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New Methods for Predicting Shock and Impact Induced Dispersal of Contained Liquids

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Fire Science and Technology Department

SAND2014-????C

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Background & Motivation

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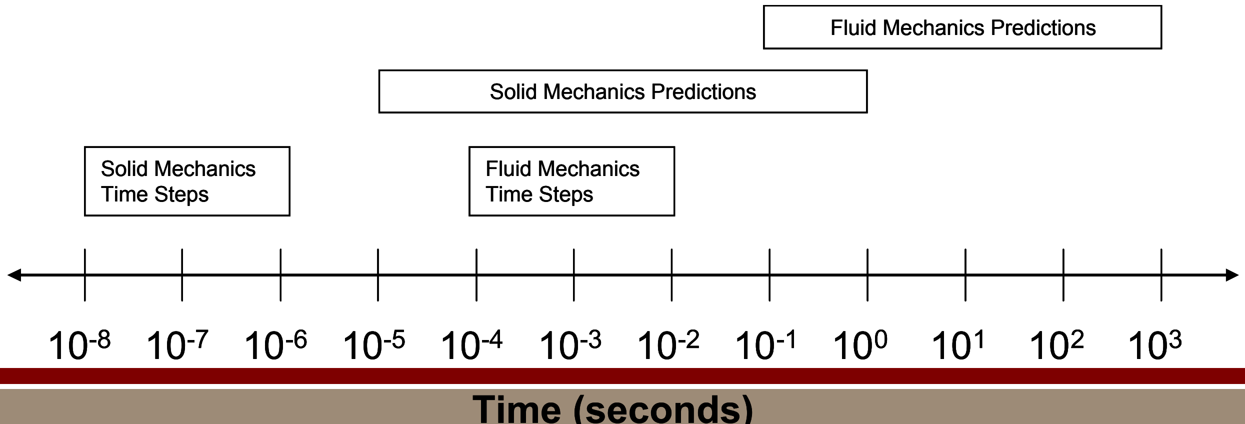
- Liquid dispersal from high-speed and detonation events are real scenarios that are challenging physical problems:
  - Thermal environments and fires resulting from aircraft and other transportation impacts
  - Dynamics of missile intercept
  - Ballistic rounds into fuel tanks and the subsequent environment
  - Use of improvised explosive devices (IEDs) to disperse chemical and biological agents (CBAs), similar accident scenarios
  - Nuclear and conventional weapons effects involving multiphase scenarios
  - In-flight aircraft response to battle or accident damage
- Challenges include:
  - Models required for wide range of length and time scales involved
  - Multidisciplinary physics regimes, changing importance of physics in each regime
  - Difficulty acquiring detailed data from such tests, survivability of instrumentation
  - Current lack of relevant validation data
  - Variety of relevant materials and their behavior in the different physics regimes

Current Status

- Tools to model liquid impact to fireball/dispersal are not mature
  - Impact and impulse physics tools are normally inadequate beyond a few seconds
  - Traditional fluid modeling tools lack the ability to model massively deforming structures
- Past work with a fluid code required data to initialize the calculations:
  - Silde, A., S. Hostikka, and A. Kankkunen, 2011, "Experimental and numerical studies of liquid dispersal from a soft projectile impacting a wall," Nuclear Engineering and Design, 241, pp. 617-624.
- Recent modeling work has focused on combining predictions from structural dynamics and fluid dynamics simulation tools



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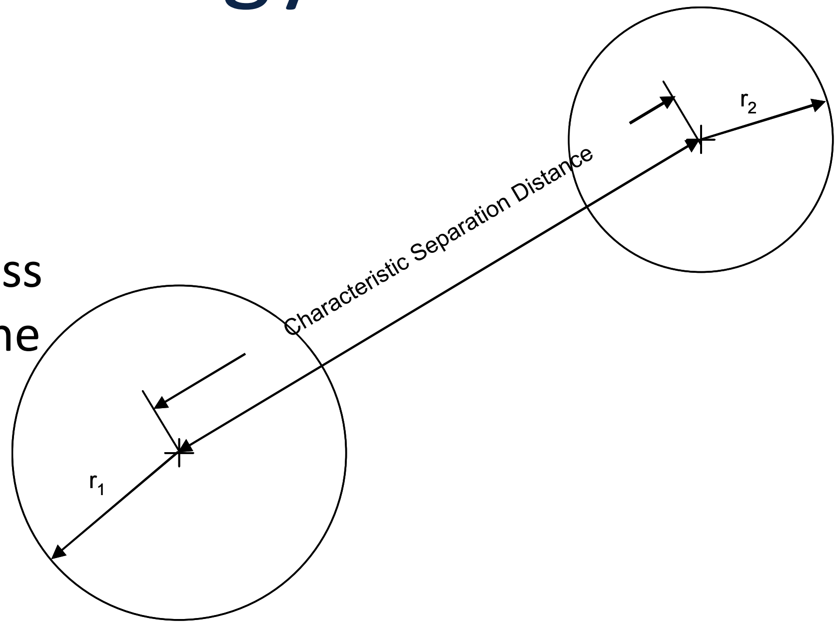
Coupling Strategy

- SPH mass/momentum conserved in a transfer between the two codes
- Mass is transferred according to an algorithm that uses a critical dimensionless particle separation distance (B_{crit}) to define transfer times:

$$B = \frac{CharacteristicSeparationDistance}{CharacteristicDropLength}$$

- All liquid mass is assumed to be spherical drops until transfer to CFD code
- Drops subsequently are predicted to distort and break-up according to the Taylor Analogy Break-up (TAB) model
- Lagrangian/Eulerian coupling employed for evaporating drops

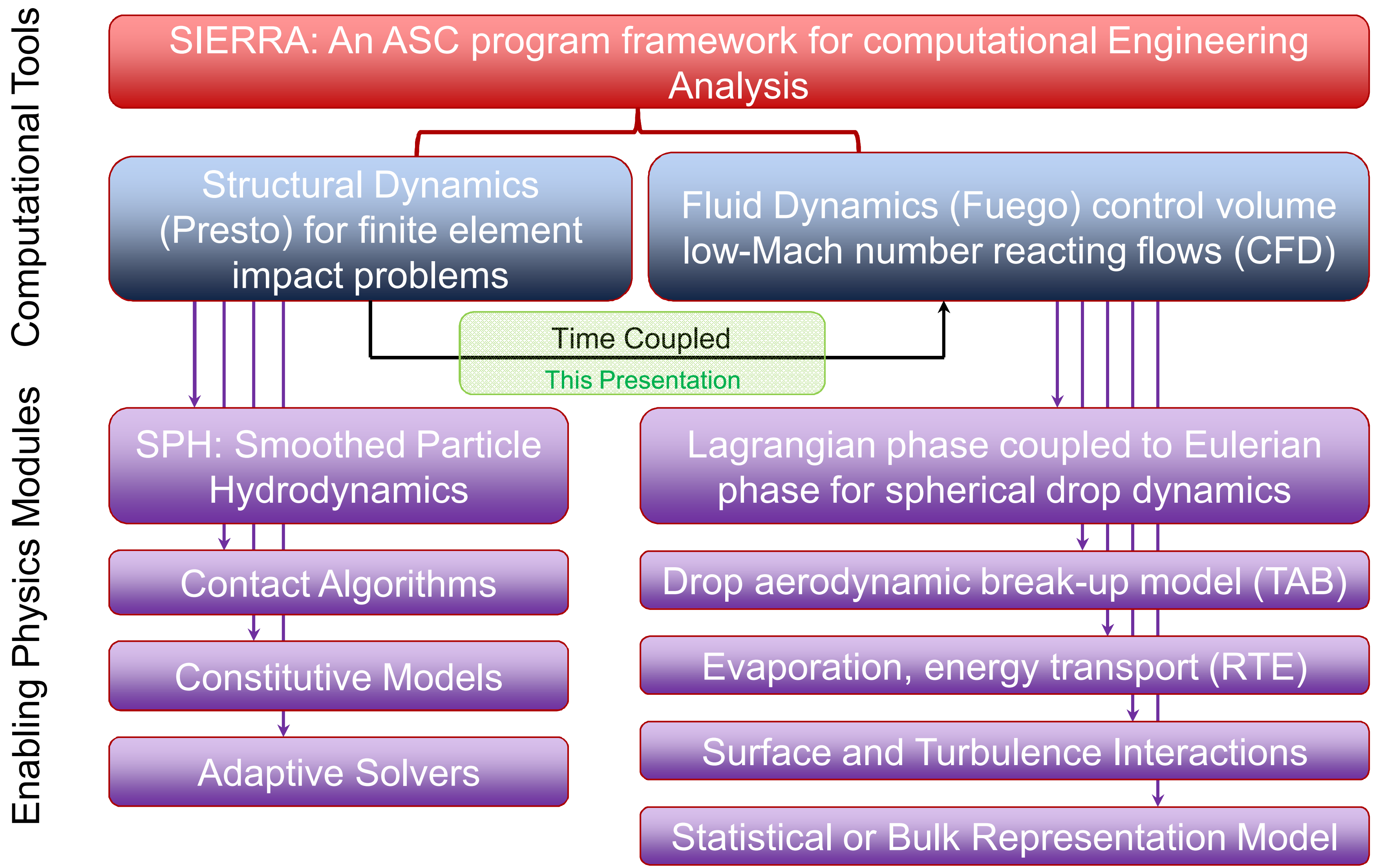


B_i assessed at each time for each particle

$$B_i = \min_{j=1\ to\ N} \left\{ \frac{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}}{d_i/2 + d_j/2} \right\}; i \neq j$$

Using this definition for B_{crit}, reasonable B_{crit} values are between 1.0 and 1.7

General Approach Schematic



Previous Studies

- This capability has been demonstrated for several scenarios:
  1. A notional 1 foot cubic tank of heptane fuel at aviation speeds into an immobile target[1]
  2. A cylindrical tank of liquid into a concrete target (for data comparisons)[2]
  3. Liquid dispersal caused by the breaking mechanism for a rocket sled (pre-test predictions for instrumenting the 2/17/13 test)[3]
  4. A detonation inside[4] a liquid tank
  5. A detonation outside[5] a liquid tank
- References:

1. Brown A.L., "Impact and Fire Modeling for Complex Environment Simulation," The 2010 Western States Meeting of the Combustion Institute, Paper # 10S-12, March 21-23, 2010, Boulder, CO, USA.
2. Brown, A.L., 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 - 021004-10, (2012).
3. Brown A.L., Metzinger, K.E., "Computational Test Design for High-Speed Liquid Impact and Dispersal," The ASME/JSME 2011 8th Thermal Engineering Joint Conference, March 13-17, 2011, Honolulu, HI, USA, AJTEC-44422.
4. Brown, A.L., C. Feng, F. Gelbard, D. Louie, and N.E. Bixler, "Predicted Liquid Atomization from a Spent Nuclear Fuel Reprocessing Pressurization Event," The 2014 ASME/AIAA Summer Conference, Atlanta, Georgia, June 16-20, 2014.
5. Brown, A.L., "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.

Objectives

- The five existing scenarios under varying conditions provide good context for evaluating the coupling capability
- There is believed to be a need for improved models relating to the last injection that circumvents the B_{crit} criteria
- This work evaluates the final injection of cases from previous work

Outline

- Introduce the five scenarios illustrating results from past work
- Show new analysis of the final injection for each case
- Discuss the grounds for formulating an additional injection criterion

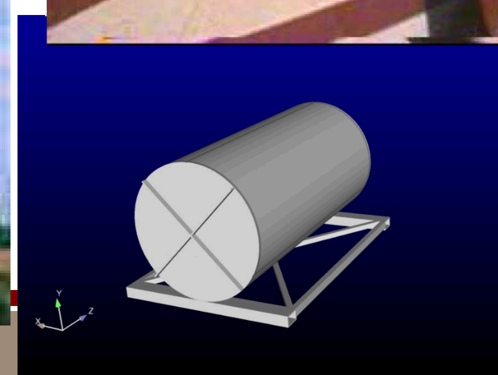
Scenarios

Scenario	Cases	SPH#	Fluid Mesh	References
Water Slug Impact	7	417K	355K	Brown et al., 2012 [6]
Aluminum Tank Impact	12	1-50K	250-2,000K	Brown, 2010 [8]
Sled Track Brake	4	320-2,500K	700-2,000K	Brown and Metzinger, 2011 [7]
Detonation Outside Tank	10	50-400K	370-2,940K	Brown, 2013 [5]
Detonation Inside Tank	2	45K	530K	Brown et al., 2014 [4]

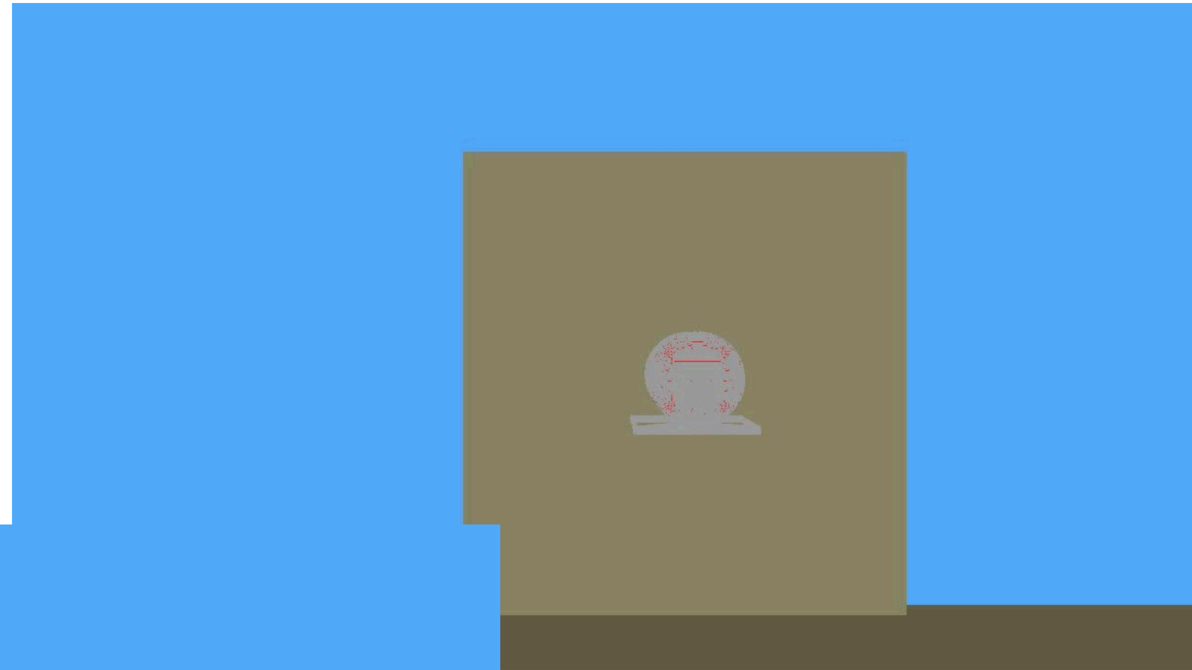
Scenario	Solid model	Parameters Varied	Fluid	Compared to data?	SM time
Water Slug Impact	SPH	Geometry Wind B_{crit}	Water	Particle Sizes Liquid Deposition Liquid Spread	120 ms
Aluminum Tank Impact	SPH	SM Mesh FM Mesh B_{crit} SM run time	Heptane	No	12-18 ms
Sled Track Brake	Finite Element	Impact Velocity Liquid Depth SM Mesh	Water	In Progress- Liquid Deposition	140 ms
Detonation Outside Tank	Finite Element	Explosive Intensity SM Mesh FM Mesh B_{crit}	Water	No	20-300 ms
Detonation Inside Tank	Finite Element	Quantity of Explosive	Nuclear Fuel Reprocessing Fluid	No	80 ms

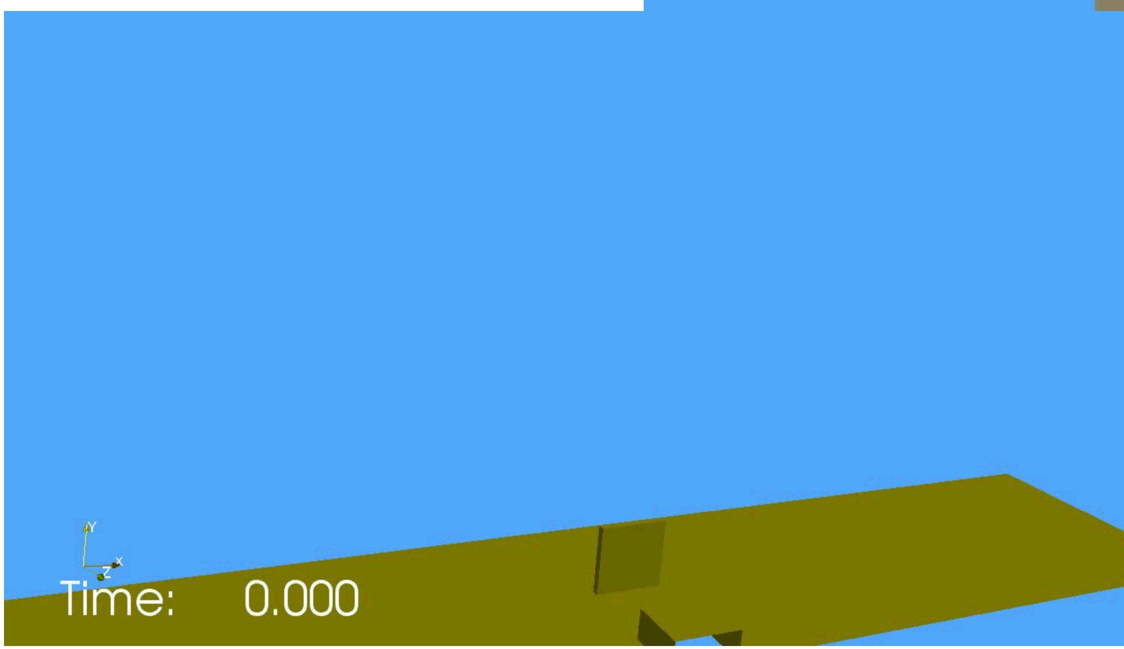
1. Water Slug Impact Validation

- Tests performed in 2002 provided data for validating liquid spread dynamics for an aluminum tank impacting a concrete slab
- Liquid deposition, particle sizing, and video data



Simulation Videos

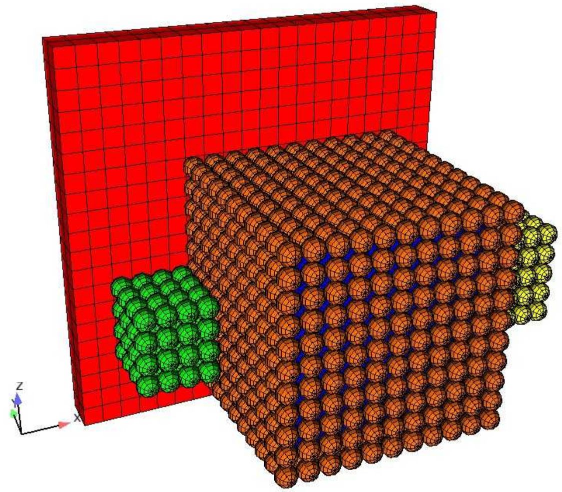




2. Aluminum Tank Impact

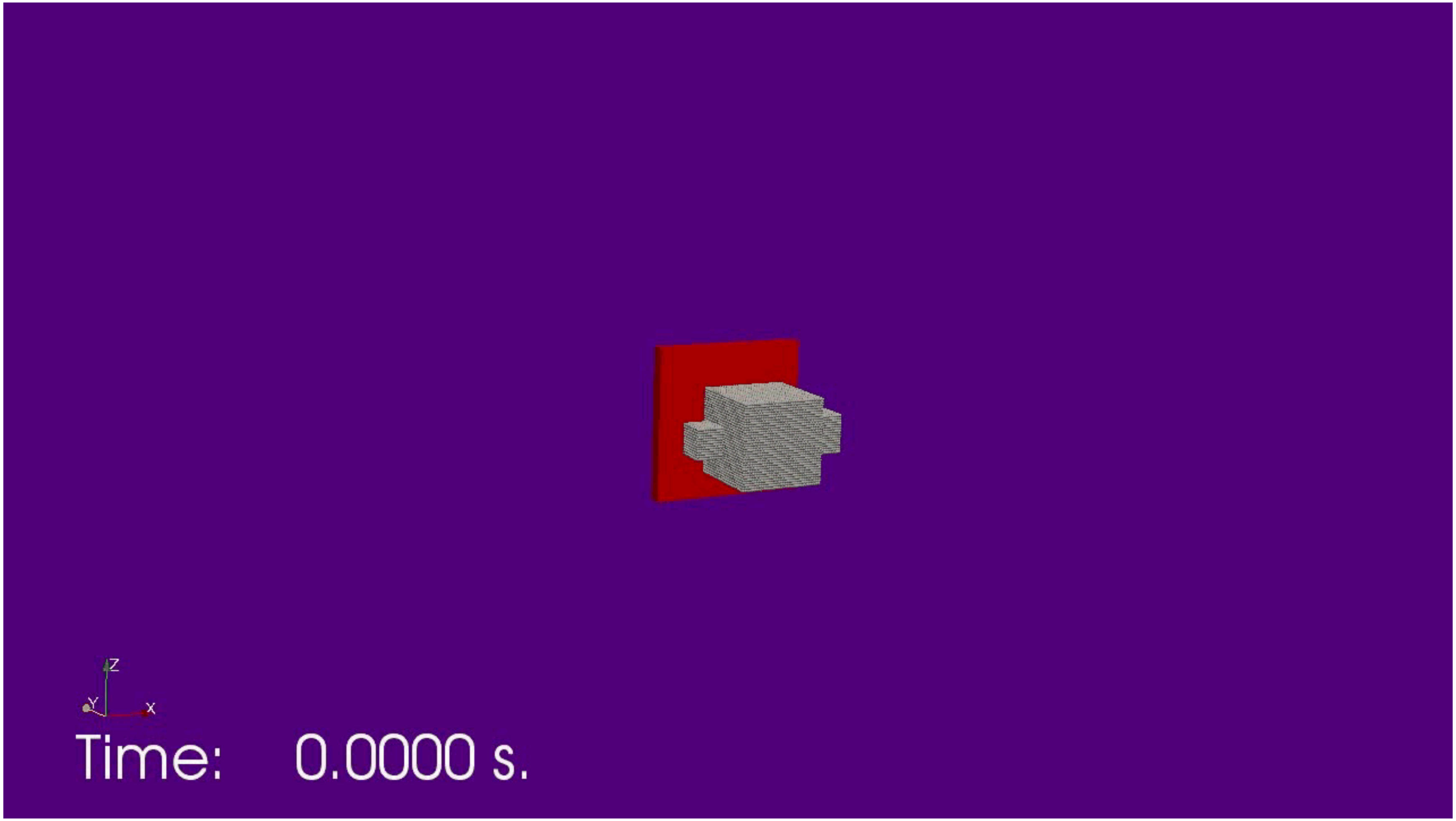
Designed to help understand discretization sensitivities

- 23 cm cube of liquid in a 2.54 cm thick aluminum tank with two adjacent cubes
  - Impact an immobile target at 182 m/s
  - Presto modeled with SPH and 4 levels of refinement
- Open air environment with ground located 6.35 m below impact point
  - Two levels of fluid mesh refinement



Medium Video

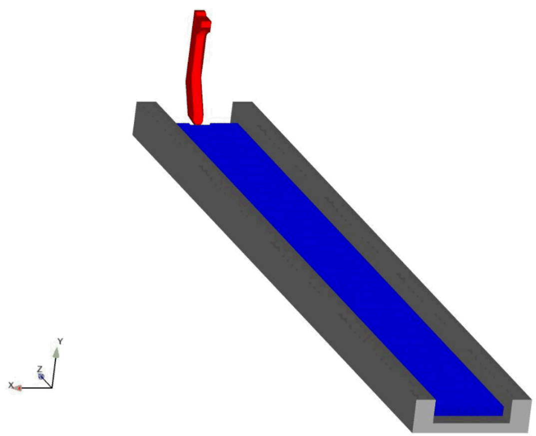
- Case mfs
- Fluid Mechanics predictions show liquid drops off-set and colored by size



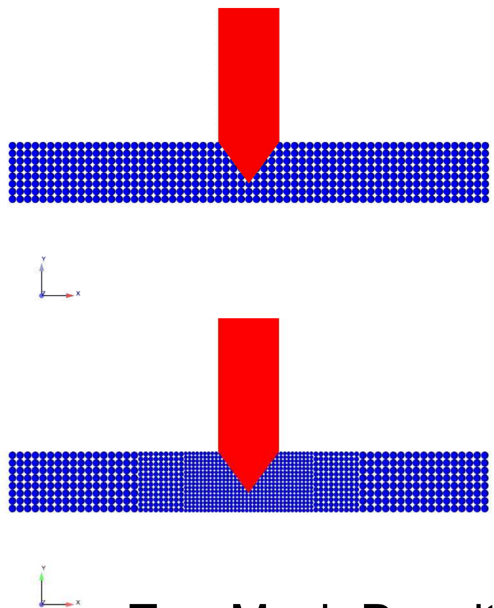
3. Sled Track Brake

These simulations are pre-test design calculations to locate instruments for validation data:

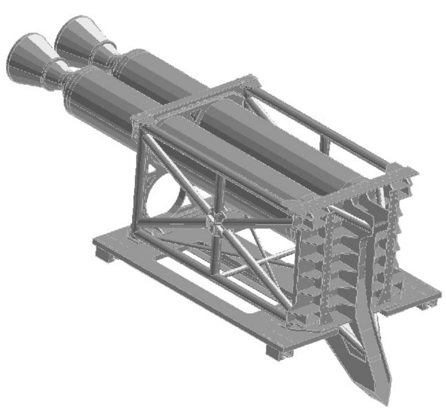
- liquid dispersal velocity (photometrics)
- local droplet size distributions and velocities (Malvern Spraytec and phase Doppler particle analyzer)
- ground level liquid deposition (catch pans)
- droplet evaporation and vapor transport (RH sensors)



Initial Presto Geometry



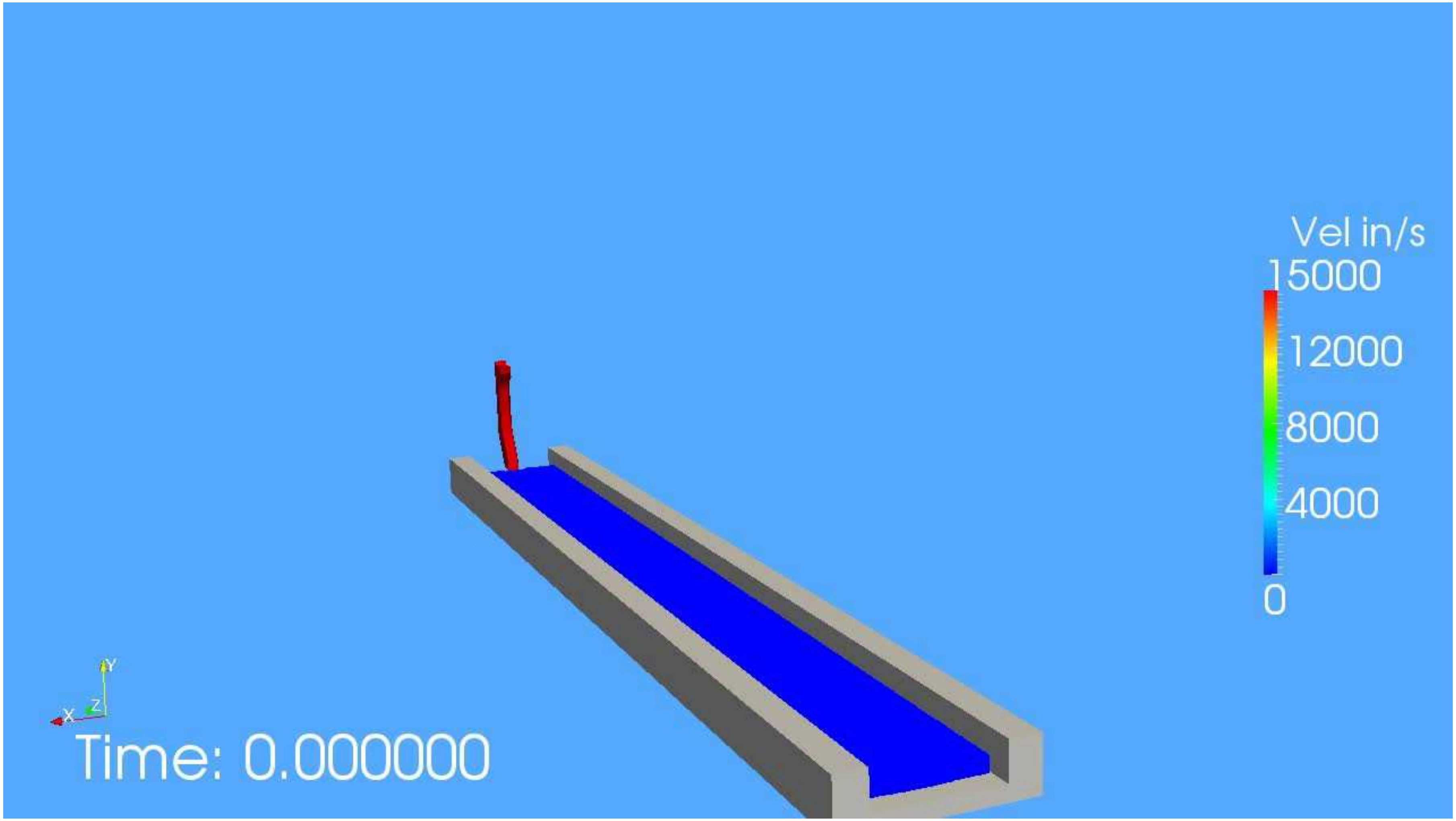
Two Mesh Densities Used



Designed Geometry

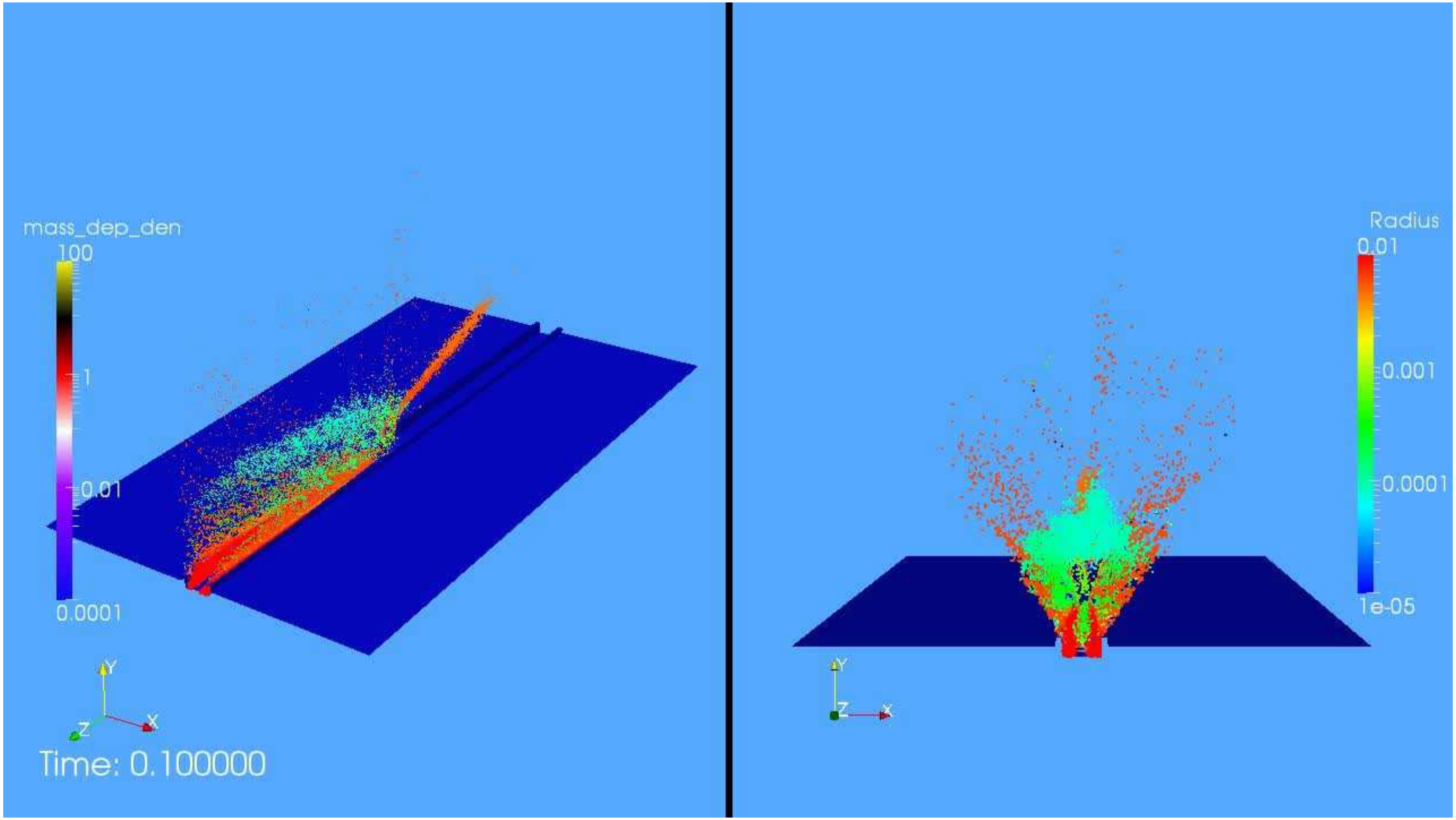
Sled Track Structural Mechanics Video

Case S3

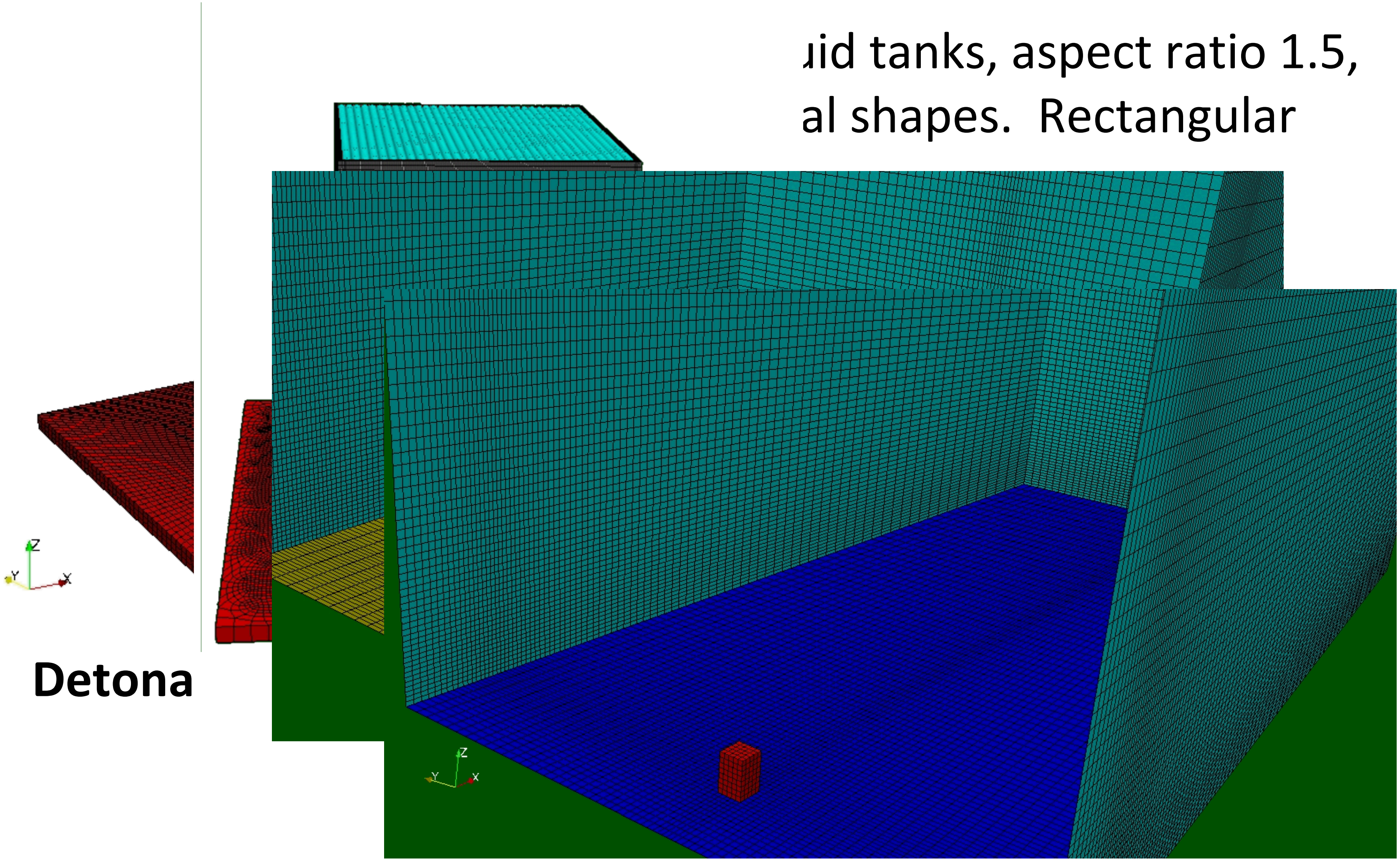


Sled Track Fluid Mechanics Video

Case F1



4. Detonation Outside Tank



- ıid tanks, aspect ratio 1.5, al shapes. Rectangular
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-
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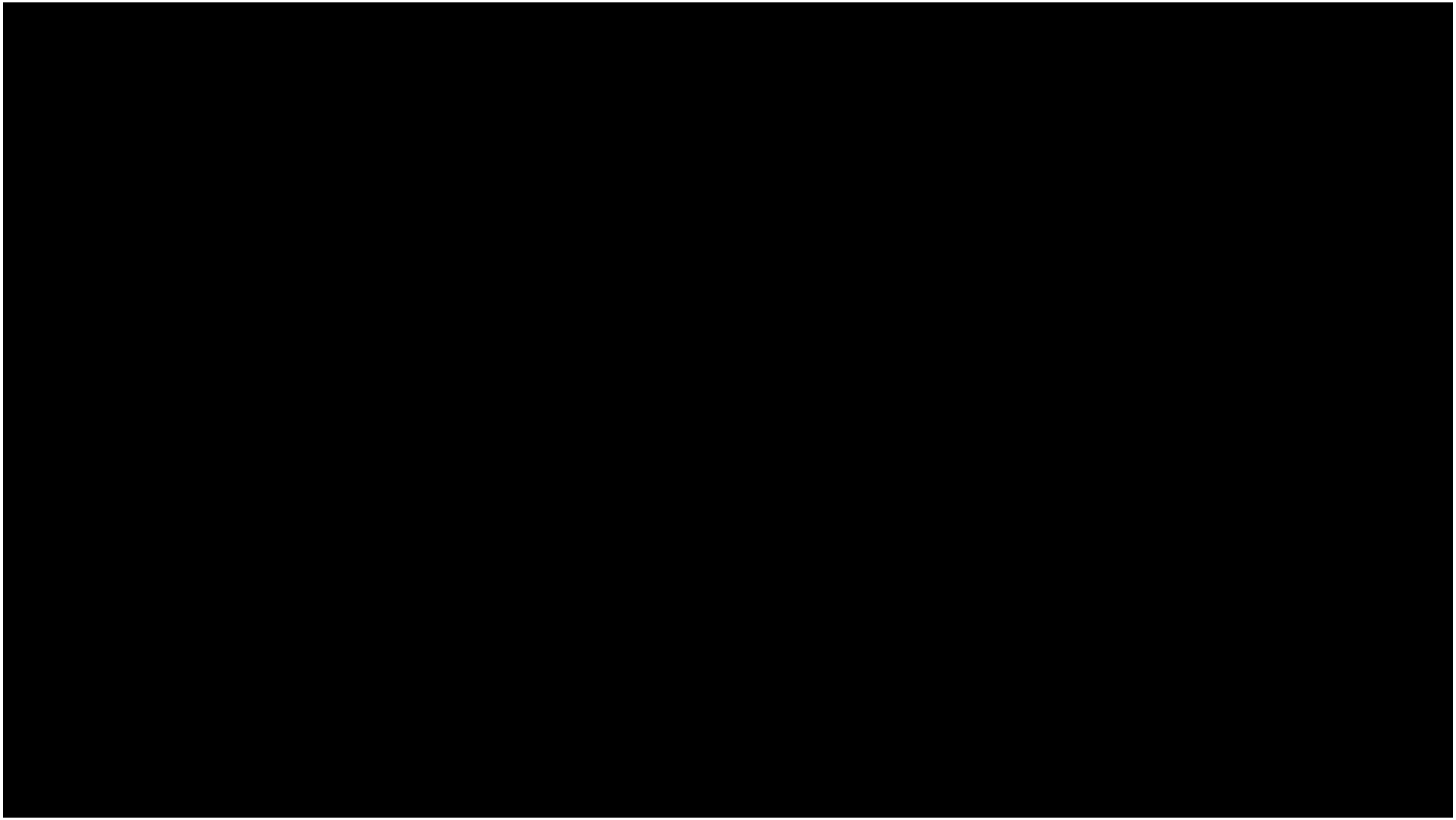
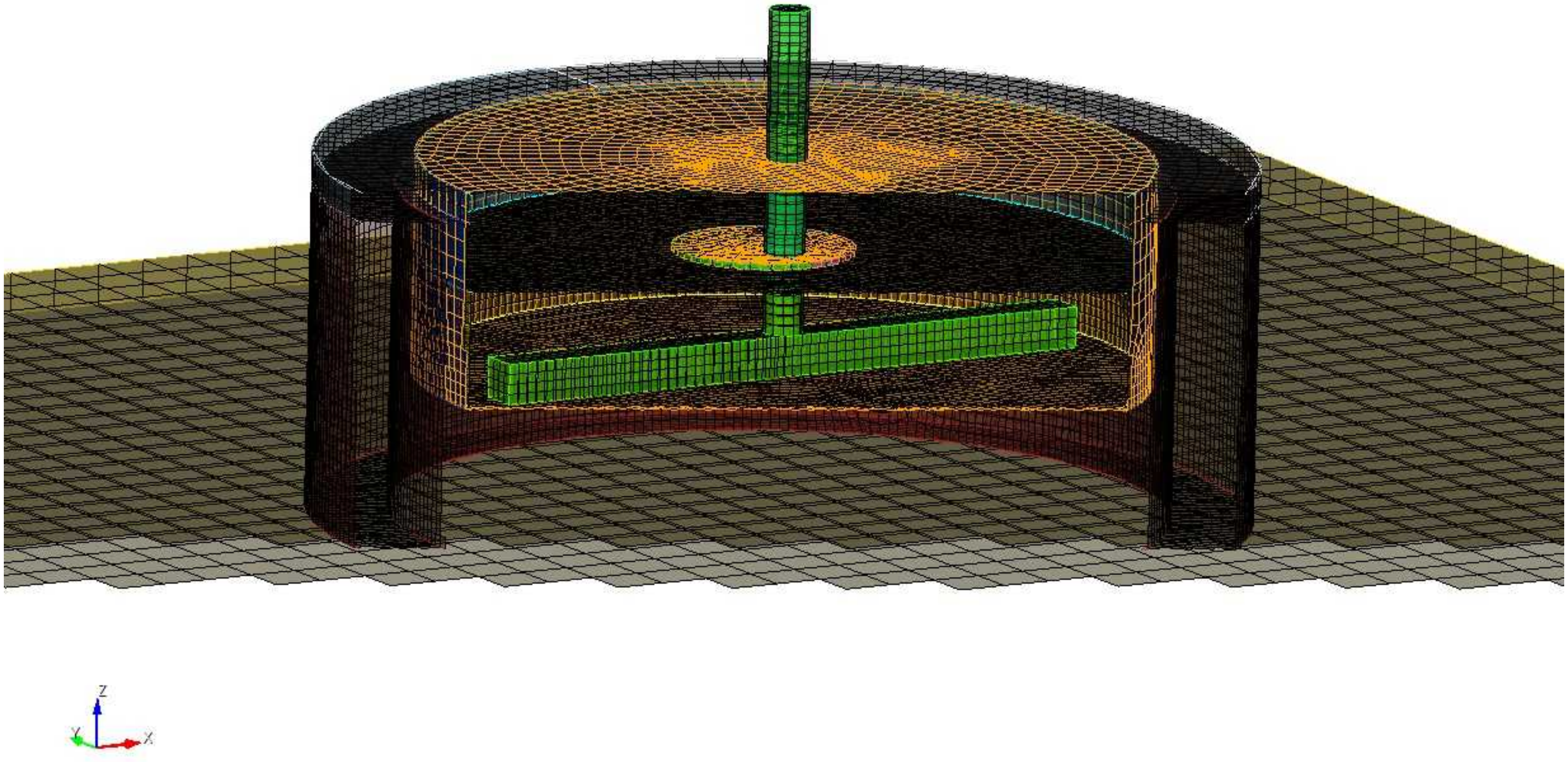
- **Detona**

Combined Video

Case 4



5. Detonation Inside Tank



Simulated Explosion and Aerosol Release in Denitrator (700 MJ)

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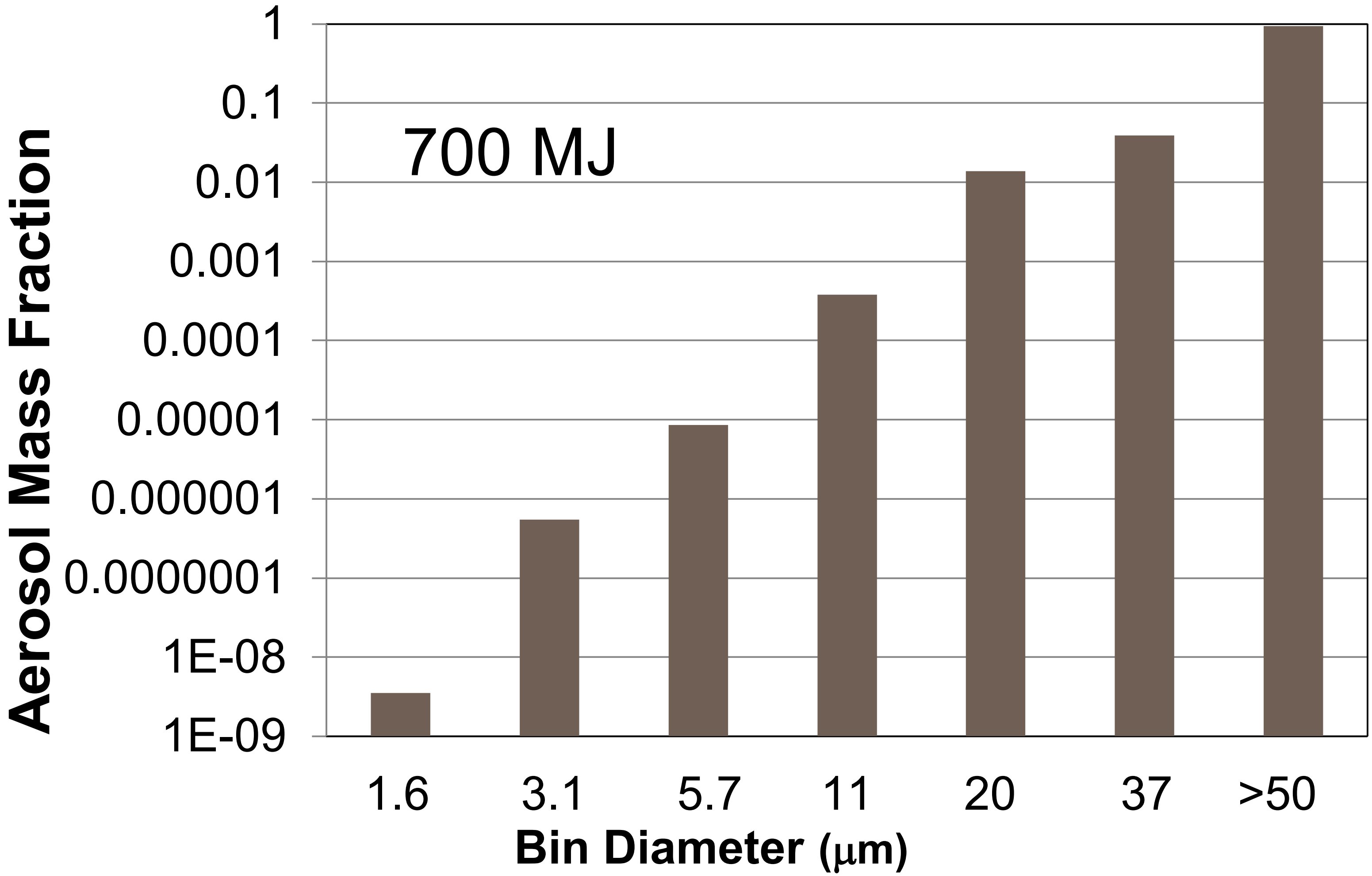
Preliminary Estimate of Aerosol Distribution 10^{-5}% Respirable (~<20 Micrometer Diameter)



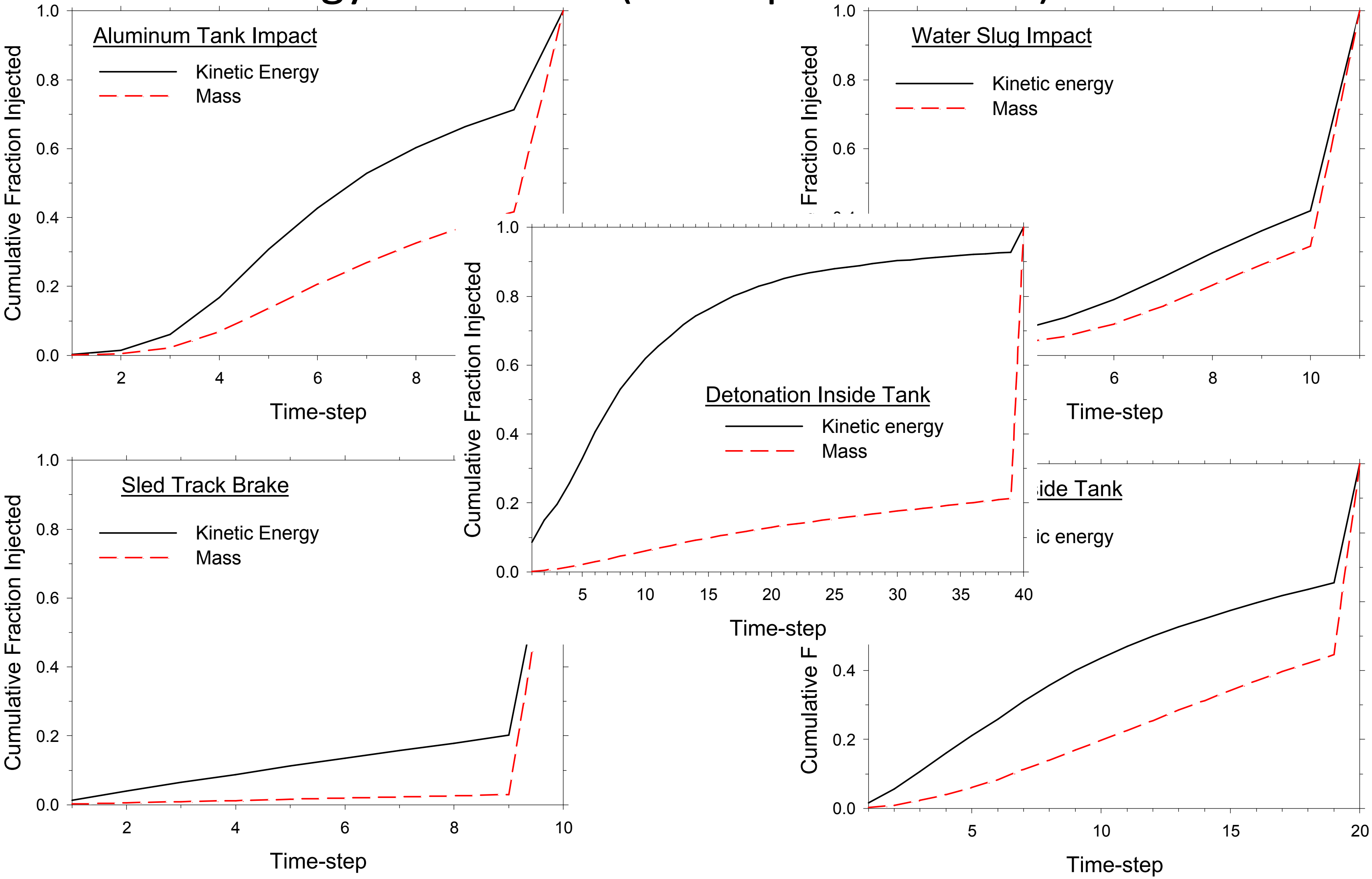
Scenarios

- A single case from each scenario is selected for subsequent analysis
  - The scenarios represent a range of application space
  - The selected cases are good representative cases
- Particular attention is paid to the last injection
  - This is normally the most stressing injection
  - Mass may be injected at this time despite violating the B_{crit} threshold
  - This is the mass that will contribute to a dense phase if such a model is implemented

Scenario	Case	B_{crit}	SPH#	Reference
Water Slug Impact	Case 7	1.5	417,792	Brown et al., 2012 [6]
Aluminum Tank Impact	cfs1.3	1.3	19,653	Brown, 2010 [8]
Sled Track Brake	S1/F1	1.3	322,016	Brown and Metzinger, 2011 [7]
Detonation Outside Tank	Hex3 (Case 5)	1.3	49,152	Brown, 2013 [5]
Detonation Inside Tank	HighE	1.5	44,813	Brown et al., 2014 [4]

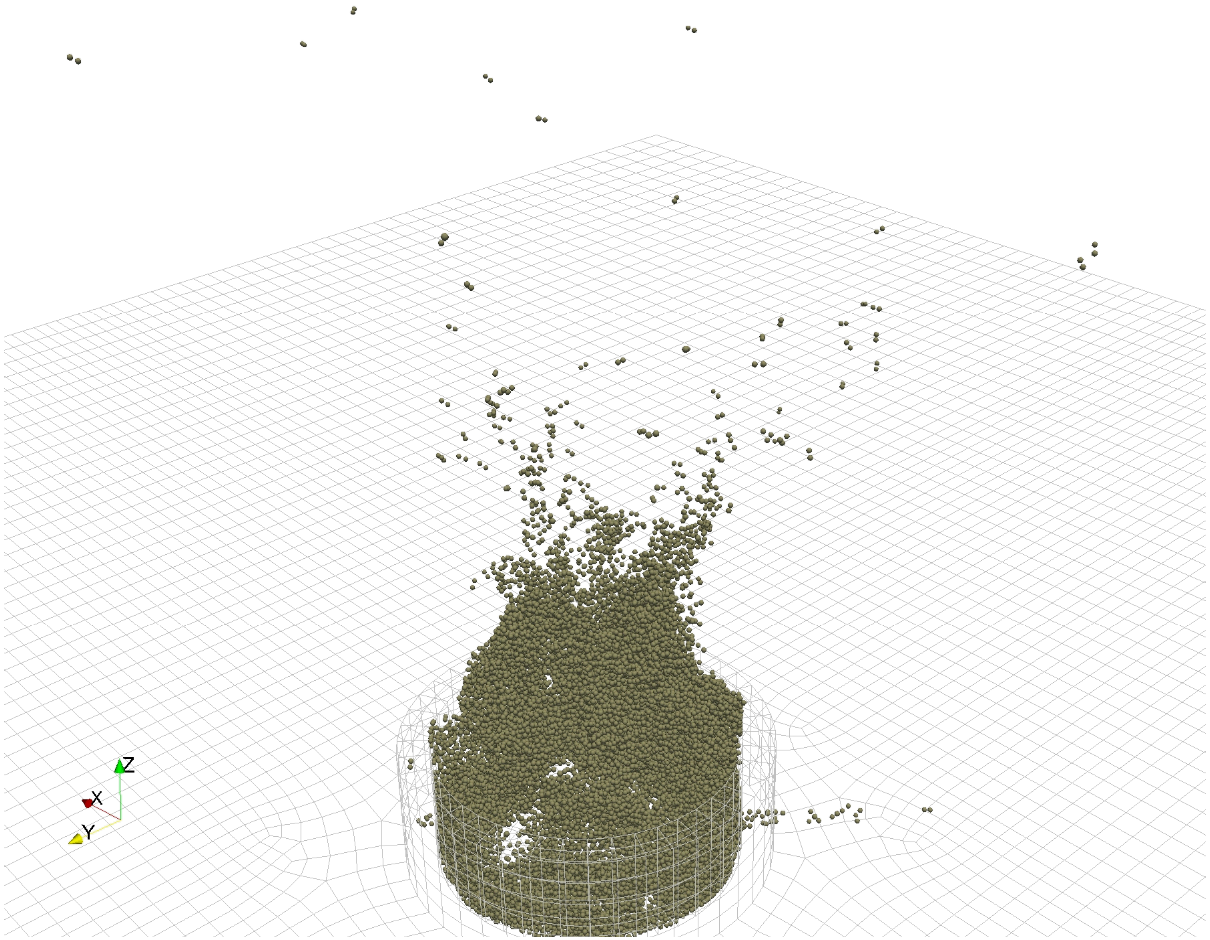
Mass and Kinetic Energy of Injections

- Kinetic energy leads mass (faster particles first)



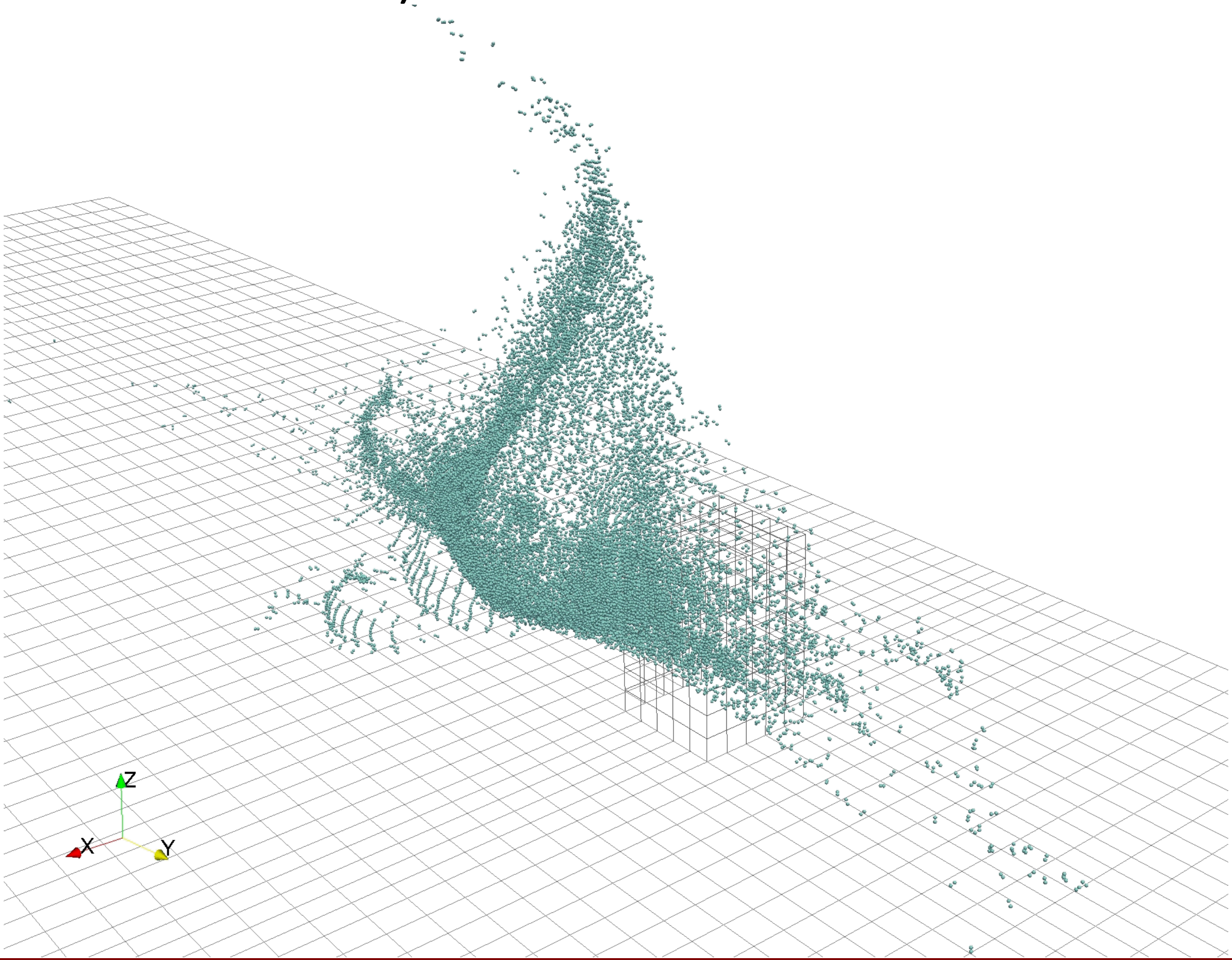
Final Injection Illustration

- The last injection is populated with pairs in many cases (detonation inside tank scenario below



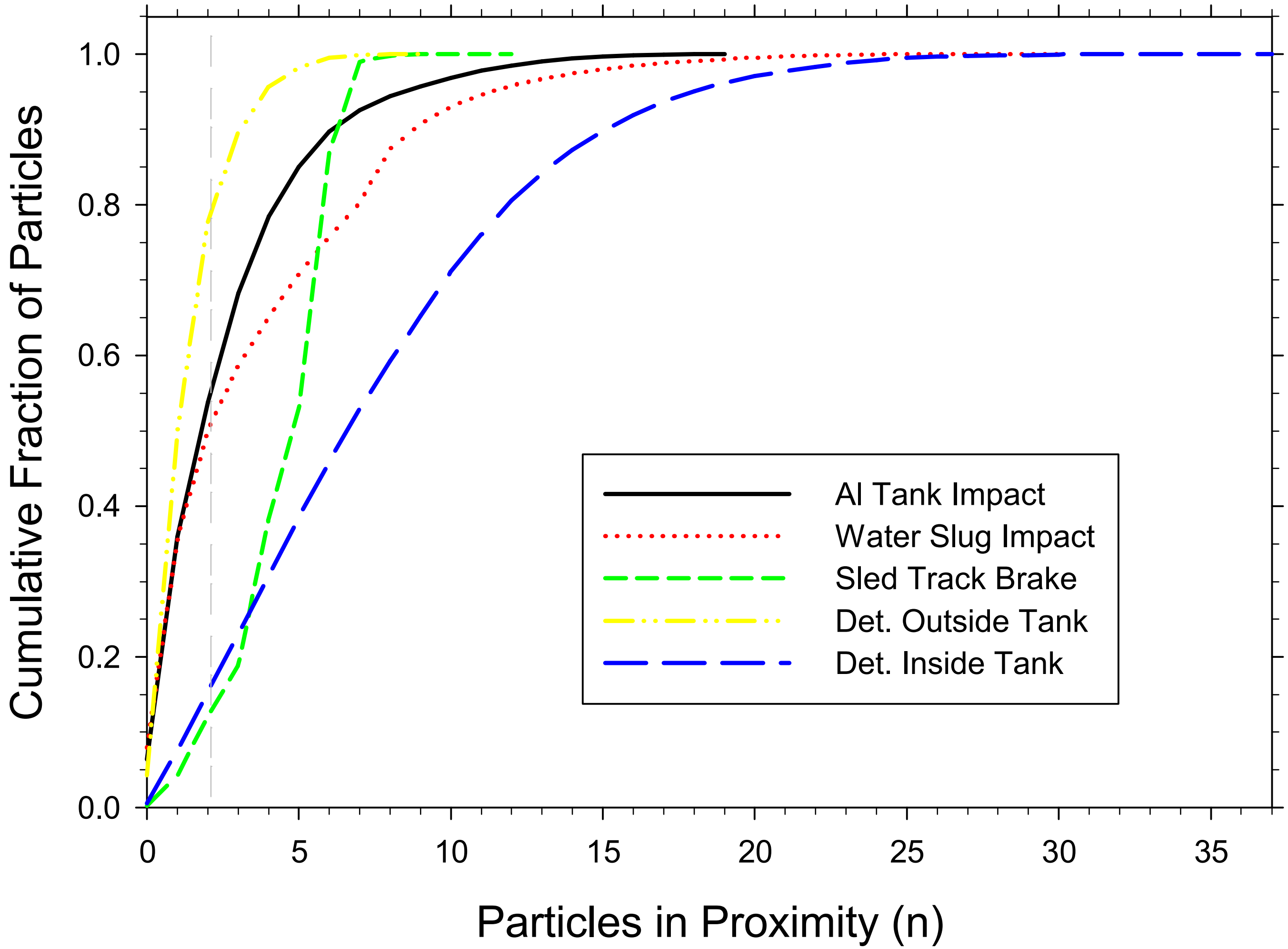
Final Injection Illustration

- Linear systems are also found in some scenarios (Detonation Outside Tank Scenario)



Cumulative B Plot

- Counting the number of particles within B_{crit} suggests the density of the mass at the end of the transfer



What does this mean?

- The injection criterion related to a B_{crit} does not capture some of the particles that may be injected
- An additional criteria are needed to capture additional mass in the transfers
- This will help, but there will still be scenarios with dense regions and mass and kinetic energy jumps at the final time step
- Improved criteria will help isolate the final injection liquid for improved modeling of the dense region of the spray

Summary

- A new capability exists to predict the dispersal of contained liquids
- The B_{crit} transfer criterion may be improved upon based on evaluations of the final injection for five existing cases
  - Linear chains of liquid
  - Binary pairs
- The various cases have significantly different dense zones at the final injection time
- Current work is aimed at improving the modeling methods for this dense spray region

Extra Viewgraphs

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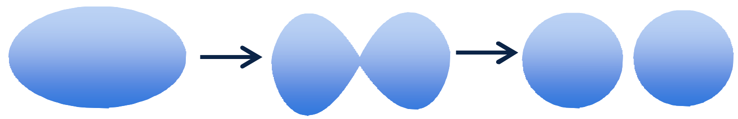
Taylor Analogy Break-up (TAB) Model

- Originally by O'Rourke and Amsden (1987)
- Approximates the drop as a damped oscillator, formulated as a second-order differential equation, with y as a deformation parameter:

$$m_d \frac{d^2 y}{dt^2} = \underbrace{m_d \frac{C_F}{C_b} \frac{\rho_g}{\rho_l} \frac{\left| u_d - u_g \right|^2}{r^2}}_{\text{Aerodynamic Forcing}} - \underbrace{m_d \frac{C_k \sigma}{\rho_l r^3} y}_{\text{Surface Energy Damping}} - \underbrace{m_d \frac{C_d \mu_l}{\rho_l r^2} \frac{dy}{dt}}_{\text{Viscous Damping}}$$

Simplified Schematic



- Discretized solution for y is:

$$y(t+\Delta t) = \frac{We}{C} + \left\{ \left(y(t) - \frac{We}{C} \right) \cos(\omega \Delta t) + \frac{1}{\omega} \left(\dot{y}(t) + \frac{y(t) - We/C}{\tau_b} \right) \sin(\omega \Delta t) \right\} \exp(-\Delta t / \tau_b)$$

$$\dot{y}(t+\Delta t) = \frac{\frac{We}{C} - y(t)}{\tau_b} + \left\{ \frac{1}{\omega} \left(\dot{y}(t) - \frac{y(t) - We/C}{\tau_b} \right) \cos(\omega \Delta t) - \left(y(t) - We/C \right) \sin(\omega \Delta t) \right\} \omega \exp(-\Delta t / \tau_b)$$

$$\omega = \sqrt{\frac{8 C_k \mu}{\rho_l d_p^3} - \frac{1}{\tau_b^2}}$$ Oscillation Frequency

$$\tau_b = \frac{1}{2} \frac{\rho_l d_p^2}{C_d \mu_l}$$ Viscous Damping Time

$$We = \frac{\rho_l d_p (u_p - u_g)^2}{\sigma}$$ Weber Number

- New drop diameters can be calculated:

$$d(t+\Delta t) = d(t) / \left[1 + \frac{C_k K}{20} + \frac{\rho_l d_p(t)^3}{8\sigma} \frac{6K-5}{120} \dot{y}(t)^2 \right]$$

- We modified the algorithm to limit break-up for new particles

Simulation Matrix

The simulation matrix involved three Presto calculations and four Fuego calculations.

Structural Test Matrix

Simulation	Water Element Size (cm)	Water Draw (cm)	Initial Scoop Velocity (m/s)
S1	1.9	10.2	146
S2	1.9	15.9	91.4
S3	0.95-1.9	10.2	146

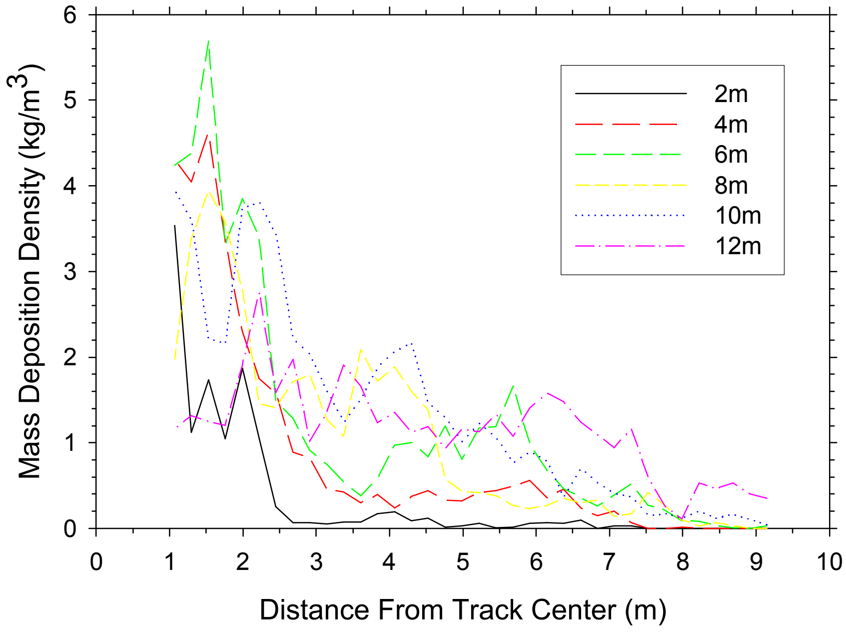
Fluid Test Matrix

Fuego Simulation	Presto Sim.	Simulation Transfer Time (s)	Number of Transfers	Fuego Mesh Elements (Thousands)
F1	S1	0.01-0.10	10	700
F2	S2	0.02-0.24	11	700
F3	S3	0.01-0.11	11	700
F4	S1	0.01-0.10	10	2,000

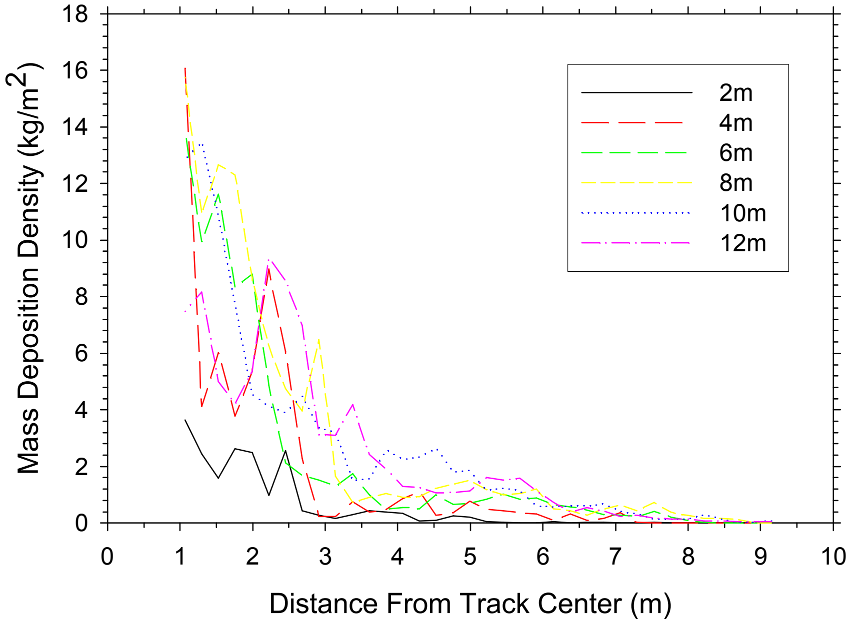
B=1.3

Predicted Environment

Ground deposition and air water vapor concentration predictions help locate instrumentation



Case F1 Deposition at Various Distances



Case F2 Deposition at Various Distances

Simulation Matrix

- Wind was not reported, so it was treated as a free parameter
- Geometry fidelity was examined, including undercarriage and cross-member for high fidelity
- Various temporal staging assumptions were analyzed

Fluid Test Matrix

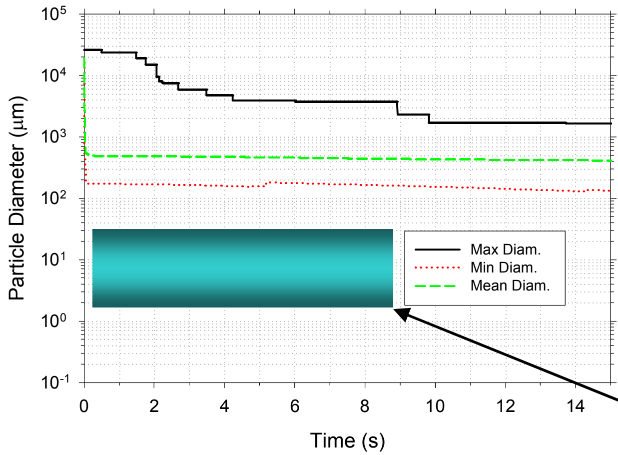
Case	Geometry Fidelity	Wind	Temporal Staging
1	Low	No	No
2	Low	No	5 times*
3	High	No	6 times**
4	Low	2 m/s	No
5	Low	1 m/s	No
6	High	No	11 times**
7	High	1 m/s	11 times**

* Dimensionless Staging Distance: 1.7
** Dimensionless Staging Distance: 1.5

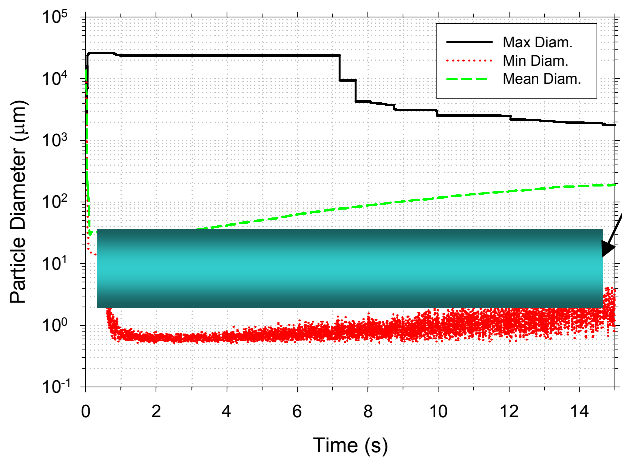
Drop size and Spread Distance Results

- Simulation matrix evaluated transfer coupling, geometry fidelity, and wind assumptions

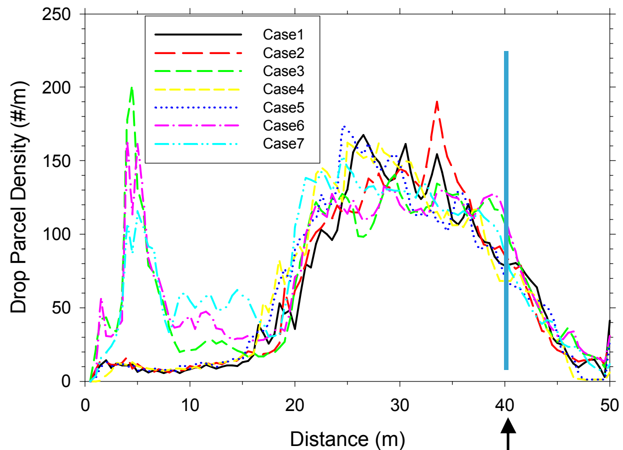
Low Geo. Fidelity



High Geo. Fidelity



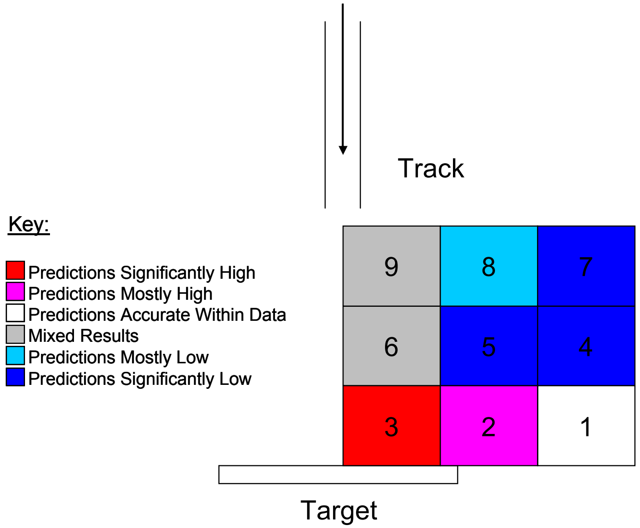
Data

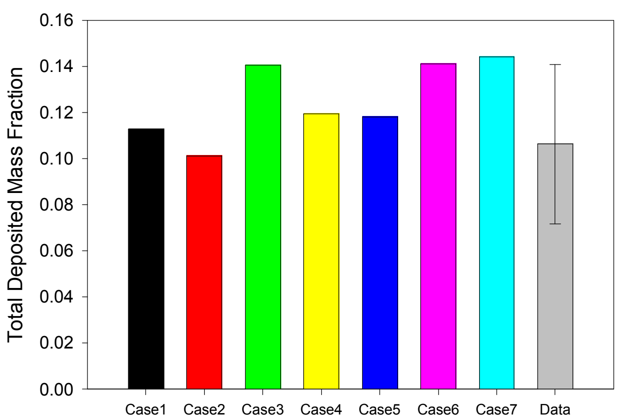


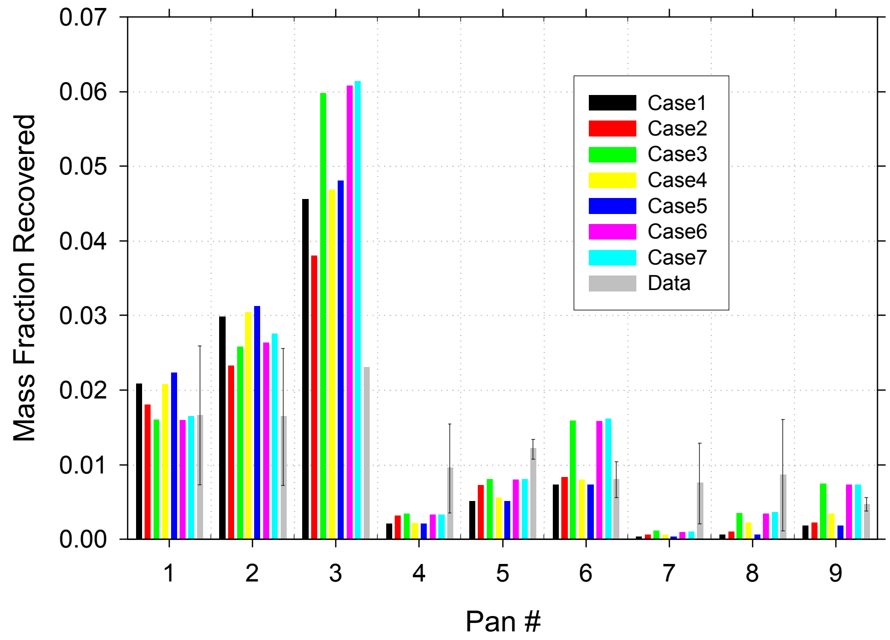
Data Peak

Liquid Deposition Results

- Geometry fidelity was found to be most significant, and coupling methodology was also important







Simulation Matrix

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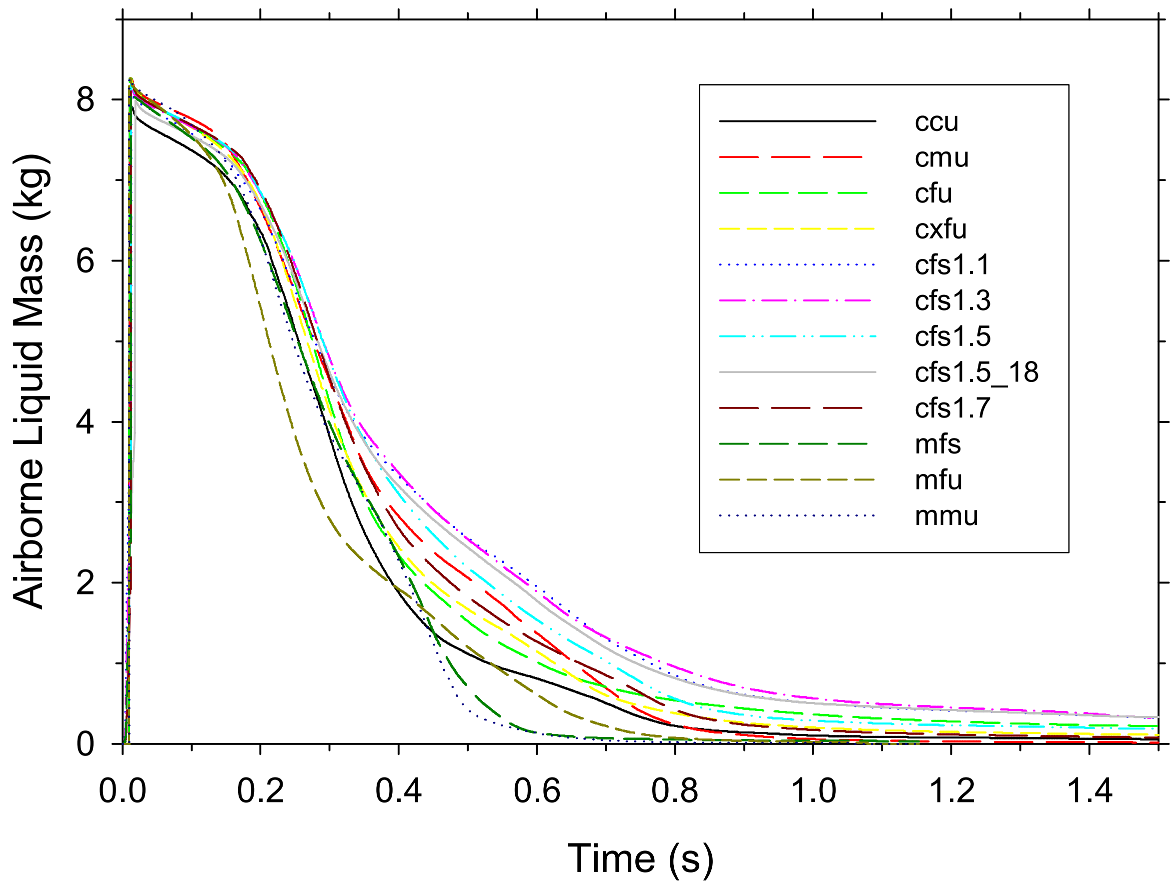
- Cases are named to indicate meshes used and staging assumptions
- Differences between cases reflect accuracies with discretization and staging

Case	Fuego Mesh	Presto Mesh	Temporal Staging	Dimensionless Spacing
ccu	coarse	coarse	No	
cmu	coarse	medium	No	
cfu	coarse	fine	No	
cxfu	coarse	xfine	No	
cfs1.1	coarse	fine	Yes	1.1
cfs1.3	coarse	fine	Yes	1.3
cfs1.5	coarse	fine	Yes	1.5
cfs1.5_18	coarse	fine	Yes*	1.5
cfs1.7	coarse	fine	Yes	1.7
mfs	medium	fine	Yes	1.5
mfu	medium	fine	No	
mmu	medium	medium	No	

*All staged cases use 1 ms steps out to 12 ms except this one, which uses 1 ms steps out to 18 ms.

Mass Results (1/2)

- Results are relatively similar, with subtle differences not well illustrated by line plots.

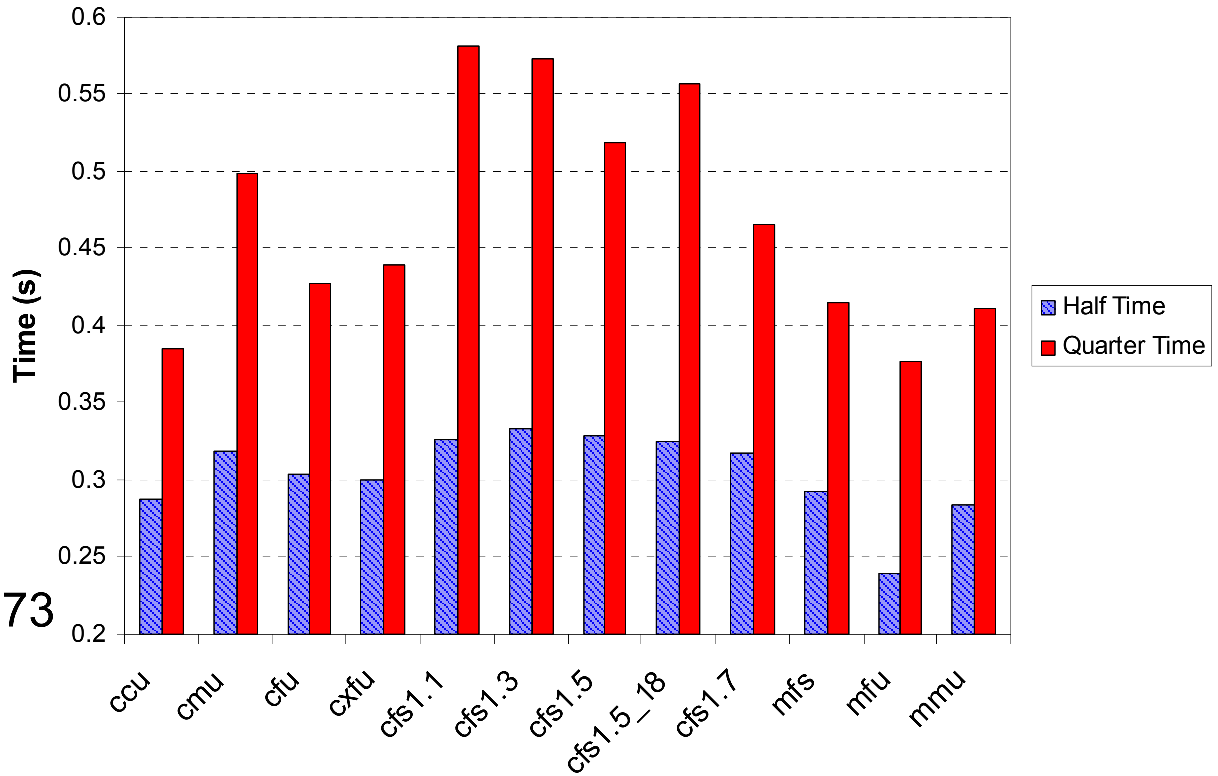


Mass Results (2/2)

- Mass loss is slower for staged predictions
- Mass loss is faster for medium Fuego mesh
- Moderate trend depending on dimensionless spacing magnitude assumed

half avg. = 0.305
half st.dev. = 0.026

quarter avg. = 0.471
quarter st.dev. = 0.073

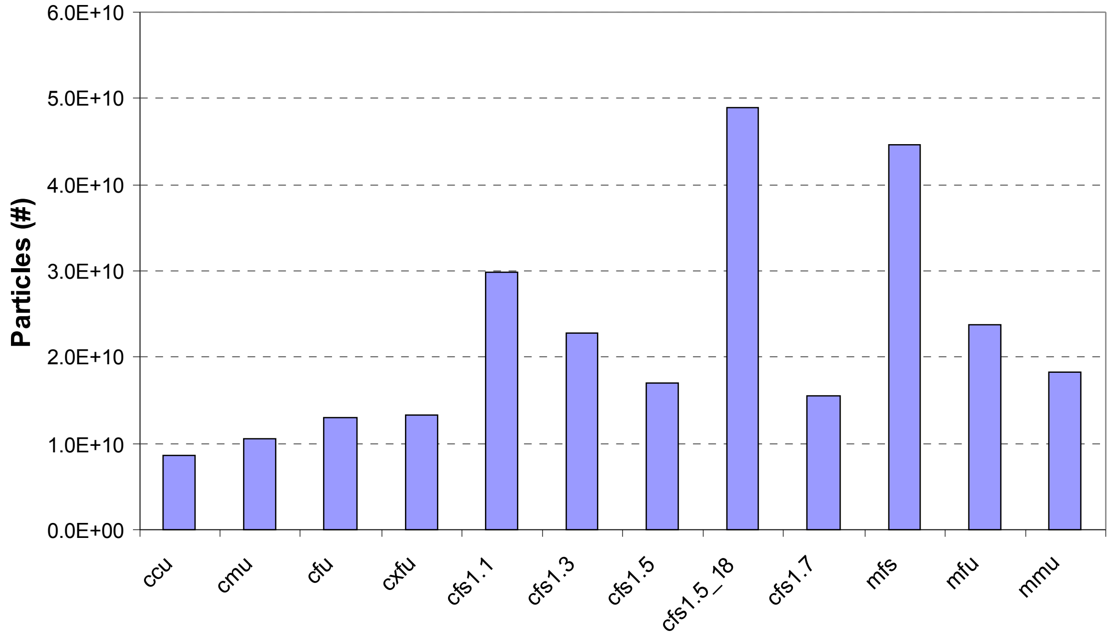


Maximum Predicted Particles Results

- Staging appears to increase break-up
- Finer Fuego mesh yields more particles
- Dimensionless spacing significant to result
- Small to moderate effect of Presto resolution
- 18 ms case results in substantially more particles

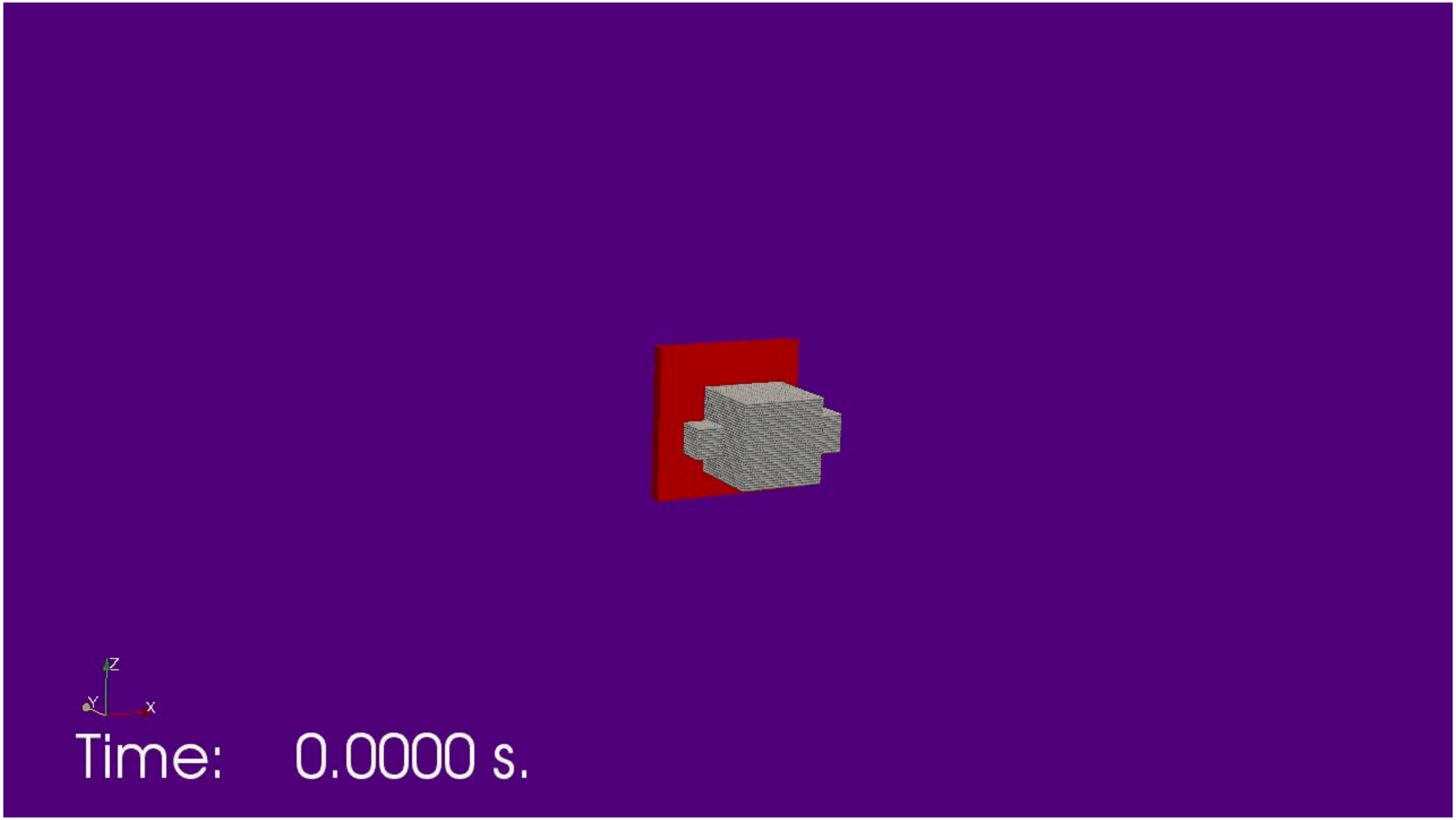
avg. = 2.2e10
st.dev. = 1.29e10

log avg. = 10.29
log st.dev. = 0.23



Coarse Video

- Case cfs1.5



Summary

- A new capability exists to predict fires from impact scenarios involving code coupling.
- Model validation work is ongoing, with existing validation suggesting the accuracy of the capability.
- Modeling resolution assumptions including discretization and coupling transfer method are analyzed, and influence prediction results.
- This work provides confidence in being able to employ these capabilities for other similar scenarios.
- Future work includes additional validation and scenarios more closely related to the application space.

Acknowledgements

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Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Approximation Details

- Low-Mach number approximation
  - It is often stated that a Mach number of 0.3 is the low-Mach number threshold for CFD predictions
  - This comes from the thermodynamic relationship and an assumption of 5% error in the density:

$$\frac{\rho_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{1/(\gamma - 1)}$$

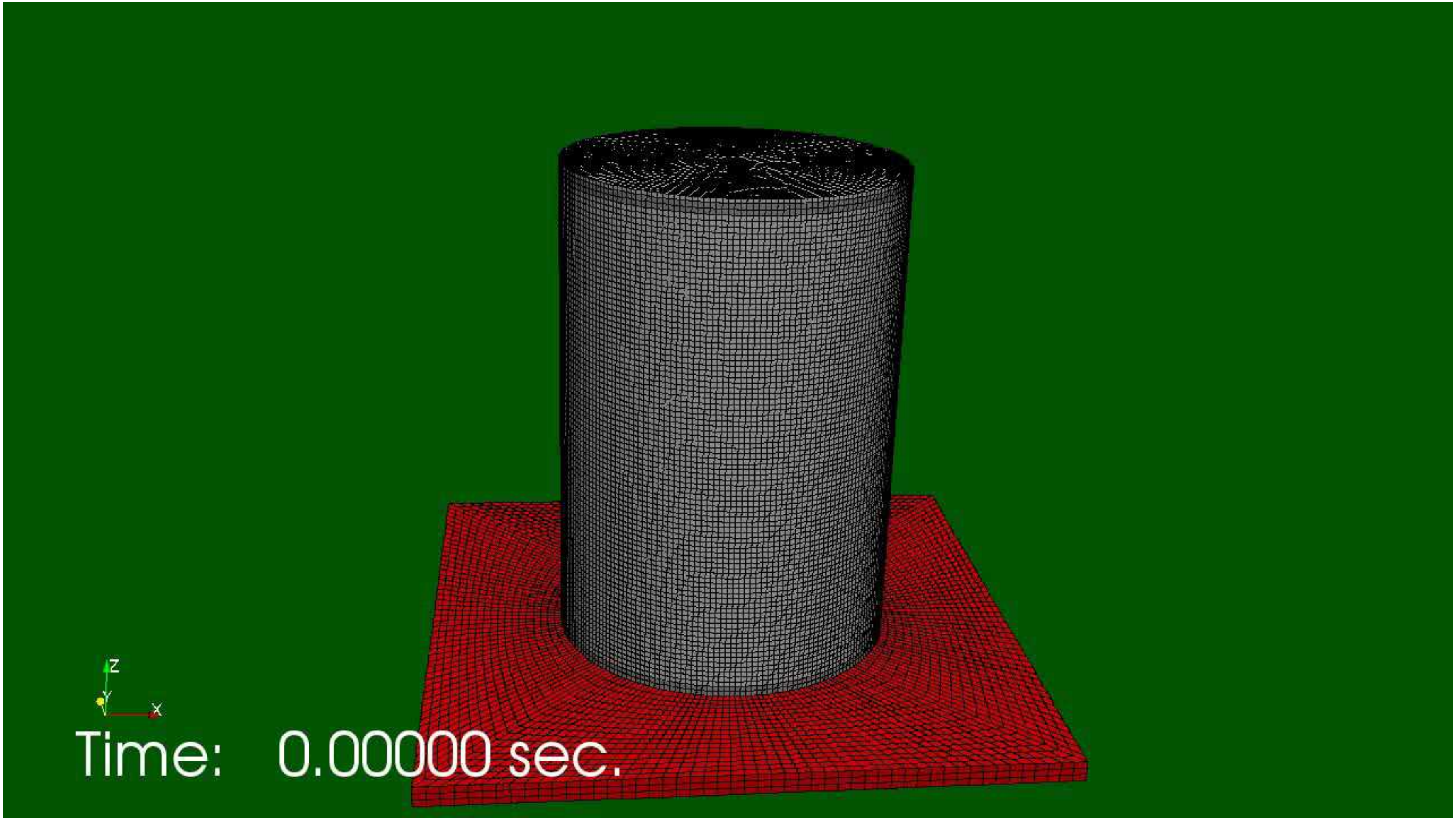
- Dilute Spray Approximation
  - Spray volume is not displaced in the Eulerian gas cell
  - Higher volume fractions have greater error
  - Also tend to instability in the solver
  - Dilute spray volume fraction is normally considered 10% and below
- Both of these approximations have typical threshold values, both of which are not hard thresholds

Test Matrix

- Tests were designed to explore a range of conditions, and to evaluate mesh refinement
- Ten cases were simulated, as defined in the table below:

Case	**Tank Geometry**	**Dim. Det. Intens.** (p/P)	**SPH elements**	**Fluid Nodes**	**B**	**Injection Step Size** *(s)*	**Number of Injections**
1	Closed Cylinder	3	50,000	370,000	1.3	variable: 0.005, 0.01	44
2	Closed Cylinder	5	50,000	370,000	1.3	0.001	20
3	Open Box	1	50,000	380,000	1.3	0.001	30
4	Open Box	1	50,000	2,940,000	1.3	0.001	30
5	Open Box	3	50,000	380,000	1.3	0.001	20
6	Open Box	3	400,000	380,000	1.3	0.001	20
7	Open Box	3	400,000	2,940,000	1.3	0.001	20
8	Open Box	5	50,000	380,000	1.3	0.001	20
9	Open Box	3	50,000	380,000	1.5	0.001	20
10	Open Box	3	400,000	380,000	1.5	0.001	20

Case 2 Video



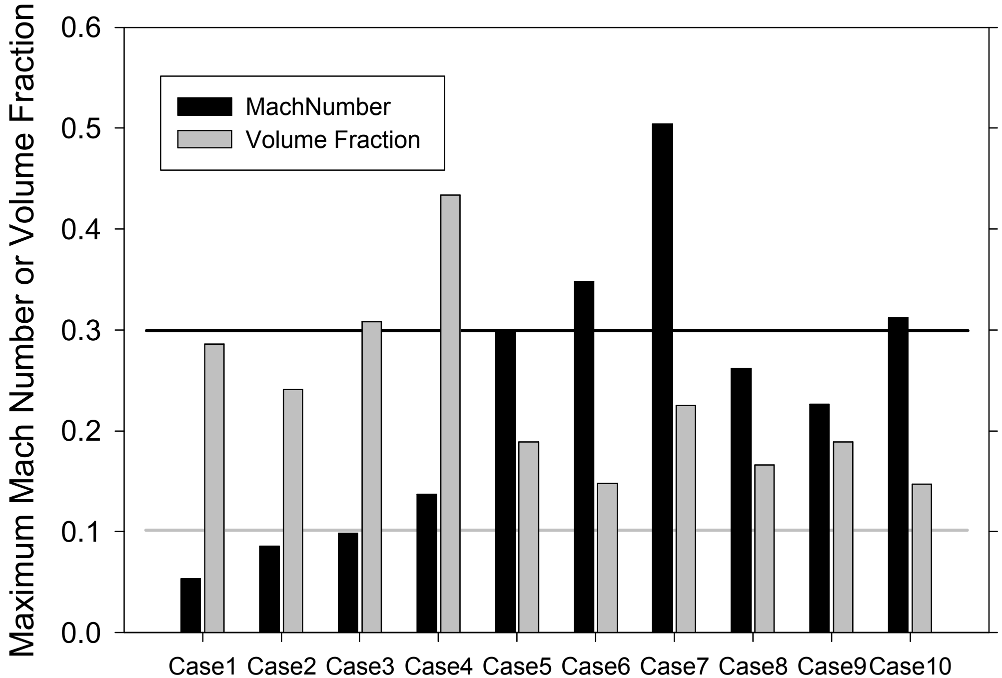
Presto SPH Simulations

- Fewer solid mechanics cases were required
- Test matrix listed below

Case	Tank Geometry	Dimensionless Det. Intensity	SPH elements	Corresponding Fuego Cases
Cyl3	Closed Cylinder	3	50,000	1
Cyl5	Closed Cylinder	5	50,000	2
Hex1	Open Box	1	50,000	3, 4
Hex3	Open Box	3	50,000	5, 9
Hex3_med	Open Box	3	400,000	6, 7, 10
Hex5	Open Box	5	50,000	8

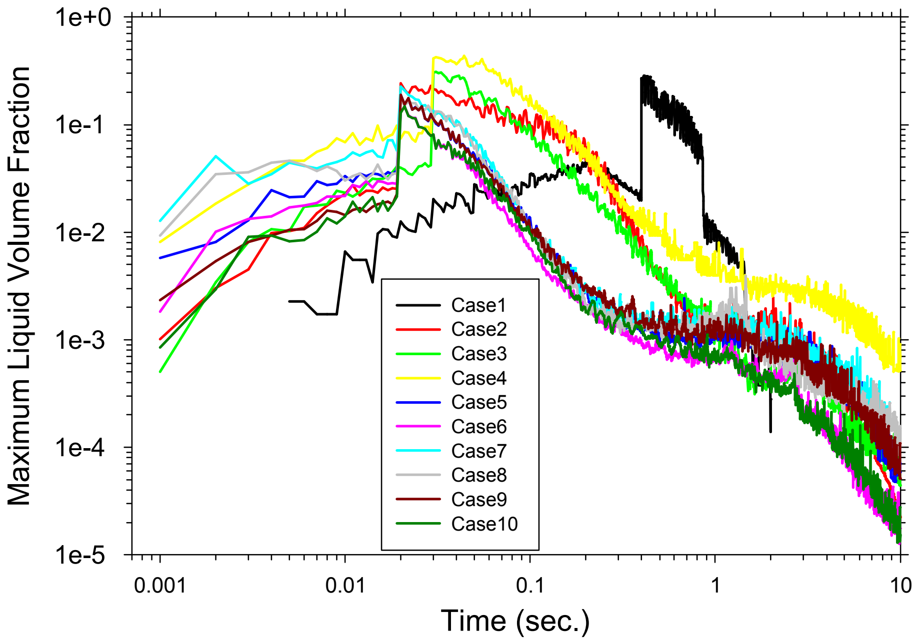
Maximum Mach and Volume Fract.

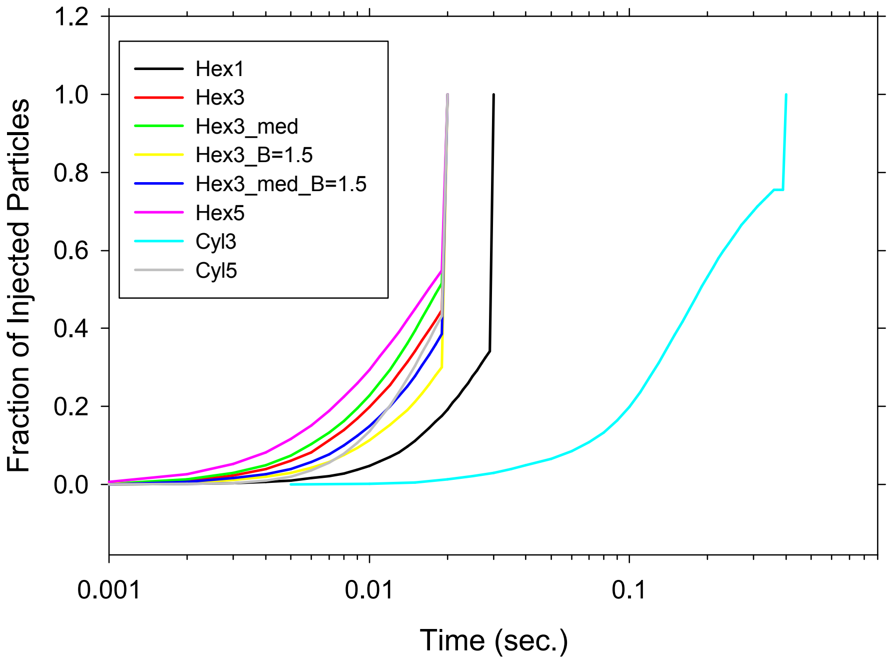
- Fluid predictions periodically violate standard approximation limits for many of the cases
- This is of concern, since we desire quantitative accuracy from our models



Volume Fraction Details

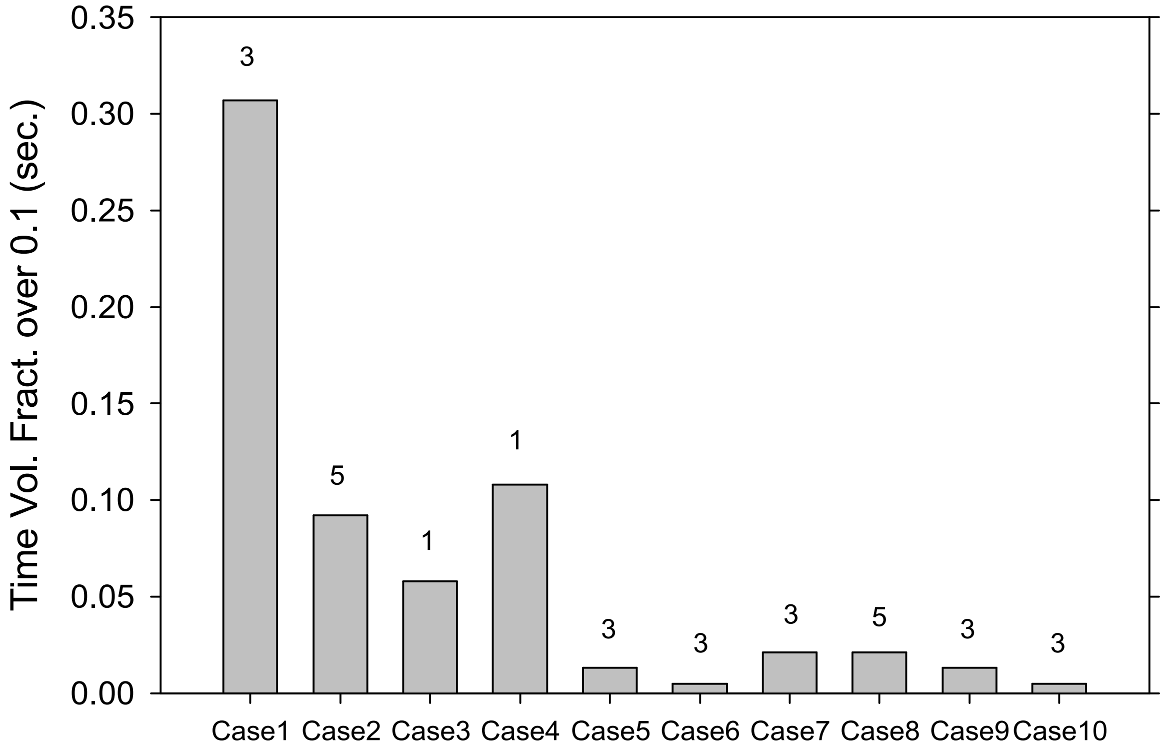
- Peak volume fraction tended to be short in duration
- Peak typically corresponded with the final particle transfer from Presto





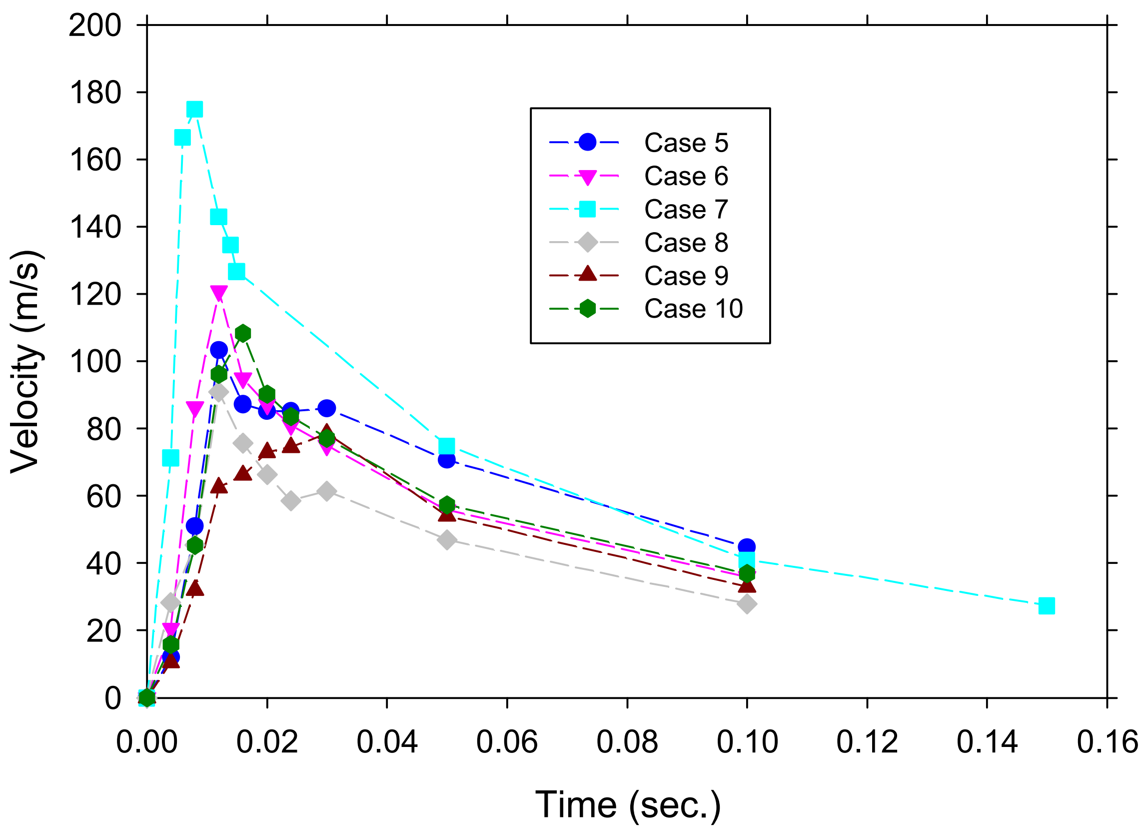
Time Exceeding 0.1

- The time that each case exceeded 0.1 volume fraction was generally quite short (plotted below)
- Dimensionless detonation intensity is labeled above each bar



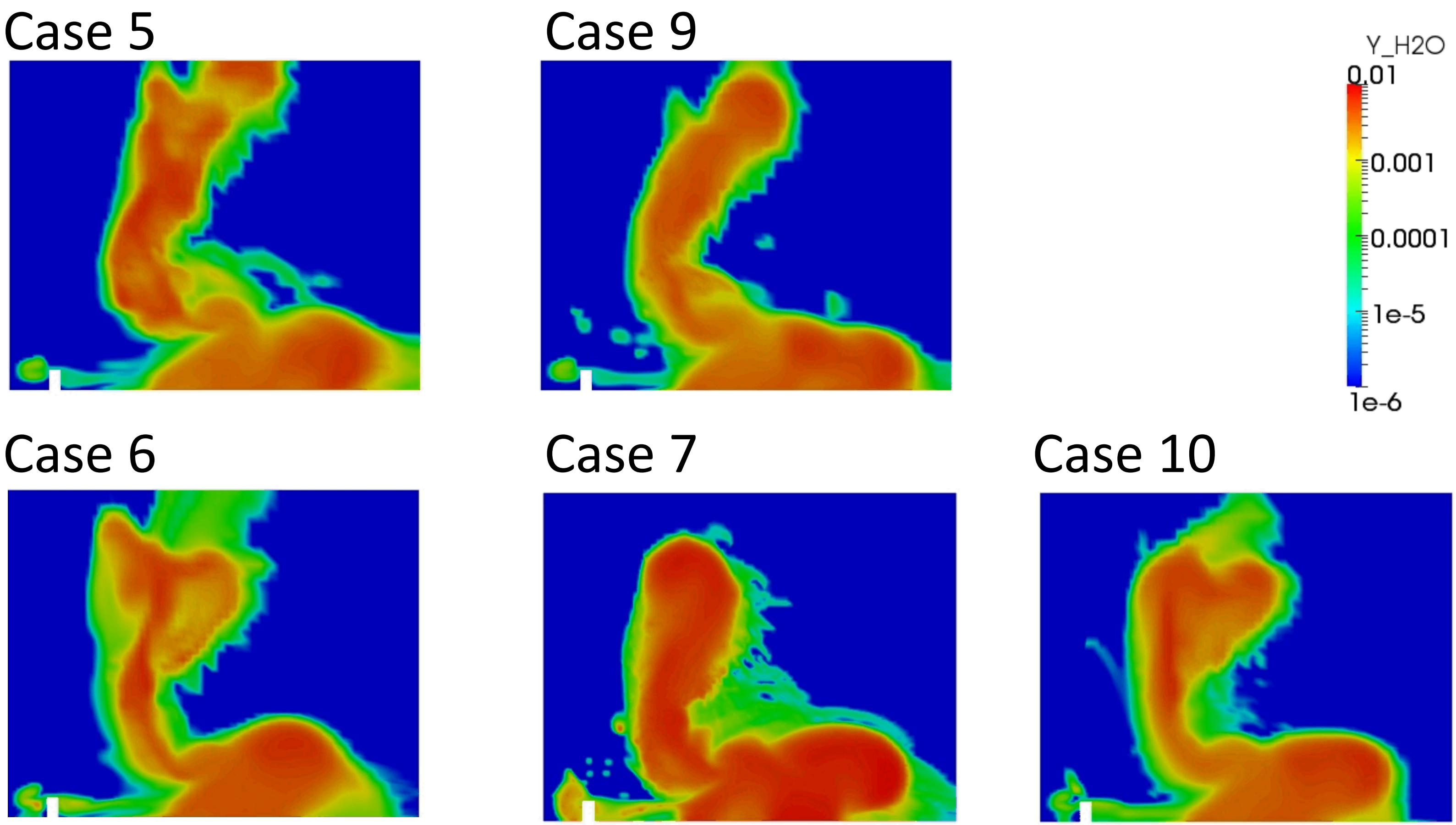
Maximum Velocity Selected Cases

- 104 m/s is M=0.3
- A few cases exceeded this for only a short time



Case Similarity

- Vapor concentration predictions for identical cases at 1 sec.



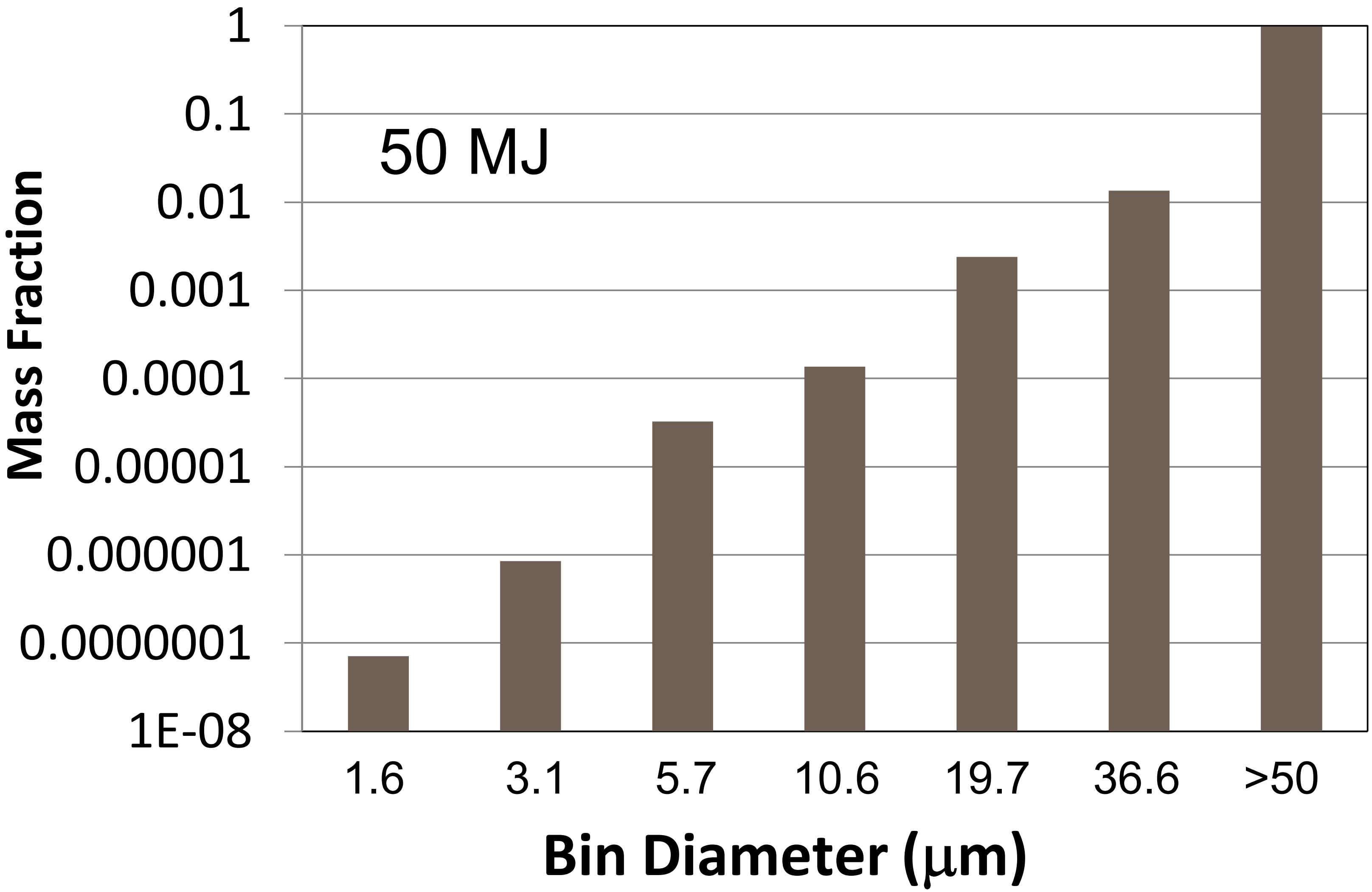
Summary

- Only minor (short-duration) violations of the low-Mach number approximation and the dilute spray approximation are found in any of the range of test cases in this study.
- Case 7, which involved highest resolution in both the Presto and Fuego calculations, exhibited the highest velocities. This suggests the potential importance of resolution parameters to the calculation. Case 1 exhibited the highest liquid volume fractions. This was different from most other cases in geometry and detonation source intensity, suggesting these as significant parameters.
- Validation testing for the modeling methods in this report would be an excellent follow-on activity since good detailed datasets for model validation are scarce.

Simulated Explosion and Aerosol Release in Denitrator (50 MJ)

Preliminary Estimate of Aerosol Distribution

10^{-7}% Respirable (~<20 Micrometer Diameter)



Comparison To Conservative Estimates from DOE Handbook 3010-94 (2000)

- DOE Handbook: "Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities: Volume I"
  - Release is a product of five factors: (1) Material-at-Risk, (2) Damage Ratio, (3) Airborne Release Fraction, (4) Respirable Fraction, and (5) Leak Path Factor. (Page 3-18 values)
  - MAR x DR = 1
  - ARF x RF = 0.2 : 0.1 : 0.07 (upper bound : median : lower bound)
- 50 MJ explosion: 10^{-9} respirable fraction (preliminary)
- 700 MJ explosion: 10^{-7} respirable fraction (preliminary)

Internal Impulse

Schematic of Denitrator (J. M. McKibben, 1976)