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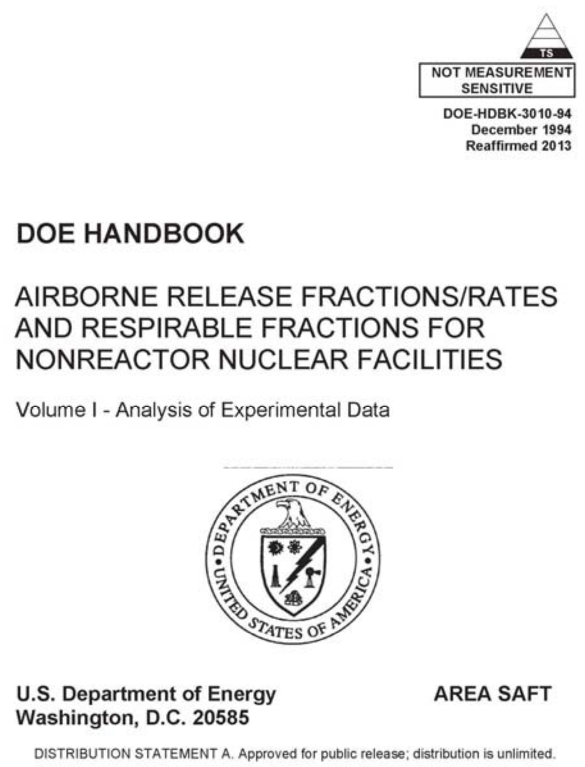
NOT MEASUREMENT SENSITIVE

DOE-HDBK-3010-94
December 1994
Reaffirmed 2013

DOE HANDBOOK

AIRBORNE RELEASE FRACTIONS/RATES AND RESPIRABLE FRACTIONS FOR NONREACTOR NUCLEAR FACILITIES

Volume I - Analysis of Experimental Data

U.S. Department of Energy
Washington, D.C. 20585

AREA SAFT

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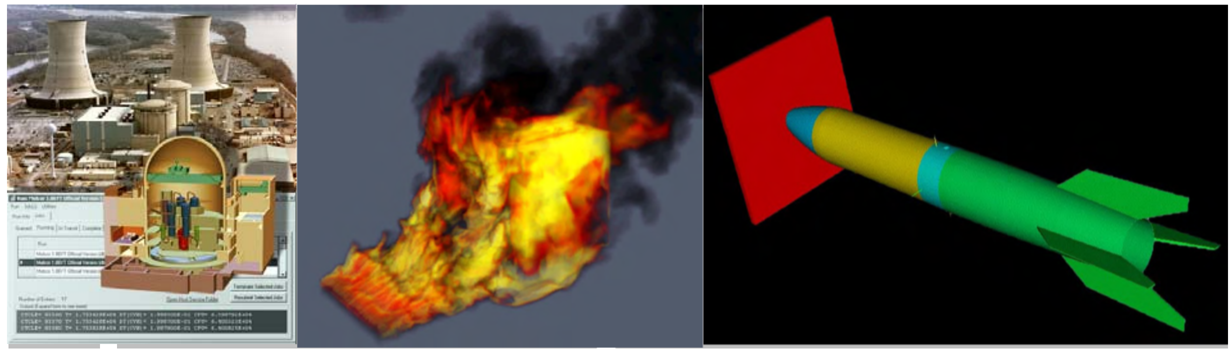

Computational Capability to Substantiate DOE-HDBK-3010 Data (NSRD-11) Status

Presented by David Louie,Ph.D.

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2016 NFS Meeting – NSR&D sub-group,
March 1, 2016

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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- Collaborators for this project include: Dr. Fred Gelbard, Dr. Alex Brown, Dr. John Bignell, Dr. Salvador Rodriguez, Dr. Flint Pierce, Dr. Tyler Voskuilen, and Mr. Victor Figueroa

Outline

- Motivation to substantiate DOE-HDBK-3010 data
- Our approach
  - Sandia high-fidelity codes
  - Substantiate the experimental data
- Year 1 accomplishment (NSRD-6)
  - Liquid fire simulations
  - Exploratory simulations
- Year 2 progress (NSRD-11)
- Year 3 proposed research

Why Substantiate the Handbook?

- Safety analysts at DOE complex rely heavily on the data provided in this Handbook to determine the source term (ST)
- Five Factor Formula
  - $\mathrm{ST} = \mathrm{MAR} \cdot \mathrm{DR} \cdot \mathrm{ARF} \cdot \mathrm{RF} \cdot \mathrm{LPF}$
    - MAR - material at risk, DR – damage ratio, ARF – airborne release fraction, RF – respirable fraction & LPF – leak path factor
- More often, analysts simply take the bounding values to perform ST calculations to avoid regulatory critique
- Derived data (i.e., ARF & RF) from Handbook:
  - Very limited table-top and bench/laboratory experiments
  - Engineering judgement which may not have adequate bases
  - Actual situation may not be represented

Technical Approach/Benefits

- To leverage the state of art 3-D integrated computer codes developed at Sandia – Sierra Code Suite to substantiate the data in the Handbook:
  - Demonstrate that our codes can substantiate table-top and laboratory experiments in the Handbook, and thus justify using codes for more accurate safety analysis
  - Provide physical insights into the events that leads to the airborne release
  - Provide data assessment for the realistic accident conditions
- The goal of this approach is to ensure the accuracy and technical defensibility of the airborne release safety analyses
  - Non-conservative data – underestimates ST – safety concern
  - Over-conservative data – overestimates ST – Substantial cost to DOE/NNSA

Sandia Sierra Code Suite

- Sierra code suite includes solid mechanics (i.e., SIERRA SM, PRESTO), structural dynamics, fluid mechanics (i.e., SIERRA FM, FUEGO) and a number of utilities that can be coupled for simulating multi-physics problems
- This code suite is compliant with DOE Order 414.1D (SAND2008-5517)
- The codes are installed on supercomputing clusters at Sandia, and readily available for use within Sandia
- There is no license fee associated with the usage
- Use and information release are subject to approval

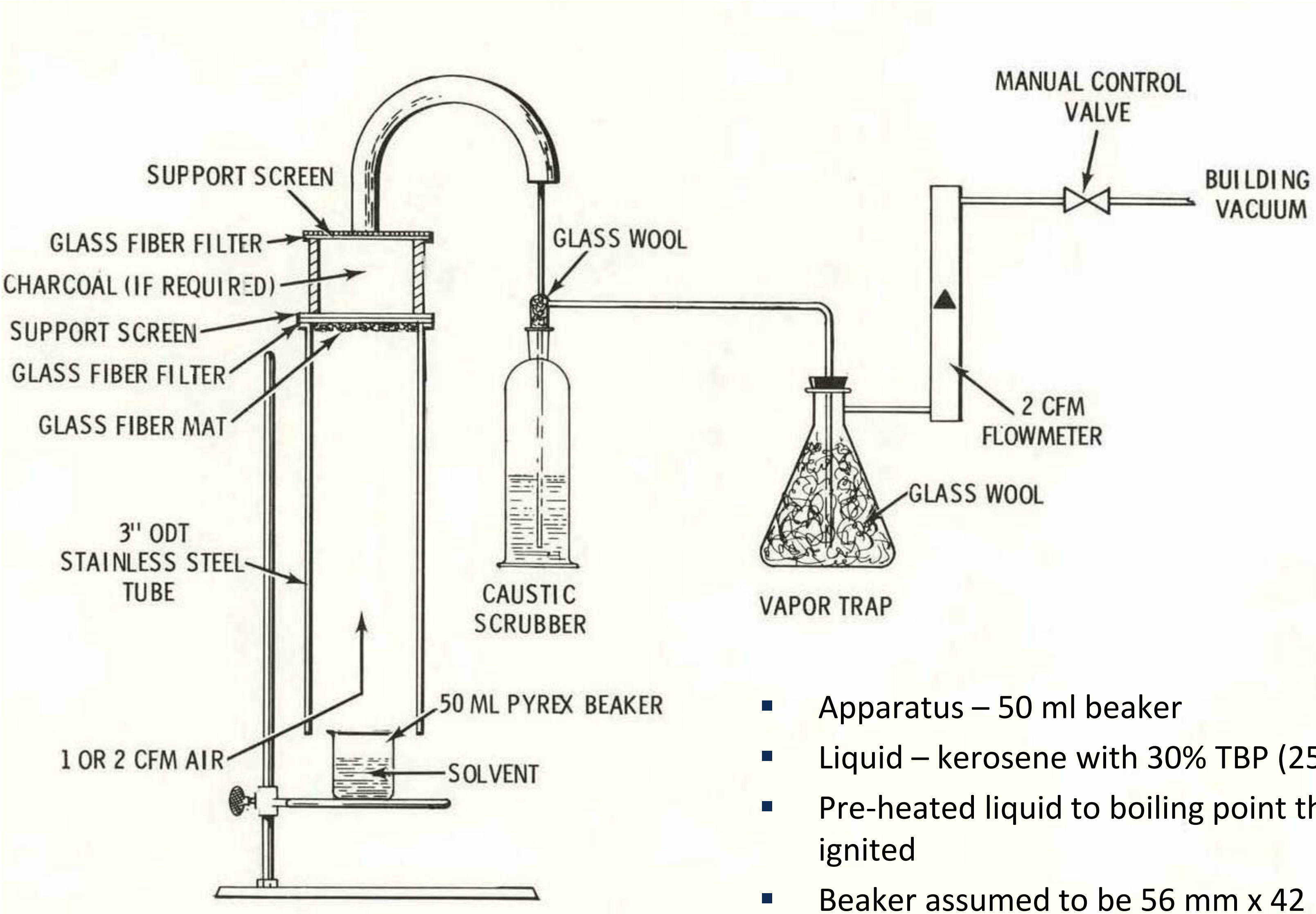
Year 1 Accomplishment

- Liquid fire experiment simulations
  - Beaker fire
  - Gasoline pool fire
  - Simulation results with experimental data
- Exploratory simulations
  - Impact on a powder can
  - Pressurized powder release
- Final report published (SAND2015-10495)
  - Recommendation for FUEGO improvement
    - Resuspension
    - Multi-component capability

Simulation of Liquid Fire using FUEGO in Year 1

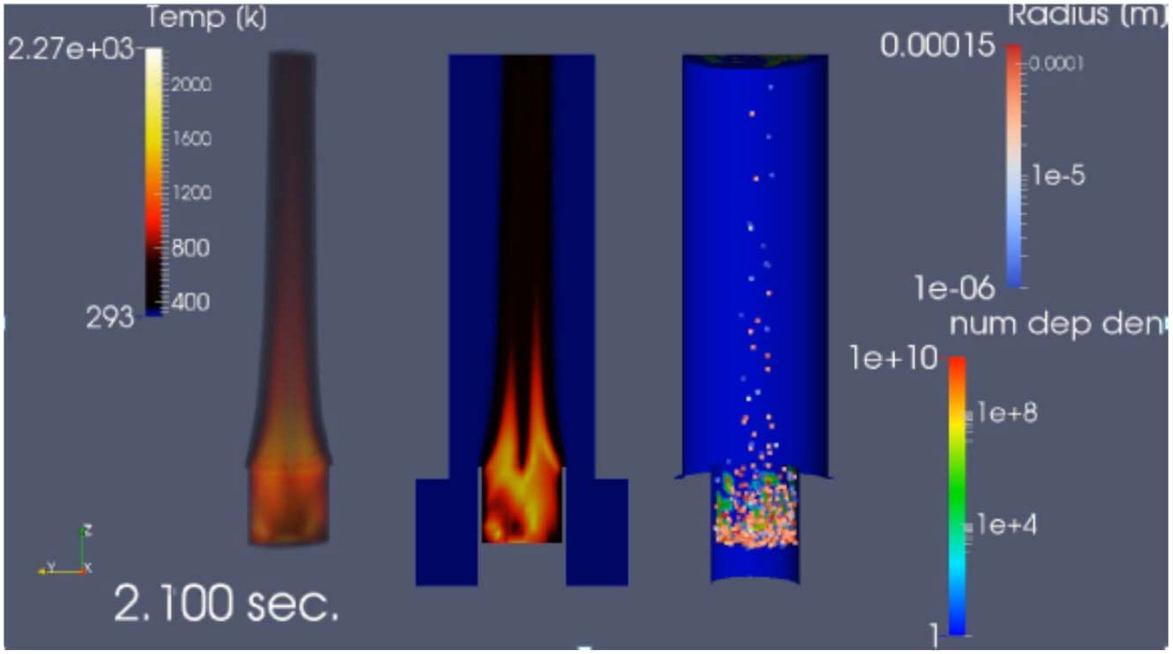
- Chapter 3 of Handbook discusses release related to liquids
- From other work, we have demonstrated that SIERRA code suite (PRESTO/FUEGO) can be used to simulate an explosion accident involving combustible liquids
  - Similarly, we believe we could simulate liquid nuclear excursion using the combination of Liquid explosion – chemical energy and by-product
  - Nuclear excursion – fission energy and fission product
- We currently simulate liquid fire experiments described in the Handbook (Section 3.3)
  - Beaker fire (BNWL-B-274)
  - Gasoline pool fire (BNWL-1732)

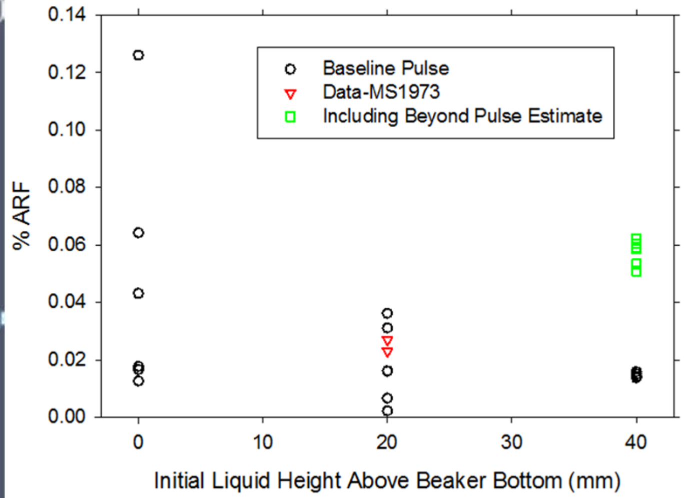
Beaker Fire (BNWL-B274)



- Apparatus – 50 ml beaker
- Liquid – kerosene with 30% TBP (25 ml)
- Pre-heated liquid to boiling point then ignited
- Beaker assumed to be 56 mm x 42 mm diameter

Beaker Fire FUEGO Simulation



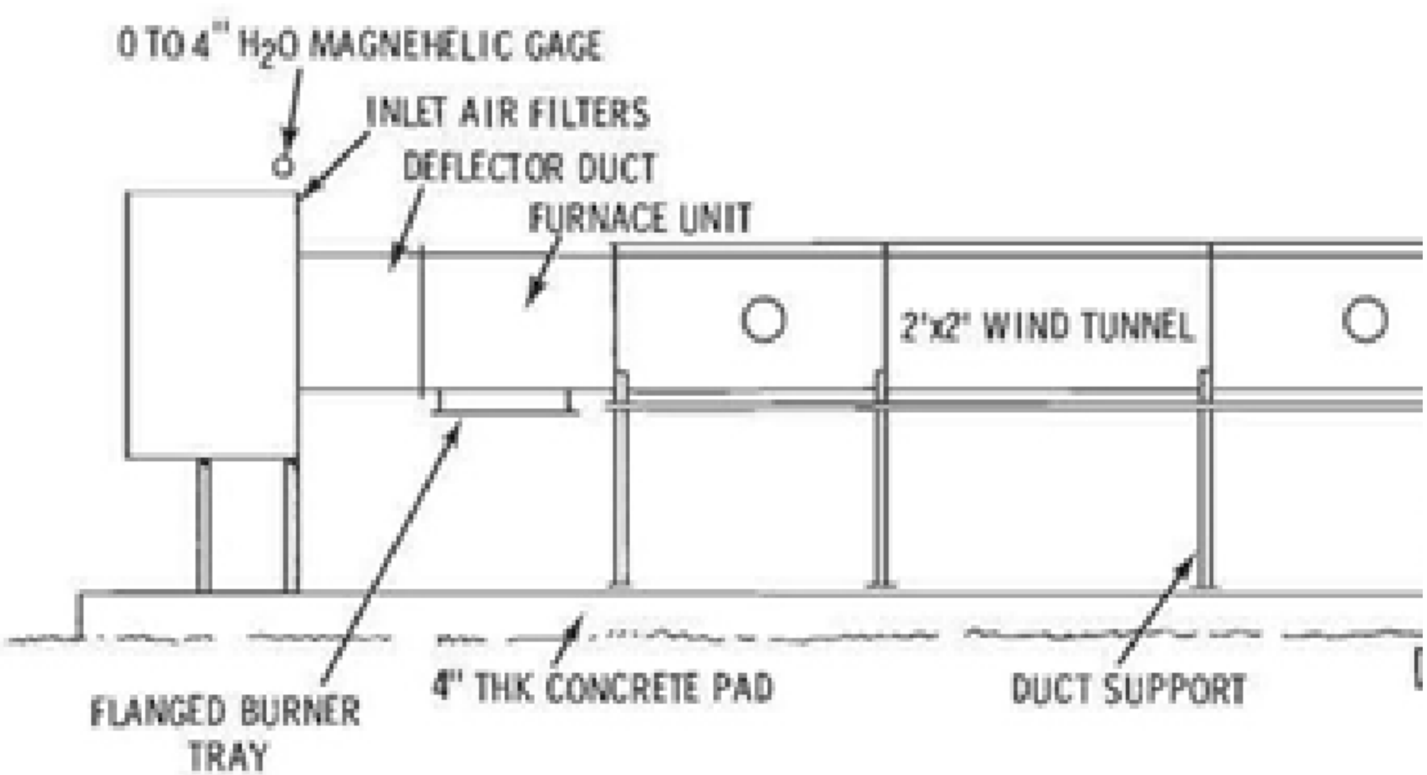


Findings:

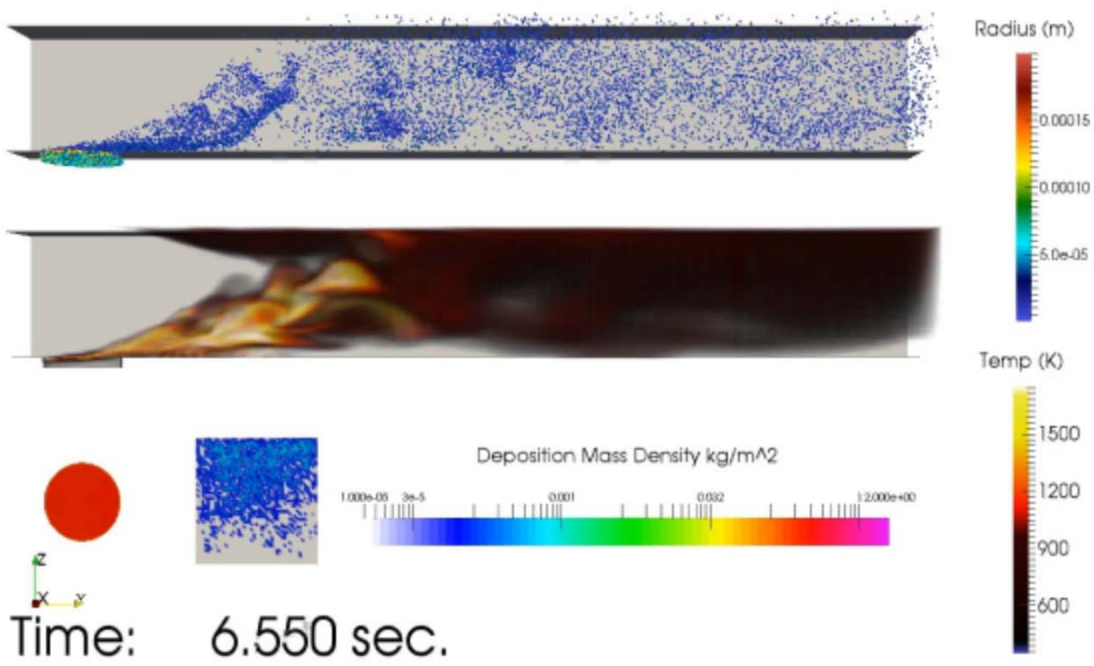
- Only a single initial liquid height was used in the experiment
- Simulation compared well with the data
- FUEGO did not have particle interaction model
- Code results can be improved with multi-component evaporation capability
    - Larger droplets tended to stay behind

Gasoline Pool Fire (BNWL-1732)

- 1 gallon gasoline onto pan surface
- UO_2 powder, 20-50 g poured before gasoline
- Pan size 15-inch diameter tray used

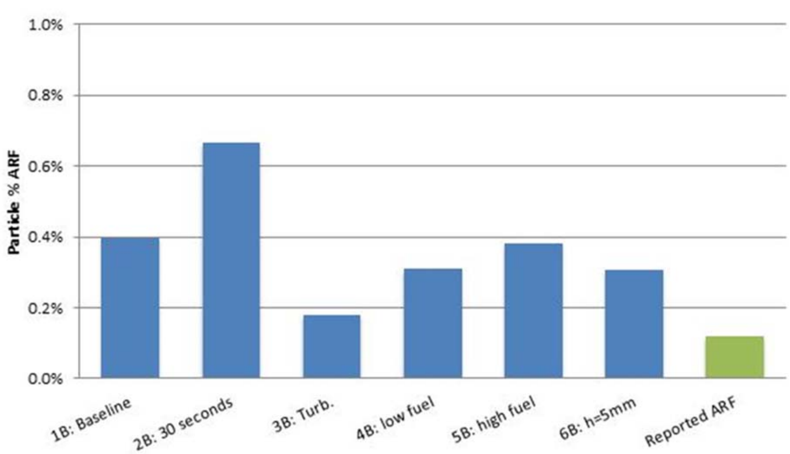


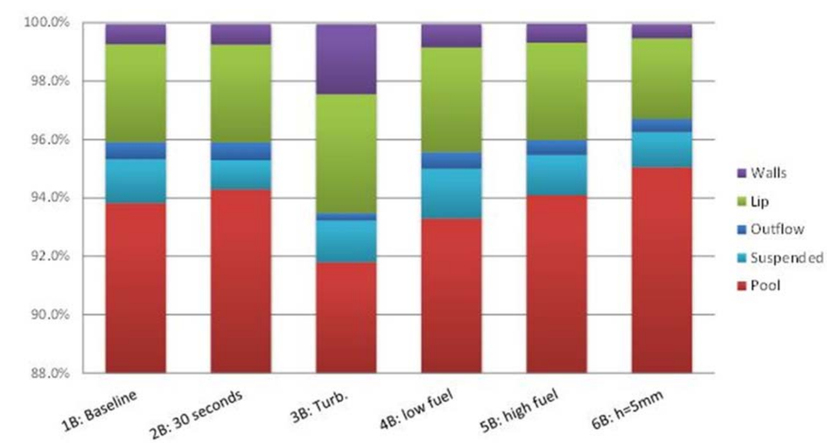
Simulation Visualization for Gasoline Pool Fire



Findings:

- Entrainment due to boiling dominates compared to the evaporation-induced in code results
- Resuspension model needs to accurately capture the residual entrainment after the fire was gone.
- FUEGO did not model particle interactions

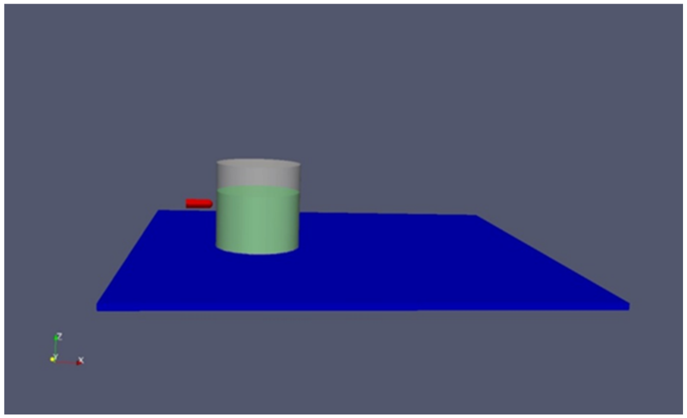


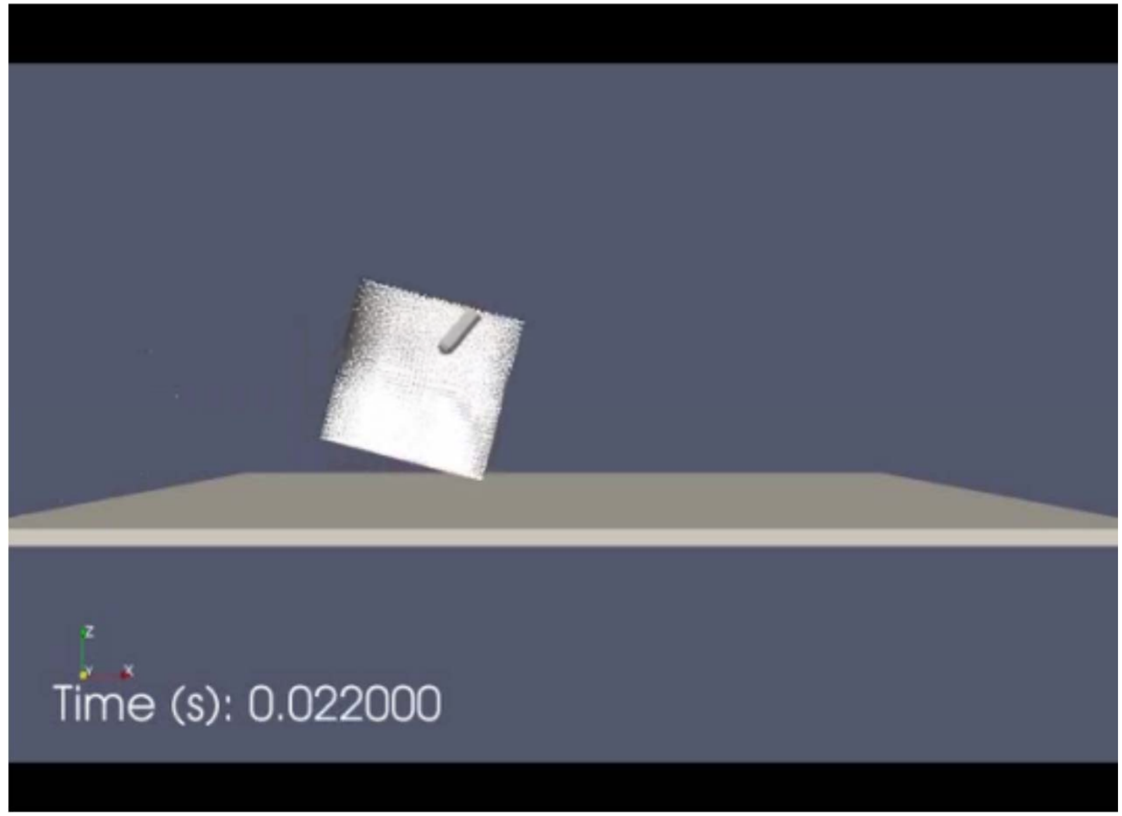


Exploratory Simulations in Year 1

- We focused on powder release in Chapter 4 of Handbook
- We selected two powder scenarios to simulate using PRESTO and FUEGO to address explosion-induced impact and pressurized dispersion
  - An object hitting a can filled with powder (Postulated) – PRESTO
  - A pressurized release of powder from a chamber into a containment volume (FUEGO)
    - Discussion on this simulation defers to Year 2

Projectile Impact Powder Can at 175 m/s





Simulation Results:

- PRESTO can be used to provide more realistic impact estimates compared to hand calculation using DOE/TIC-11268 “A Manual for the Prediction of Blast and Fragment Loading on Structures”.
- This is a demonstration, no experiment is available.

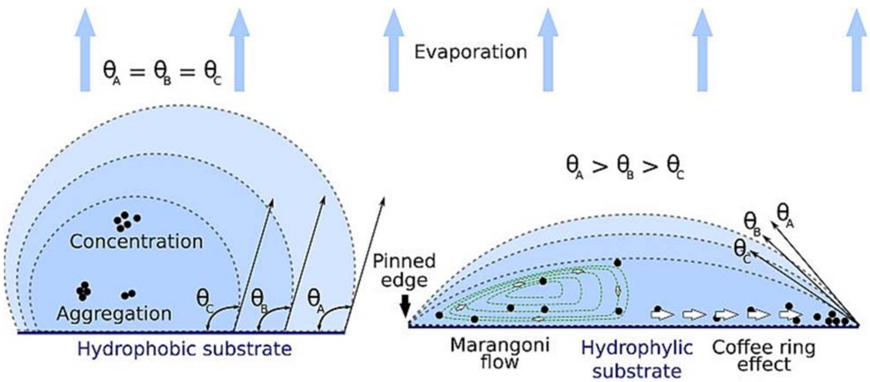
Year 2 - Progress

- Task 1 – FUEGO code improvement
  - Resuspension Model (discussed in Task 2)
  - Multi-component Model (applicable to Task 3)
- Task 2 – Validate resuspension model
  - In progress – 1967s experiment from the Handbook, and STORM experiment
- Task 3 – re-run of liquid fire simulations from Year 1
  - (not yet started)
- Task 4 – re-run the pressurized powder release simulations from Year 1
  - In progress – 50 psig case
  - Spill simulation for NSRD-10 project
- Task 5 – Fragmentation Analysis
  - In progress
- Task 6 – final report

Task 1A – Resuspension Model

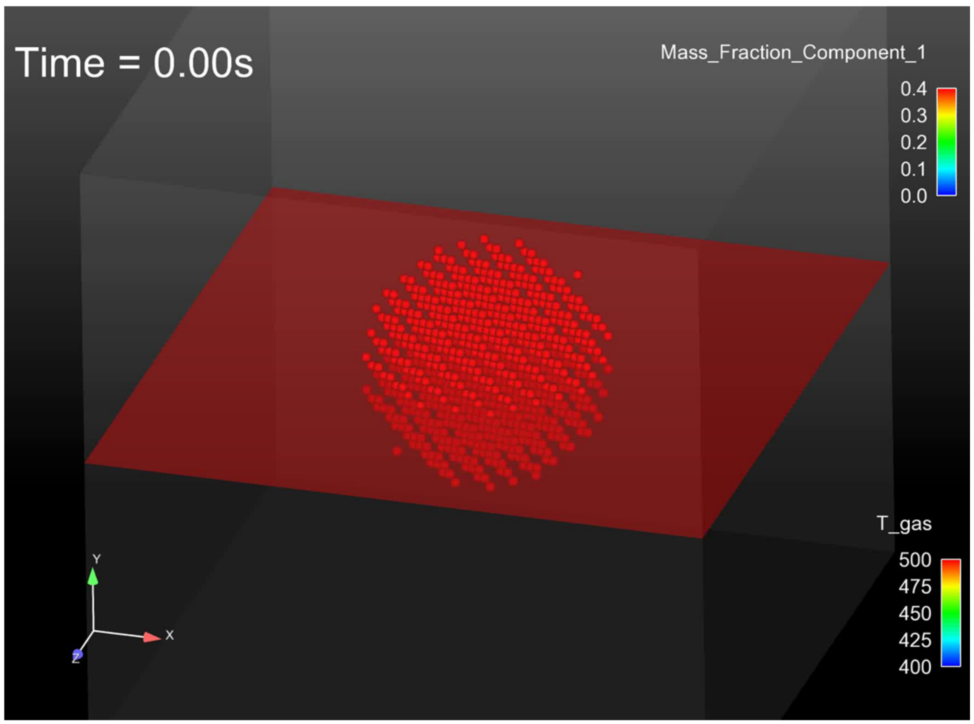
- An User function was implemented into FUEGO instead of an user subroutine
- Wichner resuspension Model is based on a similar model implemented into MELCOR (SAND2015-6119)
  - The model uses the balance forces of the lift and adhesive forces at the surface.
  - Resuspension is based on the particle size, fluid velocity, wall shear stress, surface roughness
  - This model may be good for high values of Reynolds number
  - For fires, where the fluid velocity may be low, the model has not been working successful – improvement is being developed
  - See Task 2 for test cases

Multicomponent Evaporation (Task 1B)



In FUEGO, implemented multicomponent evaporating particle model

- Particle can be composed of any number of constituent materials
  - distinct (and evolving) mass fractions
  - different physical properties
  - Inert components can be included



Simulation Example:

Spherical array of 683 evaporating liquid droplets with 2 distinct components (1, 2).

At start

- mass_fraction(1) = 0.4
- T_gas = 500 (volume and boundaries)

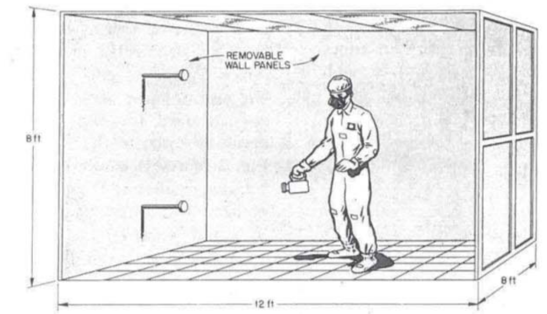
As droplets heat, A evaporates more quickly than B (distinct material properties)

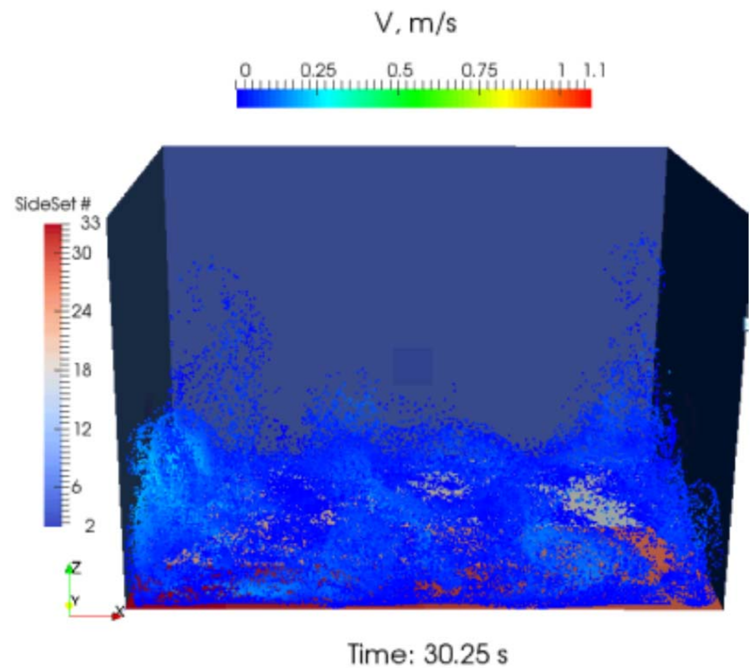
- mass_fraction(1) → 0
- mass_fraction(2) → 1

Due to evaporative cooling, T_gas near droplet array is lowered (thermal energy of gas is depleted to evaporate droplets)

Task 2 – 1967 Resuspension Exp.*

- Data used in Handbook p. 4-93 are poorly characterized
- One of the relatively better characterized experiments documented in “Redispersion of Settled Particulates,” B. R. Fish, R. L. Walker, G. W. Royster, and J. L. Thompson, 1967.
- Resuspension factor (surface concentration/atmosphere concentration, m^{-1})
  - Vigorous work-sweeping: 1.9×10^{-4} m^{-1}
  - Walking: 3.9×10^{-5} m^{-1}
  - Light work: 9.4×10^{-6} m^{-1}
  - Light sweeping: 7.1×10^{-4} m^{-1}
  - Pedestrian and equipment: 4.6×10^{-3} – 5×10^{-5}
- Preliminary FUEGO Simulation
  - Element size is sufficient to capture integral/Taylor eddies.
  - Each of 24 floor sidesets (boundaries) has time-dependent x-y-z velocity components (u, v, w velocities).
  - Floor sidesets mimic walking and sweeping motion.
  - Each sideset is activated and deactivated as man walks and sweeps through room.
  - 100,000 particles are tracked; All on floor at transient initiation.
  - Used particle “stick” option for ceiling and walls.
  - Floor has Wichner resuspension model

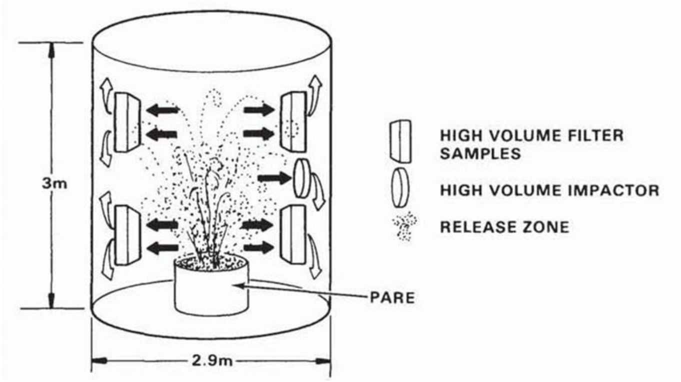


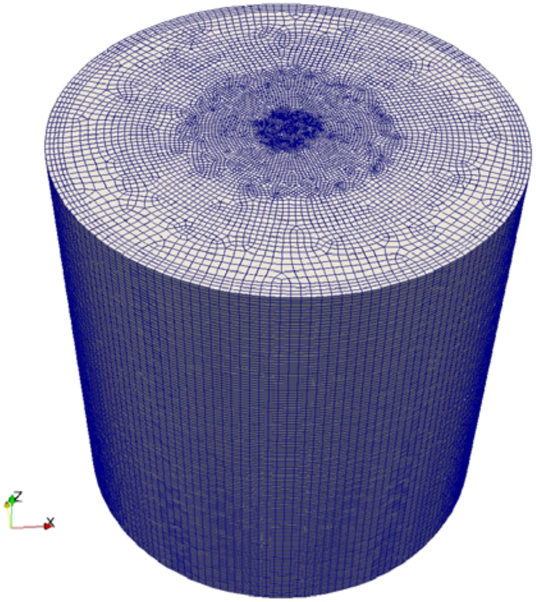


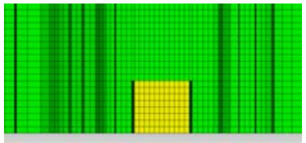
*B.R. Fish, et.al, “Redispersion of Settled Particulates,” in Surface Contamination, B.R. Fish (ed.), Pergaman Press, 1967

Task 4 - FUEGO Model

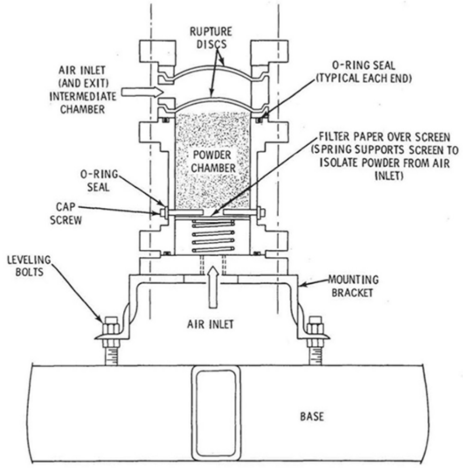
- Mesh metrics compliant with NRC, CFD journal recommendations.
- 1.03 million hexahedral elements with radial biasing near higher-velocity regions.
- Element size is sufficient to capture integral/Taylor eddies.
- Dynamic Smagorinsky LES turbulence.
- Each filter/impactor has its own time-dependent air flow boundary.
- 100,000 particles are tracked.
- Particle “stick” option for the filters and walls.
- Applications for
  - Spill case (PNL-3786)
  - Pressurized case (PNL-4566)
    - Model improved from Year 1
  - Results will also provide inputs for MELCOR model developed in NSRD-10







50 psig Pressurized Release - FUEGO (Task 4)

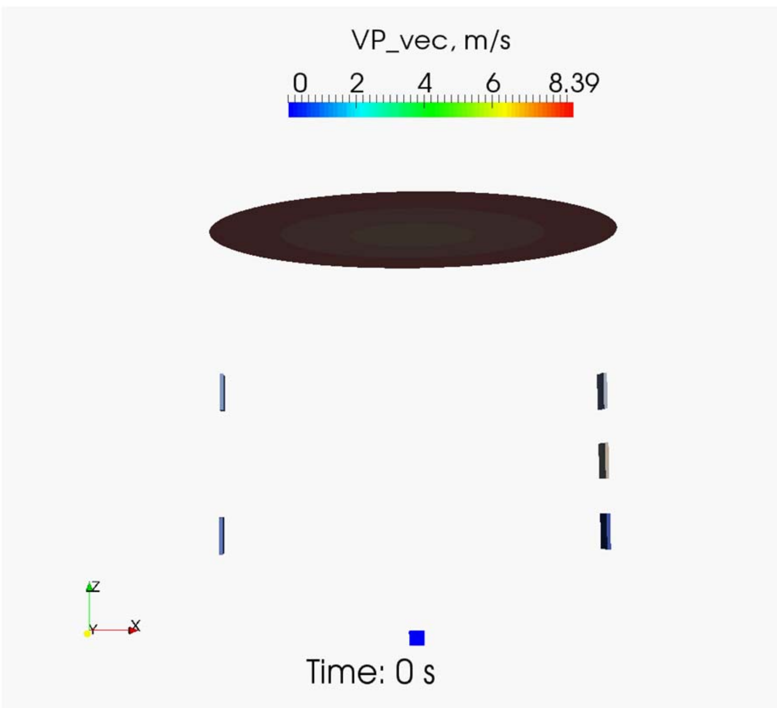


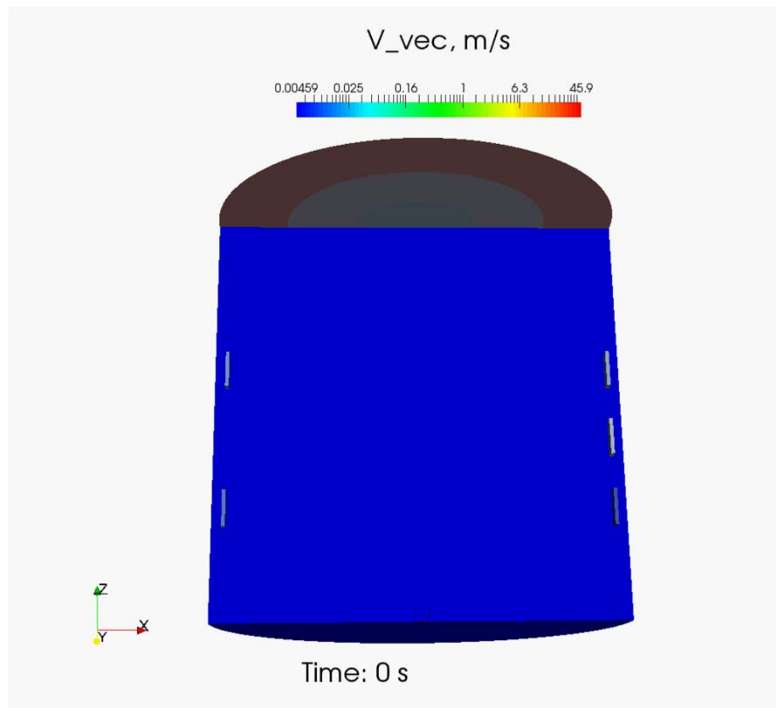
Simulation inputs:

- Rupture disk timing
  - 0 m/s @ 0.001 s
  - 643 m/s @ 0.0015 s
  - 643 m/s @ 0.015 s
  - 0 m/s @ 0.016 s

Preliminary Simulation Results

- Particle size of 1.7 μm
- Calculated fluid and particle velocity distributions (top and bottom figs., respectively).
- Ran for 100 s.
- Particles first hit top surface at 5 s.





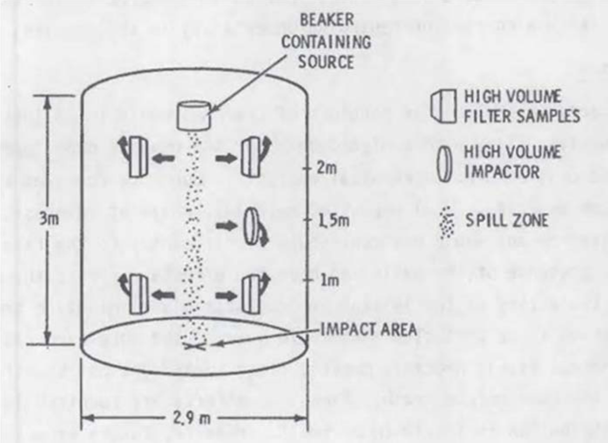
Spill Simulation – FUEGO (Task 4)

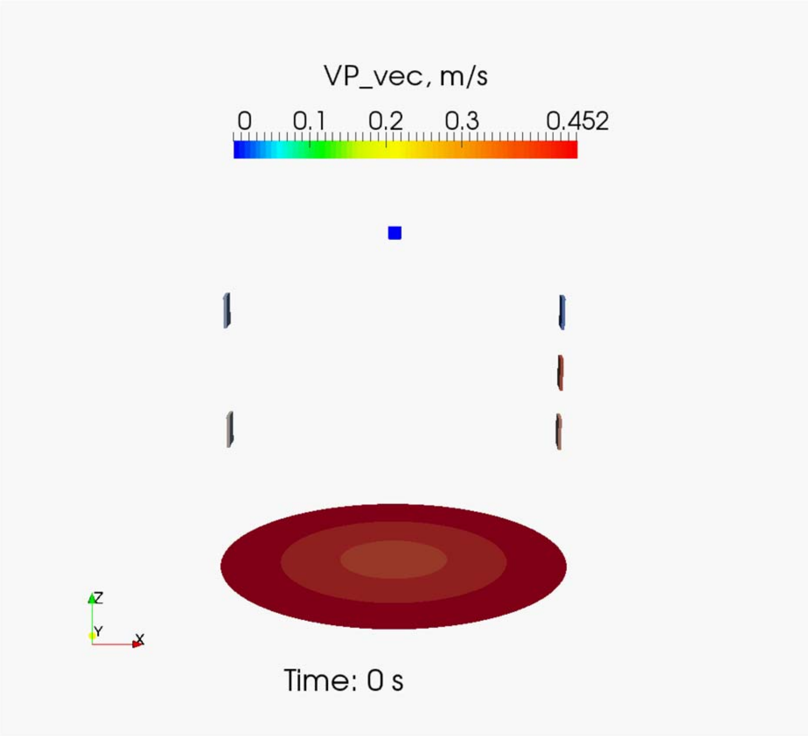
Preliminary Simulation Results:

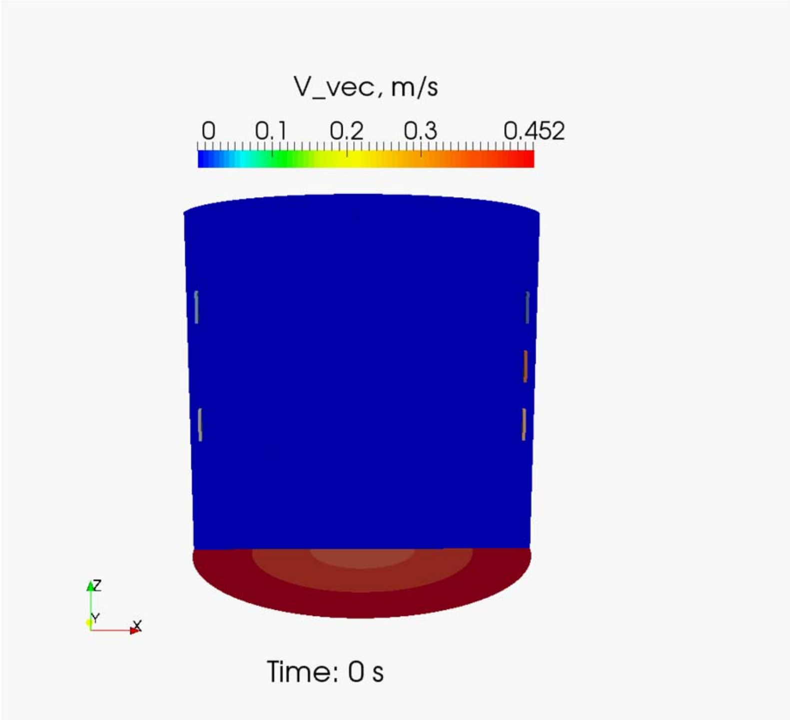
- Particle size – 1.7 µm
- Calculated fluid and particle velocity distributions (top and bottom figs., respectively).
- Simulation runs to 490 s of 30 minutes of experiment time
- The simulations show dust clusters first reached the bottom at ~50 s.

Sampling has a ramp time of 1 s

- Filters @ 0.452 m/s
- Impactor @ 0.181 m/s







Task 5 –Fragmentation Analysis

- Section 4.3.3: Non-Metallic or Composite Solids, Free-Fall Spill and Impaction Stress: ANL-82-39

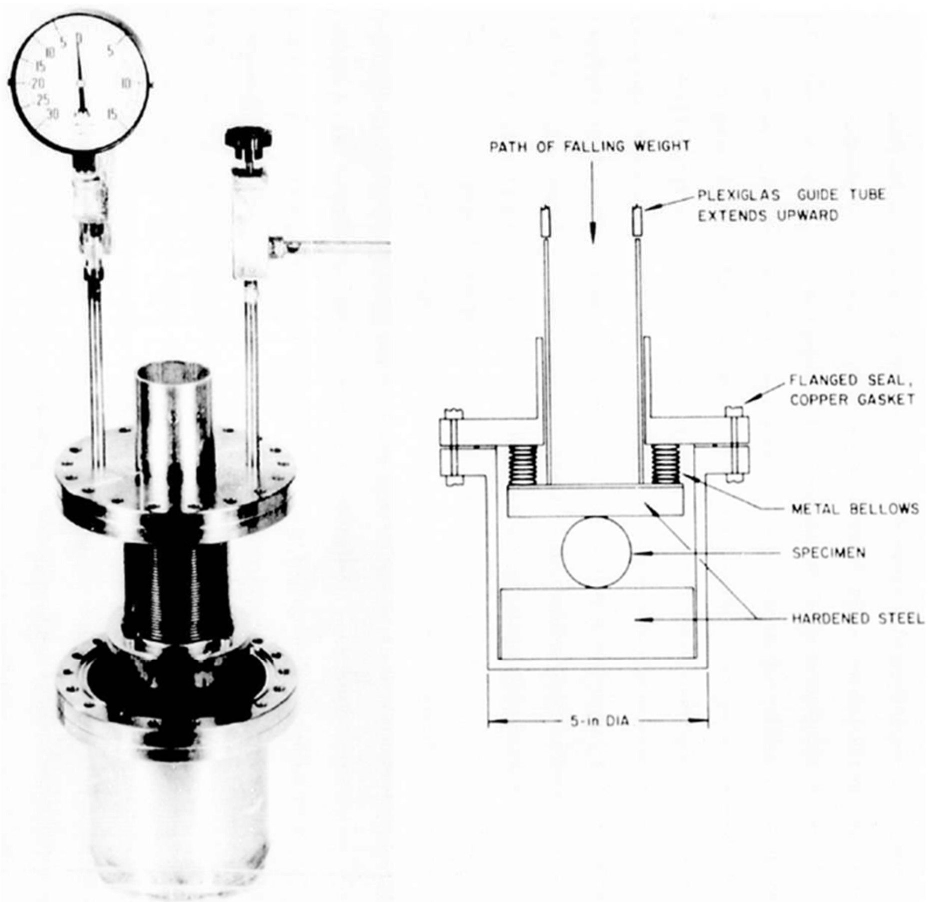


Fig. 10. Bellows Chamber for Impacting Brittle Specimens

$$ARF \; X \; RF = (A)(P)(g)(h) \quad (4\text{-}1)$$

where: ARF X RF = (Airborne Release Fraction)(Respirable Fraction)

- A = empirical correlation, 2E-11 cm^3 per $g\text{-}cm^2/s^2$
- P = specimen density, g/cm^3
- g = gravitational acceleration, 980 cm/s^2 at sea level
- h = fall height, cm.

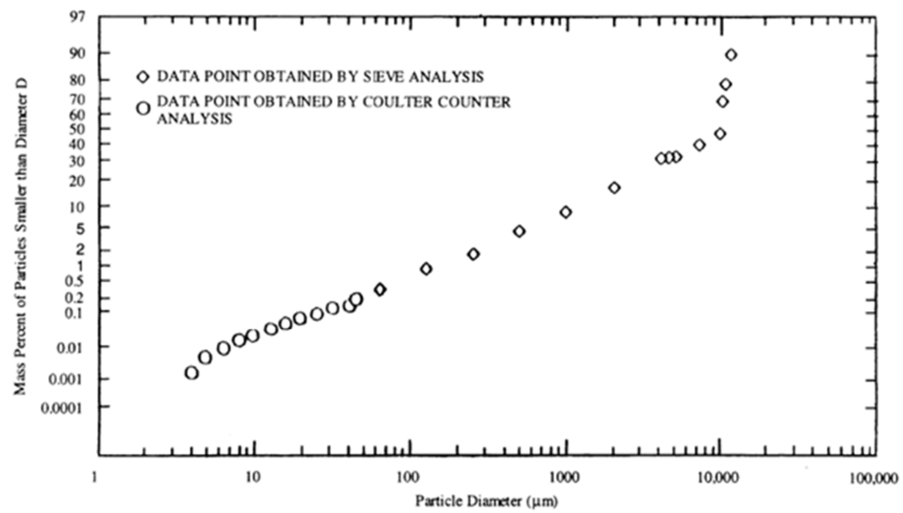


Figure 4-12. Particle Size Distribution Resulting for UO_2-2 Pellet Impact Test Data for UO_2 Specimen #2 Including Mean Grain Size of Original Crystalline UO_2 Particles. (Size Distribution 3 Pellets 13.7-mm diameter x 13.6-mm long; drop-weight 1.2 $J.cm^3$.) (Jardine, et. al. 1982)

Initial Demonstration Problem

Modeling Approach

Large Range of Length Scales Involved in Problem

- Test Specimen Geometry: 0.137 m x 0.136 m
- Particle Size of Interest < 10 μm
- Disparity in Length Scales: 4+ Orders of Magnitude

Two-Scale Model Approach

Macro-Scale → Macro-Fragmentation & Boundary Conditions

Micro-Scale → Micro-Fragmentation/Particle-Size-Distribution

Macro-Scale Model

SIERRA/SM (PRESTO) - Explicit Transient Dynamic FEA

Micro-Scale Model

Micromorphic Continuum Mechanics Approach

Elasto-Dynamic Model with Cohesive Zone Based Fragmentation Model

Test Case

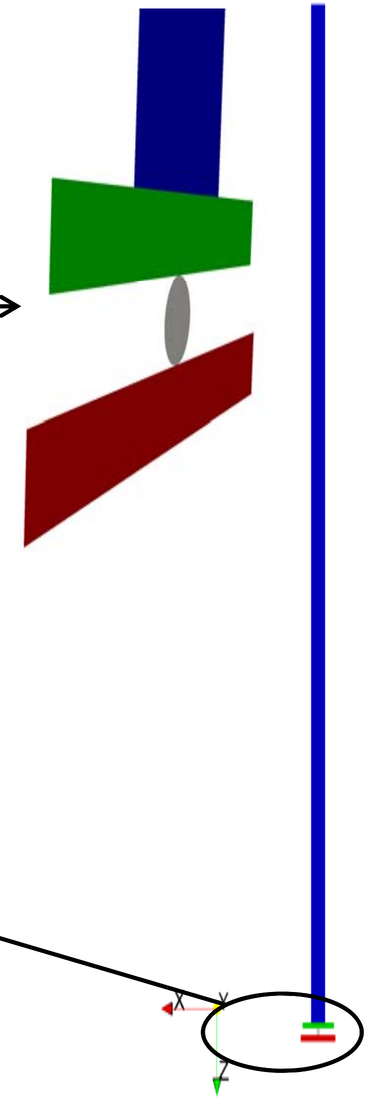
- ANL - UO_2 Diametral Impact
- 10 kg Impactor Dropped 0.0734m (1.2 J/cm^3)

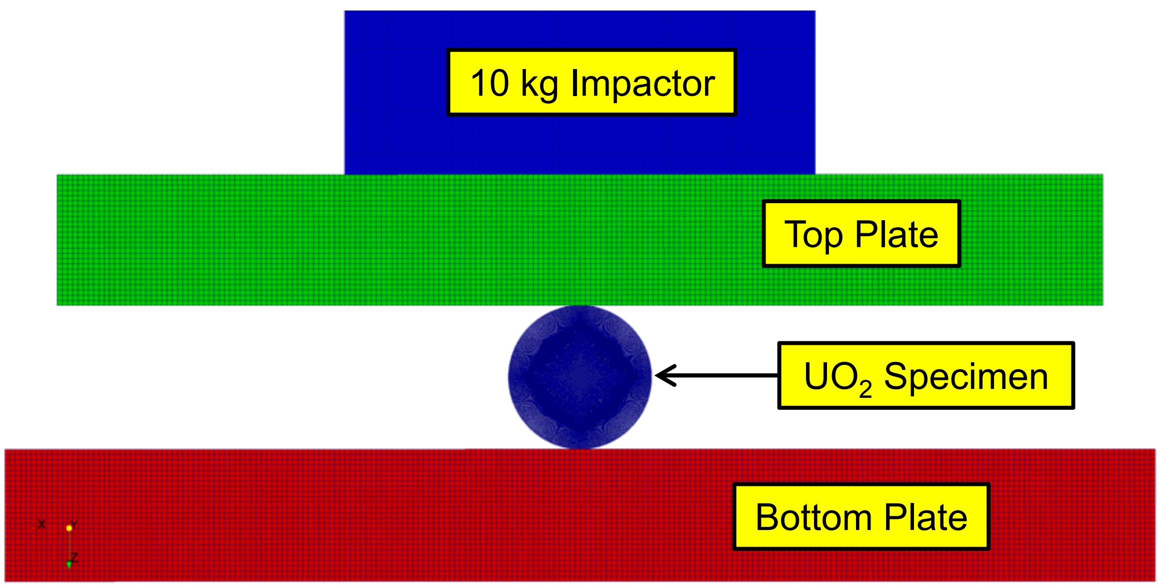
Macro-Scale Finite Element Model

- Plane Strain "Slice"

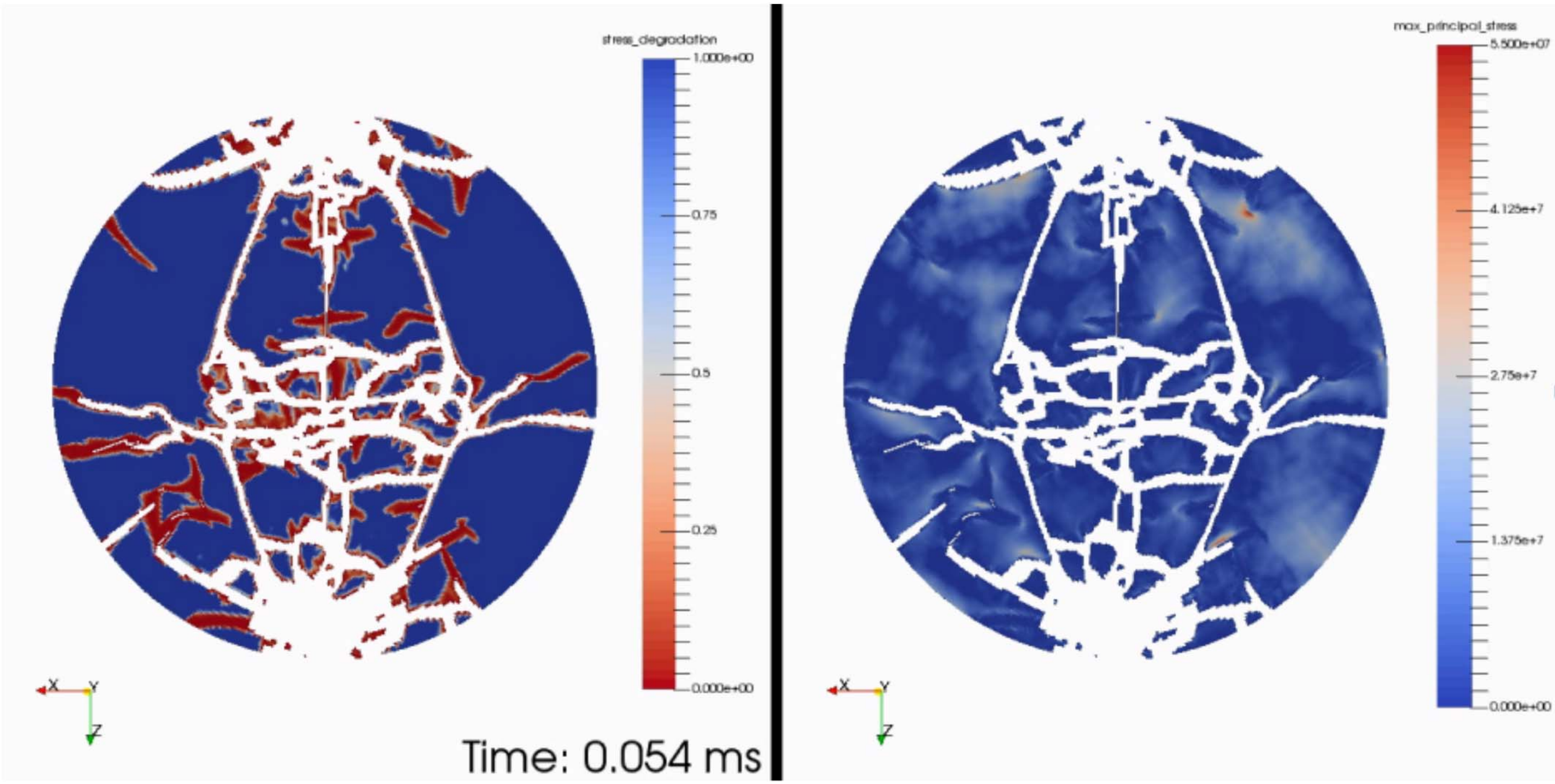
Micro-Scale Model

- 1-D Micromorphic Model with Fragmentation



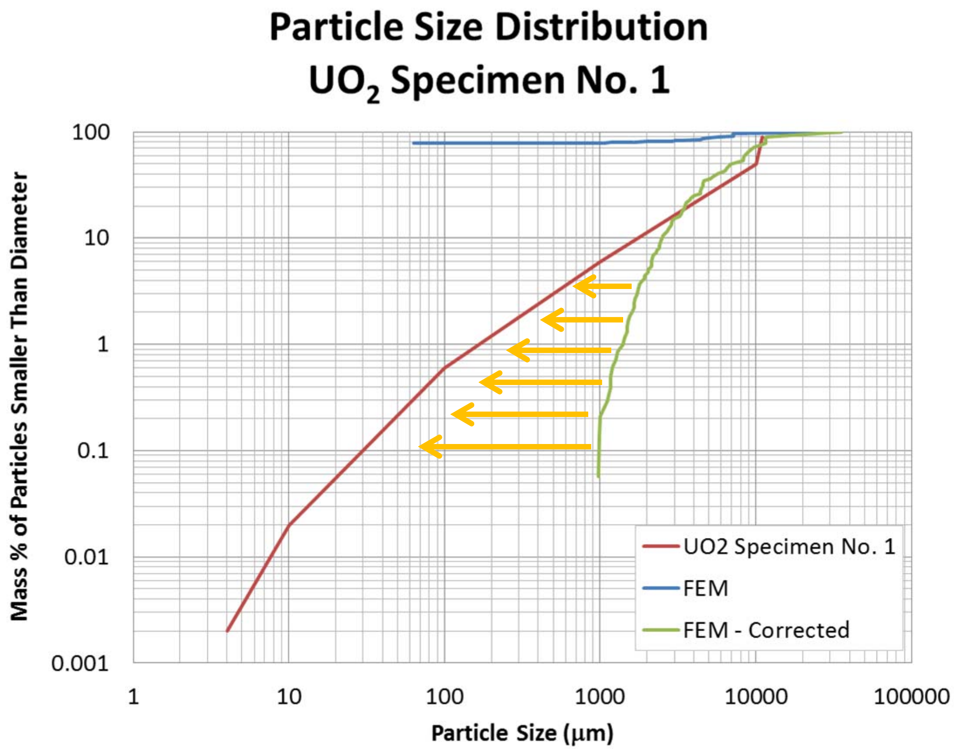


Preliminary Macro Scale Results



Micro-Scale Fragmentation

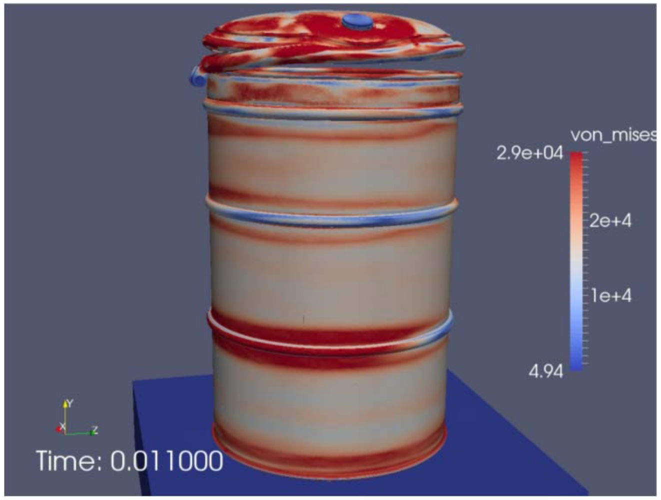
- Cohesive zone based fragmentation model to be implemented in an existing micromorphic simulation program.
- Output from the SIERRA SM (PRESTO) analyses will be used to define the boundary conditions for the micromorphic simulations.
- The particle size distribution from the macro-scale FEM will be adjusted based on the micro-fragmentation calculated by the micromorphic model simulations.



Micro-fragmentation will tend to increase the mass percentage of particles that fall below a given particle size (see arrows on plot).

Year 3 Proposed Research

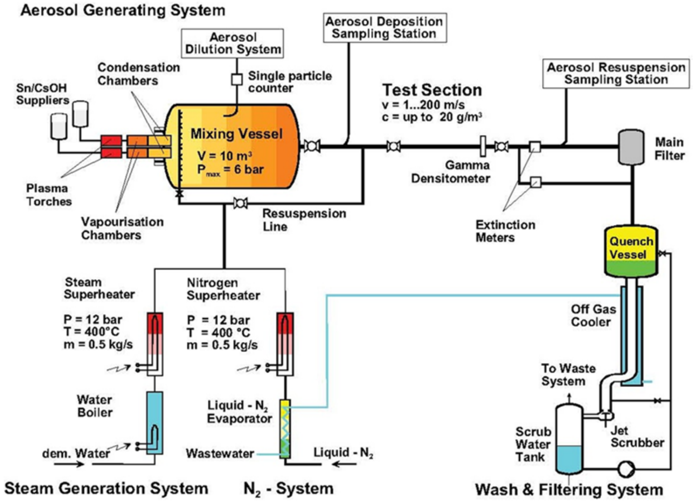
- Based on the Year 1 and Year 2 research, we demonstrate the capabilities:
  - Substantiate data for liquid material (Chapter 3 of Handbook)
  - Substantiate data for solid and powder materials (Chapter 4 of Handbook).
- In Year 3, we also like to address topics in Chapter 5 and Chapter 6 of Handbook
  - As a part of continuation in Year 2, implementation of micromorphic material model into SIERRA SM (PRESTO)
  - Revise Chapter 6 (Inadvertent Nuclear Criticality)
    - Existing data is outdated, and many references used were no longer applicable, and some irrelevant data were used
    - The revision will include updating all information to latest information available, and revisit the liquid criticality release fraction, and will simulate using SIERRA codes
- Simulate a drum release during a fire to include in Chapter 5
  - Use existing 55-gal drum model from a WIPP drum release accident analysis*
  - Capitalize the on-going drum fire experiments at Sandia and recent data for fire condition to determine the opening size of the breached drum using SIERRA SM
  - Use solid combustion models from on-going DOE project to simulate the content burn in a breached drum



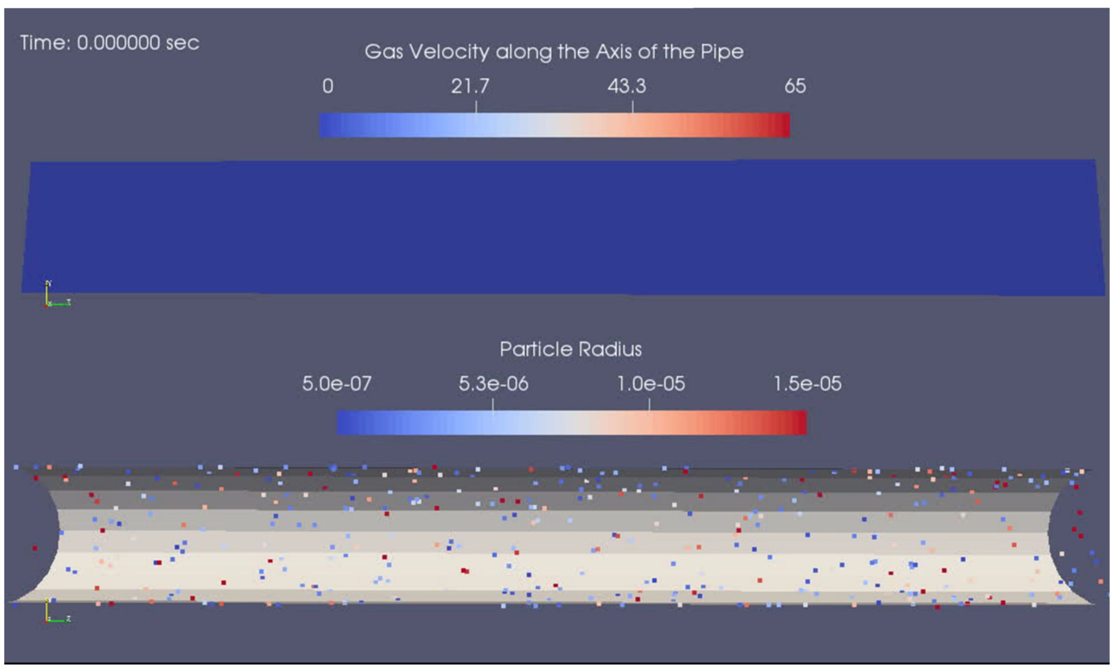
*Smith, J., Memorandum to Distribution: Mechanical Modeling of a WIPP Drum Under Pressure, Sandia National Laboratories, Albuquerque, NM, November 25, 2014

Backups

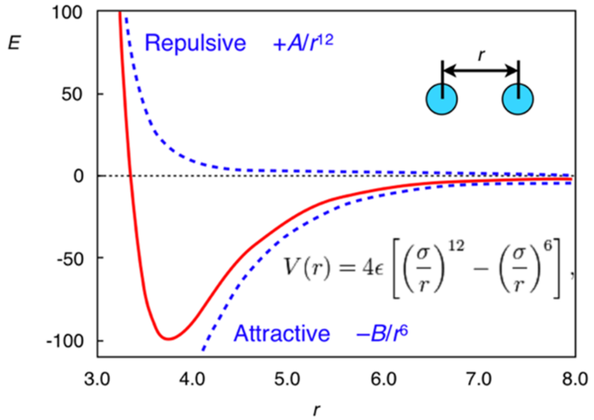
STORM SR-11 Resuspension Phase



Resuspension Model



Particle Interactions (not part of NSRD-11)



Simulation Example:

- 5 vertically suspended liquid droplets are released at start of simulation
- Lower droplet impacts rebounding surface at bottom of simulation domain
- Subsequently, other 4 droplets impact and coalesce with growing droplet
- Final agglomerate moves around on lower boundary due to velocity of immersing gas (fluid) phase
- Any number of scenarios is possible from droplet agglomeration to breakup to liquid flow

- In FUEGO, implemented modified Lennard-Jones interaction to model liquid-like materials (droplets)
  - Central force (van der Waals type), binding energy, repulsive core (modified spring-like for stability)
  - LJ Parameters map directly to liquid surface tension
- Sufficient for particle agglomeration and breakup
- Granular materials would require additional terms (non-central forces) but could be implemented without great difficulty