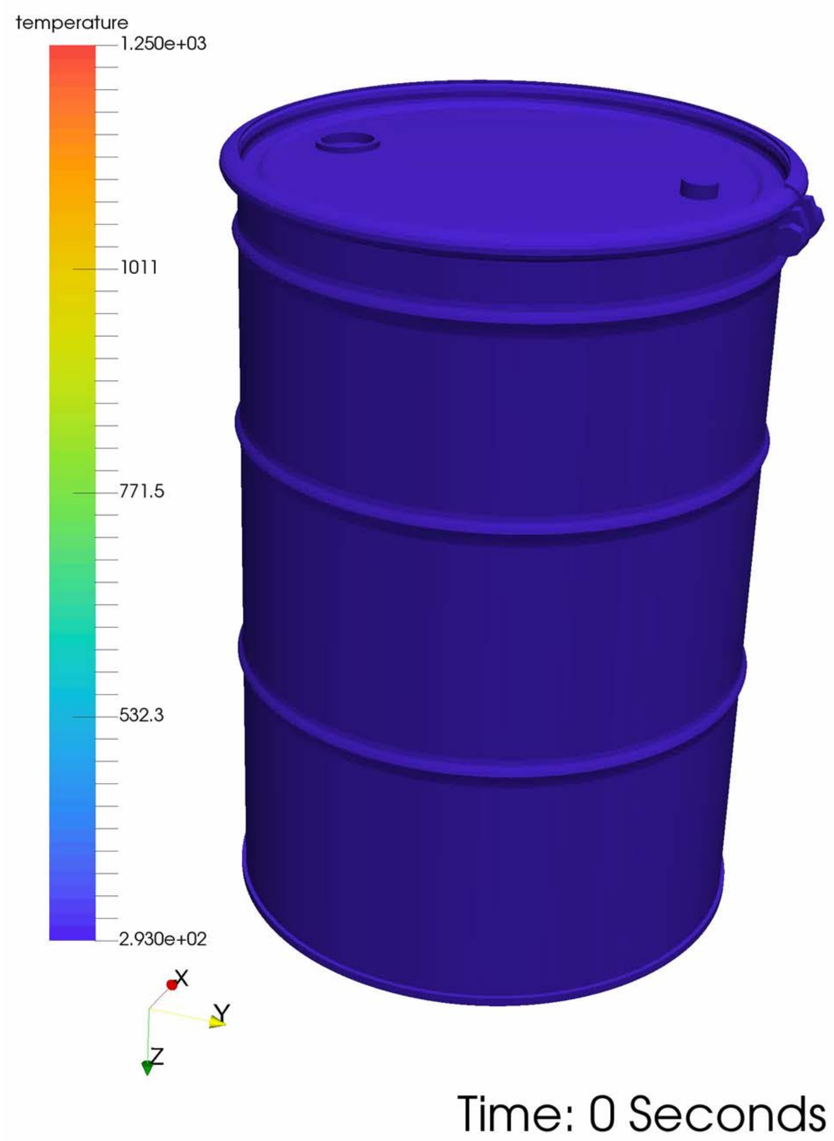


Thermal-Mechanical Simulation

- Path-Finder Simulation
  - Coupled Aria-Presto Analysis (Arpeggio)

- Aria used to calculated material temperatures and internal volume pressure.
  - Heat flux BC representing fire applied to drum outer surface.
  - Radiation and convection BCs applied to internal and external surfaces of drum.
  - Internal volume (filled with air) represented as bulk fluid node (without venting). Ideal gas law used to calculated change in pressure with change in temperature and volume.

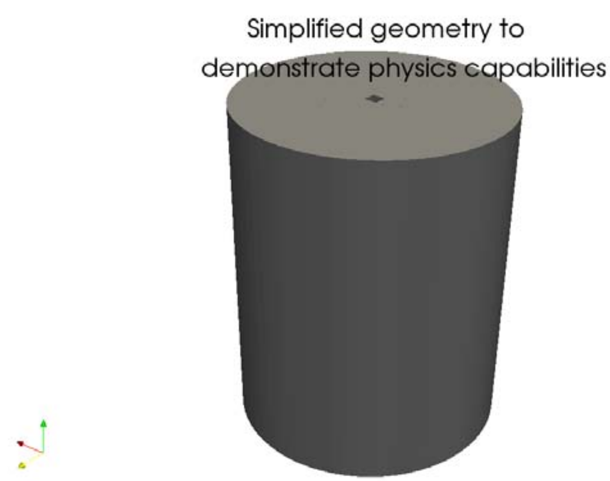
- Presto used to calculate thermal-mechanical response.
  - Temperature dependent material properties (including stiffness, yield strength, hardening, and failure) defined for all materials.
  - Material thermal expansion/contraction parameters also defined for all materials.
  - Tightening of closure ring simulated during first 100 seconds of simulation.



Preliminary Thermal-Fluids Simulation (Task 3)

- Standing up capabilities with simplified model
  - Coupled Fluid-Mechanics (Fuego)/Heat-Transfer (Fuego) using Sierra coupling capabilities
  - Eventually coupling to Aria/Presto/Fuego for the final simulation
- One Sierra Fluid-Mechanics region used to calculated thermal conduction and material temperatures.
  - Fire modeled as a heat flux BC on drum external surface.
  - Modeled radiation and convection thermal transport on the internal and external surfaces of drum.
  - Material modeled as homogeneous steel
- Separate Sierra Fluid-Mechanics region used to calculate thermal-fluid response.
  - Internal fluid region used to predict pressure and temperature.
  - Heating of drum leads to an internal pressure increase due to the ideal gas law principles and material decomposition.
  - Trash and contaminant represented by Lagrangian reacting particles

Simulation demonstrates particle distribution and entrainment capabilities for a simplified drum geometry. Particles release after reaching a decomposition threshold.



Summary and Recommendations

- NSRD-11 accomplishment is provided
- NSRD-15 progress has been provided
  - Fragmentation model in SIERRA/SM will allow two-way coupled (feedback) and morphoric modeling
  - Revision of Chapter 6 of 3010 is in progress with up-to-date information
  - Drum fire failure extracted from existing POC experiments conducted in Sandia's FLAME facility is in progress
    - Eventual couple of Aria, Presto (SIERRA/SM) and Fuego will be demonstrated to fail the drum to estimate ARF/RF based on the drum opening
- Proposed next year works include:
  - Adding temperature and porosity in the morphoric model of Task 1 , including updating Equation 4-1
  - Develop damage ratios of container breach due to free-fall spill and impact, and puncture stresses

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Fragmentation Model Improvements

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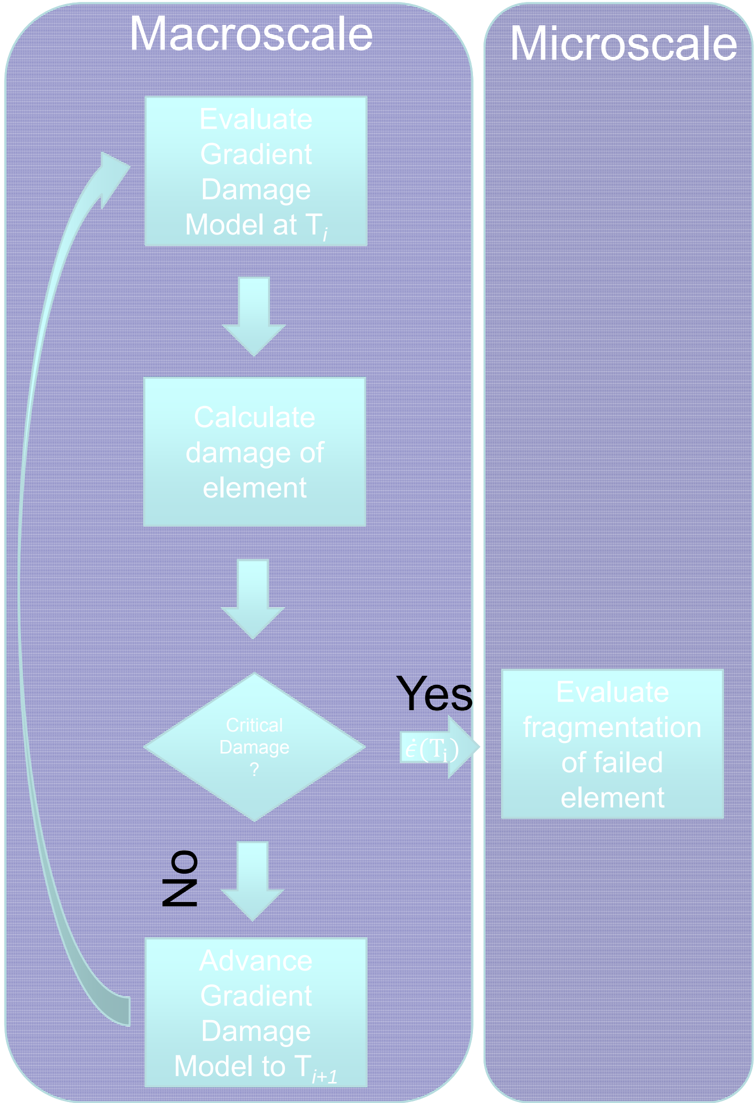
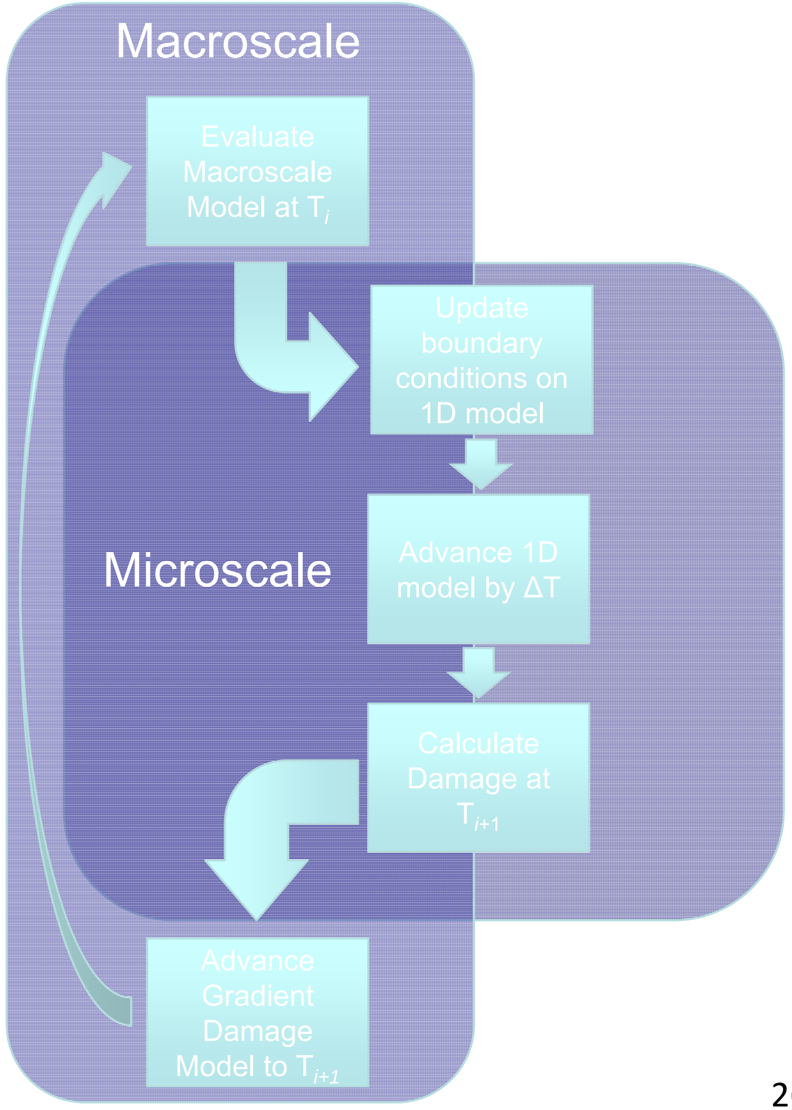
Present Integrated Two-scale Model



Advanced Integrated Two-way Coupled Model



Remaining objectives

- Refine Thermal-Fluids region to the higher-fidelity drum model from Thermal-mechanical simulation
- Model seal degradation vent paths
- Include a model for drum paint decomposition
- Refine trash decomposition and entrainment models
  - Representing cellulosic and plastic trash, along with contaminant
  - Decomposition gases will contribute to drum pressurization
- Tighter coupling between Thermal-Mechanical and Thermal-Fluids

Decomposing seal