

Meso-scale and continuum simulations for Arrhenius reactive burn model calibration of initiation in hexanitrostilbene (HNS)

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Motivation

- Predictive capability.
- Direct comparison of experiment and simulation.
 - Shock to detonation transition in thin film cutback study.
- Calibration and validation of EoS's and reactive burn models.

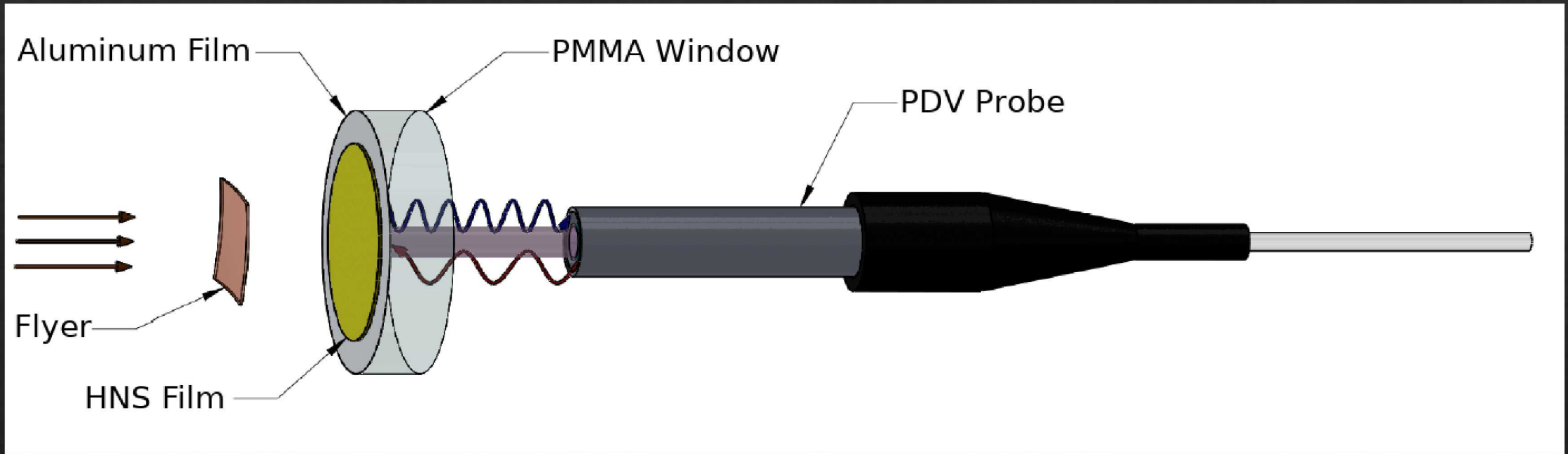
FOCUS: Use experimental data for direct linkage between experiments and simulations.

Computational

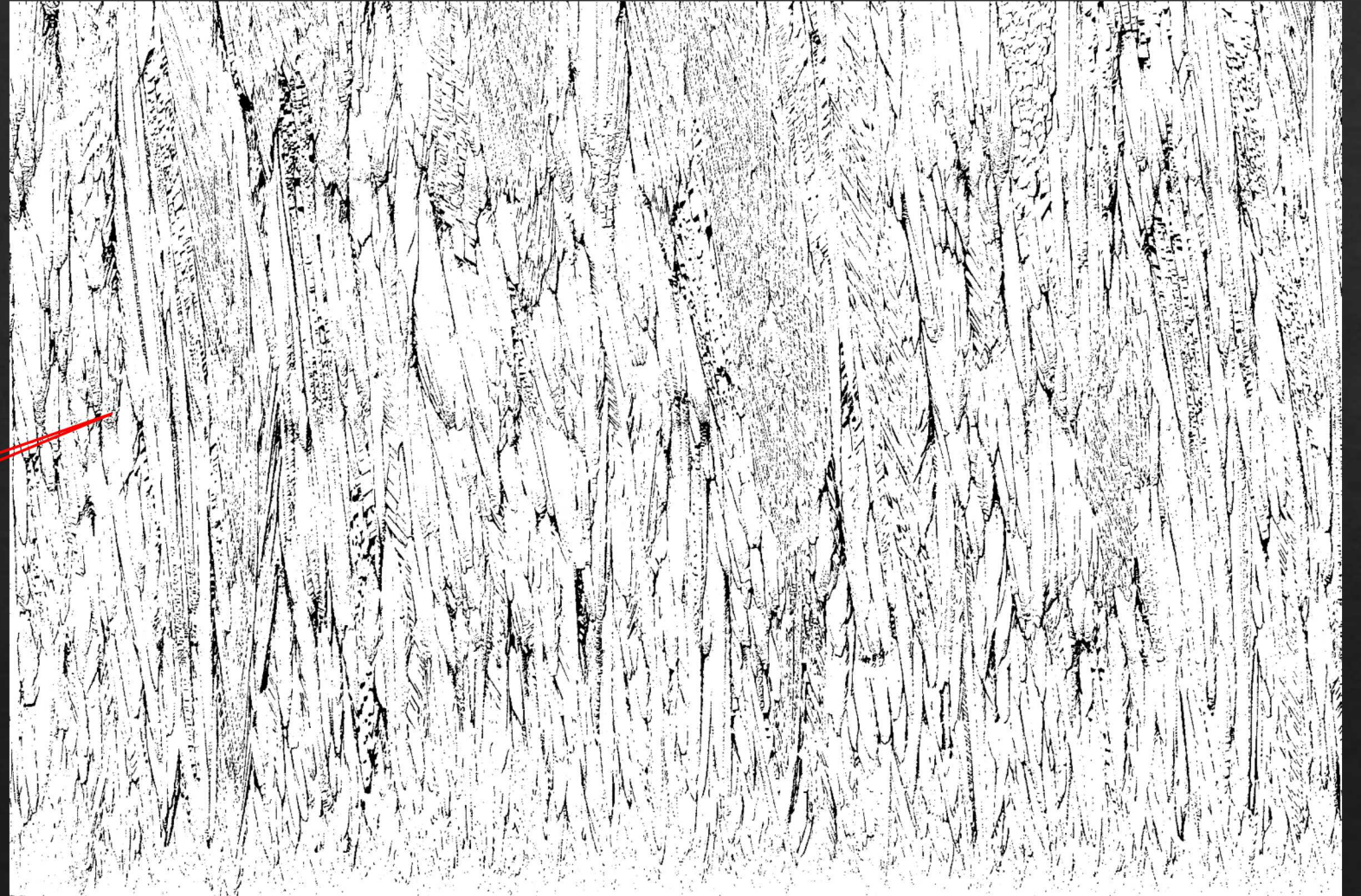
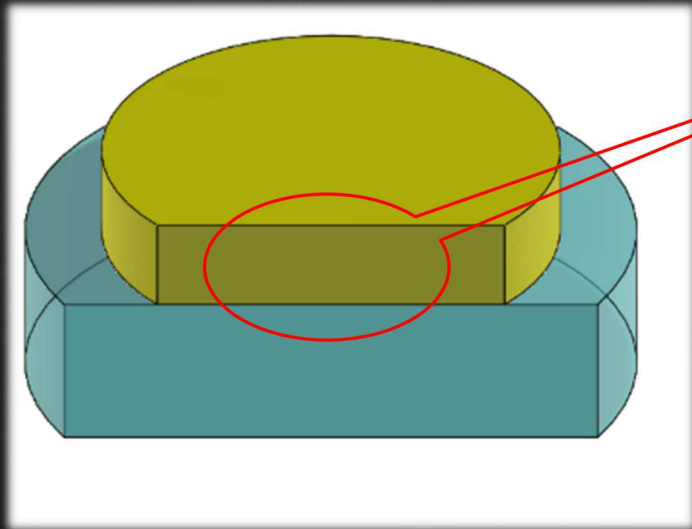
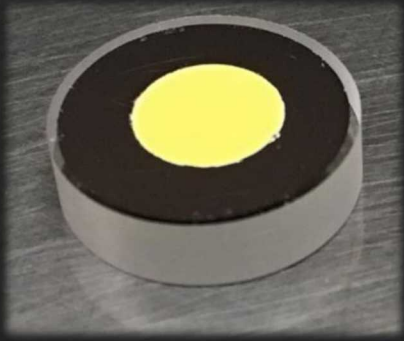


Experimental

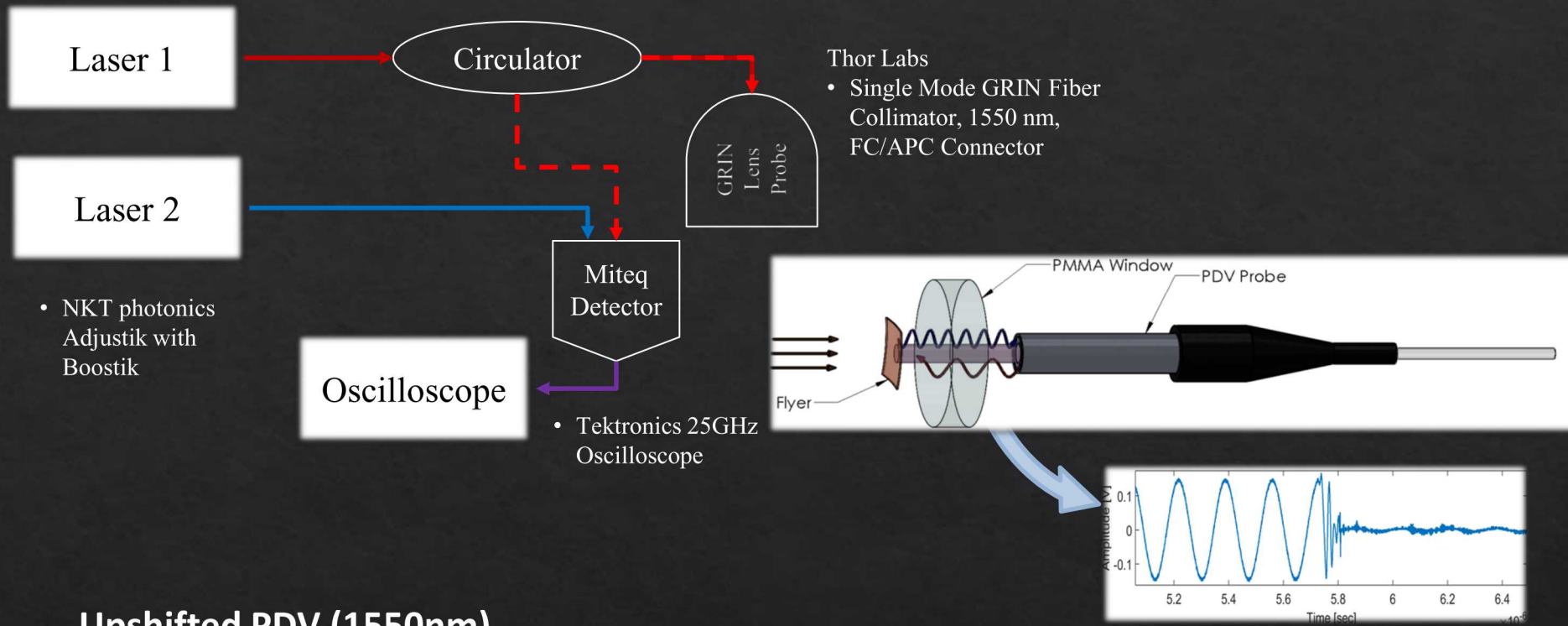
Schematic of experiment



Thin film HNS samples



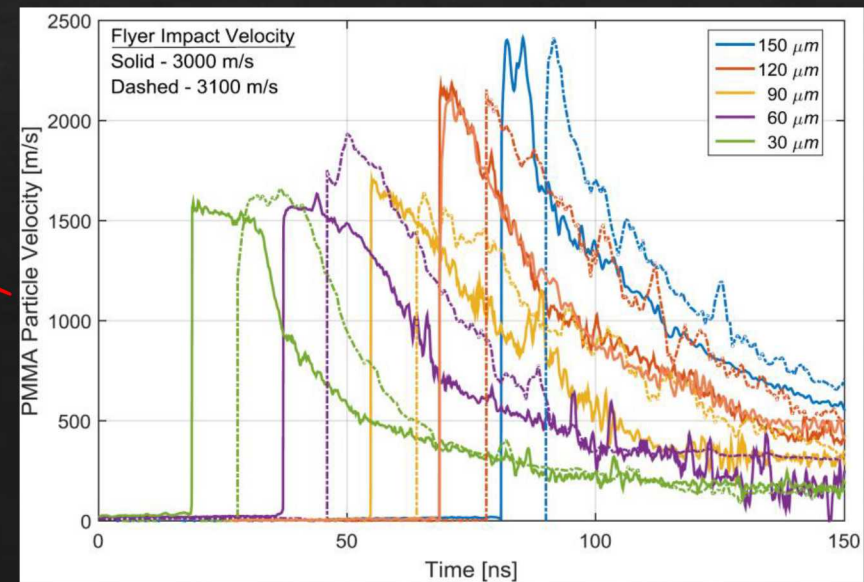
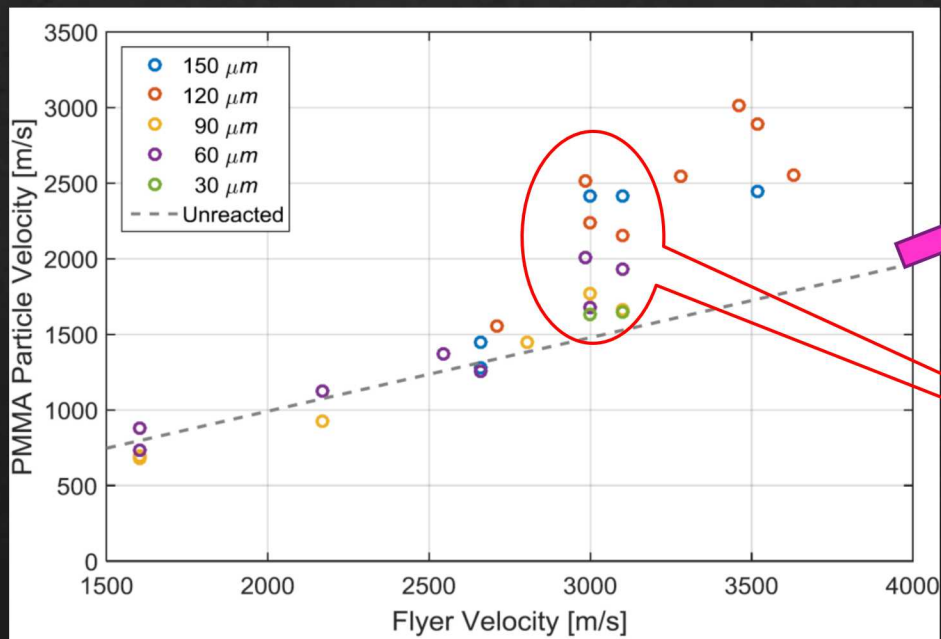
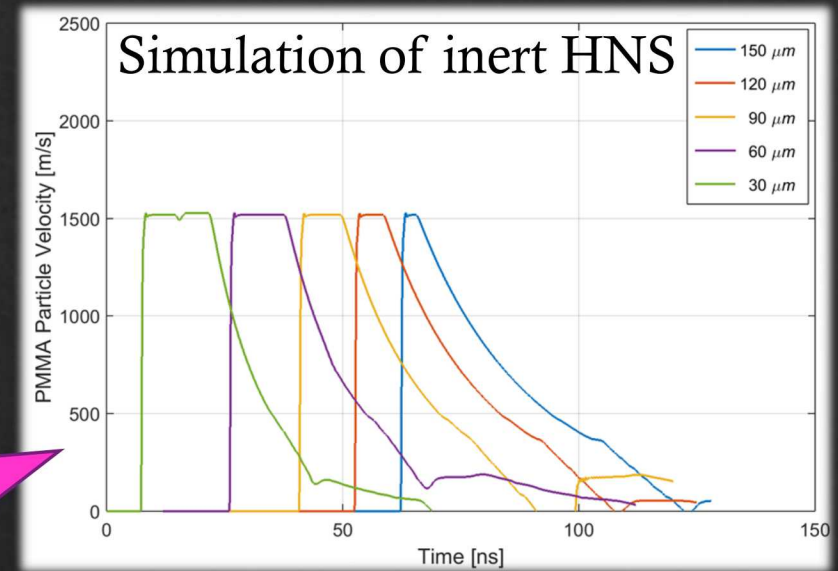
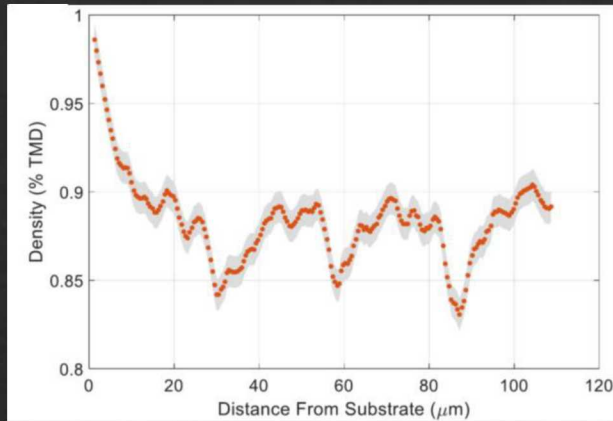
Velocity measurements



Upshifted PDV (1550nm)

- One laser is used as a reference beam and the other is sent to the target, beat frequency is produced and measured with the oscilloscope
- Single mode collimated Graded-Index (GRIN) lens probe sends and receives light from target
- Post processing of signal is done using Short-time Fourier Transform (STFT)

Experimental results



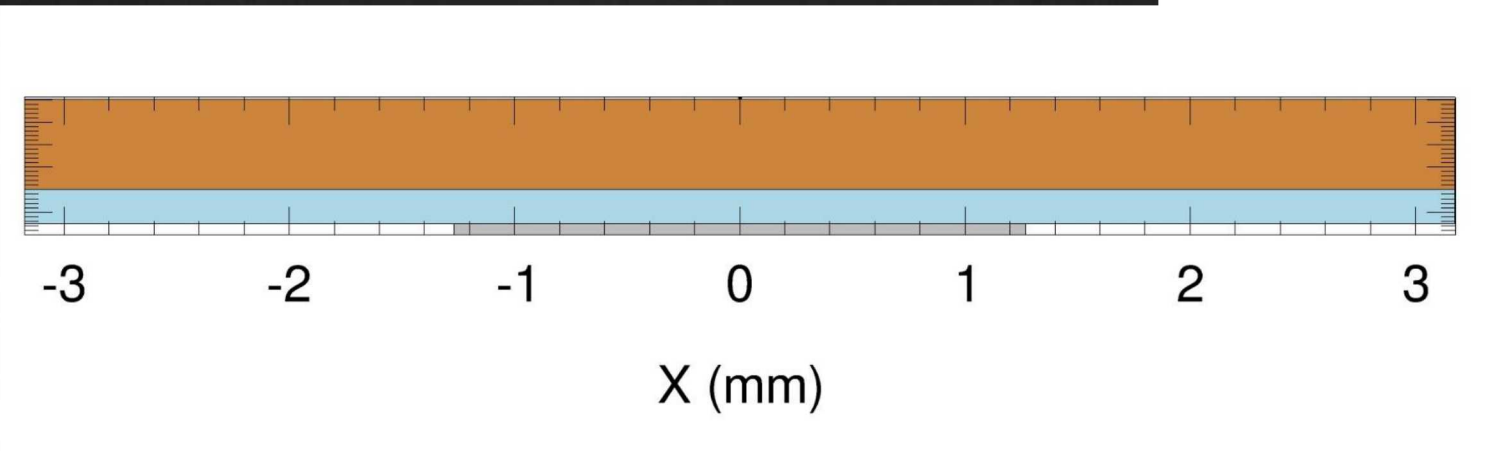
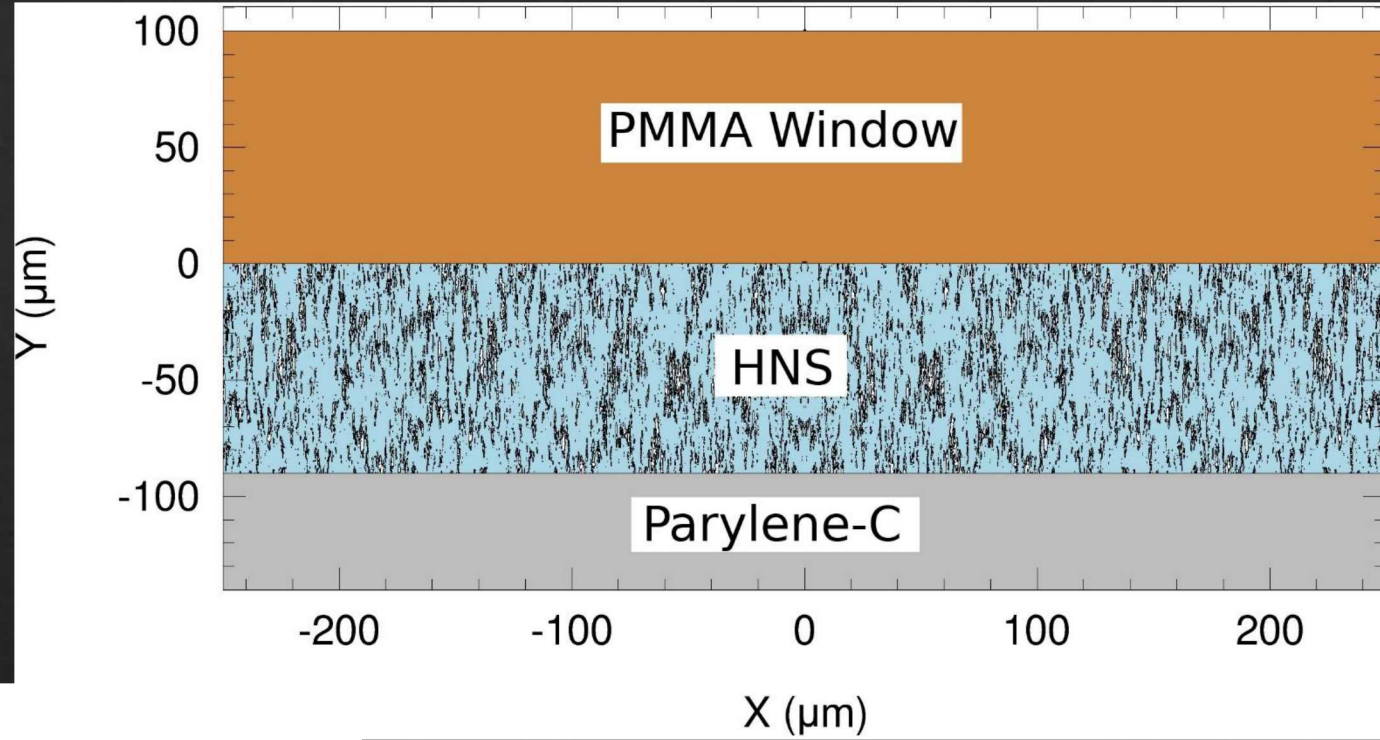
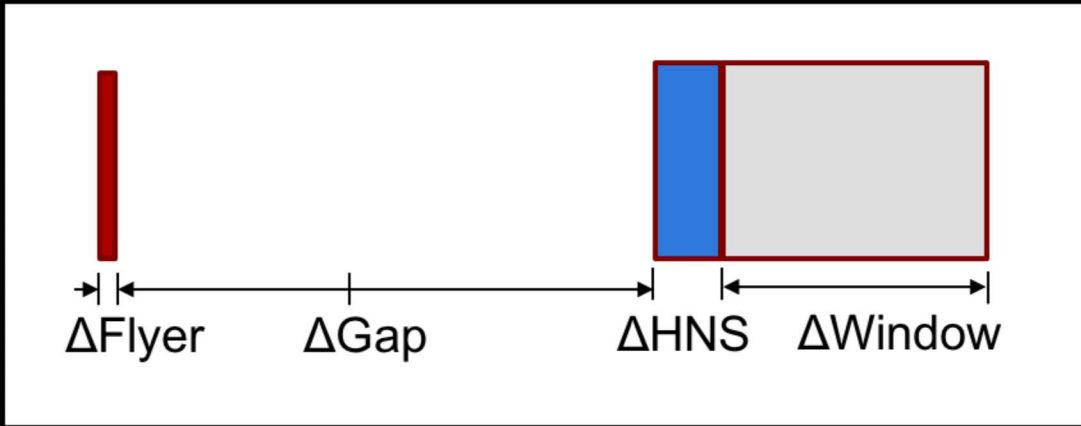
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Observations of shock-induced chemistry with subnanosecond resolution

Appl. Phys. Lett. 114, 214102 (2019); <https://doi.org/10.1063/1.5092230>

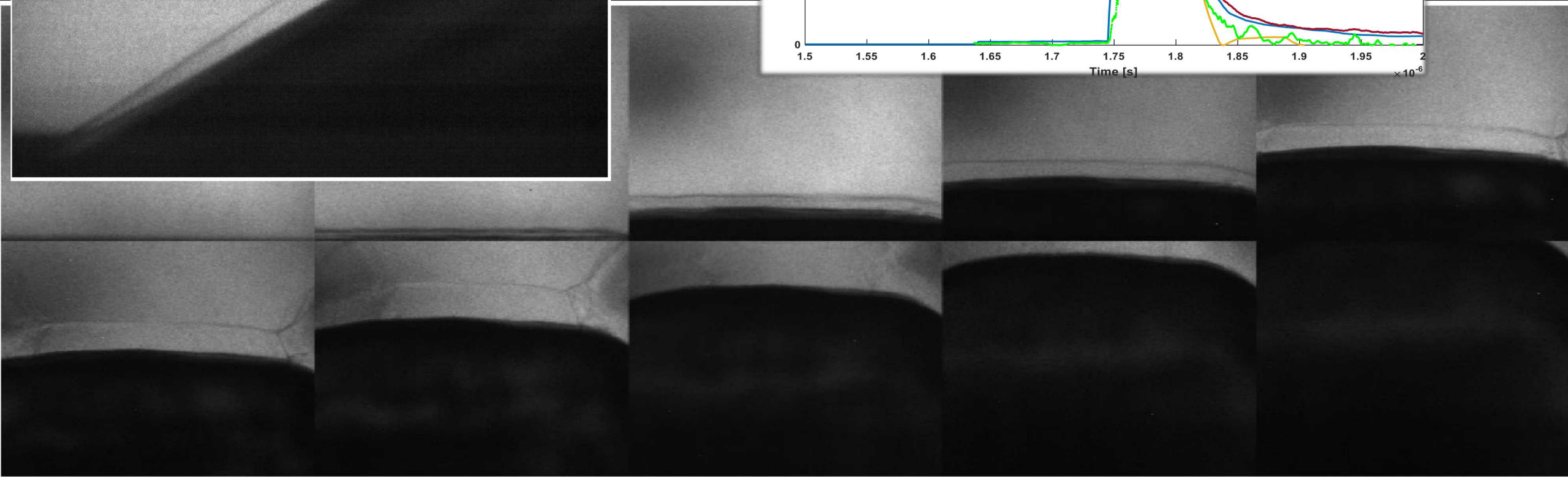
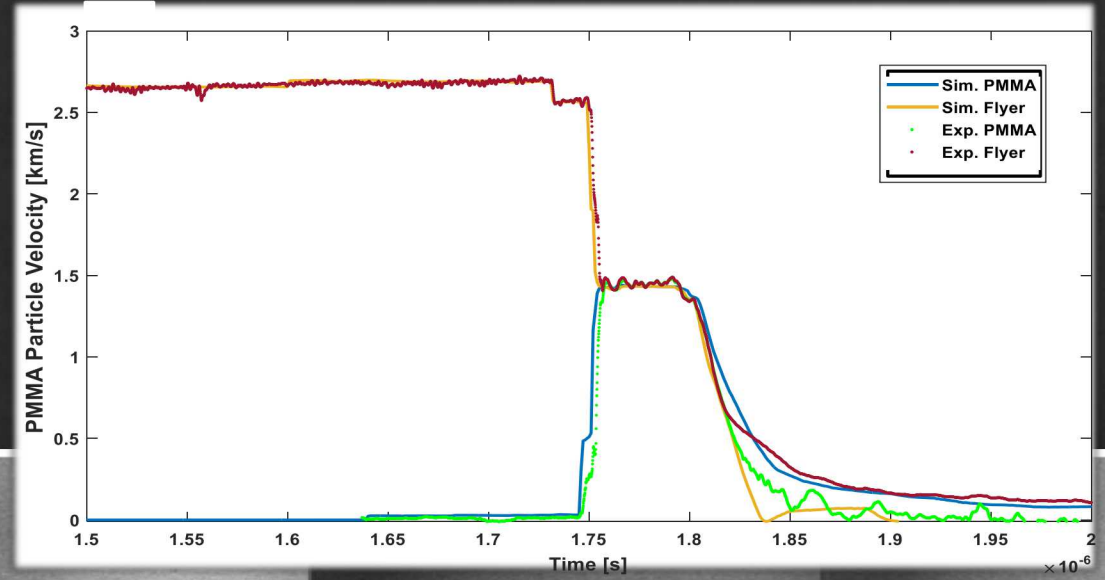
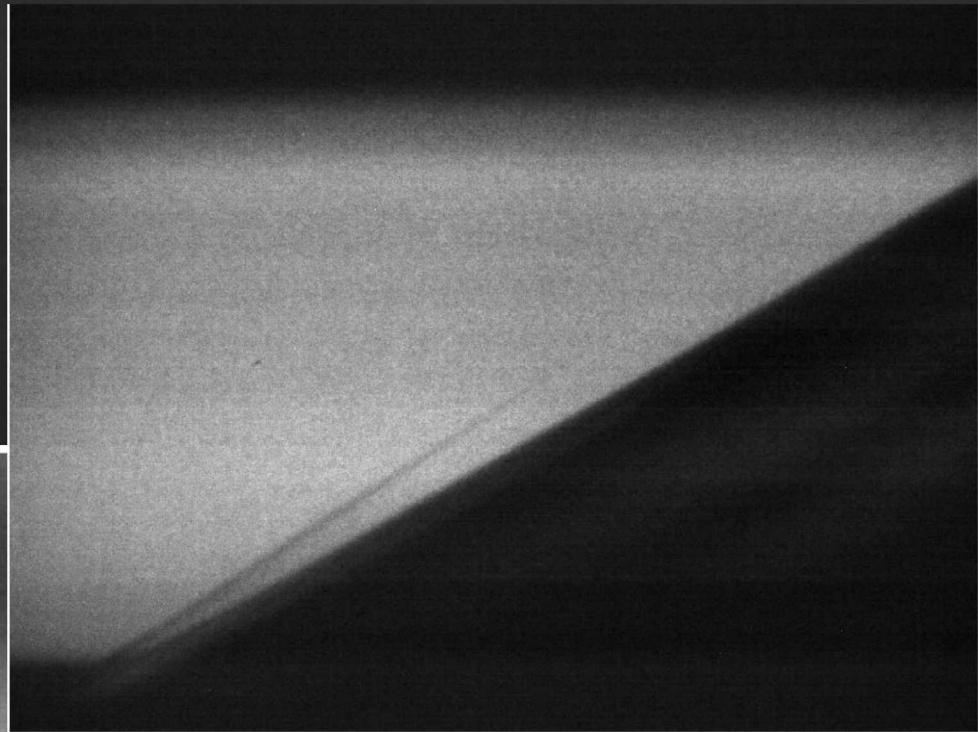
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Simulation geometry

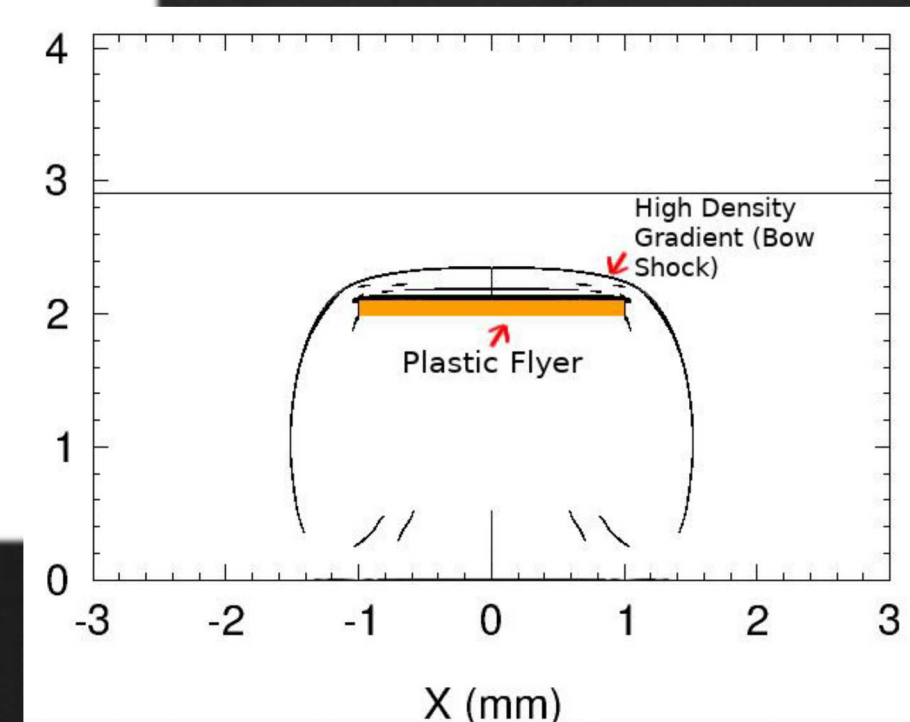
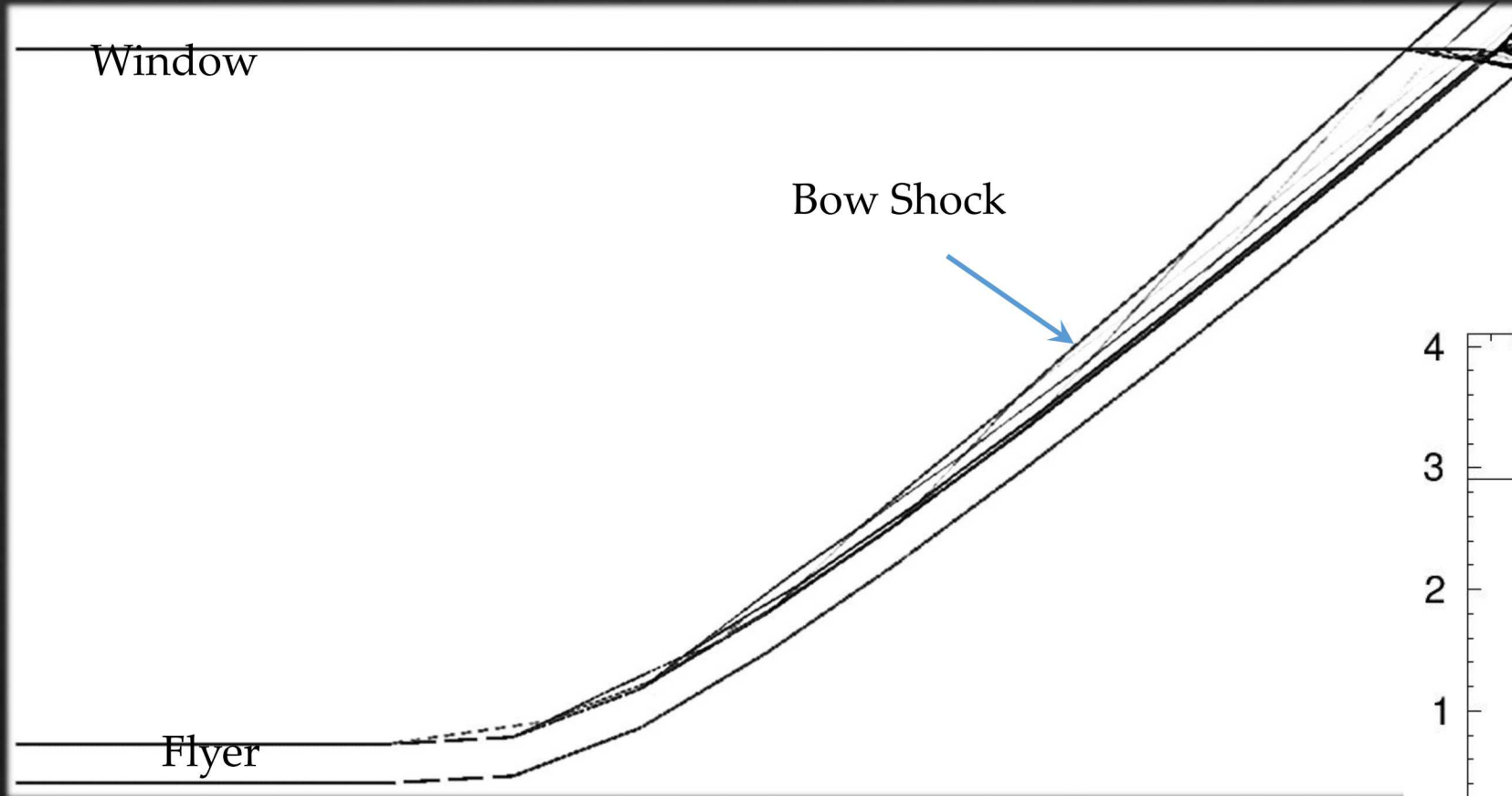


CTH Input Geometry Sketch

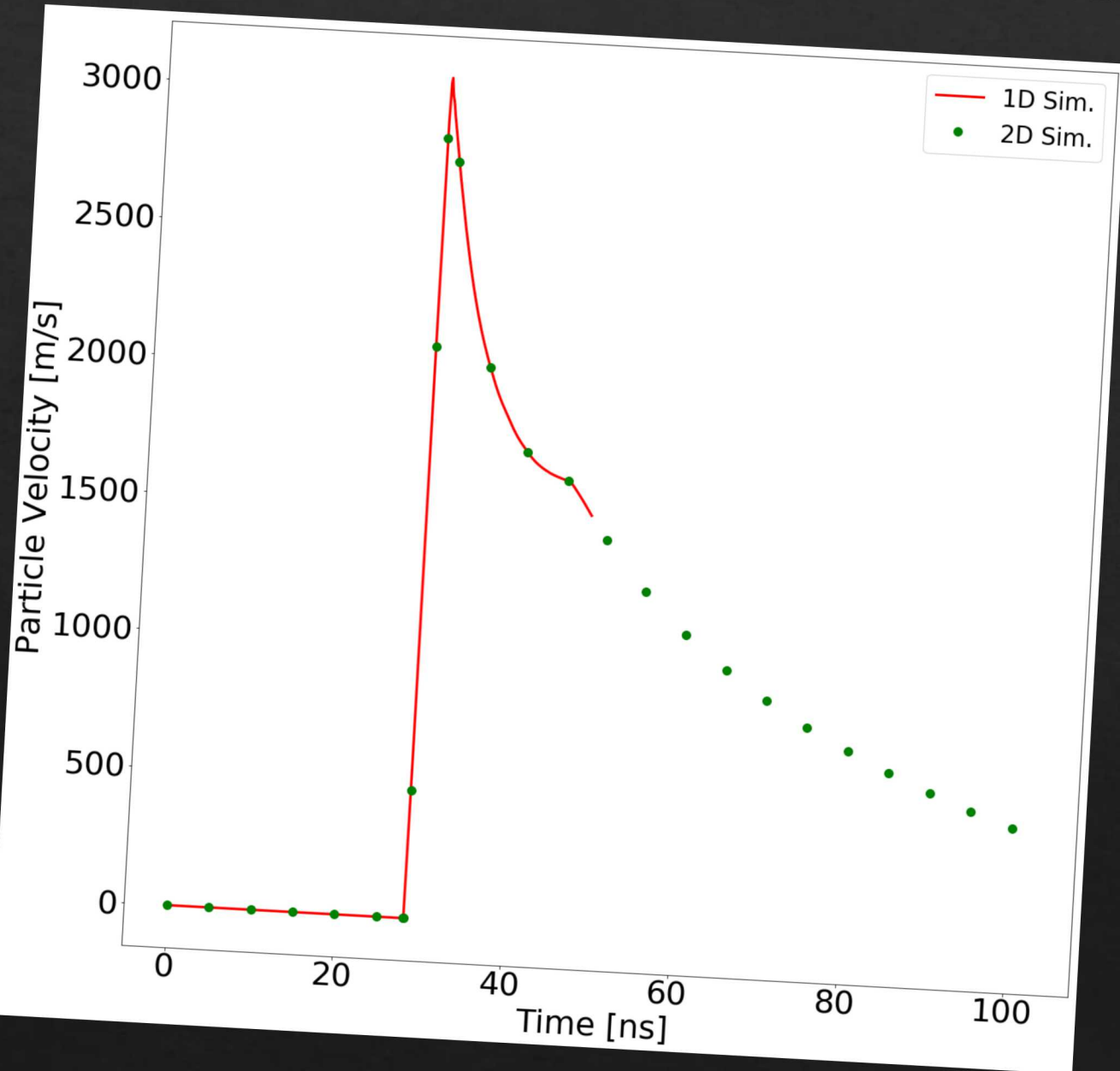
Simulation geometry



Simulation geometry



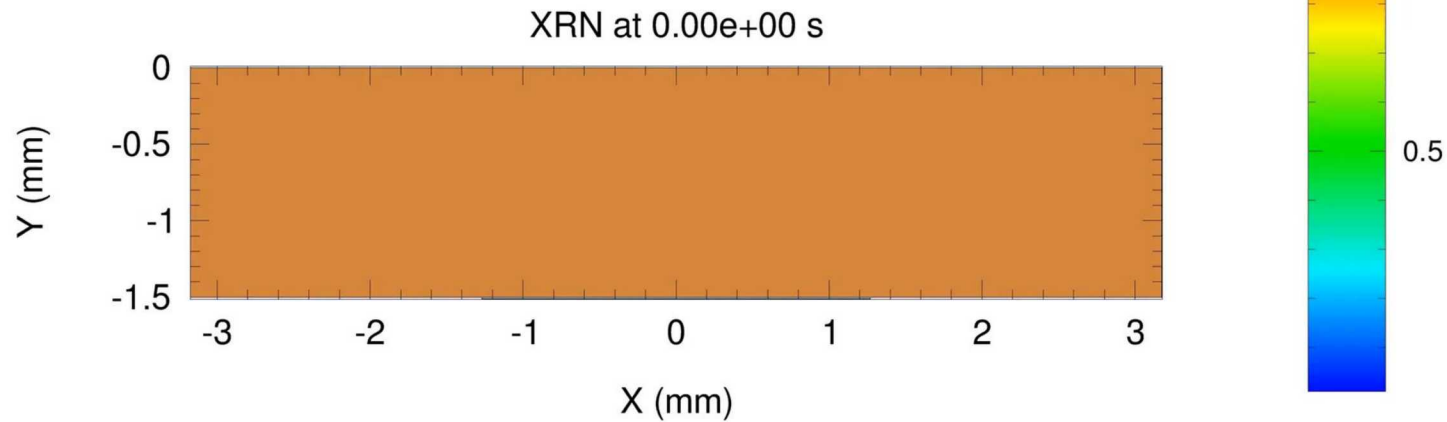
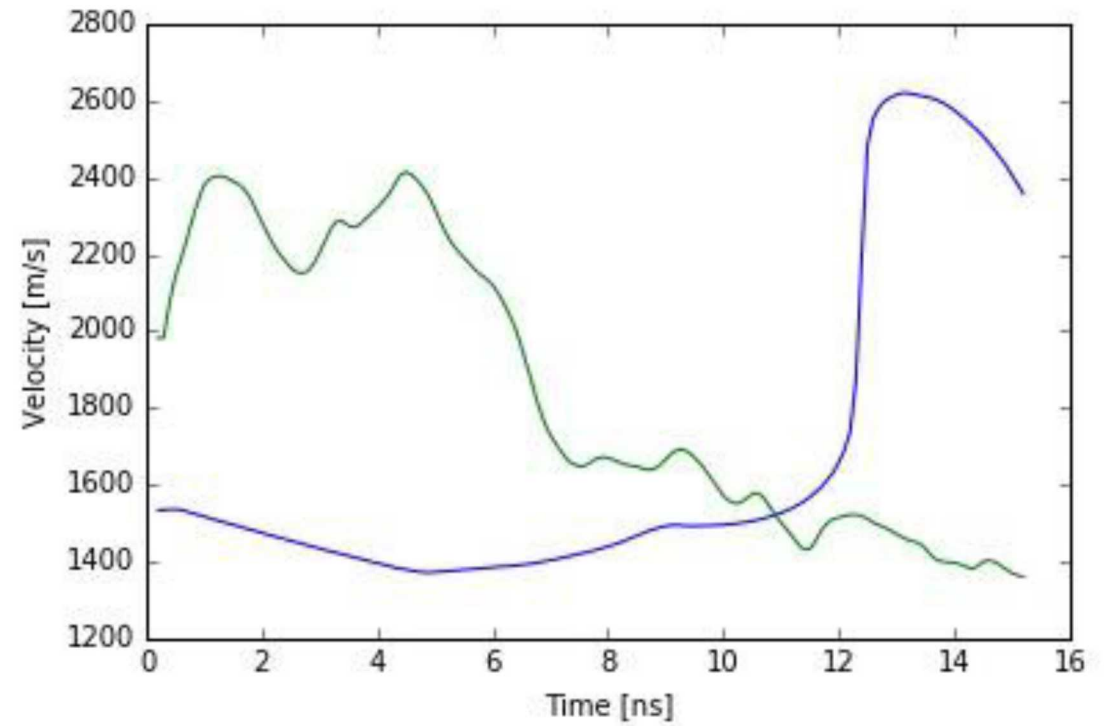
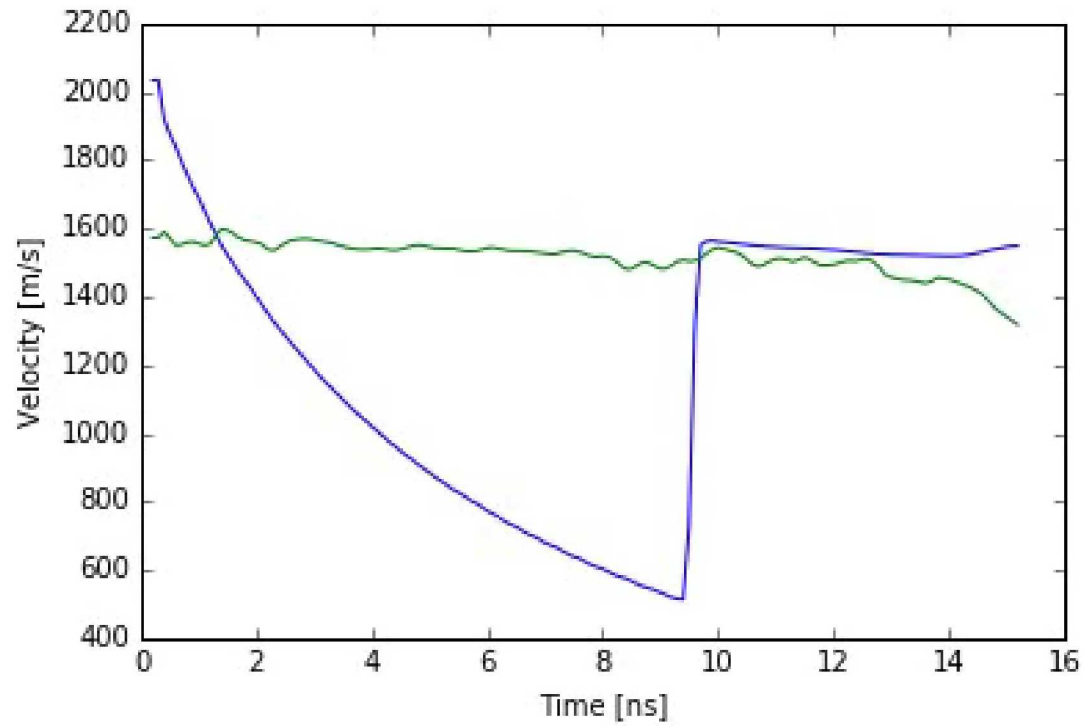
Simulation



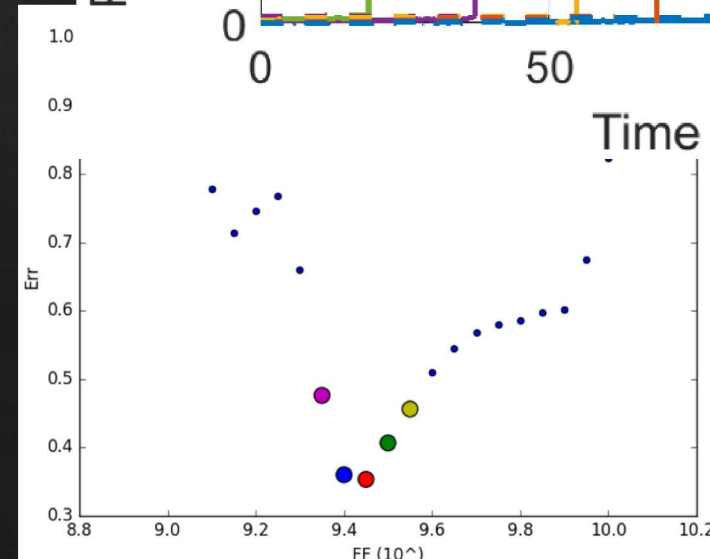
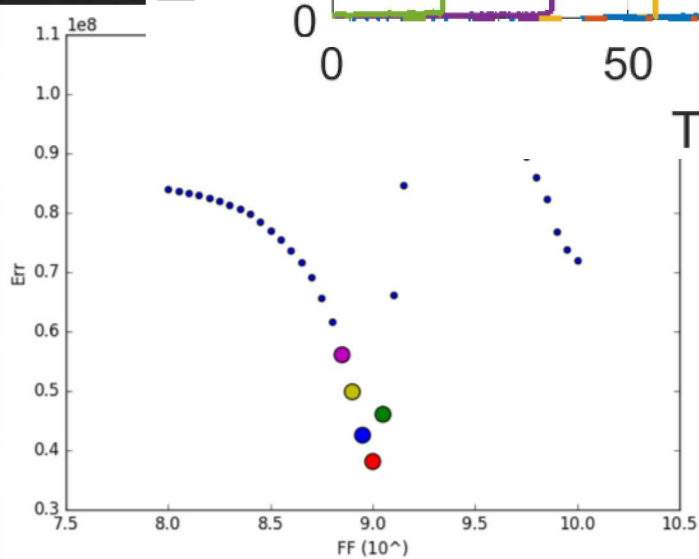
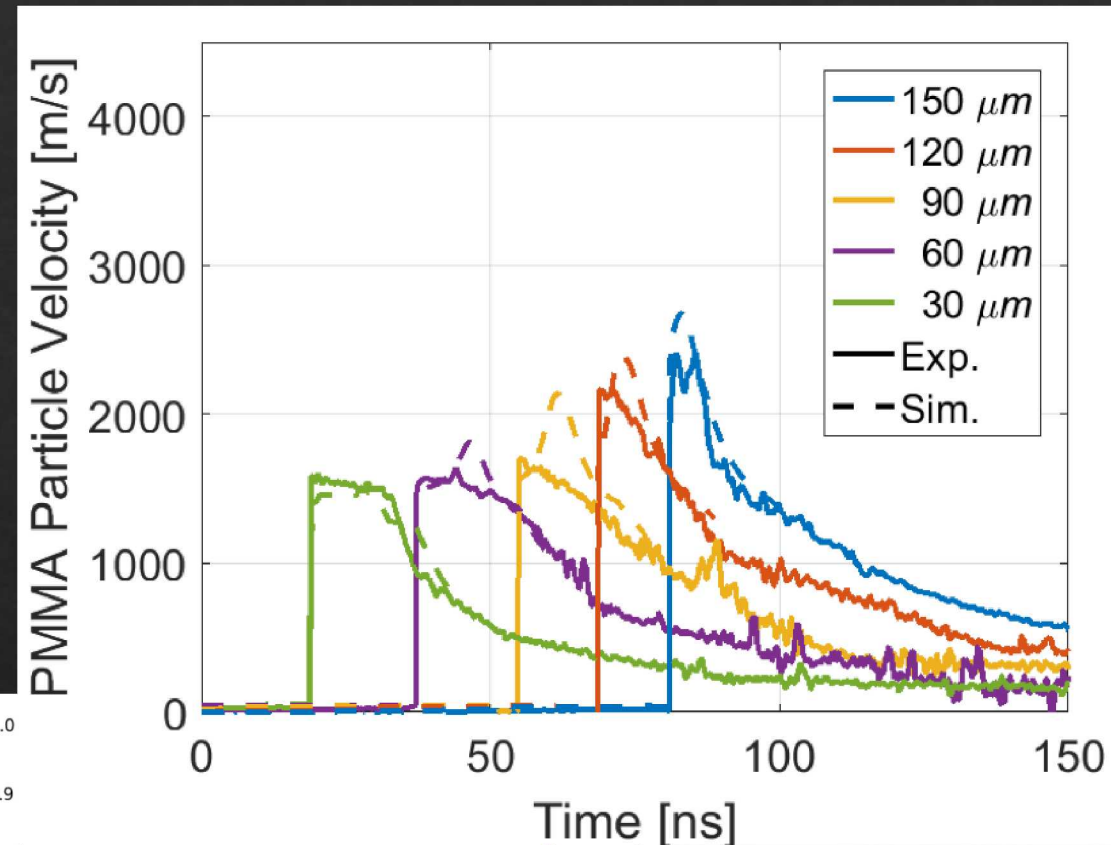
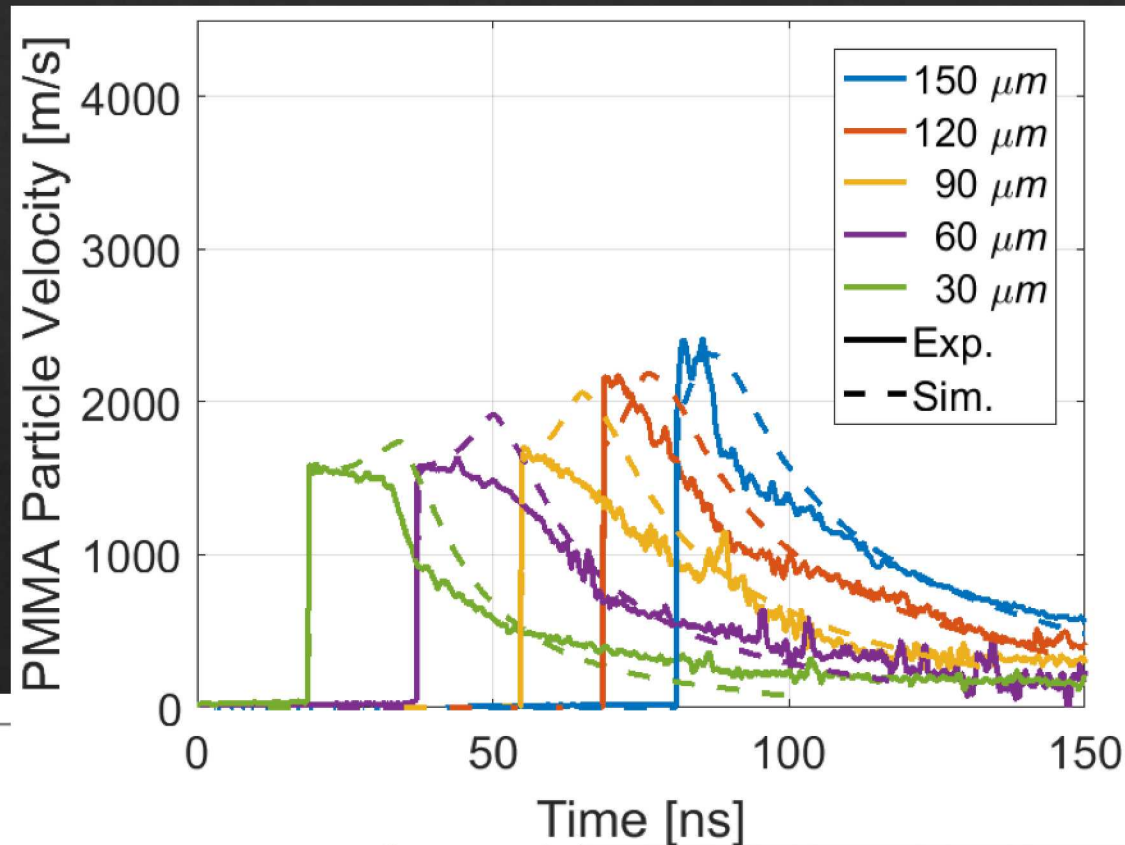
*Arrhenius
reactive burn*

$$k = FF e^{(-AT/T)}$$

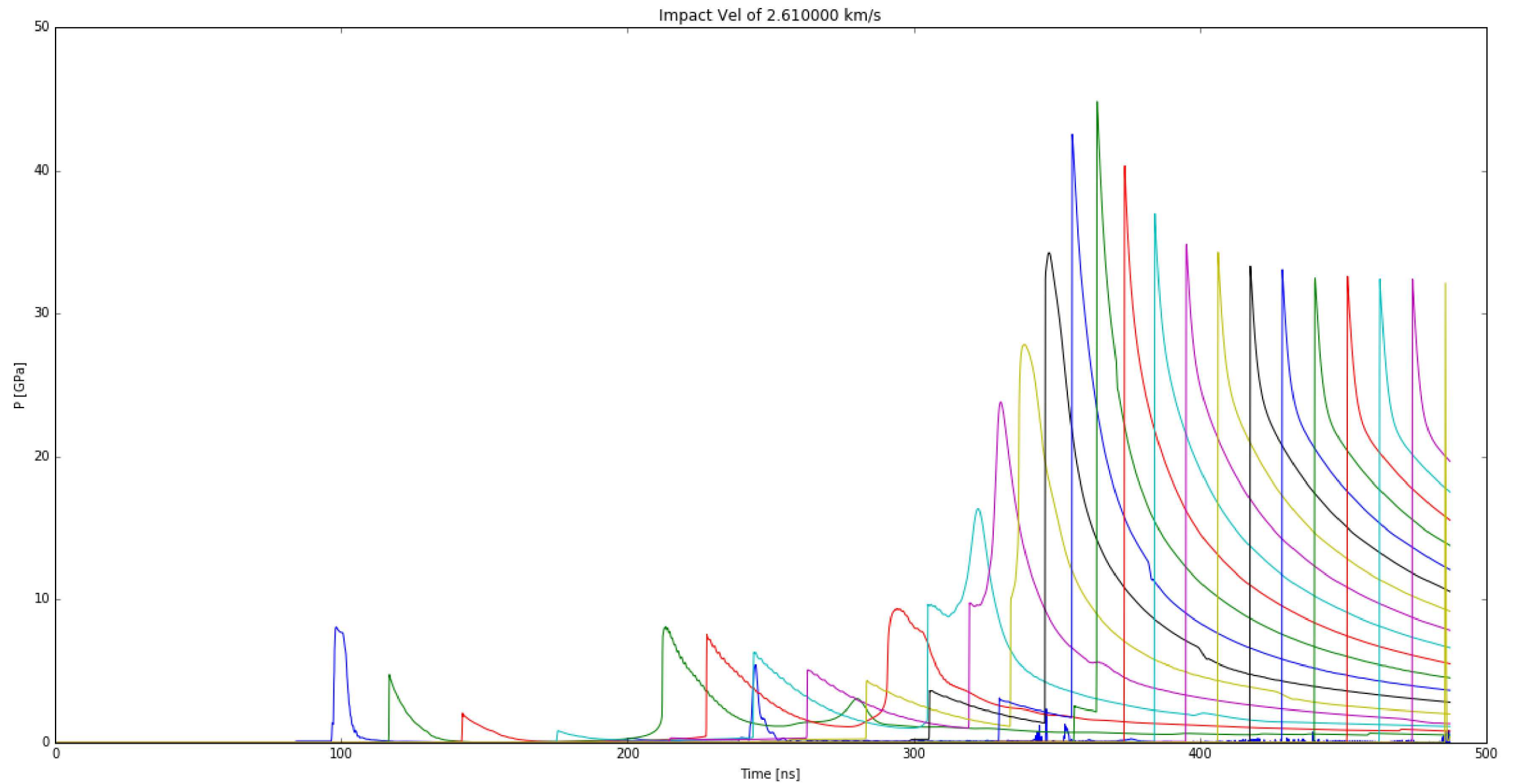
Simulation results



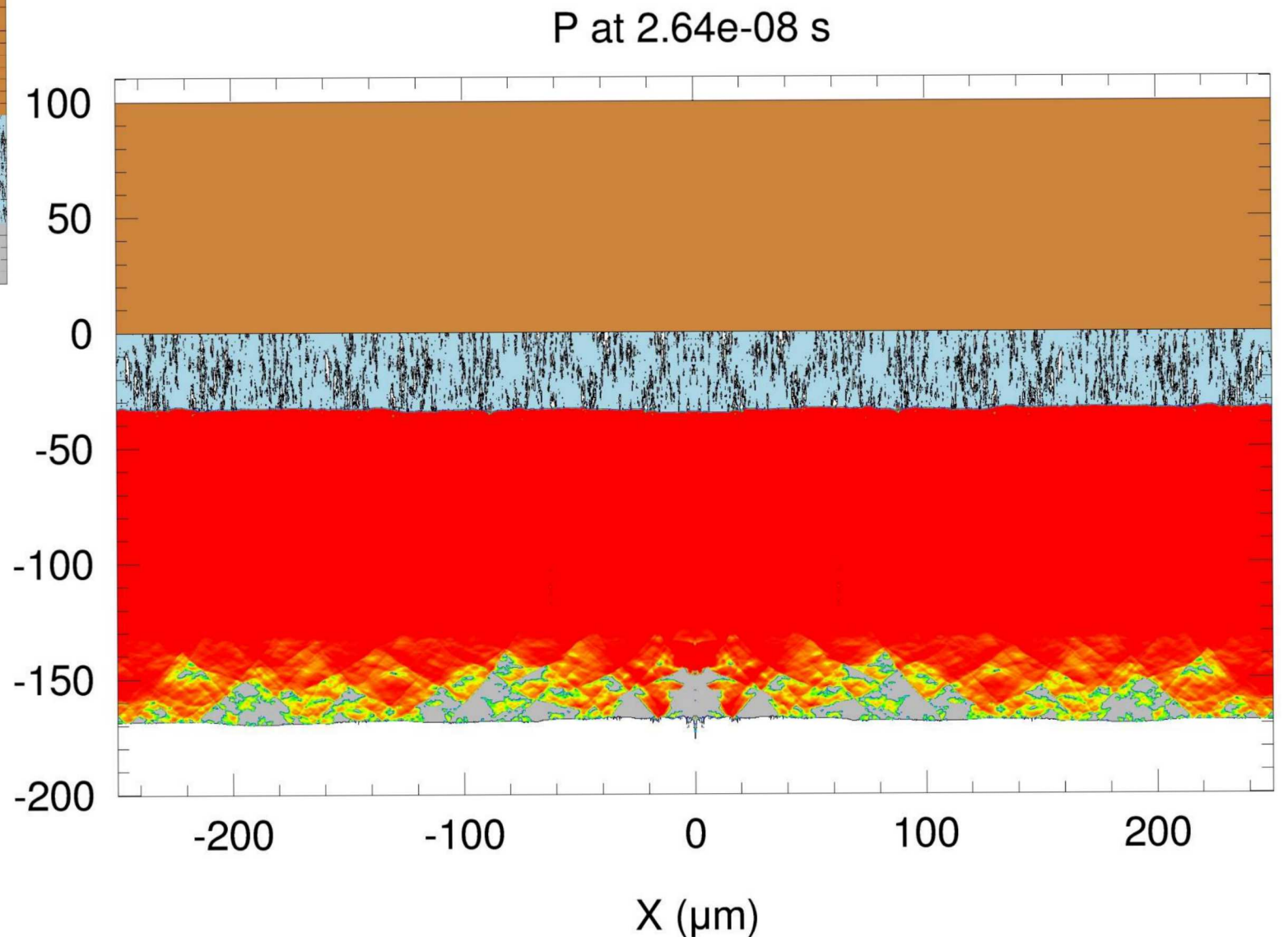
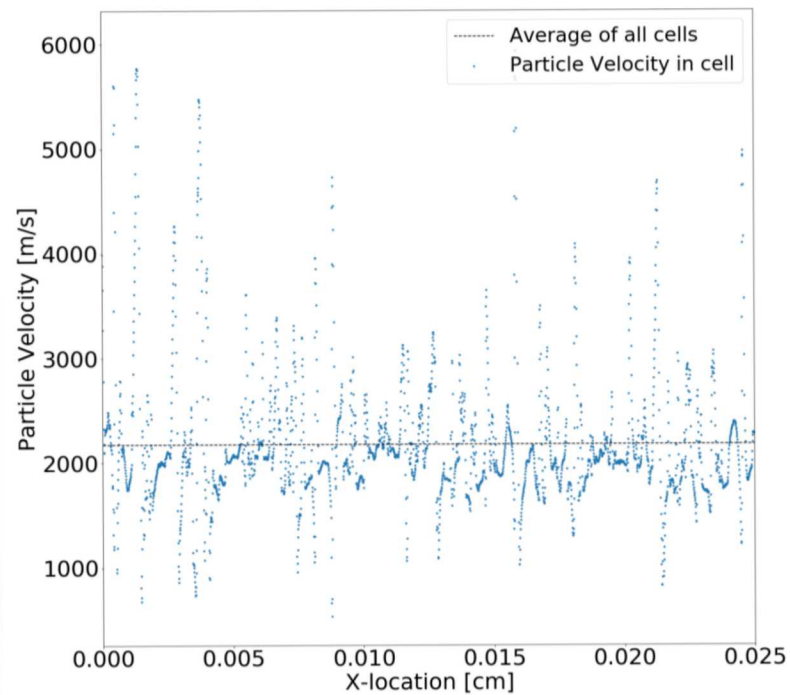
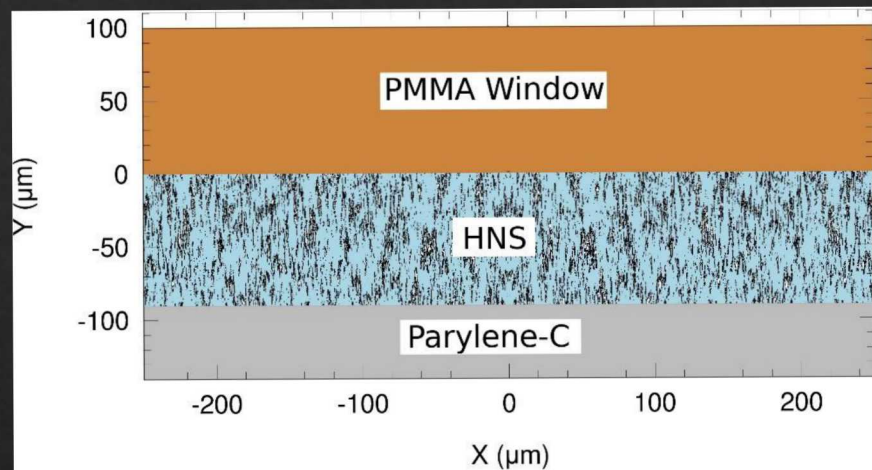
Simulation results



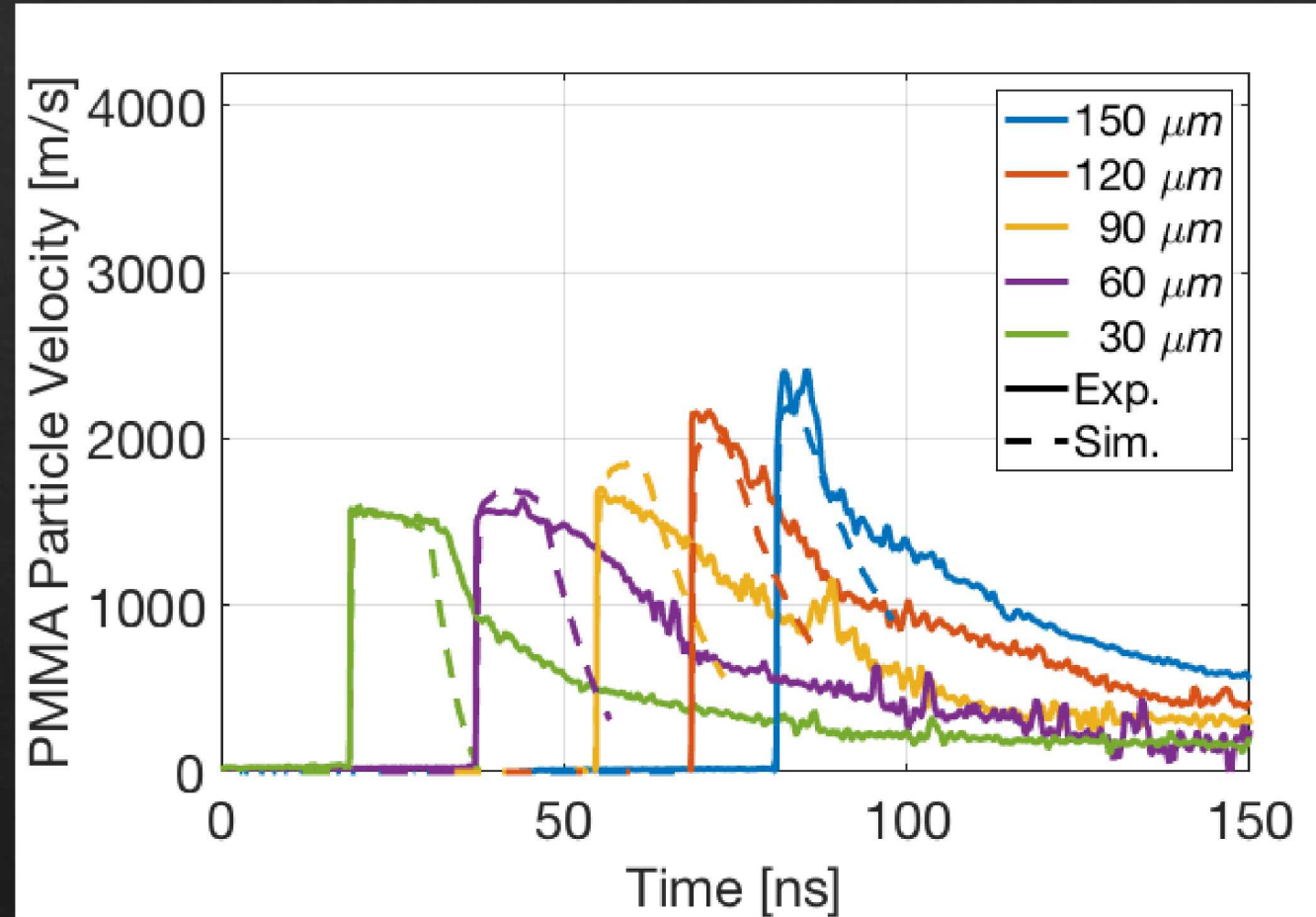
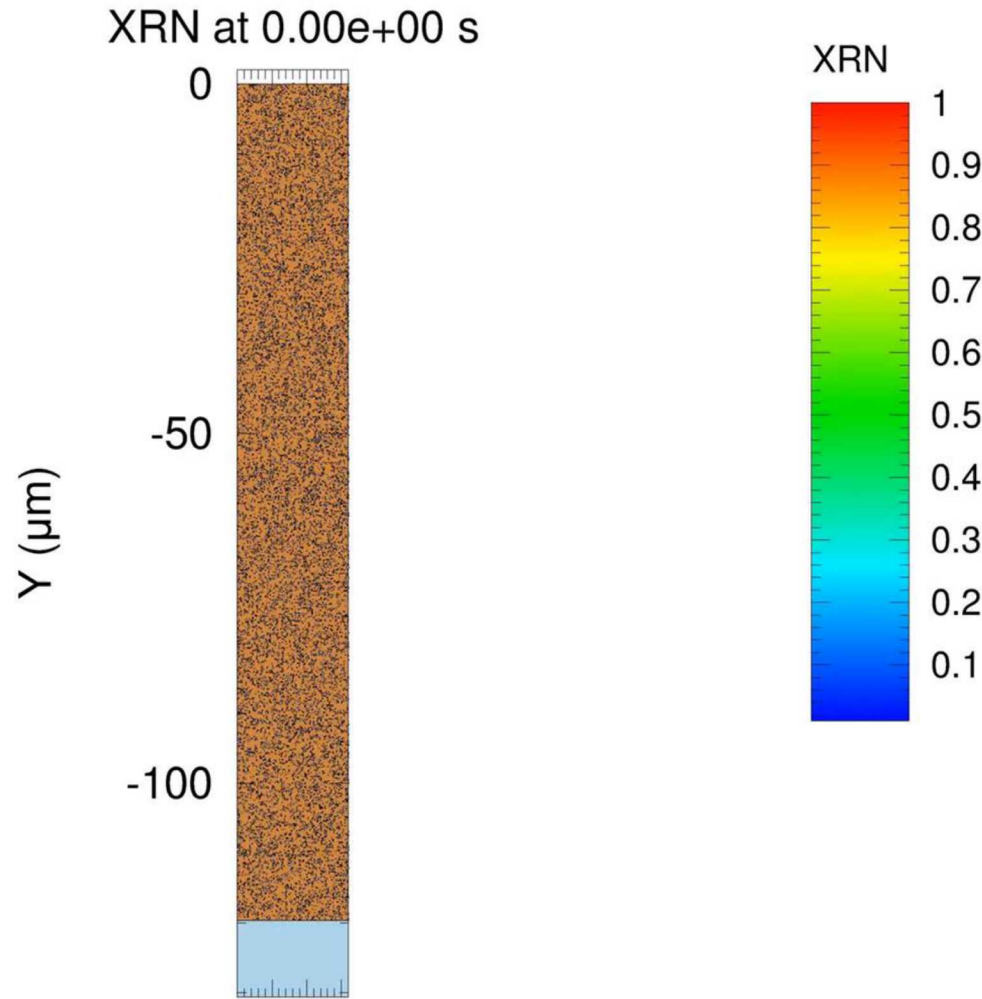
Simulation results



Simulation results



Simulation results



Summary

- Direct simulation of experiments.
 - Advantageous due to use of HNS – short run to detonation length
- Continuum and grain-scale (meso-scale) simulation
 - Continuum: vacuum or air
 - Reactive burn parameters optimized



Extra Slides

PDV Analysis Process

Interactive Spectrogram and Analysis

