



Investigation of Mixing Law Efficacy for Hydrodynamic Simulations and Associated Compressibility Implications

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Abstract

A computational simulation of various mixing laws for gaseous equations of state (EOS) using planar traveling shocks for multiple mixtures in three dimensions (3D) is analyzed against nominal experimental data. Numerical simulations utilize the Sandia National Laboratories (SNL) shock hydrodynamic code CTH and other codes including the SNL thermochemical equilibrium code TIGER and the uncertainty qualification (UQ) and sensitivity analysis code DAKOTA. The mixtures are: a 1:1 and a 1:3 molar mixture of helium (He) and sulfur hexafluoride (SF_6). The mixing laws to be analyzed are the ideal gas law, Amagat's Law, and Dalton's Law. Examination of the experimental data with TIGER revealed that the shock strength should not be strong enough to turn the mixture non-ideal as the compressibility factor, z , was essentially unity ($z \approx 1.02$). Strikingly however, experimental results show that neither Dalton's nor Amagat's Law are able to accurately predict the properties of the shocked mixture. A methodology is being developed to possibly optimize the various mixing laws with computational results for the data set investigated. Lastly, a framework for future sensitivity and uncertainty quantification analysis will be established.

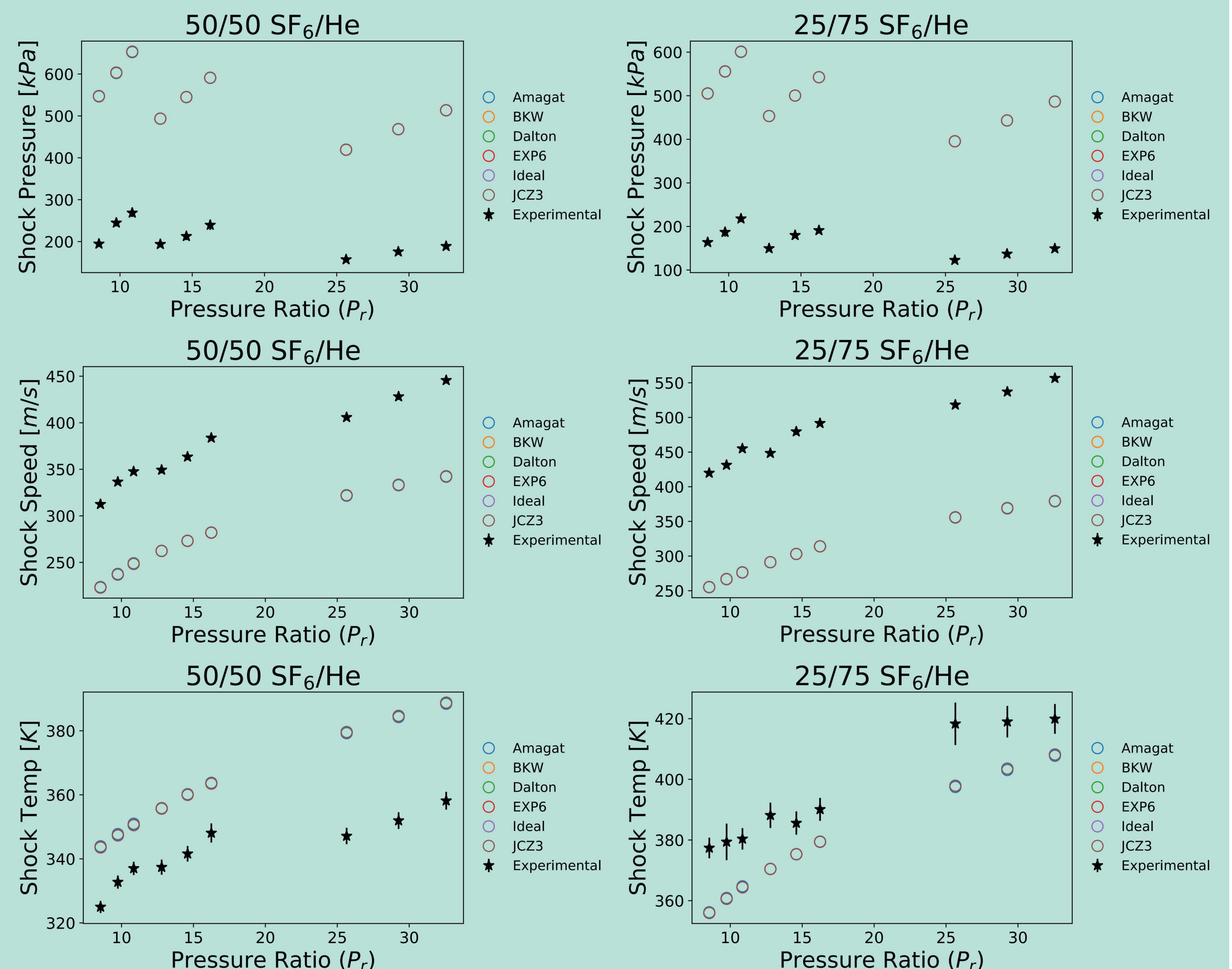
Gas Shock Tube Simulations

- N_2 & SF_6/He Mixture
 - N_2 used as driver gas
- Mixing EOS's
 - Amagat, Dalton, Ideal
 - BKW, JCZ3, EXP6
- Mixture Ratios
 - 1:1 & 1:3 SF_6/He
- Driver Pressures (N_2)
 - 1,006 kPa, 1,145 kPa, & 1,282 kPa
- Driven Pressures (SF_6/He Mixture)
 - 39.3 kPa, 78.6 kPa, & 118 kPa
- Shock Tube Dimensions
 - 7.62 cm square cross-sectional area
 - 122 cm Driver Section
 - 320 cm Driven Section

Sensitivity & UQ Framework

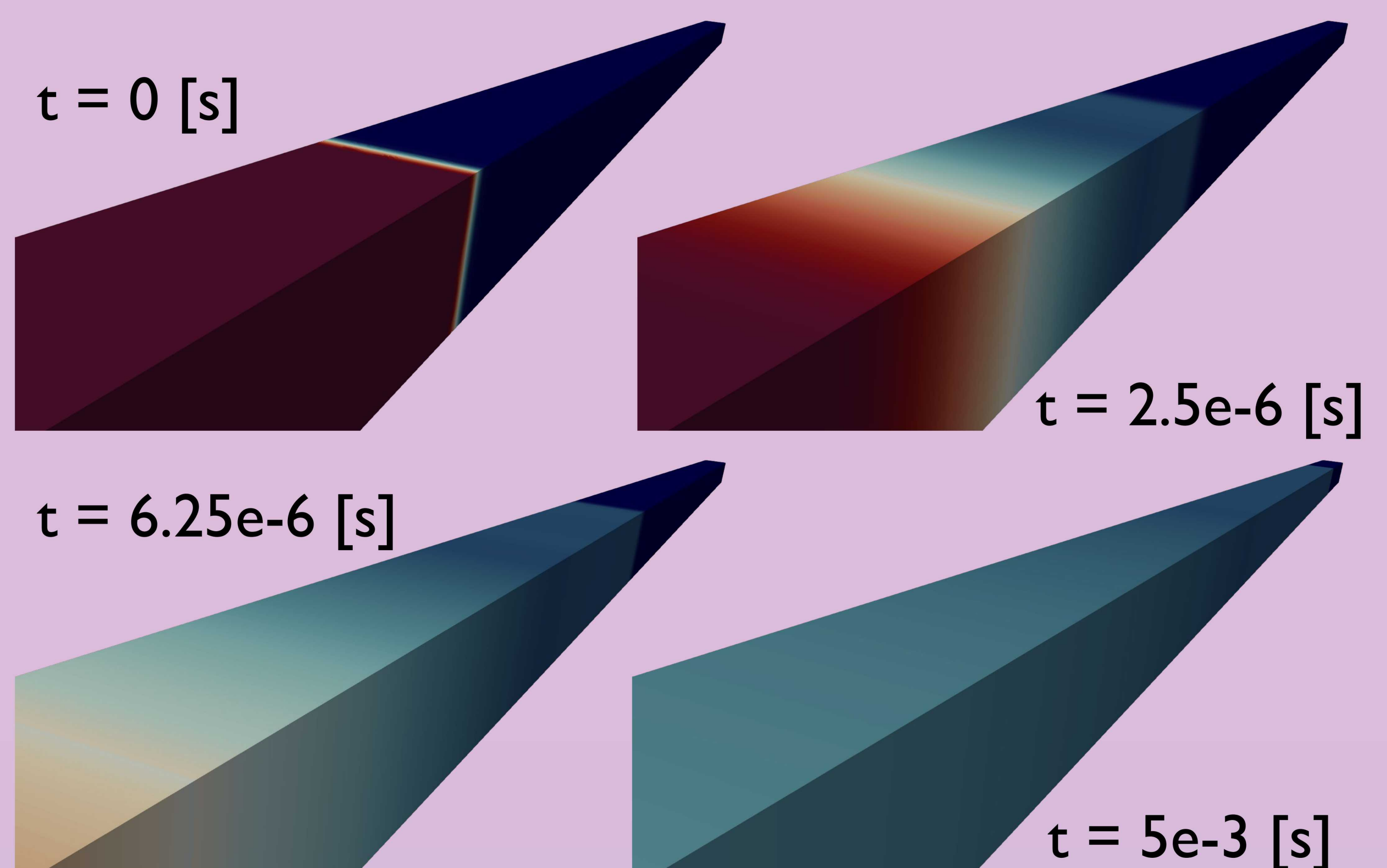
- Sensitivity Analysis
 - Incremental LHS via DAKOTA[2]
- Representative Uncertainty Distributions
 - Gaussian (Normal)
 - Triangle
 - Uniform (Rectangular)
 - Log-Normal
- Potential variables to perturb
 - Driver & Driven Pressures
 - N_2 & SF_6/He Mixture Temperatures
 - Mixture Ratios
 - Tracer Locations

Results



Simulation vs. Experimental[1] data for the various mixing EOS's and mixture ratios. The pressure ratio is defined as $P_r = P_{driver}/P_{driven}$. The results from all six EOS's are coincident which is further proof that the shock strength is not strong enough to turn the mixture non-ideal. The computational model is currently unable to accurately predict the experimental properties of the mixture, however, the general trends are matched and the shifts could be explained through various unknown sources of error.

Pressure Contours



Pressure contours depicting the planar shock for a mixture ratio of 1:1, JCZ3 EOS, driver pressure of 1,282 kPa, and a driven pressure of 39.3 kPa (corresponding to the max pressure ratio). It should be noted that the shock boundary is significantly faster than the material boundary (not depicted).

[1] Wayne, Patrick John. "Characterization of single- and multi-phase shock-accelerated flows." (2019). https://digitalrepository.unm.edu/me_etds/170
 [2] Adams, B.M., Bauman, L.E., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hough, P.D., Hu, K.T., Jakeman, J.D., Stephens, J.A., Swiler, L.P., Vigil, D.M., and Wildey, T.M., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.0 User's Manual," Sandia Technical Report SAND2014-4633, July 2014. Updated May 2019 (Version 6.10)