SAND2018-8651C

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Sandia National Laboratories

Computational Capability to Substantiate DOE-HDBK-3010 Data

Acknowledgement

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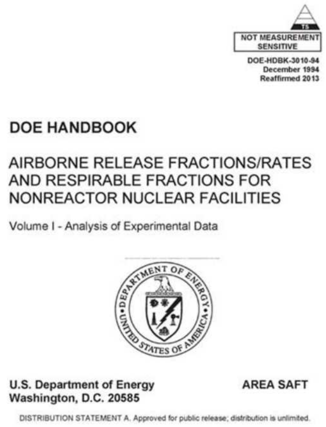

NOT MEASUREMENT SENSITIVE

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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David L.Y. Louie, Ph.D.

Presented to 2018 EFCOG NFS Conference

August 11-17, 2018

SAND2018-xxxx

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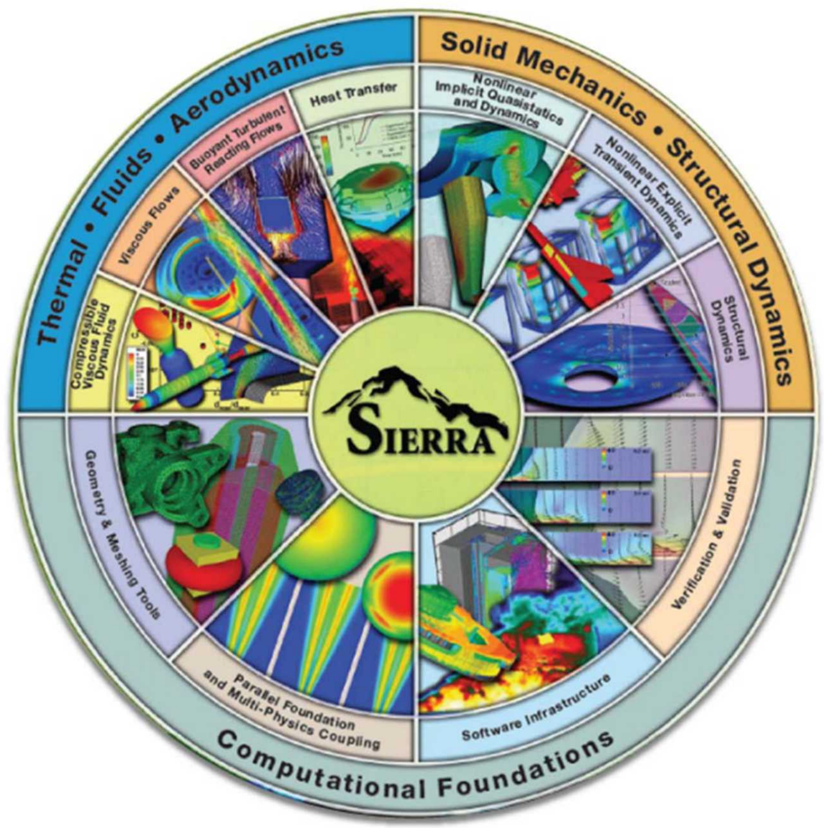
Outline

- SIERRA Engineered Tool
- Research tasks simulated since FY15
- Highlights of past accomplishment
- Progress of tasks in FY18
- Summary and Conclusion

Sandia's SIERRA High Fidelity Code Suites

Sandia National Laboratories

- 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 Tasks

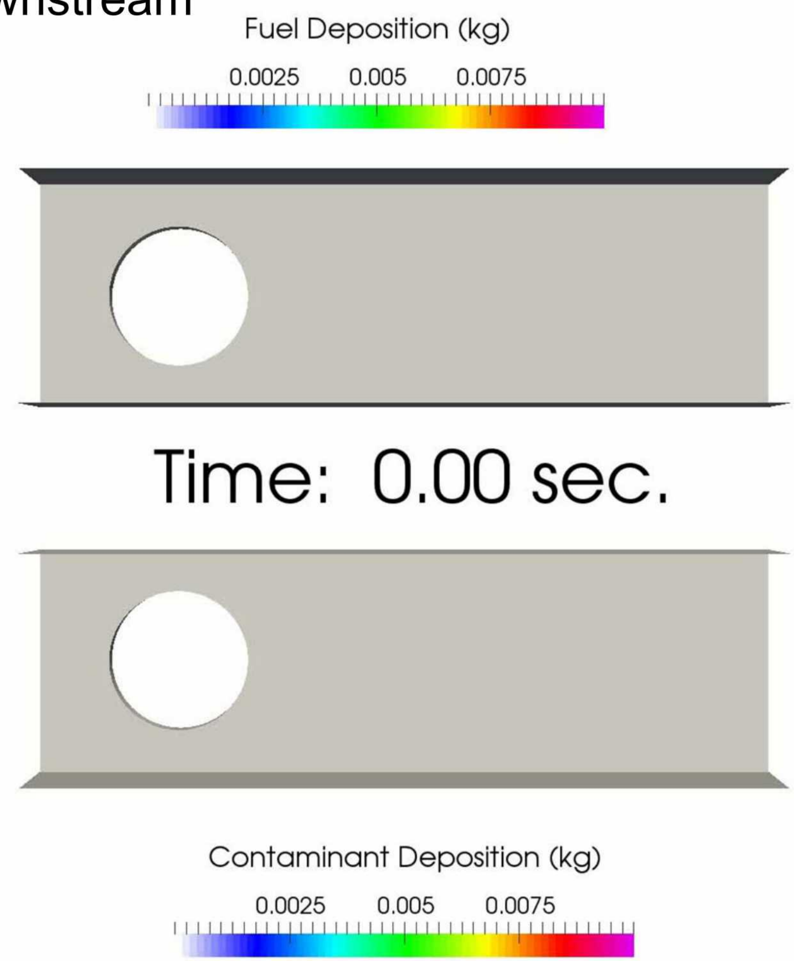
Research Task	Status
Exploratory simulations of energetic impacts using Presto/Adagio (SIERRA/SM).	• A simulation model of a bullet hitting a can filled with small particles has been simulated and formulated such that we could use a non-export version of the SIERRA/SM (see [SAND2015-10496] for more details). • 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].

Research Tasks

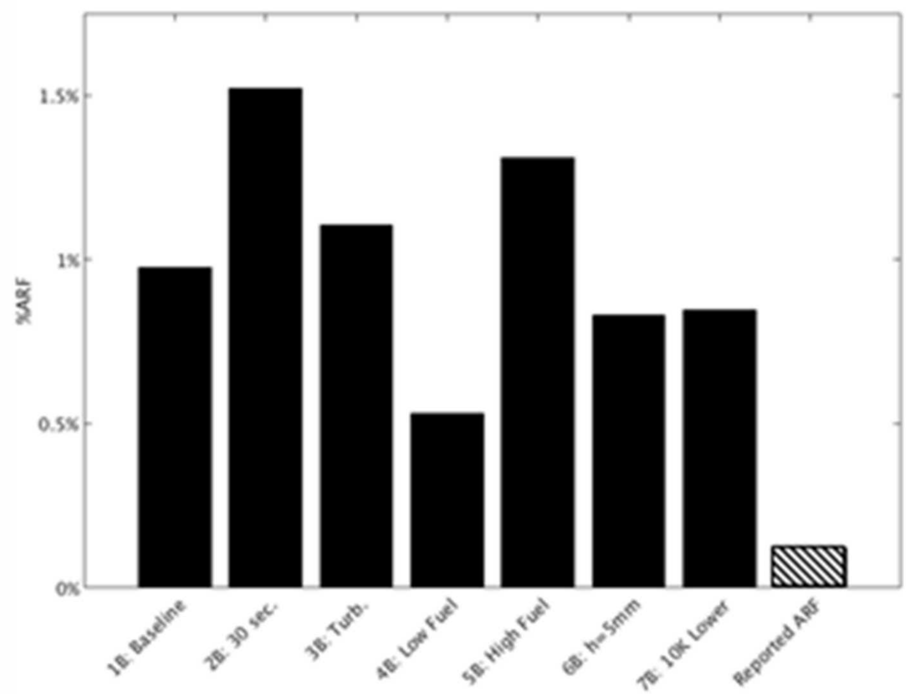
Research Task	Status
Investigation of particle resuspension using Fuego – A resuspension model [SAND2015-6119] has been added to Fuego [SAND2016-12167].	• Particle resuspension is an important phenomenon in particle transport. Many resuspension experiments were used to simulate this phenomenon. See SAND2016-12167 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 be improved 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 model needs to be developed.

Simulation Visualization and Results

Boiling Entrainment , Multi-component Evaporation(1B): The fuel deposits closer to the pool, while the lighter contaminant particles carry further downstream



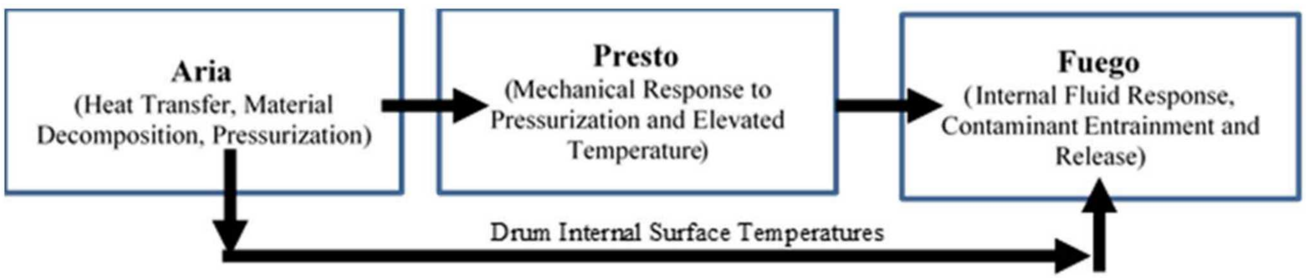
Fuego Results on Gasoline Pool Fire Experiment



Drum Fire Release Simulation (Task 3)

Motivation and Approach

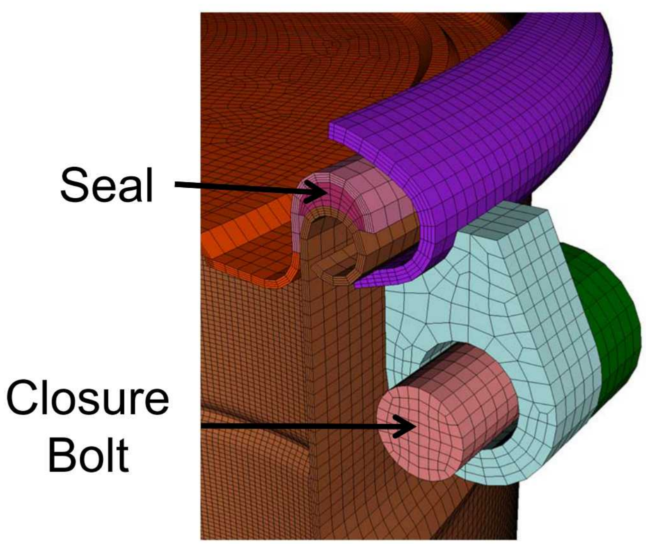
- Estimate airborne release fraction (ARF) and respirable fraction (RF) using SIERRA analysis tools for a type 7A waste drum exposed to a fire accident scenario.

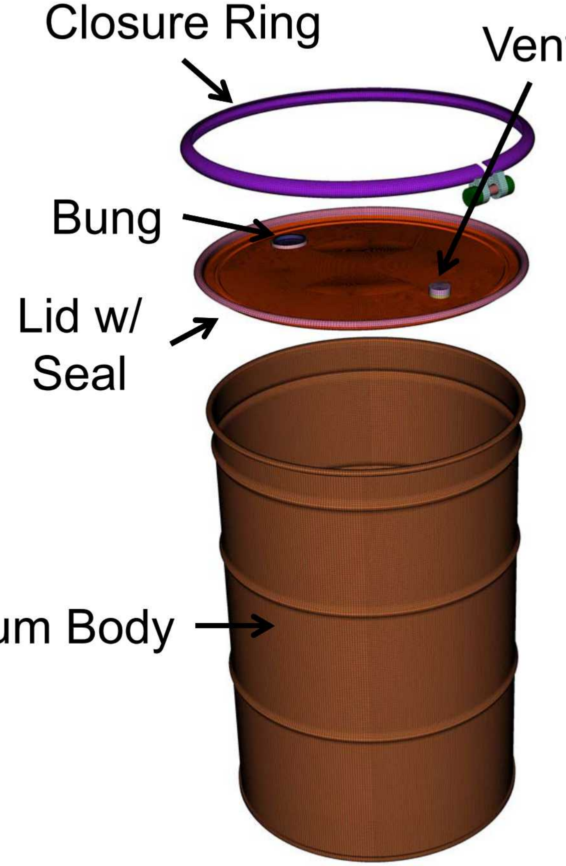


Material	FLAME Experiment (2016)	RART Experiment (1973)
Cardboard	Included in paper weight	17.5% (15.7-20.9%)
Paper	17.6% (4.98 lbs.)	41.1% (31.7-43.9%)
Plastic	75.7% (21.47 lbs.)	9.7% (8.0-14.4%)
Rubber	6.7% (1.9 lbs.)	2.4% (1.8-4.2%)
Miscellaneous (Rags, Oil, Tape, Other)	None	29.3% (23.8-38.2%)

Presto Simulations

- Calculate thermal-mechanical response of drum and determine breach area.
- 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.
- Seal decomposition modeled using element deletion (at a temperature of 675 K).
- Tightening of closure ring simulated during first 10 seconds of simulation.
- Two simulations: w and w/o depressurization

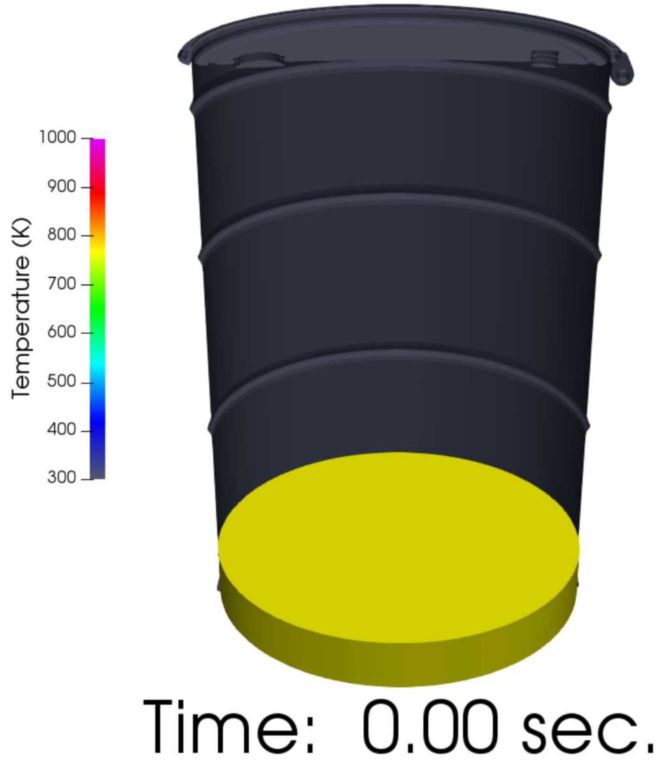


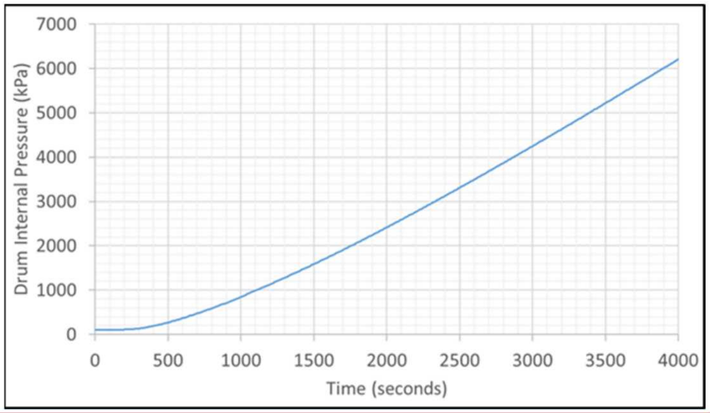


Aria Simulation

Aria used to calculated material temperatures and internal volume pressure.

- Mesh identical to Thermal-Mechanical, but included meshed interior
- 55 kW/m^2 heat flux BC representing fire applied to drum outer surface, based on experimental values[1].
- Radiation and convection BCs applied to internal and external surfaces of drum.
- Internal volume represented by 2 regions: Air and Trash (without venting). Ideal gas law applies.
  - Cellulose which decomposed with temperature based on a two-step Arrhenius equation.
- Trash mass loss after a half-hour fire predicted to be 1.8 kg, whereas the experiment recorded 2.0 kg.
- Temperatures in the air region could be predicted by a cubic function with respect to time
- Pressure and temperature values used as input data for the Thermal-Mechanical model

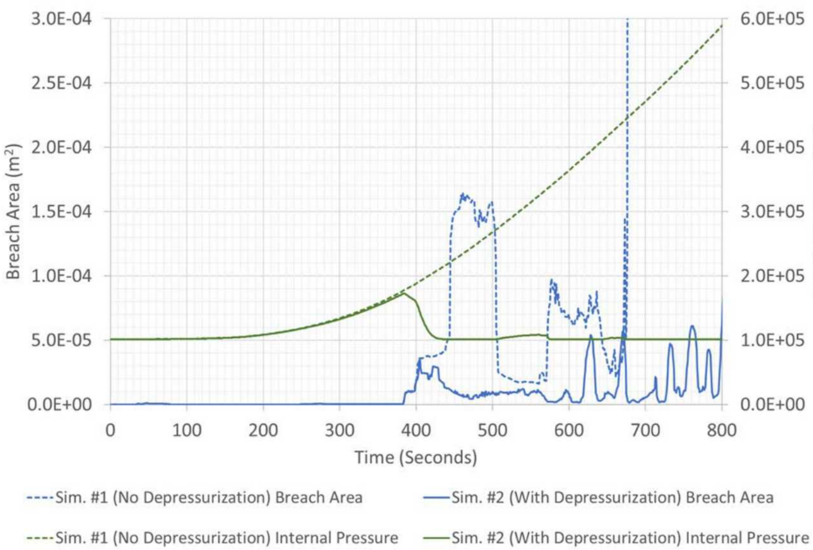




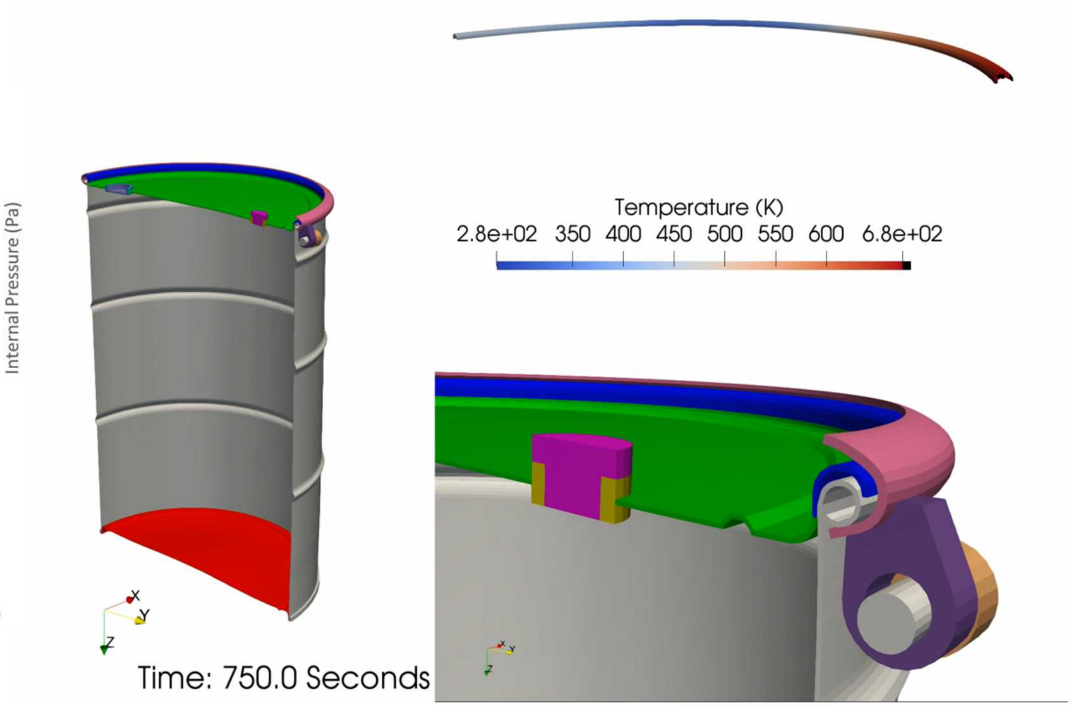
1. Figueroa, V., et al., "POC Pool Fire Experiments", Sandia National Laboratories, 2017.

Sim. #2 (With Depressurization)

- Simulation #2 (With Depressurization)
  - Breaching of the drum predicted in Sim. #1 used to calculate new pressure-time relationship used in Sim. #2.
  - Resulting breaching of drum calculated in Sim. #2 used in subsequent Fuego simulation.

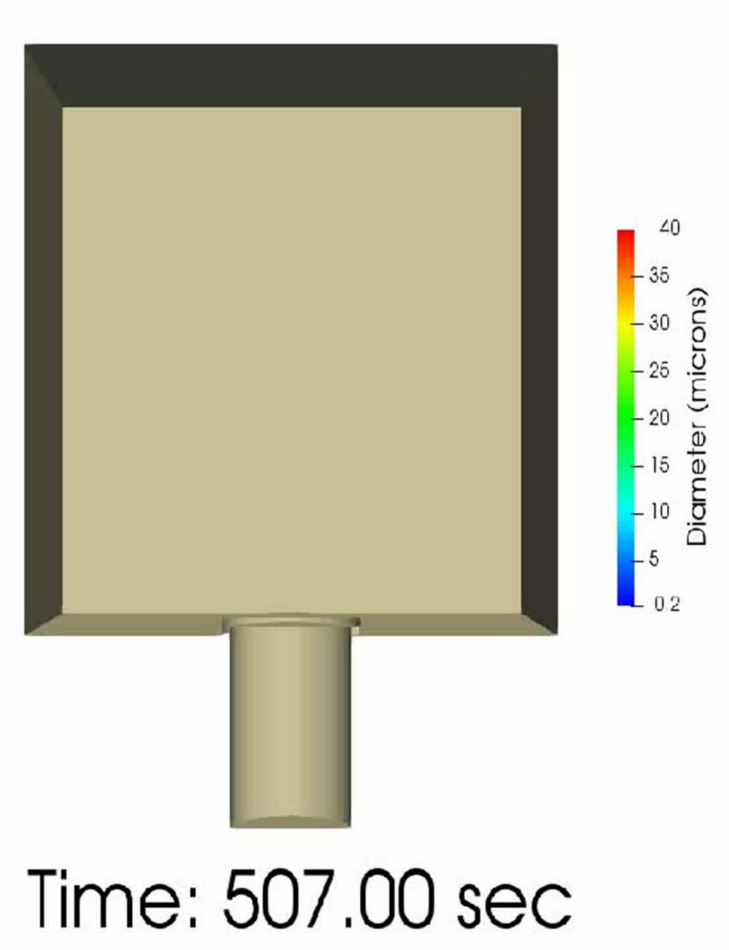


Sim. #2 (With Depressurization)



Fuego Simulation and Results

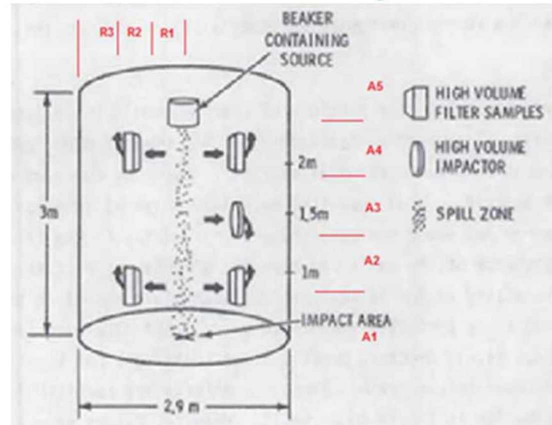
- Calculate contaminant particle release
  - Lagrangian particles coupled to Eulerian flow
  - Vented area 2E-3 m^2 as time did not permit the refinement required by the reduced area (1E-5 m^2) calculated by Presto simulation #2
- Inner surface temperature from Aria results mapped onto the Fuego drum surface as a BC
- All surfaces 'stick' boundaries; which collect parcels as they collide with that boundary.
  - Total deposited mass and total number of particles were recorded on the boundary nodes.
- All released particle diameters were below 10µm, resulting in an RF of 1.0.
- Only a small fraction (4%) of contaminant was entrained from decomposing trash into the drum volume prior to venting

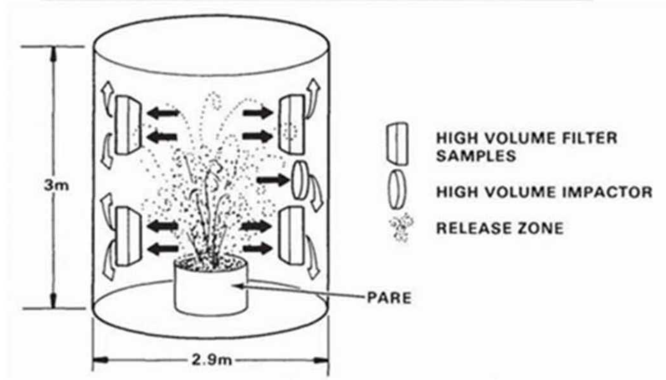


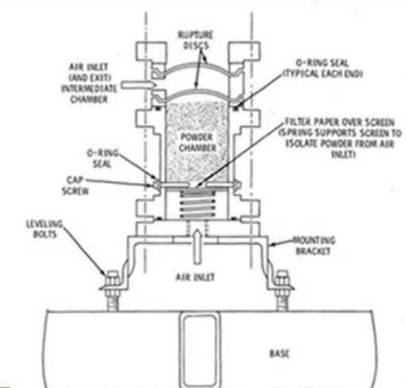
Parcel Deposition Location	Mass Deposition (kg)	Mass Fraction (%)
Drum Walls	0.0113	99.49%
Released (DRxARF)	5.85×10^{-5}	**0.02%**

Powder Release Exp (Sutter 1981)

- Cylindrical chamber (RART): 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
- TiO_2 (100 g) particles with 1.7 µm, using a distribution as described from experiment
- 100,000 particles modeled for both spill and pressurized release cases
- Only 50 psig pressurized release (in PARE) can be modeled using Fuego. 250 psig case can be modeled using Adagio/Fuego

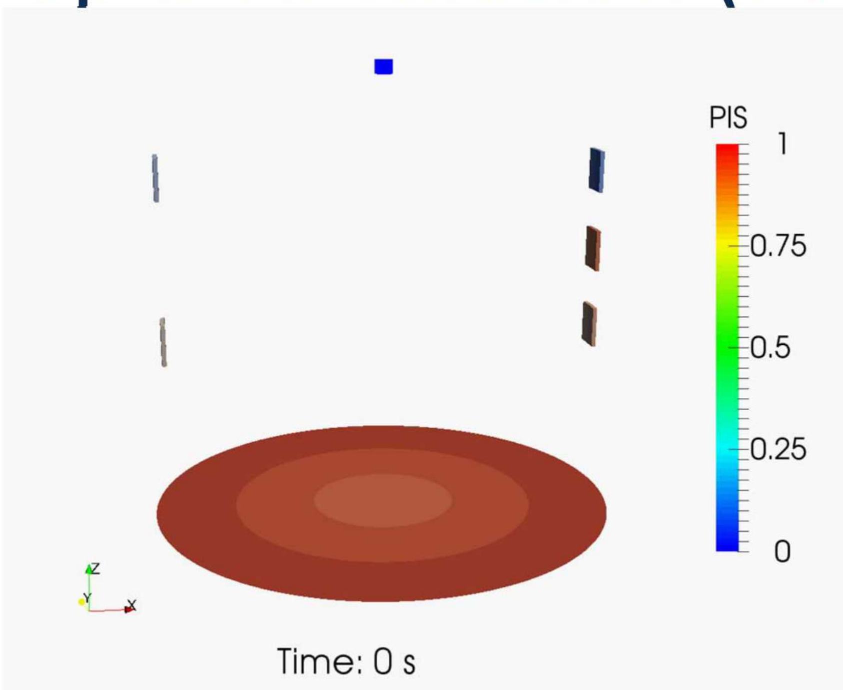


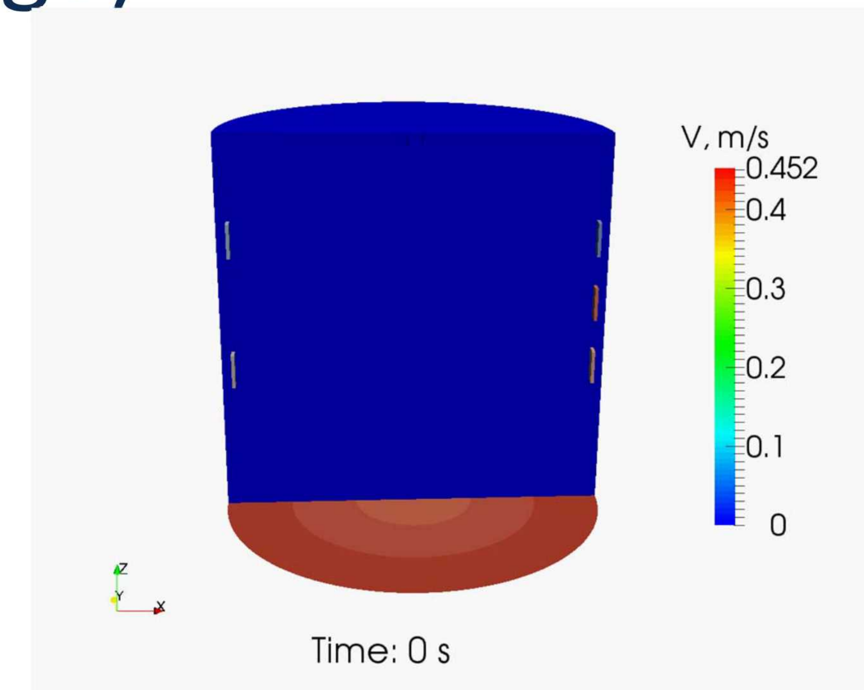


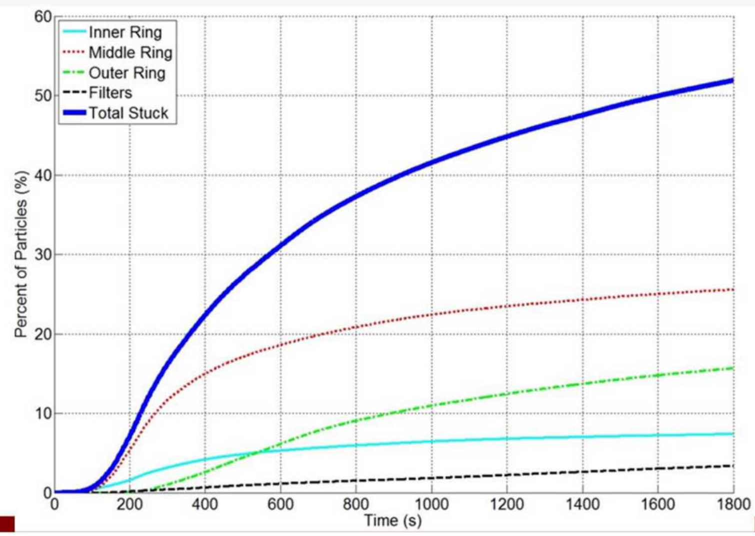


PARE

Spill Simulation (Fuego)



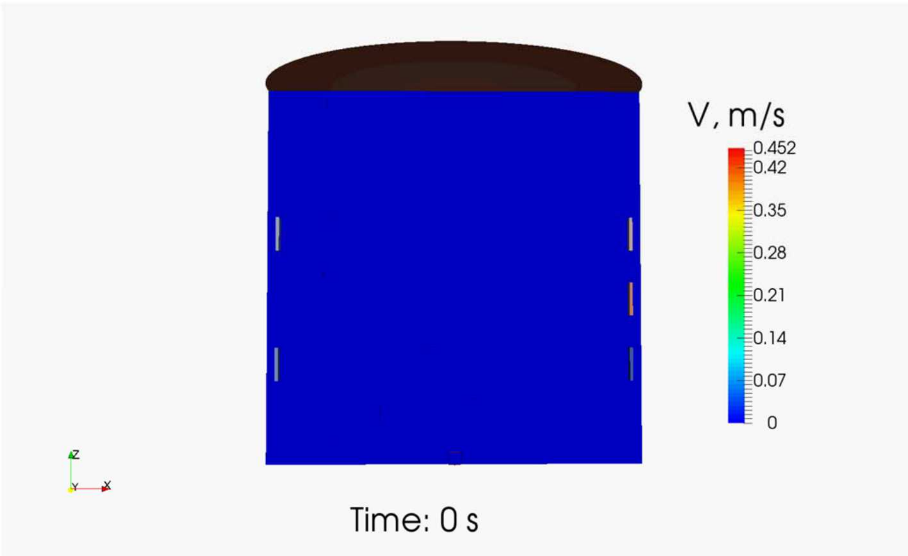


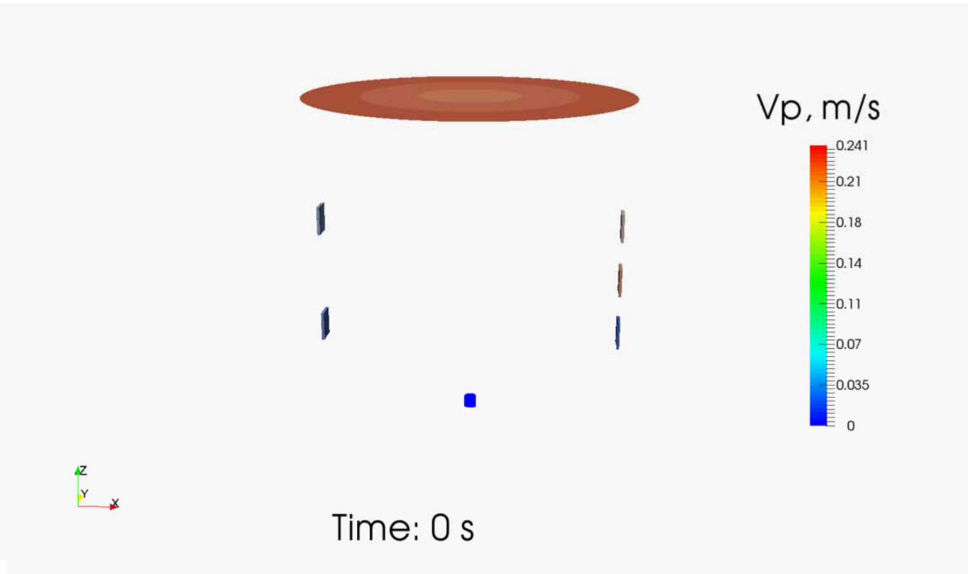


Particle "clusters" comprised of the larger particles first reached the bottom of the chamber at around 50 s.

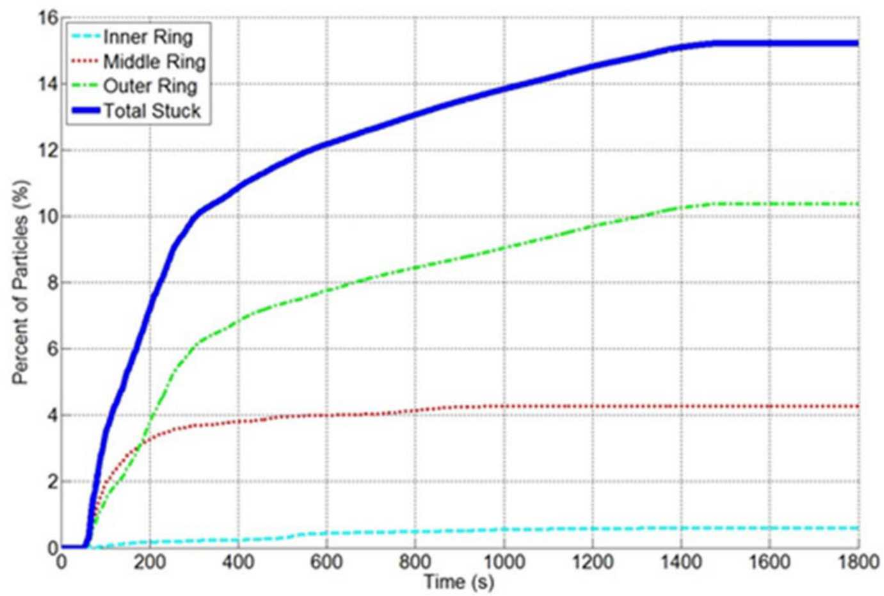
The lighter particles first reached the floor at 200 s and continued settling on the floor for the duration of the transient.

50 psig (0.34 Mpa) Pressurized Release Simulation (Fuego)

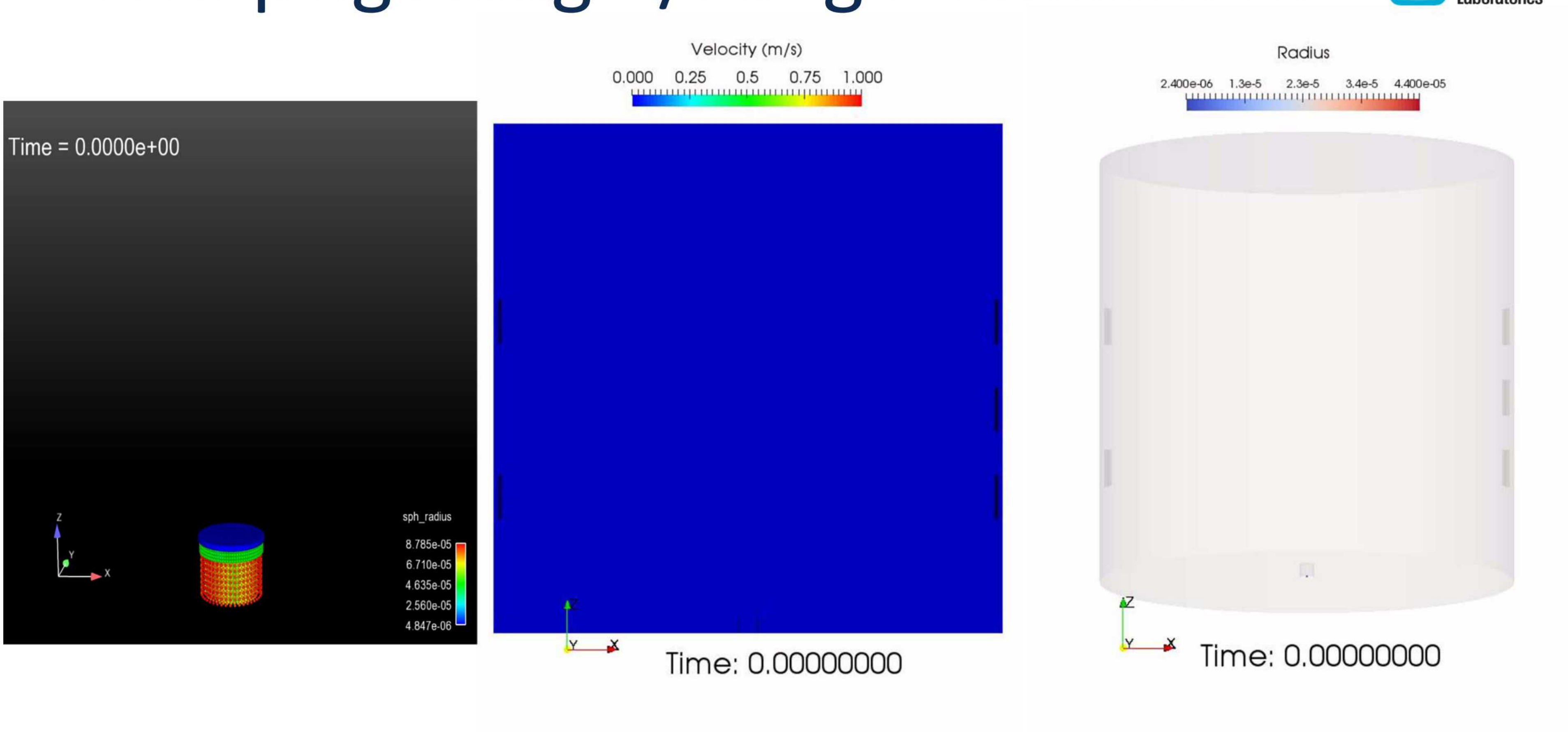




Fuego Results of Ceiling Deposition



250 psig Adagio/Fuego Simulation



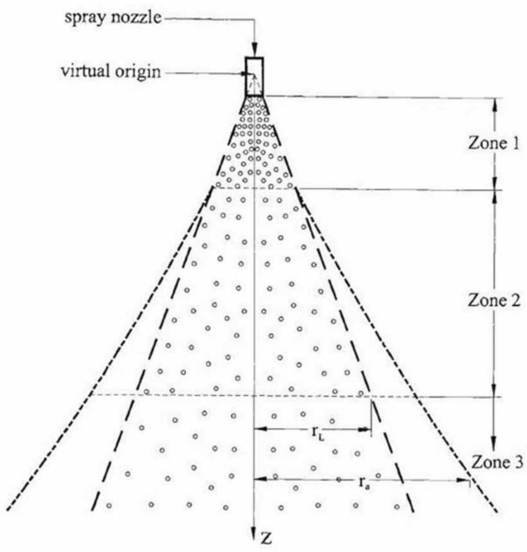
- Multi-SPH models used for Adagio to create sufficient particle flows
- One way couple method use: Adagio results translate into Fuego inputs
- This capability is demonstrated so that particles lose kinetic energy to induce fluid flow

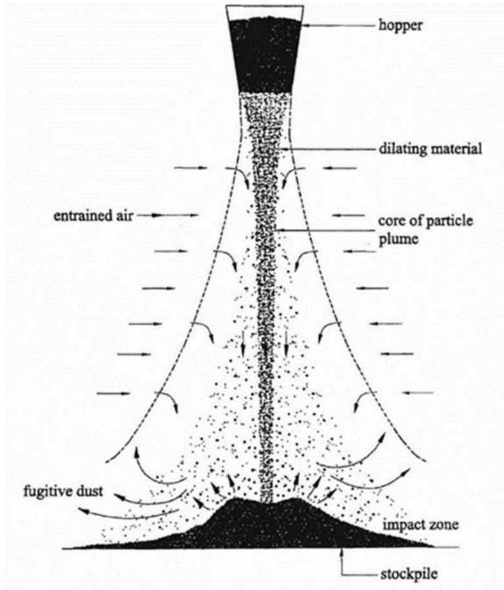
NSRD-16 (FY18) Tasks

- Task 1 – Revise Sections of Chapters 4 and 5 (3010) on powder release and solid impact sections using recent literatures (Louie, Gordon, Bignell)
  - Examine literature in free fall powder and impact of solids (i.e., ceramics)
- Task 2 – Provide drop and impact of containers to determine the DR values (Le, Bignell, Gordon)
  - Review waste stream data from LANL
  - 7A drum
  - 2^{nd} container (i.e., SWB)
- Task 3 – Based on Task 1 of NSRD-15 on the fragmentation model, develop an improved equation better than existing Eq(4.1) in the Handbook (Gilkey, Bignell, Dingreville)
  - Collect and tabulate experimental data available and calibrate concurrent fragment model – including micromorphic (ε, T, d_{gr})
  - Perform simulations of the concurrent model to vary micromorphic parameters using DAKOTA.
  - Revise Equation 4-1

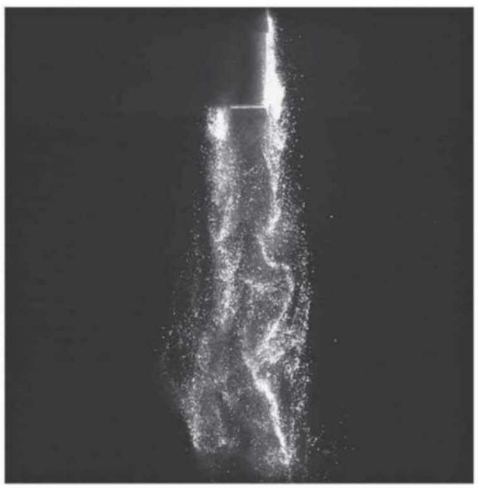
Literature on Free Fall Powders

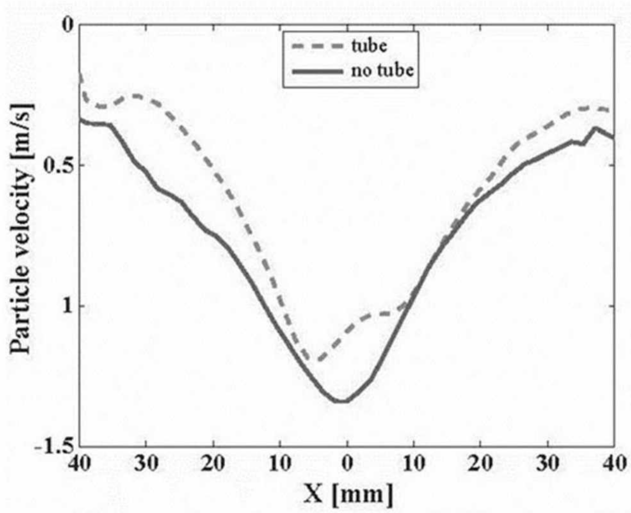
- Air entrainment in free falling bulk materials [Liu 2003]
  - Summarized particle velocity and air entrainment models and conducted validation experiments to models
  - Use 3-Zone droplet models to explain the particle velocities
  - Useful to develop air entrainment for MELCOR, substantiate NSRD-11 free fall CFD/MELCOR simulations





- Dust emission by powder handling: Influence of the hopper outlet on the dust plume [Ansart 2011]
  - Study the effect of obstruction, such as tubing on particle fall velocity
  - Study the similar phenomena on free fall powders as [Liu 2003]

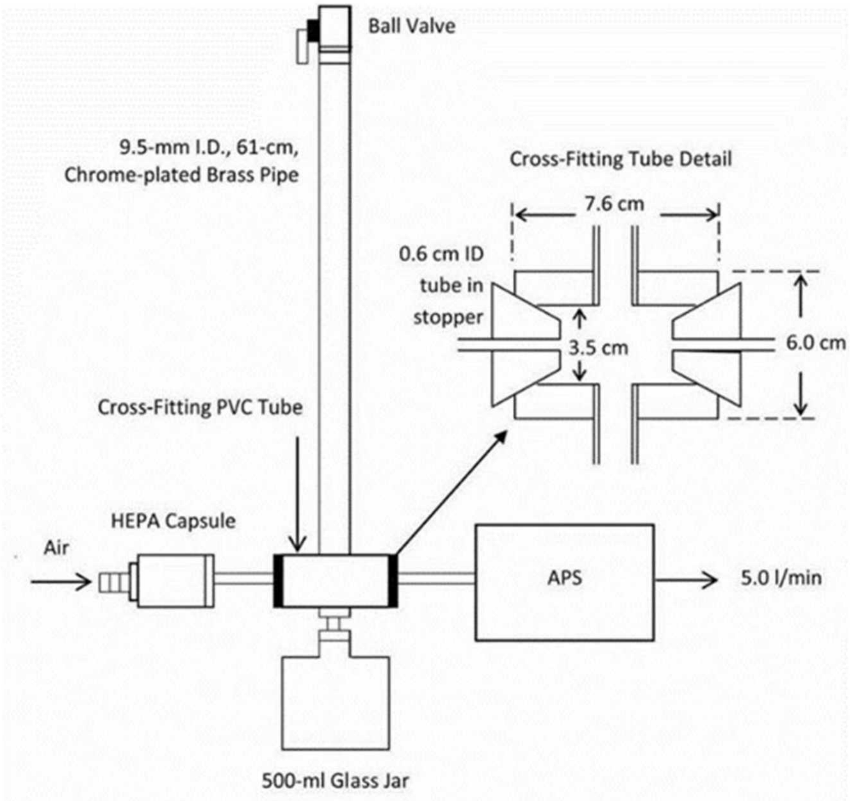




Literature on Free Fall Powders (concluded)

A novel device for measuring respirable dustiness using low mass powder samples [O'Shanughnessy 2012]

- Use single drop of 15 mg nm powder
- Use low mass dustiness tester including the use of APS –counting particle size channels
- Use sample rate of 5 liter/min (<0.1 m/s)
- 3 trials were conducted for each powder type



Results:

- indicates the nm powder to agglomerate into µm due to van der Waals, other electrostatic forces
- Develops a regression model and classification scheme based on the powder measurements

Powder	Medium Size (nm)	Count Median Diameter (µm)	Mass Median Diameter (µm)	Geometric Standard Deviation (µm)	Respirable Dustiness (mg/kg)
Al_2O_3	10	3.9	0.24	0.05	40.4±0.7
Al_2O_3	50	3.9	1.28	0.07	16.5±1.5
Carbon black	14	2.0	0.56	0.07	42.9±6.0
Cu	25	8.9	0.25	0.01	3.9±1.3
Fe_2O_3	35	5.2	1.20	0.70	8.1±0.8
SiO_2	20	2.2	0.03	0.20	121.4±14.6
TiO_2	5	4.3	0.26	1.08	60.4±5.7
TiO_2	21	4.3	0.12	0.19	45.3±8.5

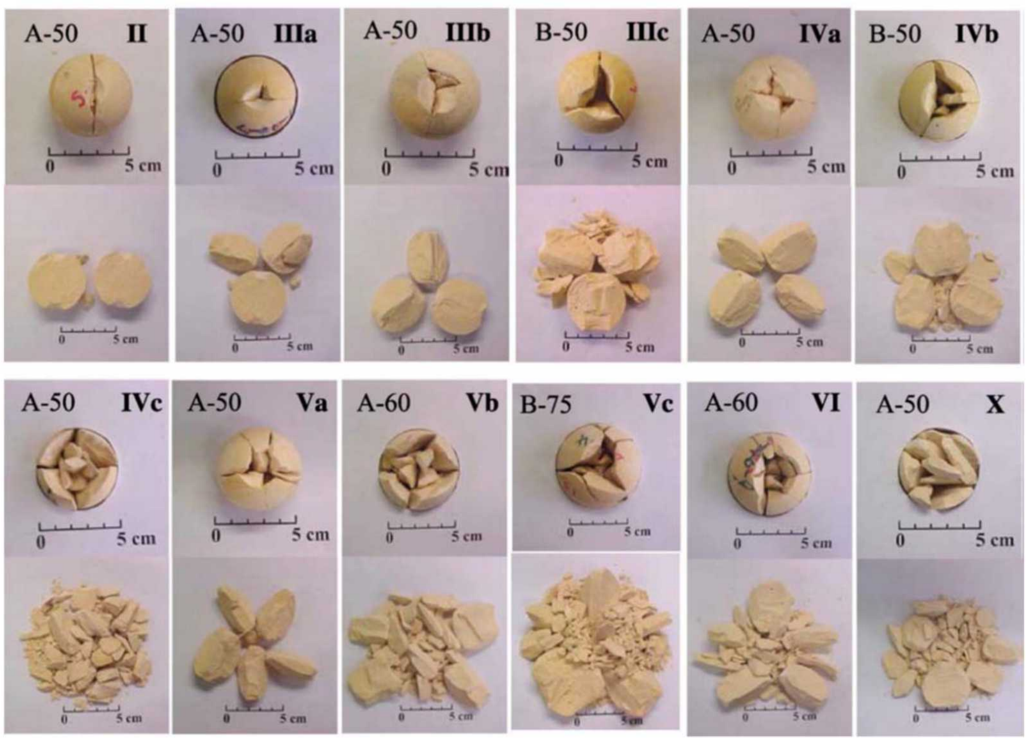
Fragmentation of Brittle Spheres

Wu, S.Z., et al., “Crushing and Fragmentation of Brittle Spheres under Double Impact Test,” Powder Technology 143-144, page. 41-55, 2004.

Crushing and fragmentation of brittle spheres under an impact test using spherical samples of brittle materials.

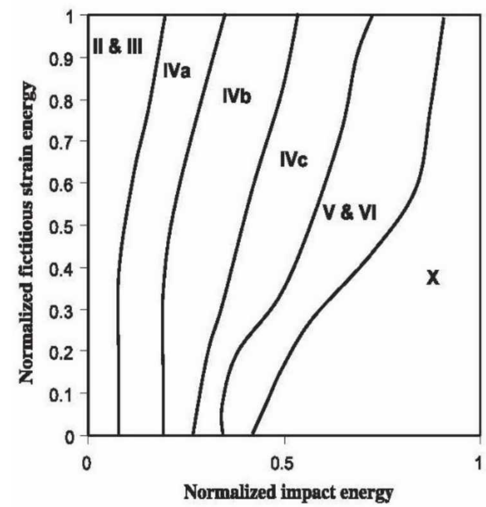
Samples made of plaster.

Impact energies: 8 to 310 J.



Typical Failure Modes Observed.

Experimental Apparatus



Failure Modes of Spheres as Function of Normalized Fictitious Strain Energy Versus Normalized Impact Energy

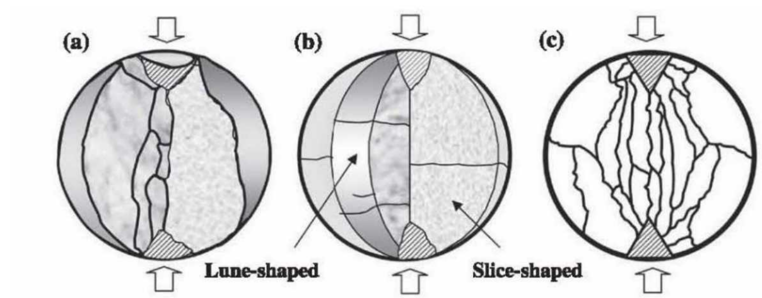


Illustration of Internal Cracking Patterns. (a) Crushing of Internal Core to Form Lune-Shaped Fragments (b) Substantial Transverse Cracking (c) Typical Cross-Section of Crushed Sphere.

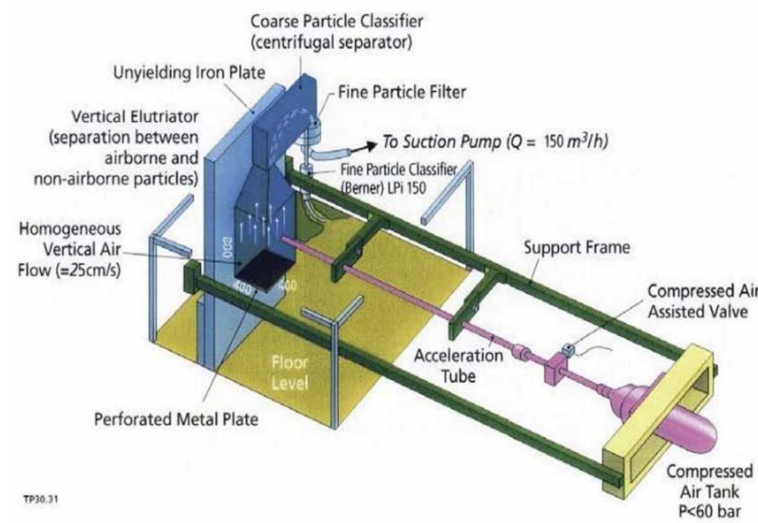
Pellet Fragmentation

Koch, W., et al, "Determination of Accident Related Release Data," 14th International Symposium on the Packaging and Transportation of Radioactive Materials (PATRAM 2004), Berlin, Germany, September 20-24, 2004.

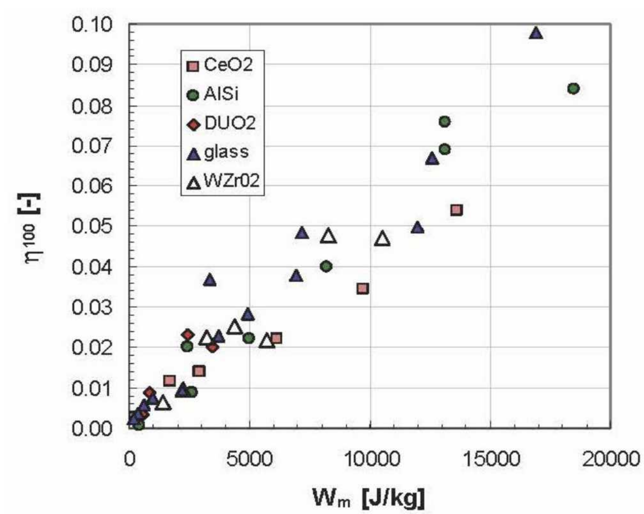
Impact brittle material into unyielding iron plate using an acceleration tube. Material is composed of pellets of ceramic materials and glass.

The relationship $\eta_{100} = C1 + C2\ W_m$ was fitted, where Wm is kinetic energy.

Additionally a cumulative size distribution was determined to fit the experimental data. $Q_3(\chi_{AED}) = a\ \chi_{AED}^{\mu}$



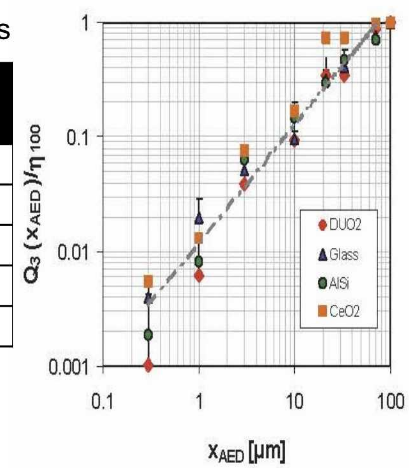
Acceleration Tube.



η_{100} has a linear relationship with kinetic energy.

Fitted C1 and C2 Constants for different impact materials

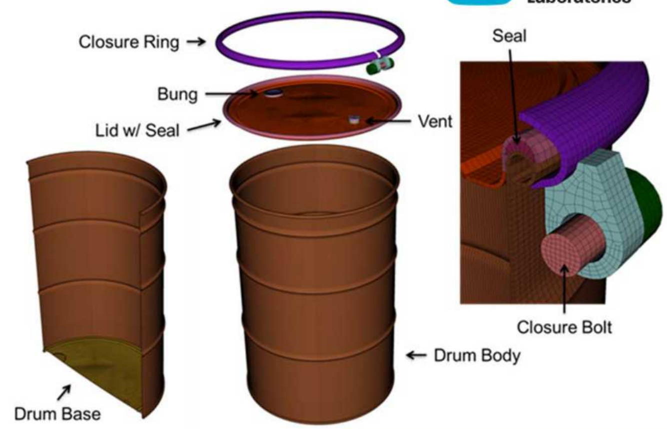
Impact material	C1 [-]	C2 [kg/J]	ρ_m [g/cm^3]
AlSi	9.27E-04	4.93E-06	1.6
Glass	3.77E-03	5.15E-06	2.2
CeO2	2.77E-03	3.56E-06	6.8
WZrO2	1.92E-03	4.69E-06	10.3
DUO2	2.82E-03	6.08E-06	11.0

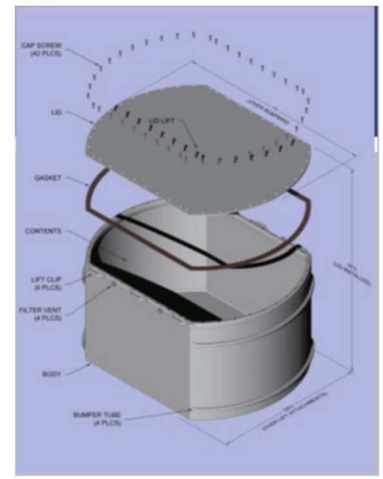


Cumulative Size Distribution

Task 2 – Damage Ratio (DR) Study on Container Breach

- Develop a test matrix for the DR study
  - Utilize the TRU waste stream data from LANL
  - Determine the second container to be simulated (i.e. SWB)
- Develop 7A drum DR for free fall and puncture cases
  - Using existing 7A drum model from NSRD-15 work
  - Run simulations according to the test matrix
- Develop a second container model to be simulated the same cases as in 7A.
  - Develop a SWB model
  - Run simulations according to the test matrix
- Document the models and correlation, including the development of DRxARFxRF relationship examples





Free-Fall Impact –Analysis Combinations

- **<u>55-gal Drum</u>**
- Content Type (3)
  - Heterogenous Debris Waste
  - Solidified Inorganics
  - Contaminated Soil/Debris Waste
- Drop Height (4)
  - 2.5, 5.0, 10.0, 20.0 m
- Content Mass/Weight (1)
  - Max or Limit
- Orientation (5)
  - Pitch Range: 0 to 180 degrees
  - Increment: 45.0 Degrees
- Total # of Analyses:
  - 3 x 4 x 1 x 5 = 60

<u>SWB</u>

Content Type (1)

Heterogenous Debris Waste

Drop Height (4)

2.5, 5.0, 10.0, 20.0 m

Content Mass/Weight (1)

Max or Limit

Orientation (5 x 1 = 5)

Pitch Range: 0 to 180 degrees

Pitch Increment: 45.0 Degrees

Roll Range: 0

Total # of Analyses:

1 x 5 x 1 x 4 = 20

Puncture –Analysis Combinations

55-gal Drum

Content Type (3)
- Heterogenous Debris Waste
- Solidified Inorganics
- Contaminated Soil/Debris Waste

Content Mass/Weight (1)
- Max or Limit

Impactor Mass/Weight (1)
- Fork Lift

Constraint (2)
- Free to Move
- Constrained From Motion (Backed)

Impact Location (3)
- Lid-Center, Side-Lid, Side-Middle

Impactor Shape (1)
- Fork Lift Tine

Impactor Speed (3)
- 0.5, 2.5, 5.0 m/s

Total # of Analyses
- 3 x 1 x 1 x 2 x 3 x 1 x 3 = 54

SWB

Content Type (1)
- Heterogenous Debris Waste

Content Mass/Weight (1)
- Max or Limit

Impactor Mass/Weight (1)
- Fork Lift

Constraint (2)
- Free to Move
- Constrained From Motion (Backed)

Impact Location (3)
- Lid-Center, Side-Lid, Side-Middle

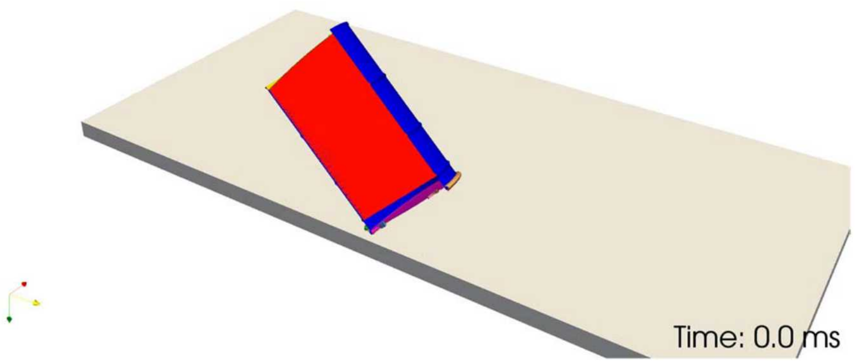
Impactor Shape (1)
- Fork Lift Tine

Impactor Speed (3)
- 0.5, 2.5, 5.0 m/s

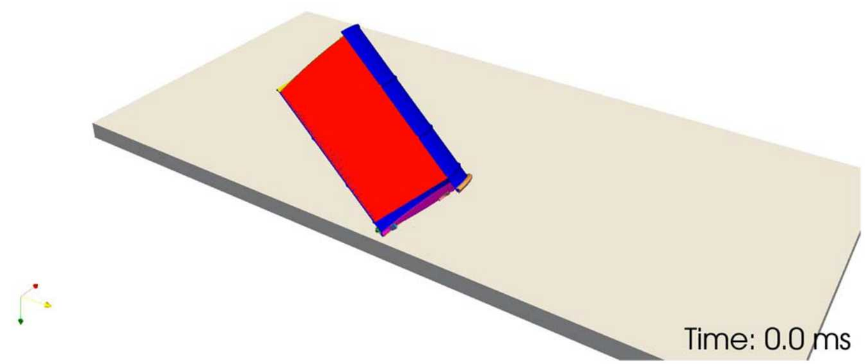
Total # of Analyses
- 1 x 1 x 1 x 2 x 3 x 1 x 3 = 18

7A Drop Cases

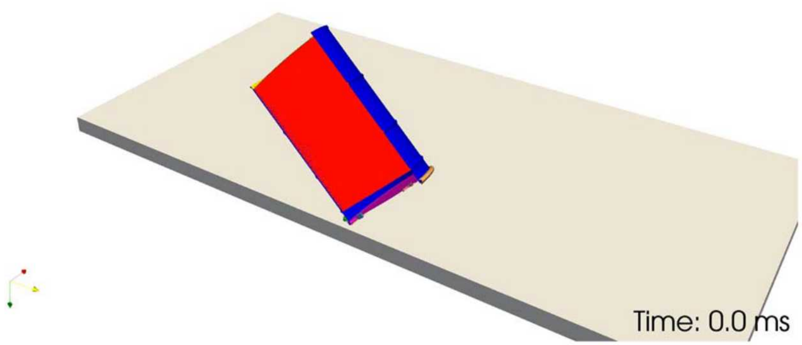
135 deg 20 m drop HS



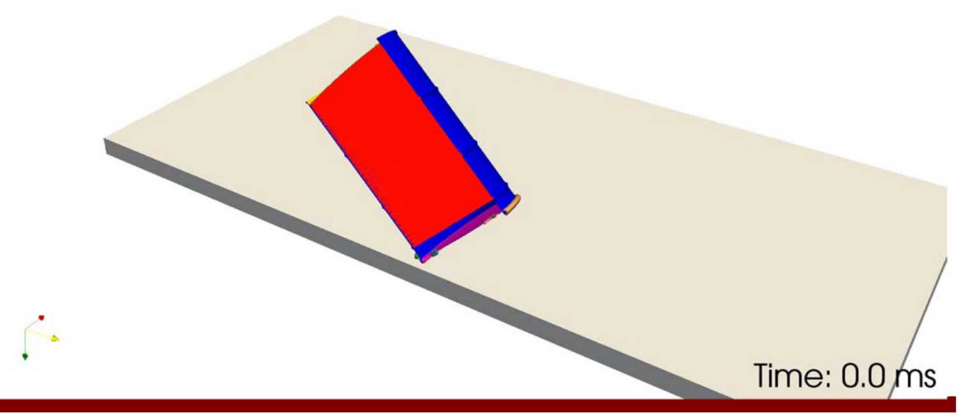
135 deg 10 m drop HS



135 deg 2.5 m drop HS

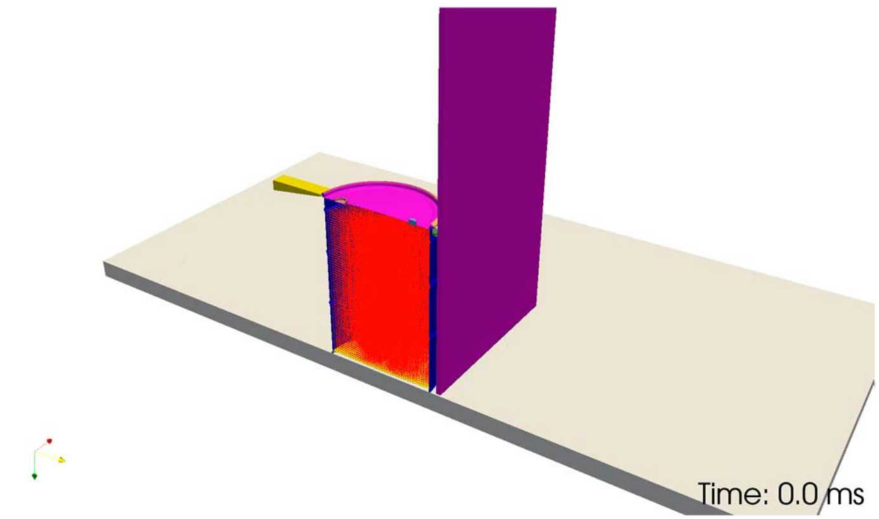


135 deg 5 m drop HS

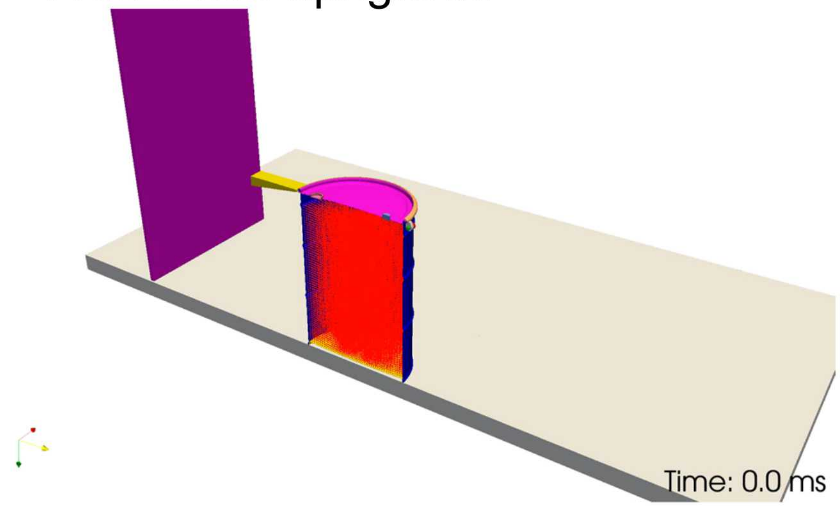


7A Puncture Cases – tine puncture

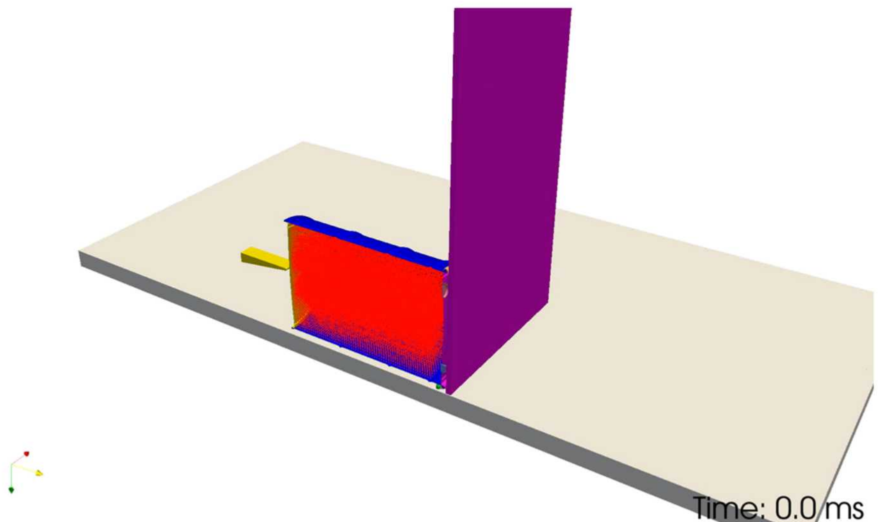
Fixed 5 m/s upright lid



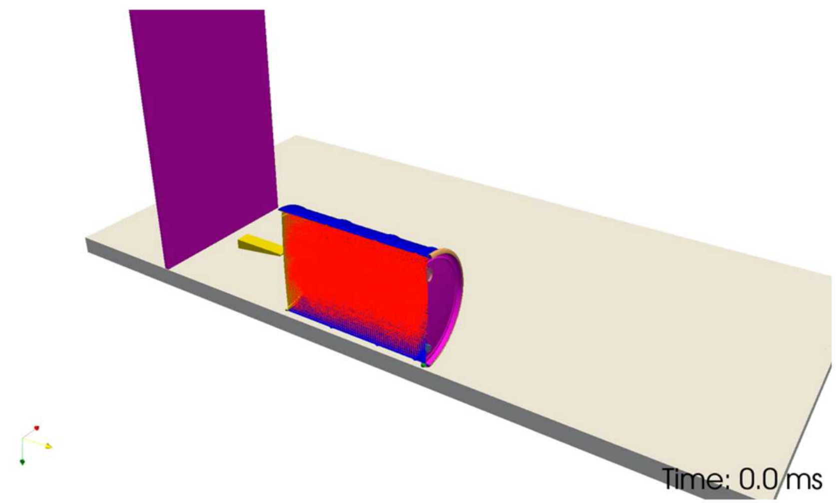
Free 5 m/s upright lid



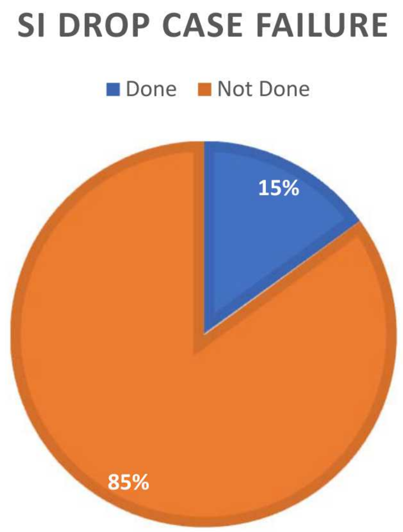
Fixed 5 m/s side bottom

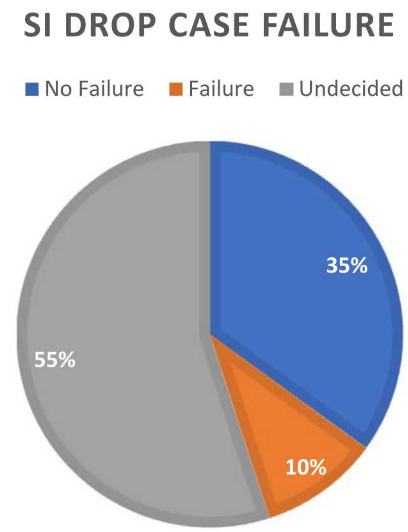


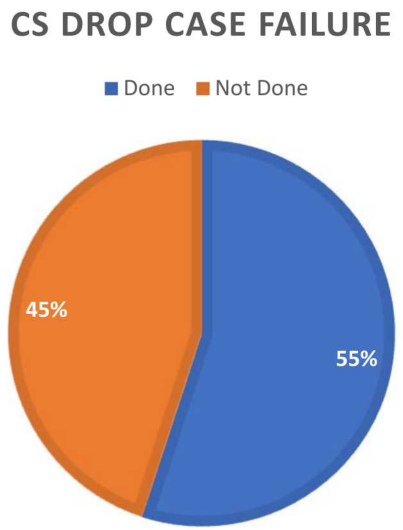
Free 5 m/s side bottom

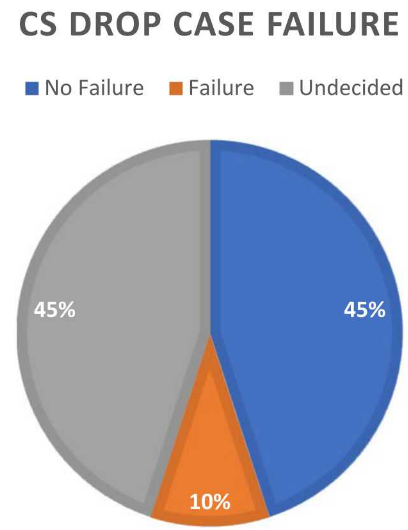


7A Drop Status and Results

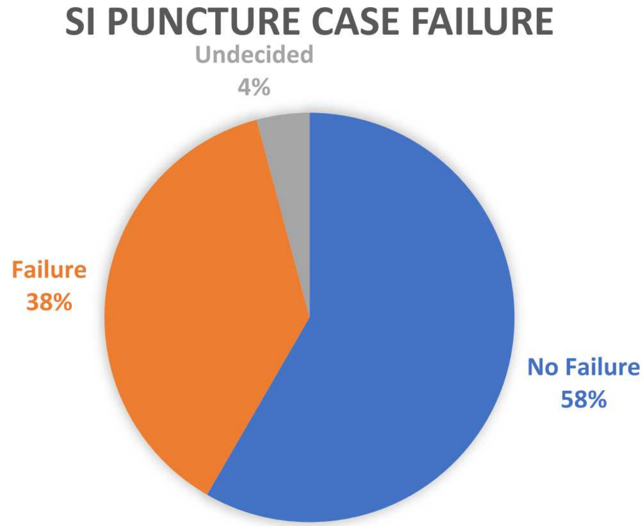


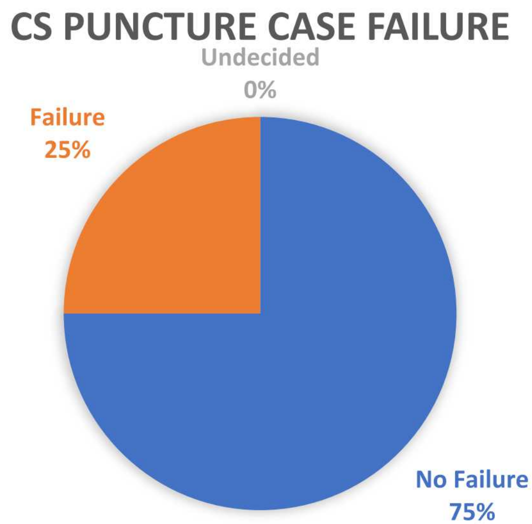






7A Puncture Results

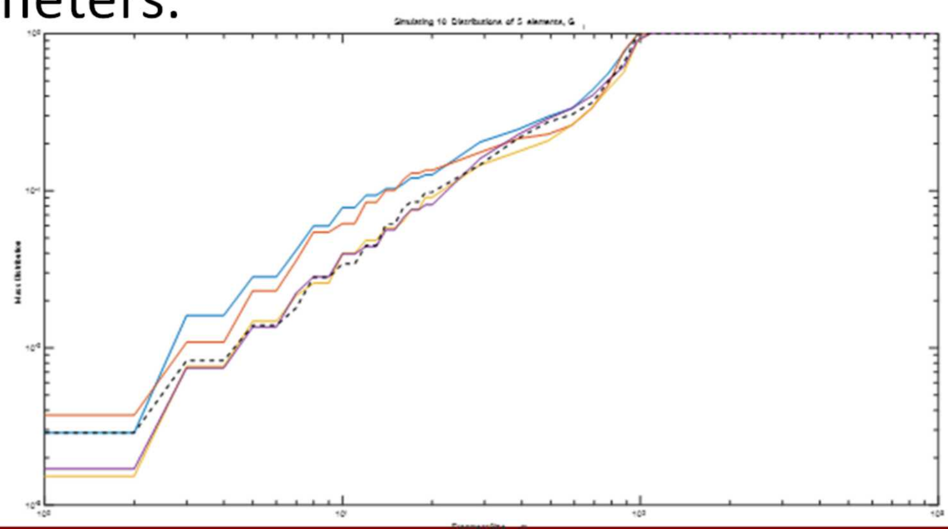




Task 3: Current Progress (1)

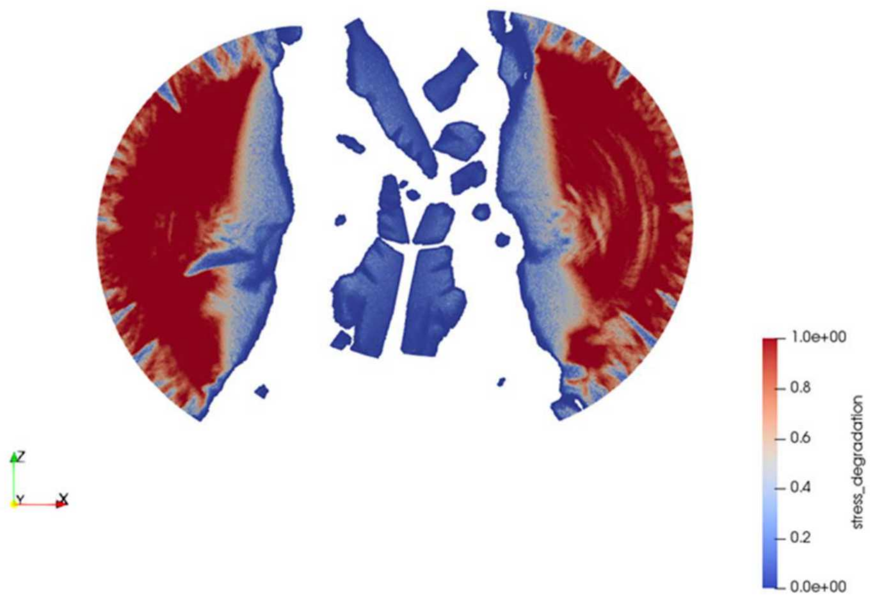
- Distributions of microscale parameters (Gi, sigmaci, thetai) have been implemented in microscale model. Parameters at microscale determine macroscale Fracture Energy and Critical Stress values (1D bar at microscale is assumed to break at weakest node, which should be also reflected by the macroscale parameters).
- Parameter sweeps have been implemented with Dakota coupled to the model in Sierra. Model appears to be insensitive to changes in the microscale parameters.
  - Debugging is being performed.

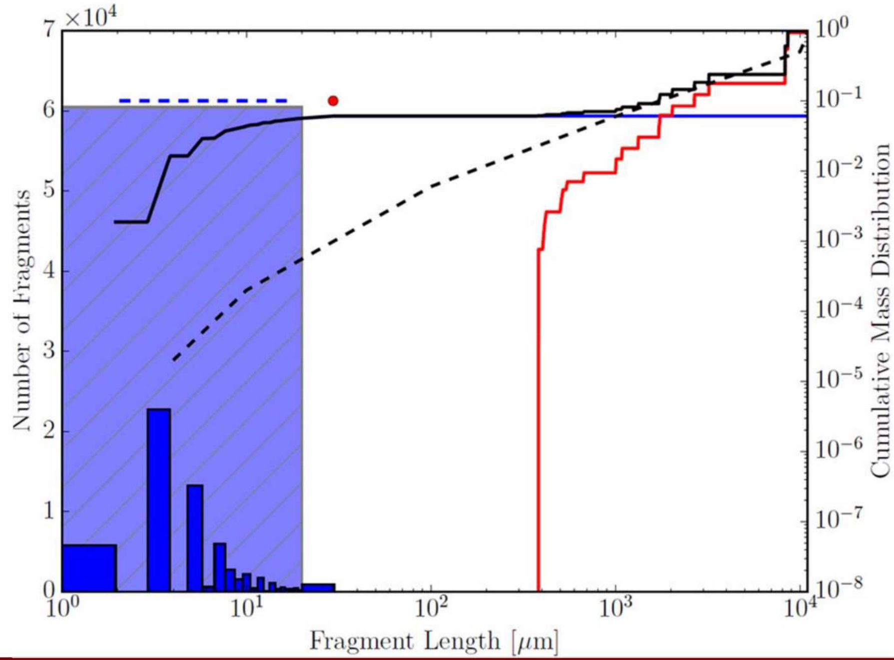
Changing Gi has a small effect on the distribution of mass at the microscale.



Task 3: Current Progress (2)

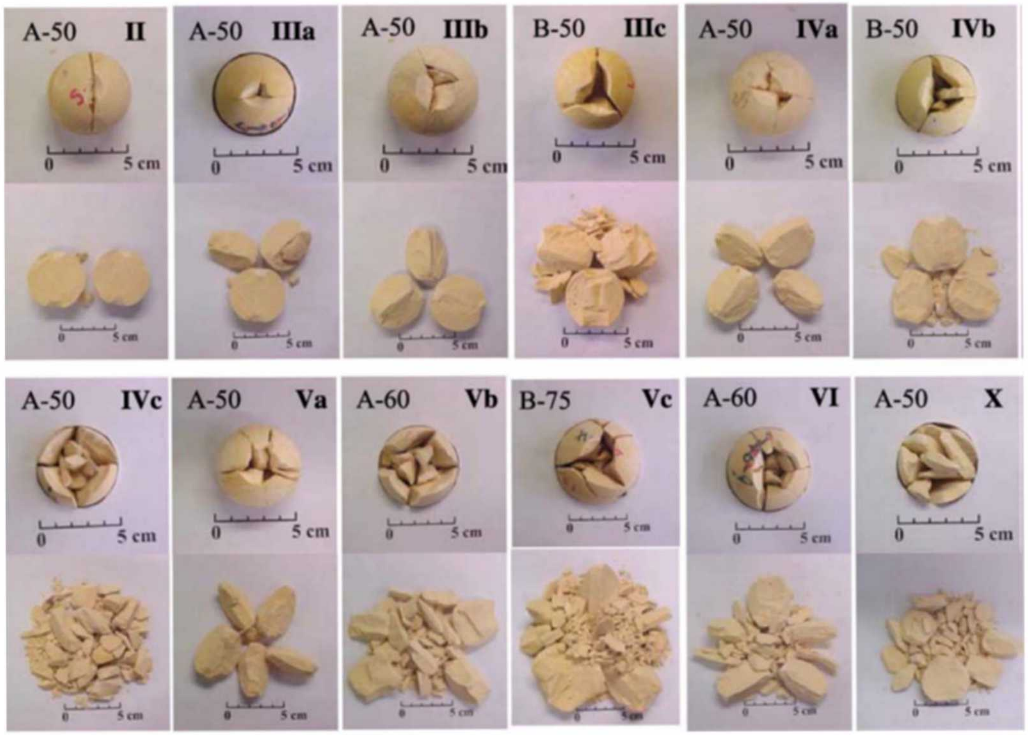
- Model is matching at the macroscale more closely now than previously, however too many small fragments are being produced as a result of an increased number of elements reaching the degradation criterion.
  - Debugging this now.





Task 3: Validation

- Fragmentation of Brittle Spheres
  - Crushing and fragmentation of brittle spheres under an impact test using spherical samples of brittle materials.
  - Simulation of this experiment is planned once issues with model have been debugged.



Summary and Conclusion

- In Task 1, we identified recent literatures that can add values to the Handbook in free fall powder and solid impact
- In Task 2, we began to simulate 7A drops based on the recent TRU waste stream information provided by LANL, and selection of the scenarios identified from the test matrix
  - 2nd container has been identified as SWB
- In Task 3, we have improved the concurrent fragmentation model to start to integrate the feedback and micromorphic model
  - To ensure the conservation of energy
  - This model is an improvement over the sequential fragmentation model discussed last year (NSRD-15)

Sandia National Laboratories

Back ups