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Fire Science & Technology

7th International Seminar on **Fire and Explosion Hazards**

5–10 May, 2013
Renaissance Hotel, Providence, R.I., USA



Predictive Impulse Dispersal of Liquid Employing a Code Coupling Methodology

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SAND2013-????



Introduction

- We have recently developed methods using coupled Sierra architecture tools to simulate liquids dispersed by an impact.
- Some problems of national security interest involve an impulse dispersal; similar, but different.
- Sierra/Presto (structural mechanics) can accurately model short-term liquid dispersal with finite element and SPH.
- Sierra/Fuego is a low-Mach number reacting CFD code with Lagrangian particle capabilities.
- This effort is designed to explore the potential for using this same coupling method for detonation driven liquid dispersal

- 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
 2. A cylindrical tank of liquid into a concrete target (for data comparisons)
 3. Liquid dispersal caused by the breaking mechanism for a rocket sled (pre-test predictions for instrumenting the 2/17/13 test)

- 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.

Coupling Strategy

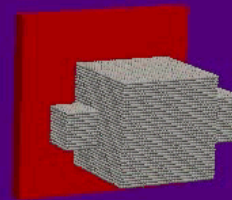
- SPH mass/momentum conserved in a transfer between the two codes
- Mass is transferred according to an algorithm that uses a critical dimensionless particle separation distance to define transfer times:

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

- 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

Presto	Phenomena	Fuego
✓	Gravity Force	✓
✓	Structural Deformation	
✓	Mass Conservation	✓
✓	Momentum	✓
~	Energy Conservation	~
✓	Structural Material Interactions	
~	Sensible Energy	✓
	Surface Tension Forces	~
~	Liquid Phase Viscous Forces	~
~	Gas Phase Transport	✓
~	Multiphase Interactions	~
	Chemically Reacting Flows	✓
~	Wind	✓
	Turbulence	✓
~	Thermal Response of Materials	✓

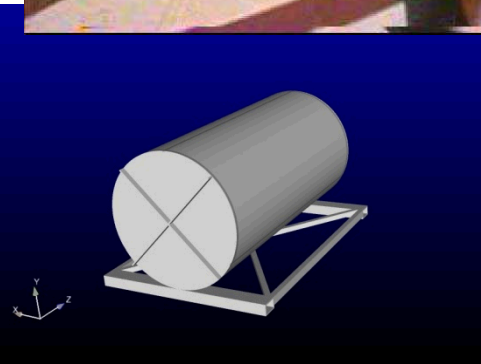
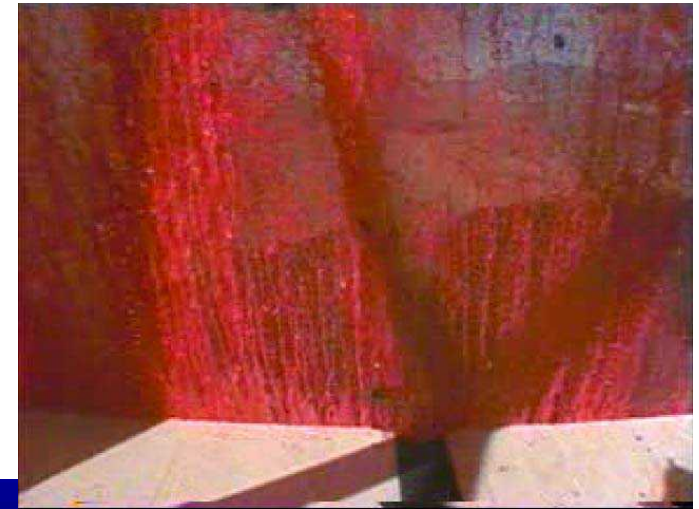
Heptane Tank Example Visualization



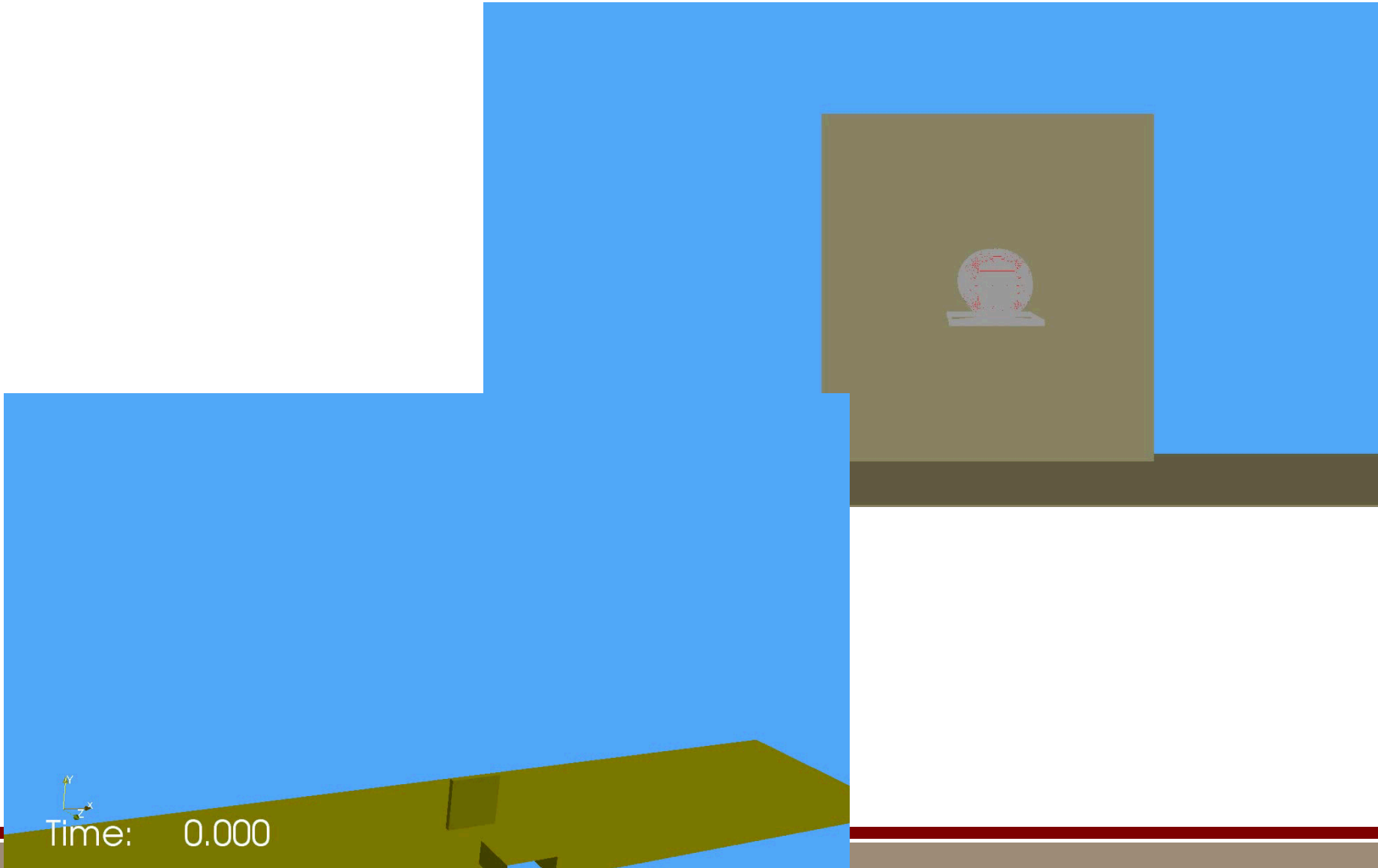
Time: 0.0000 s.

Water Tank Impact Validation Example

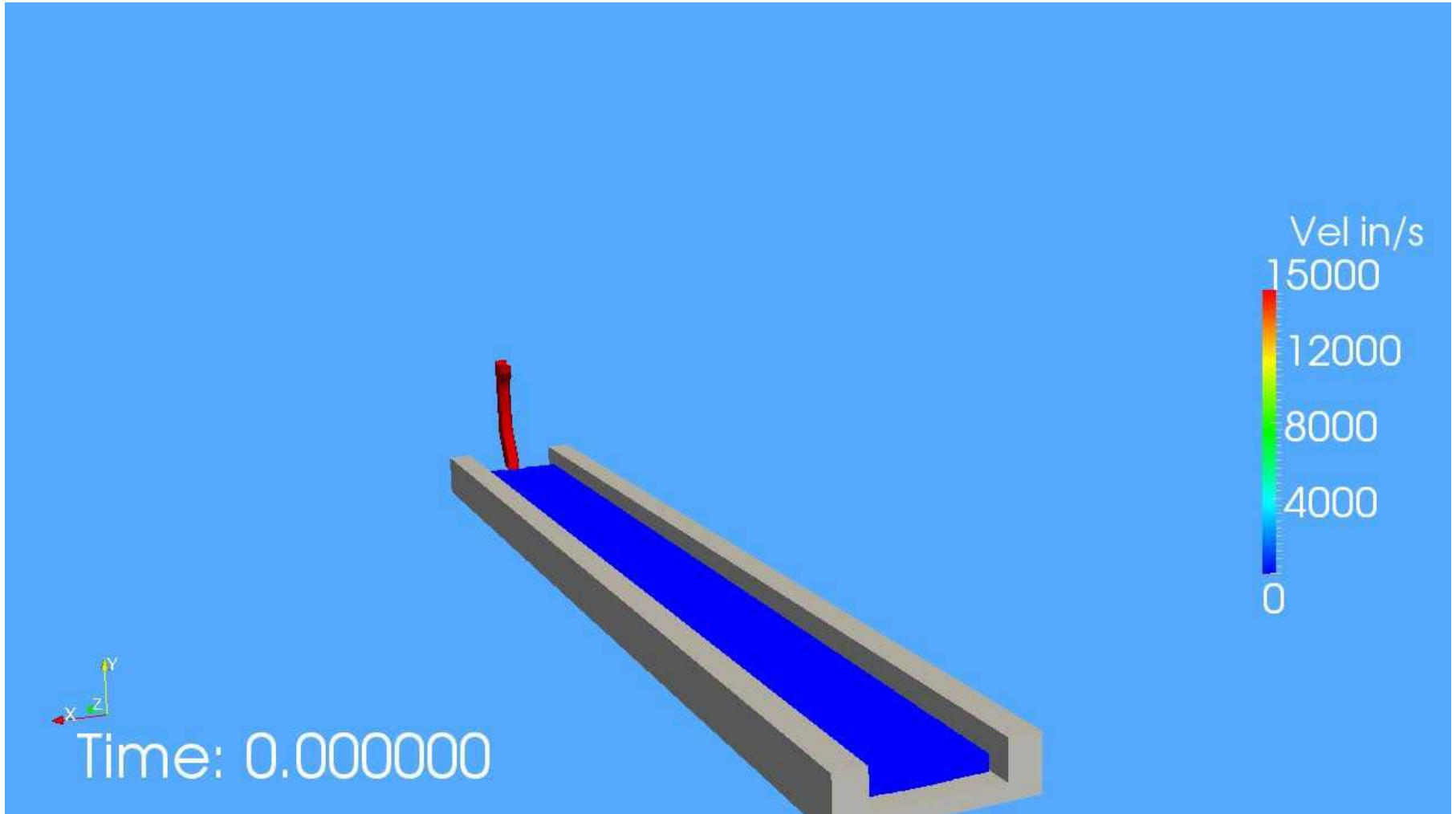
- Tests performed in 2002 provided data for validating liquid spread dynamics for an aluminum tank impacting a concrete slab
- Liquid deposition, particle sizing, and video data



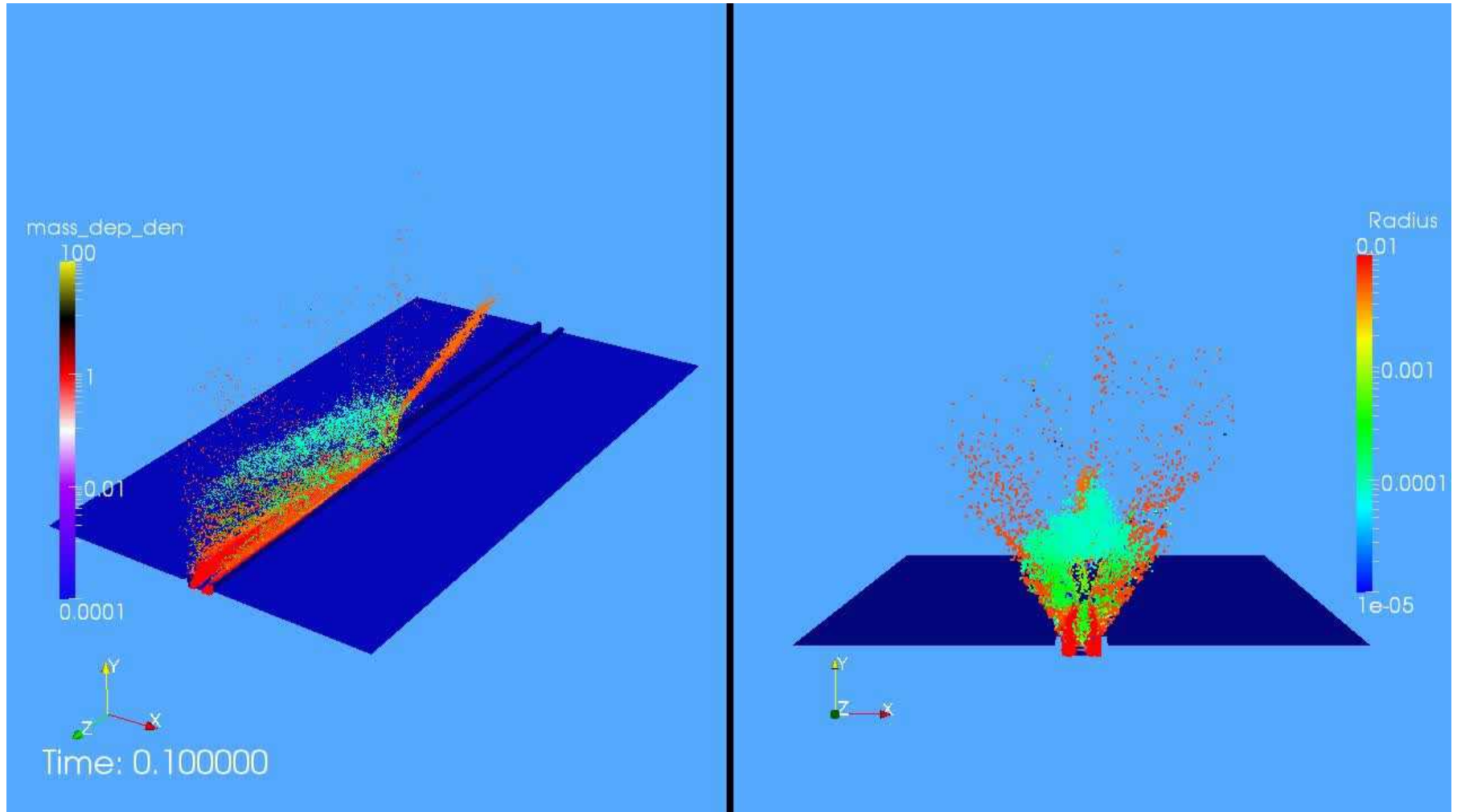
Tank Impact Validation Coupling



Example Sierra/Presto prediction



Example Sierra/Presto prediction



Motivation for Study

- Sierra/Presto can simulate detonations using various methods, one (subject of this study) being a spherical propagating shock wave from a source point
- Sierra/Fuego does not simulate shock waves (incompressible), but may be adequate for the subsequent dispersal provided:
 - Impulse primarily interacts with a solid body, then the liquid
 - Range of validity is not significantly exceeded
- Approximations of interest to this study:
 - Low-Mach number approximation
 - Dilute Spray Approximation
- This study examines a notional detonation scenario to assess whether the predictions maintain reasonable accuracy with respect to the approximations of interest

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:

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

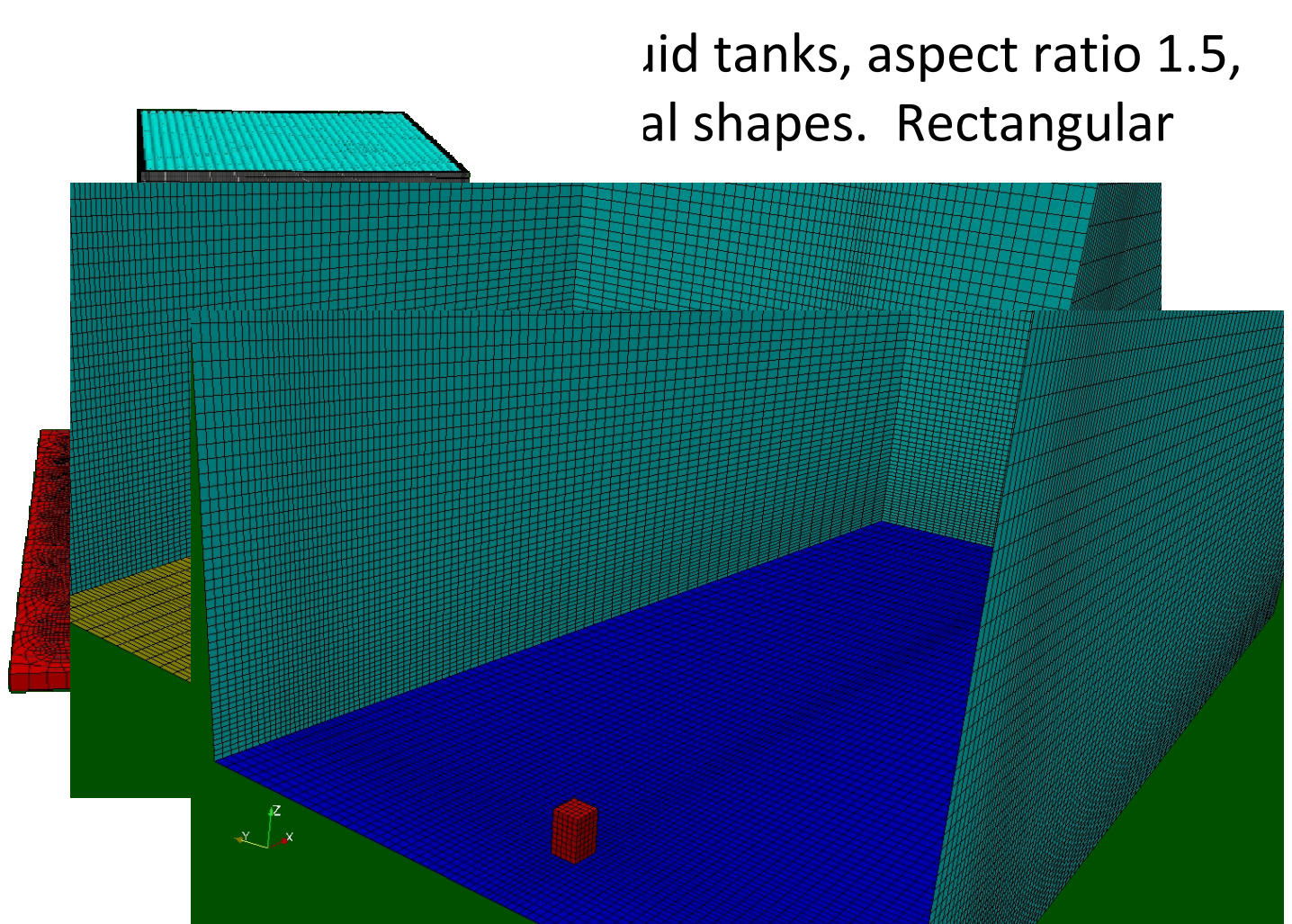
- Dilute Spray Approximation

- 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

Simulation Details

igid tanks, aspect ratio 1.5,
al shapes. Rectangular

-
-
-
-
- **Detona**

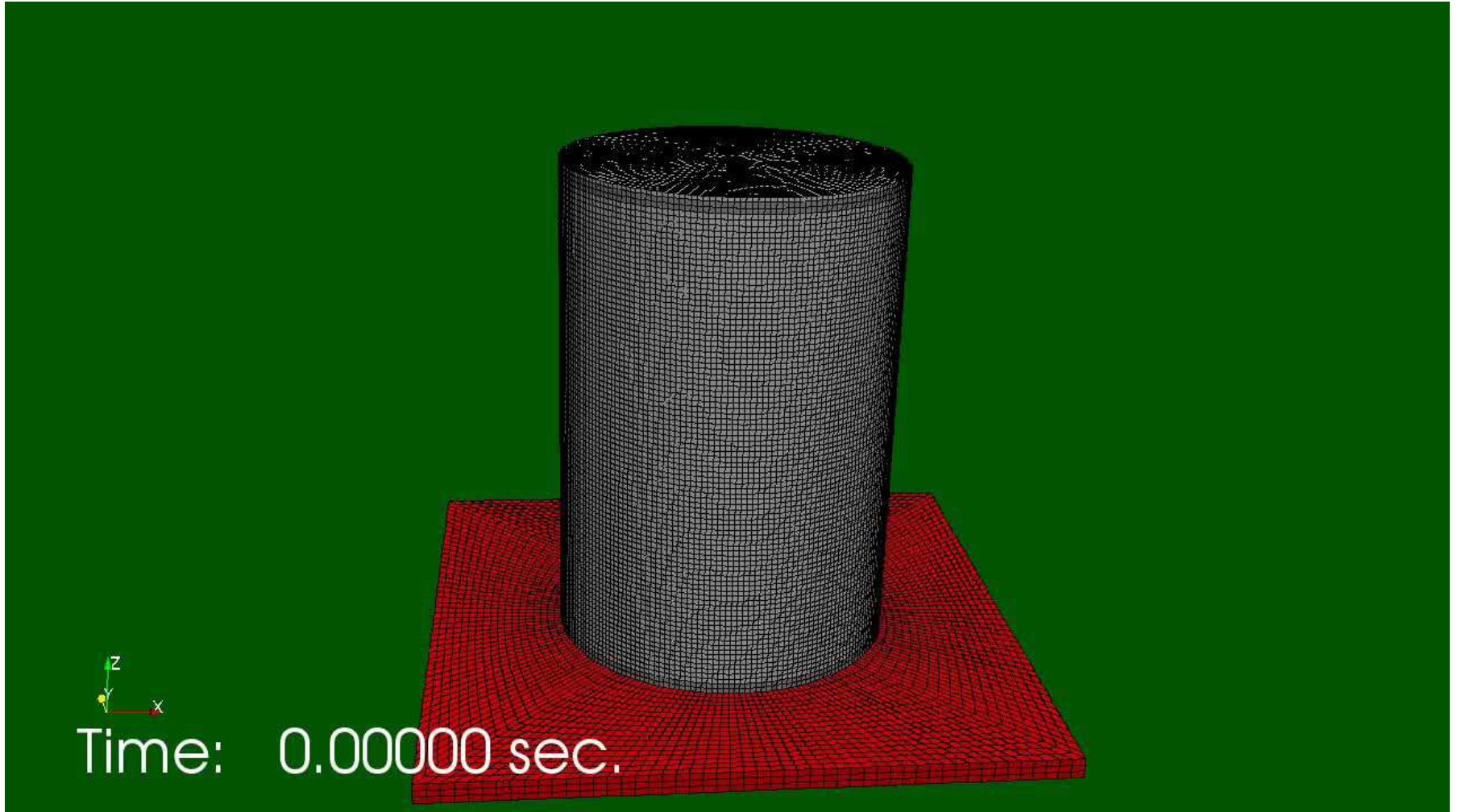


Test Matrix

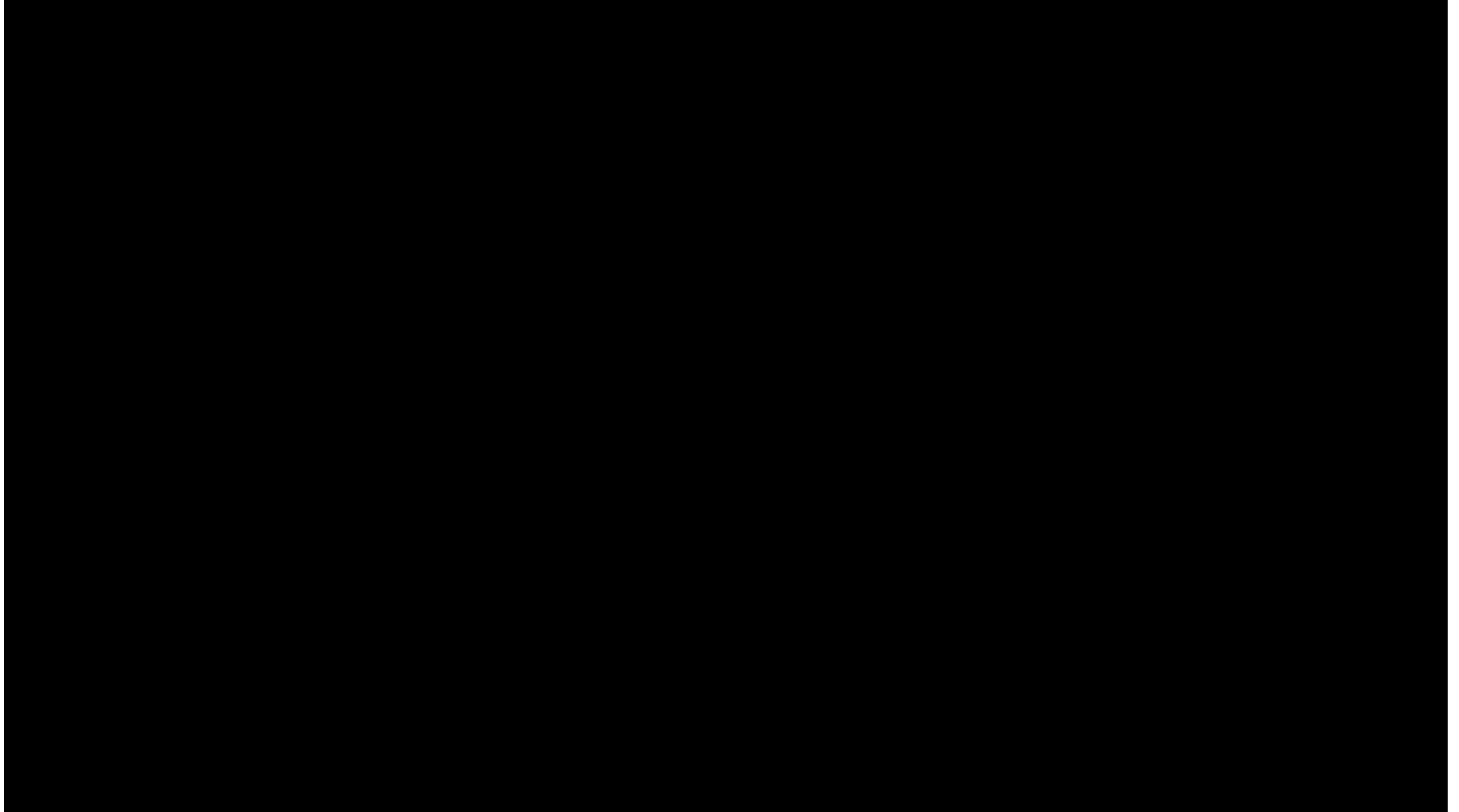
- Tests were designed to explore a range of conditions, and to evaluate mesh refinement
- Ten cases were simulated, as defined in the table below:

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



Case 4 Video



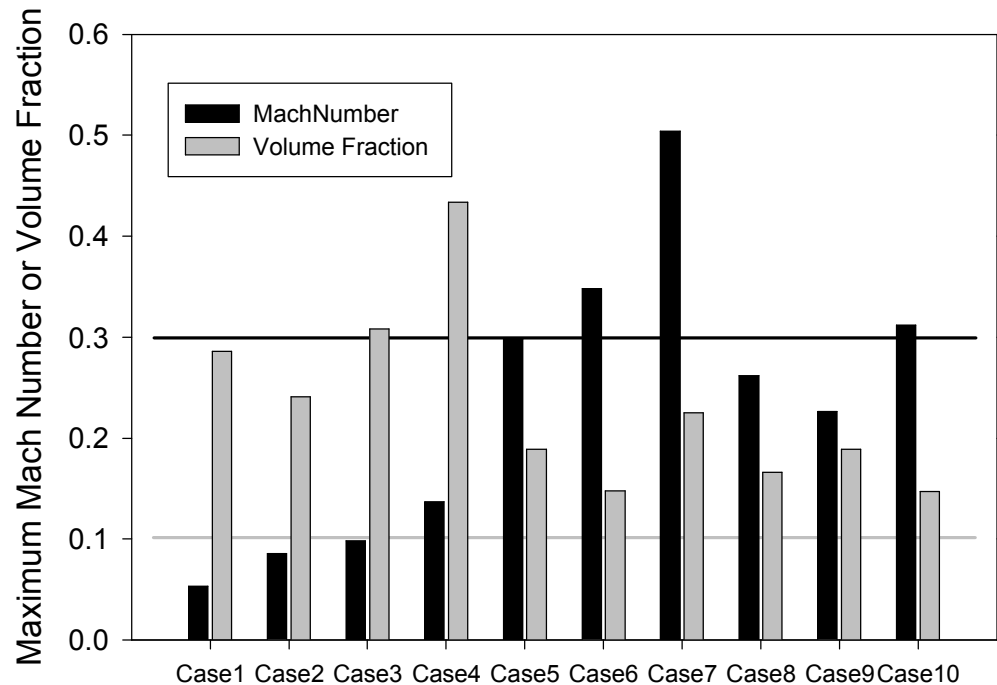
Presto SPH Simulations

- 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

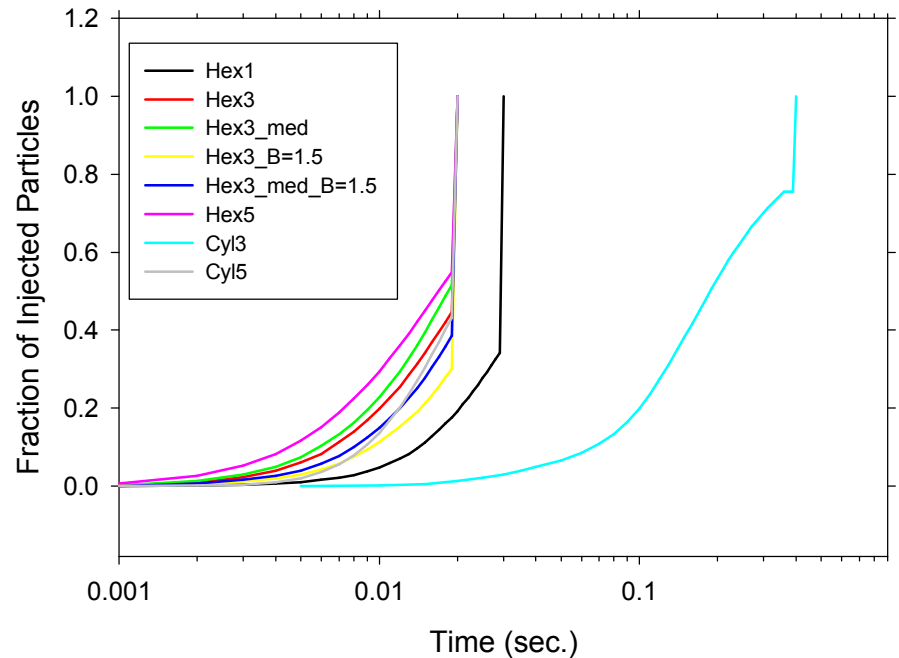
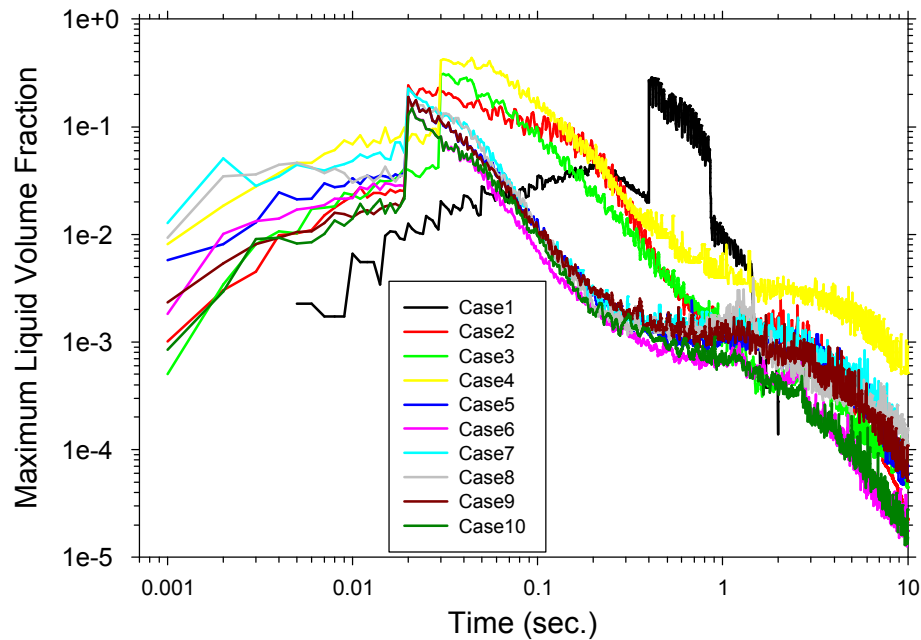
Maximum Mach and Volume Fract.

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



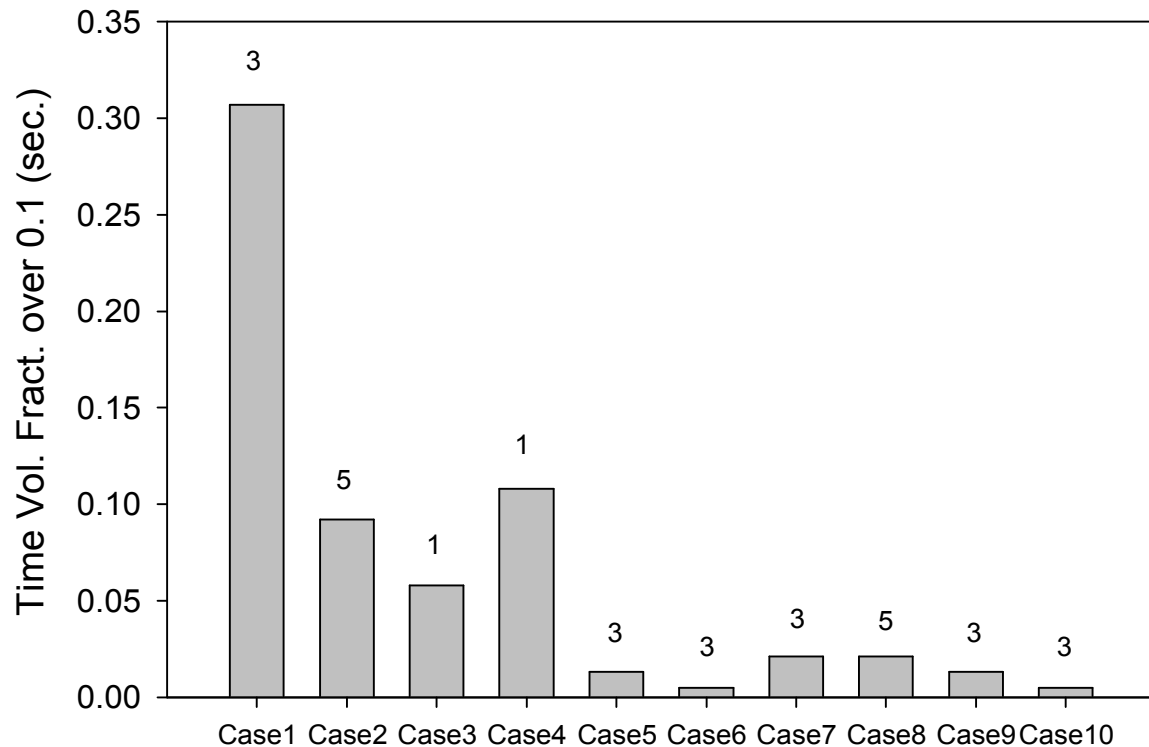
Volume Fraction Details

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



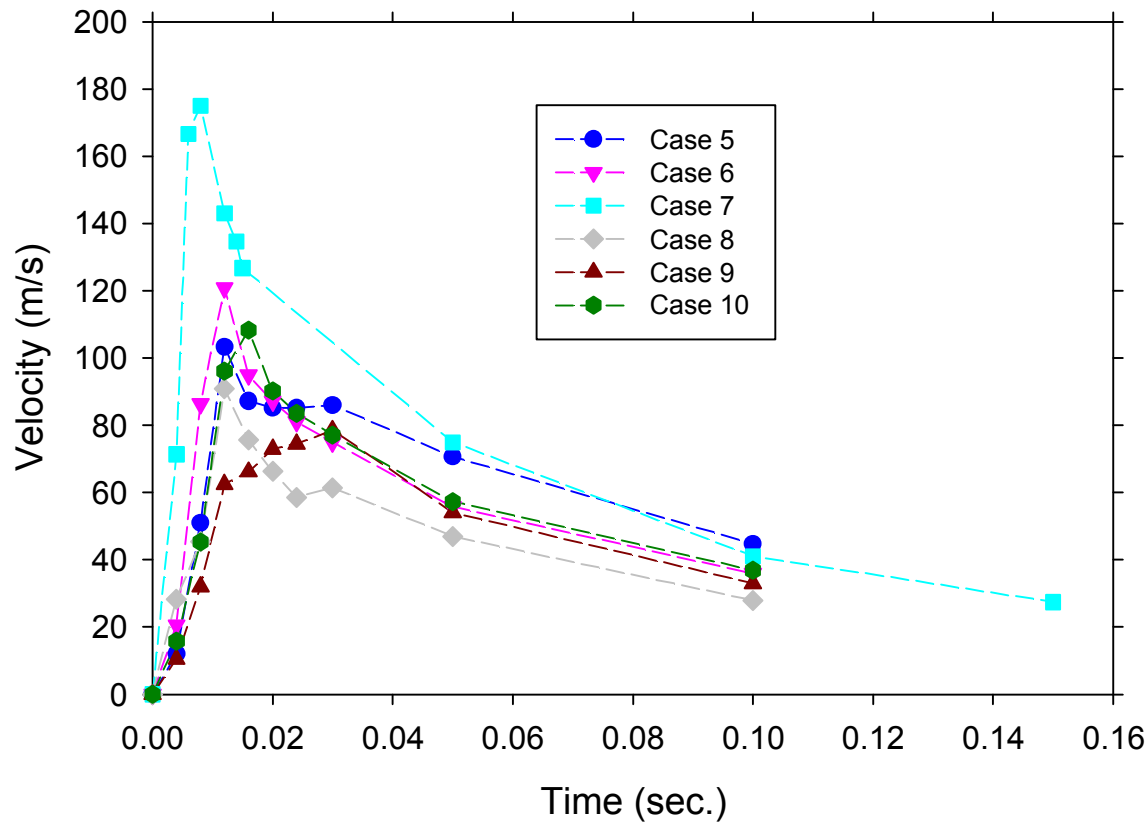
Time Exceeding 0.1

- 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

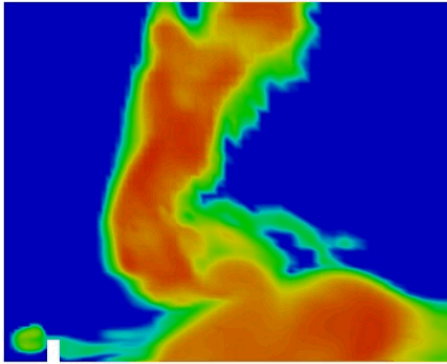
- 104 m/s is $M=0.3$
- A few cases exceeded this for only a short time



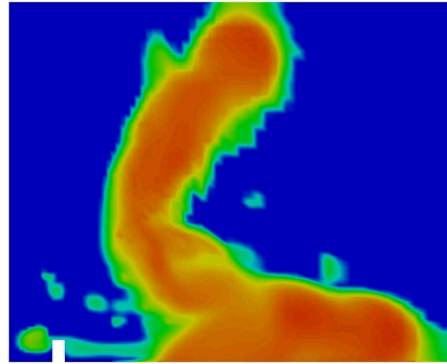
Case Similarity

- Vapor concentration predictions for identical cases at 1 sec.

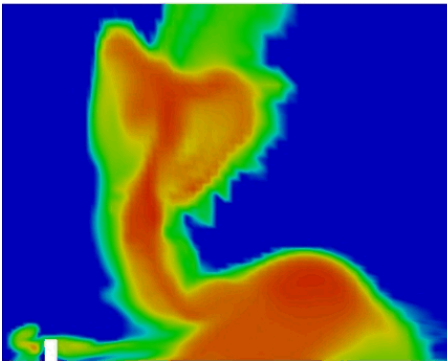
Case 5



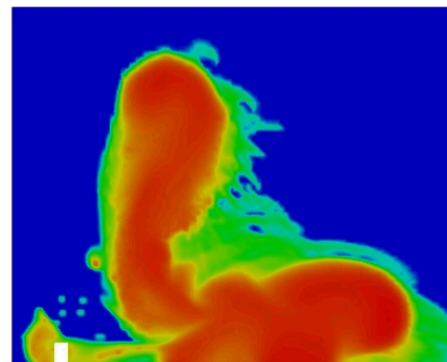
Case 9



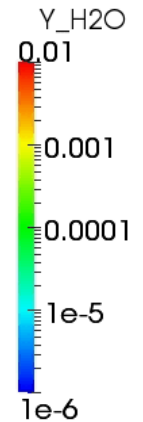
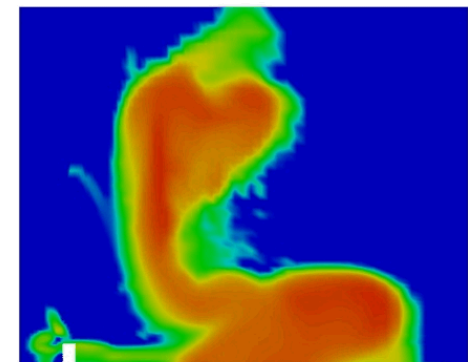
Case 6



Case 7



Case 10



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.

Acknowledgements

Document reviews by Fred Gelbard, Rich Jepsen, Kurt Metzinger, and Randy Watkins are appreciated.

Support from the ASC P&EM program is appreciated.

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.