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Title: Detailed Validation of Ejecta Transport Models

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Detailed Validation of Ejecta Transport Models

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PEM Mix and Burn FY 21 Update – October 21, 2021

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LA-UR-21-XXXXX

LANL Ejecta Experiments

- 2017 Experiments → study ejecta transport in inert and reactive gases
  - Solid ejecta

- 2019 Experiments → Repeat 2017 experiments with liquid ejecta

- Target thicknesses:
  - 2017 Tin: $2\ mm$
  - 2017 Cerium: $3\ mm$
  - 2019 Cerium: $1.75\ mm$

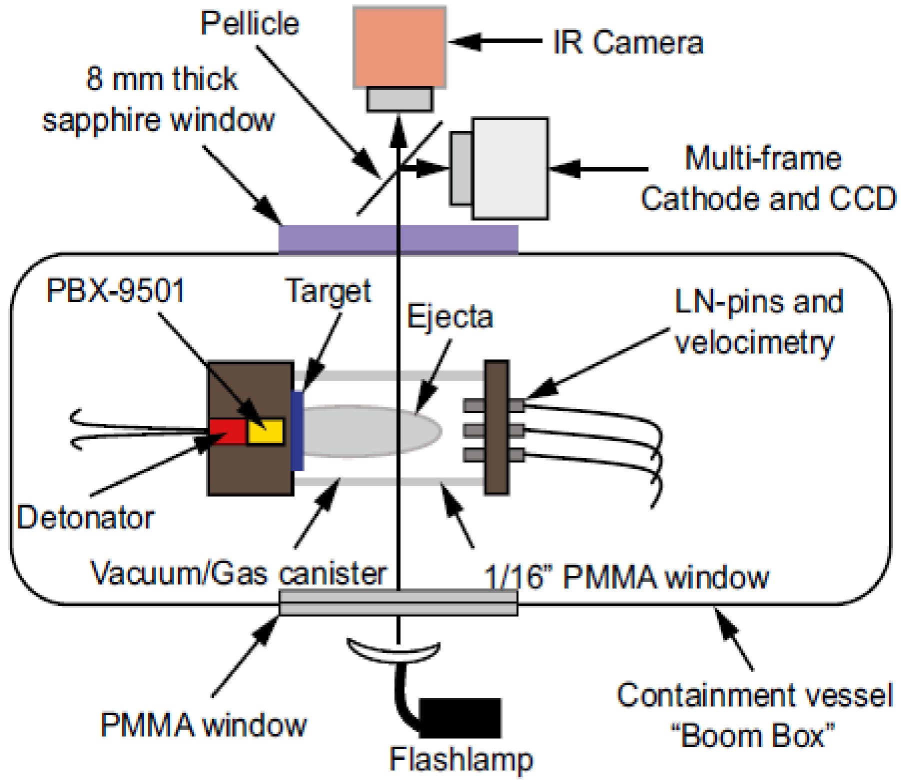


Figure 1: Figure 3 from [1] showing the ejecta experiment configuration and diagnostics

[1] Buttler, W. T., Lamoreaux, S. K., Schulze, R. K., Schwarzkopf, et al. (2017). Ejecta Transport, Breakup and Conversion. *Journal of Dynamic Behavior of Materials*, *3*(2), 334-345.

LANL Ejecta Experiments

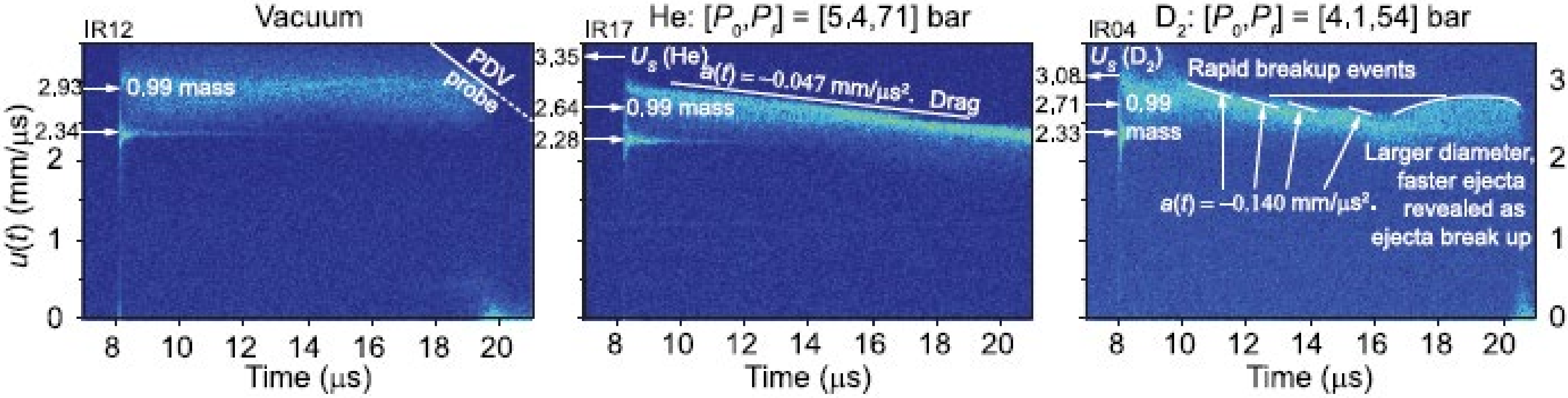


Figure 2: Figure 6 from [2] shows ejecta velocities over time while propagating in a vacuum (left), an inert gas (center) and a reactive gas (right)

- Reacting ejecta show a staged rapid break-up phenomenon not seen otherwise
- Schwartzkopf and Schulz developed initial “0D” models of solid ejecta phenomena
  - did not account for spatial variations in gas or particle cloud temperatures

<u>Overall goal for work</u>:

1. Develop a 2D simulation to that enables accurate validation with experiments
2. Build a melt based break-up model on top of this 2D simulation and try to reproduce the new staged breakup behavior

[2] Buttler, W. T., Schulze, R. K., Charonko, J. J., Cooley, J. C., Hammerberg, J. E., Schwarzkopf, et al. (2021). Understanding the transport and break up of reactive ejecta. *Physica D: Nonlinear Phenomena*, *415*, 132787.

Melt Dispersion Mechanism

- Searched aluminum combustion literature for analogous behaviors
- In the "melt dispersion mechanism" [3], if an initially solid particle melts at a fast heating rate while surrounded by an oxide shell, it will generate stresses which will fracture the shell and possibly cause cavitation due to an unloading wave
- Preliminary calculations using the physical constants for cerium and its hydride showed that this phenomenon, if present, may cause cavitation in the ejecta so long as $r_{ejecta} < 0.653\ \mu m$

Table 1: Results from sample calculations used to determine the potential feasibility of cavitation in the ejecta particles from the experiments

Crystal Structure	M (C1)	$\delta(nm)$ (C1)	$P(t_s, R)$ (MPa)	$v(t_s, R)$ (m/s)	P_m (MPa)	v_m (m/s)	P_{cr} (MPa)	Cavitation?
CeF_2	2.9752	84.0290	365.953	85.464	-4679.546	240.095	-56.000	Yes
FeS_2	4.5678	54.7311	371.339	86.773	-4751.347	243.770	-56.000	Yes
AlB_2	3.8808	64.4192	362.940	84.732	-4639.369	238.038	-56.000	Yes
CeB_2	4.7389	52.7548	363.974	84.984	-4653.147	238.743	-56.000	Yes
$R_{max}(nm)$	652.733	-						

- Since, for us, the ejecta are initially liquid, but may form a crust afterwards, it is unclear how relevant this mechanism is.
  - Left open the possibility that this phenomenon could be occurring locally and cause the hydride shell to flake off rather than universally fracture

[3] Levitas, V. I., Asay, B. W., Son, S. F., and Pantoya, M., 2007. "Mechanochemical mechanism for fast reaction of metastable intermolecular composites based on dispersion of liquid metal". Journal of Applied Physics, 101(8), p. 083524

Particle Energy Equation: Numerical Stability

- Discovered a numerical stability issue in the implementation of the particle temperature update of the hydride model
- Tested with a single, small tin particle transporting in helium,
  - Initial method was semi-implicit: $\frac{\Delta e_p}{\Delta t} = \frac{Nu^n}{2}\frac{c^m}{\tau_T^n}\left(T_\infty^n - T_p^{n+0.5}\right)$
  - Writing this as $T_p^{n+1} = aT_\infty^n + bT_p^n$, an additional stability criterion was found by enforcing $a + b = 1$ and $a, b > 0$ → $\boldsymbol{\Delta t < \frac{4\tau_T^n}{Nu^n}}$
- Reformulated particle energy update with a fully implicit method

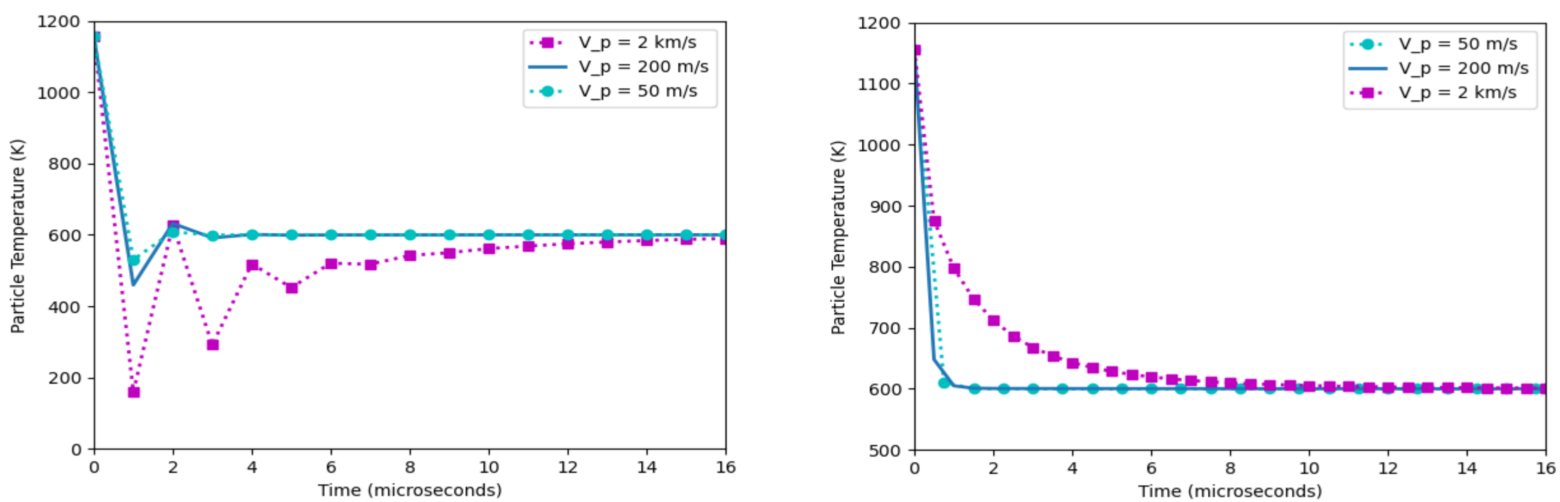


Figure 3: Temperature of a 1 μm diameter tin particle cooling in helium from 1183 K to 600 K without (left) and with (right) the semi-implicit time step restriction at various particle velocities

Hydrocode Governing Equations

Continuum Phase Governing Equations [3] → Discretized Staggered Mesh Equations

$$\rho \frac{d(\rho^{-1})}{dt} - \boldsymbol{\nabla} \cdot (\boldsymbol{v}) = 0$$

$$\rho \frac{d\boldsymbol{v}}{dt} + \boldsymbol{\nabla} P = 0$$

$$\rho \frac{de}{dt} + P\boldsymbol{\nabla} \cdot (\boldsymbol{v}) = 0$$

Trivially satisfied

$$m_p \frac{d\boldsymbol{v}_p}{dt} + \sum_{Z(P)} \boldsymbol{f}_Z^p = 0$$

$$m_Z \frac{de_Z}{dt} - \sum_{P(P)} (\boldsymbol{f}_p^Z \cdot \boldsymbol{v}_p) = 0$$

Lagrangian Particle Equations:

$$\frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{u}_i$$

$$M_i \frac{d\boldsymbol{u}_i}{dt} = \boldsymbol{F}_{drag}$$

$$M_i C_i \frac{dT_i}{dt} = \dot{Q}_c$$

Additional Code Utilities:

- ALE relaxers to avoid mesh tangling
- Particles tracked as computational superparticles

[3] Fung, J., Harrison, A. K., Chitanvis, S., & Margulies, J. (2013). Ejecta source and transport modeling in the FLAG hydrocode. *Computers & Fluids*, *83*, 177-186.

Ejecta Models

- Ejecta Sourcing: Richtmyer-Meshkov Source Model [4]
  - Solves ODEs for bubble/spike velocities based on shock emerging from donor material and imparting a free-surface velocity to a perturbed surface
  - Ejecta velocities: Set to the spike tip velocity
  - Ejecta diameters: Based on perturbation wavelength and areal fraction of spikes on surface
  - Ejecta thermodynamic properties initialized by using values from target material 2 zones inward from sourcing face*

- Particle-Fluid Momentum Transfer: Parmar drag correlation

$$\boldsymbol{F}_{drag} = \frac{1}{8}\pi d_p^2 \rho_f |\boldsymbol{u}-\boldsymbol{v}|(\boldsymbol{u}-\boldsymbol{v}) C_D(Re_p, M_p)$$

  - Formula for C_D given in [5]

- Particle-Fluid Heat Transfer: Hydriding model (currently minus the reaction term)

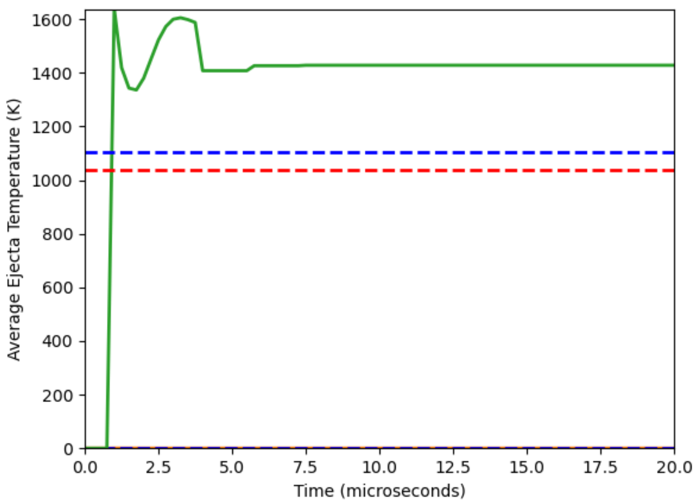
$$\dot{Q}_c = \dot{Q}_{conv} = \pi d_p k Nu\left(T_g - T_p\right)$$

$$Nu = 2 + 0.6 Re_p^{0.5} Pr^{\frac{1}{3}}$$

[4] Buttler, W. T., Oró, D. M., Preston, D. L., Mikaelian, K. O et al. (2012). Unstable Richtmyer–Meshkov growth of solid and liquid metals in vacuum. *Journal of Fluid Mechanics*, *703*, 60-84.
[5] Parmar, M., Haselbacher, A., & Balachandar, S. (2010). Improved drag correlation for spheres and application to shock-tube experiments. *AIAA Journal*, *48*(6), 1273-1276.

Modified Ejecta Initialization

- Early flyer plate test simulations with a geometry similar to the experiments showed an issue with the ejecta temperatures being reported from the simulations



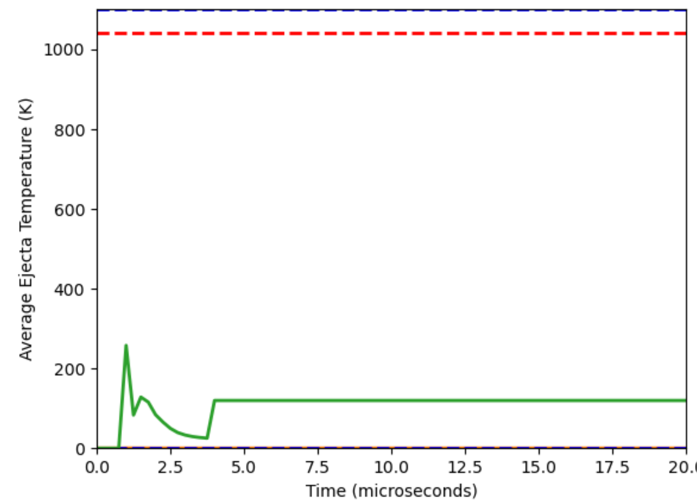


Figure 4: Average ejecta temperatures for axisymmetric, 18 x 99 zone (left) and 36 x 198 zone (right) simulations

- No heat transfer → particle temperatures were constant after ejecta creation
- This led us to investigate the method being used to initialize certain ejecta properties

Modified Ejecta Initialization

- Originally, ejecta density, pressure, temperature and bulk modulus were all initialized to the values of the donor material in the zone immediately behind the generating face (i.e. z=1)

- A problem arises as these properties can be unphysical in simulations near a material interface

- Solution was to modify the code to make ejecta initialize these properties from a zone layer which is user-specified in the input deck
  - Exactly as existing treatment for shock speed and melt state calculations

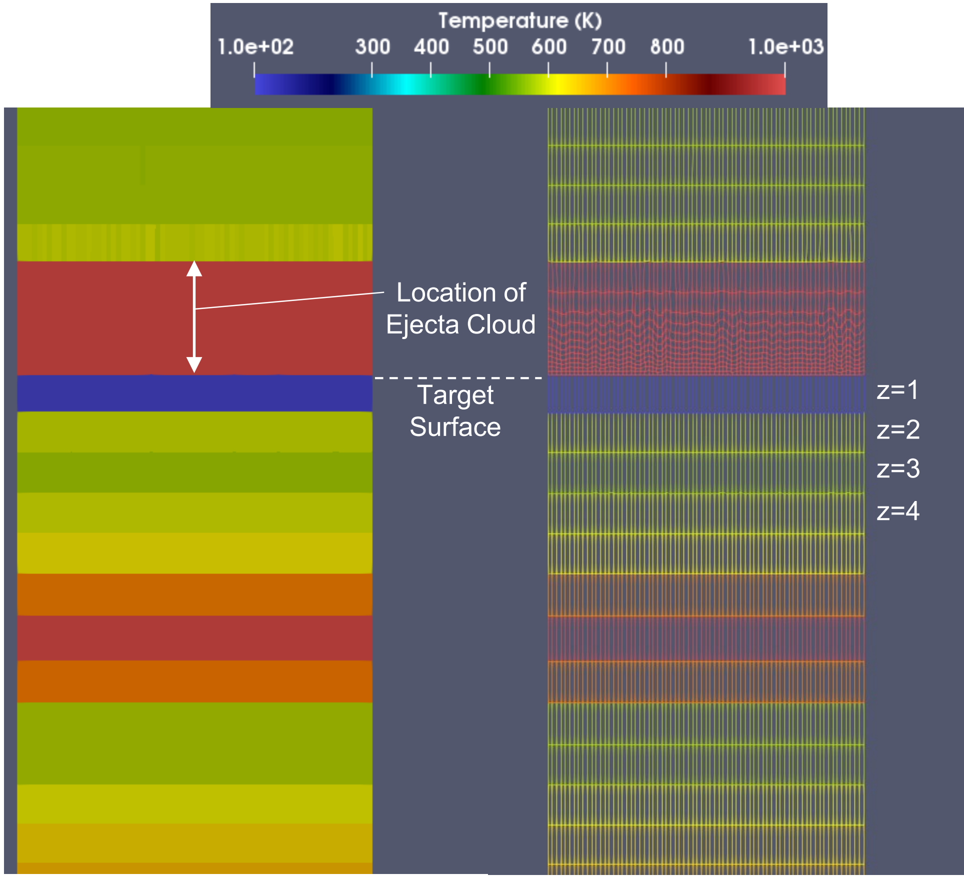


Figure 5: Surface and wireframe contours of zonal temperatures $1\mu s$ after ejecta are produced at a tin target surface for illustration of zone depths

Modified Ejecta Initialization

- Results with new initialization were satisfactory and provided accurate ejecta temperatures

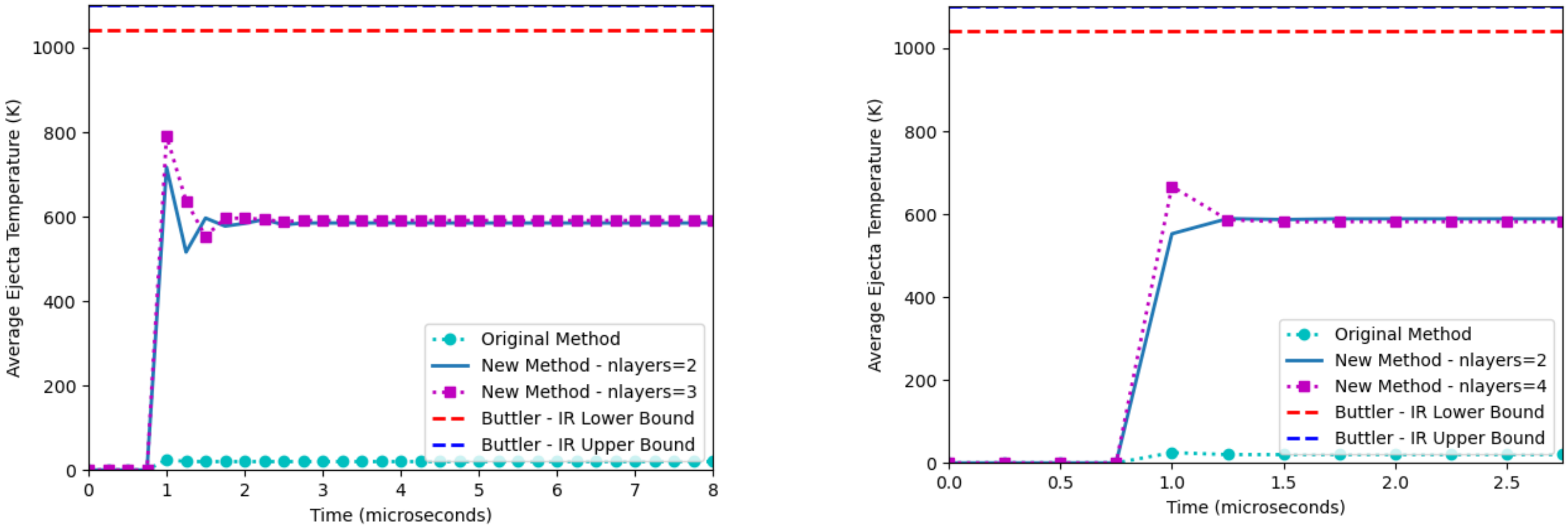


Figure 6: Average ejecta temperatures for axisymmetric, 36 x 198 zone (left) and 72 x 396 zone (right) simulations

- These changes have recently been merged into the main code repository

Simulation Setup and Initialization

- The target and flyer plate are both set to be tin.
- Flyer plate is used to avoid computationally modeling the HE from the experiments
- Flyer plate is initialized to the jump velocities reported in [2]
- The gas is initialized to the ambient state also reported in [2]

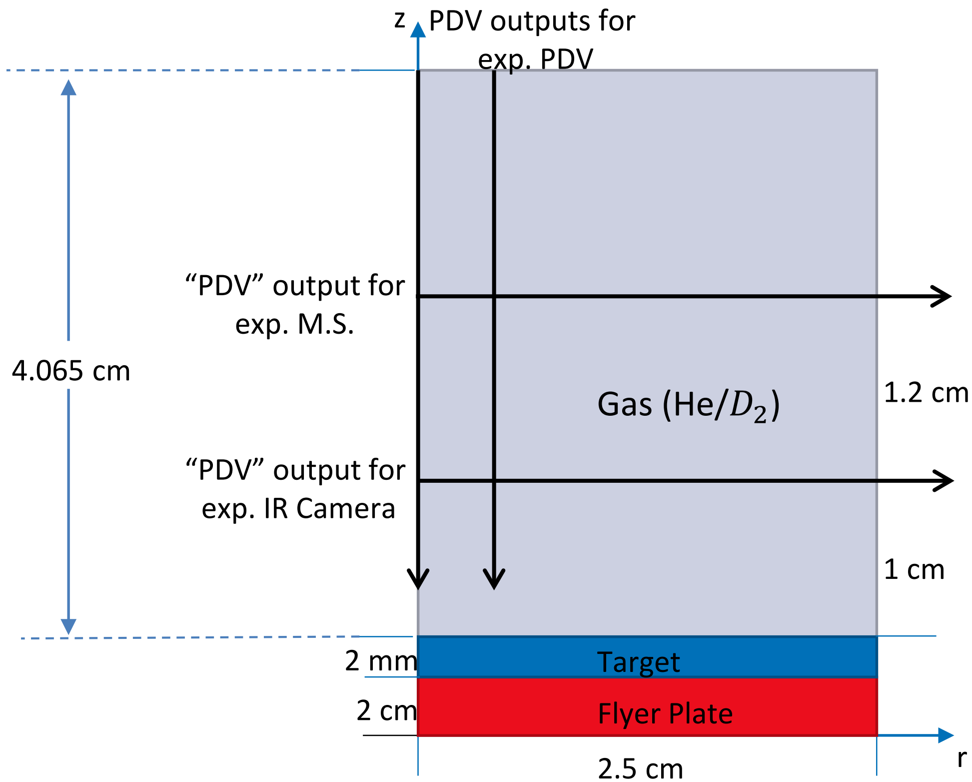


Figure 7: Simulation Configuration for 2017 Tin Cases

[2] Buttler, W. T., Schulze, R. K., Charonko, J. J., Cooley, J. C., Hammerberg, J. E., Schwarzkopf, et al. (2021). Understanding the transport and break up of reactive ejecta. *Physica D: Nonlinear Phenomena*, *415*, 132787.

Simulation Matrix: Inert Experiment Comparisons

Table 2: Initial conditions for the ambient gases in the simulations for each case considered

Case	Gas	$\rho_o \ (mg/cm^3)$	$P_o \ (KPa)$	$h_o \ (\mu m)$	$\lambda \ (\mu m)$
SN3 - 2017	He	0.325	2.03	2.05	39.8
SN5 - 2017	He	1.520	9.45	2.05	40.6
SN6 - 2017	D_2	1.310	8.11	2.15	39.5
SN7 - 2017	D_2	0.327	2.03	2.20	43.8
CE3 - 2019	He	0.866	5.40	2.75	50.0

- SN 5/6 give comparisons to reported post-shock gas properties and jump velocities
- SN 5/6/7 are to compare results to LDV and IR imaging data from the experiments
  - Gives comparisons of ejecta velocities and temperatures
- CE 3 is meant to compare to Mie-Scattering experimental data for ejecta sizes

Grid Convergence Study

Table 3: Description of meshes used to study effect of grid refinement on simulated post-shock properties

Mesh	N_r	$\Delta r\ (\mu m)$	N_z	$\Delta z\ (\mu m)$	N_{tot}
1	360	69.5	102	614.2	36,720
2	540	46.3	152	412.2	82,080
3	792	31.5	210	298.3	166,320

- Early simulations using 2D-axisymmetric configurations show that $\frac{\Delta z}{\Delta r} \approx 9$ lead to the most stable runs

- Goal: Refine the initial mesh until simulations for Cases Sn5 and SN6 gave comparable post-shock gas conditions and jump velocities to those in [2]

[2] Buttler, W. T., Schulze, R. K., Charonko, J. J., et al. (2021). Understanding the transport and break up of reactive ejecta. *Physica D: Nonlinear Phenomena*, *415*, 132787.

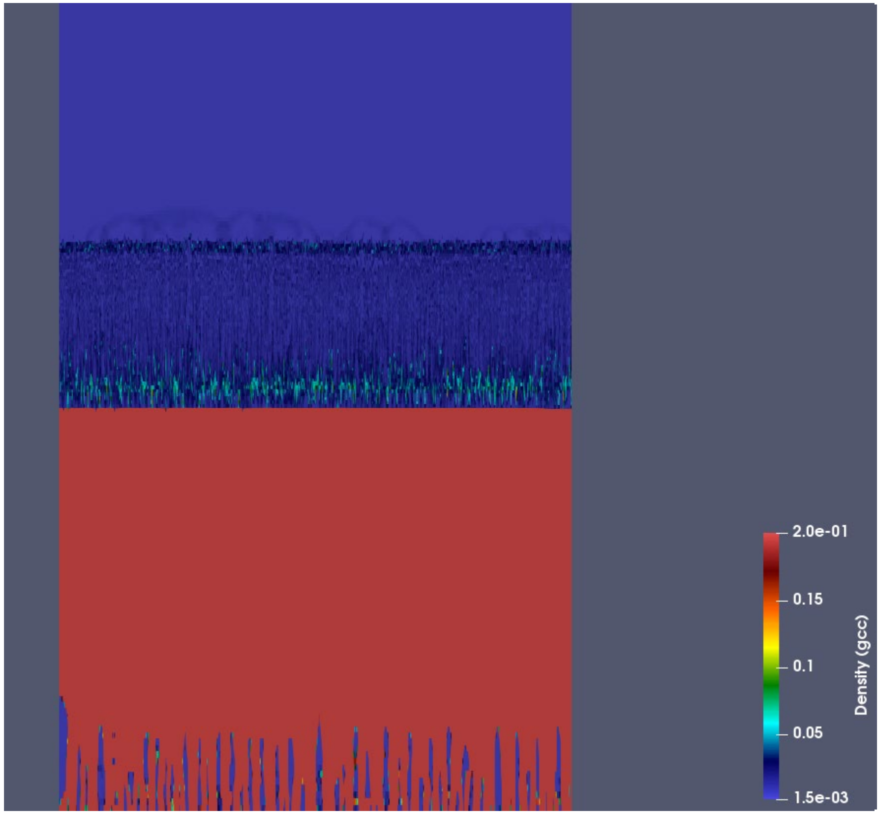
Grid Convergence Study

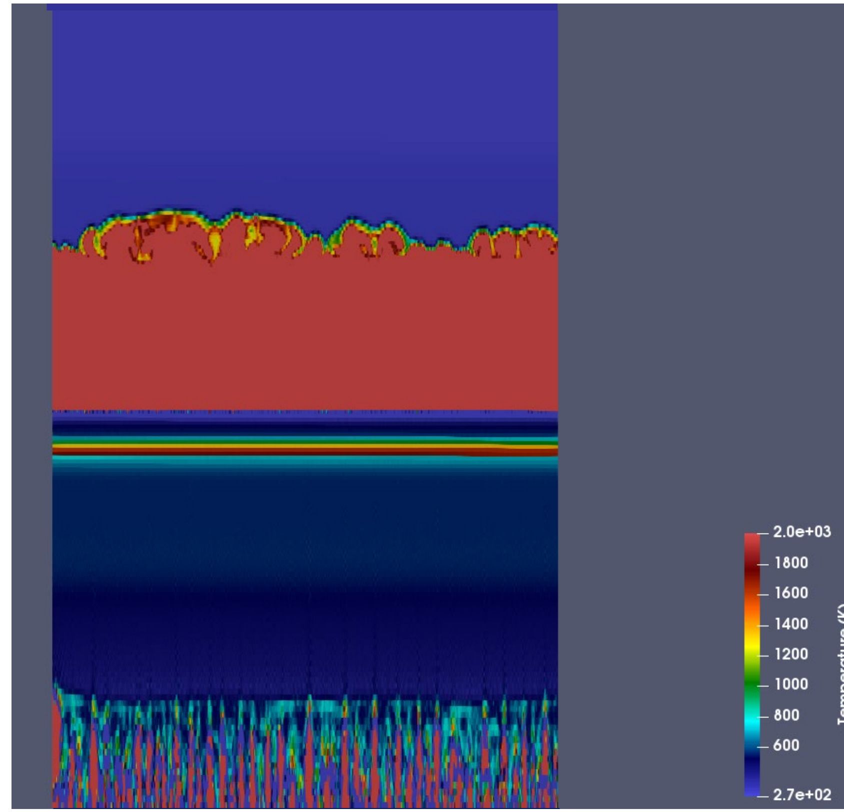
Table 4: Simulation post-shock gas values and associated errors for Case SN5

	Buttler	M1	M2	M3	Error 1	Error 2	Error 3
$u_j\ (\frac{mm}{\mu s})$	1.920	1.927	1.923	1.920	0.39%	0.18%	0.01%
$\rho_{ps}(\frac{kg}{m^3})$	4.430	4.480	4.476	4.472	1.12%	1.04%	0.96%
$P_{ps}(MPa)$	9.500	9.492	9.461	9.435	-0.09%	-0.41%	-0.68%
$T_{ps}(K)$	1030.0	1027.2	1024.7	1022.6	-0.27%	-0.51%	-0.71%

- The 166,320 zone mesh was able to yield post-shock values within $\approx 1\%$ of the reported values (values from SN6 omitted for space)
- This mesh was chosen for the simulations discussed in the remainder of the talk

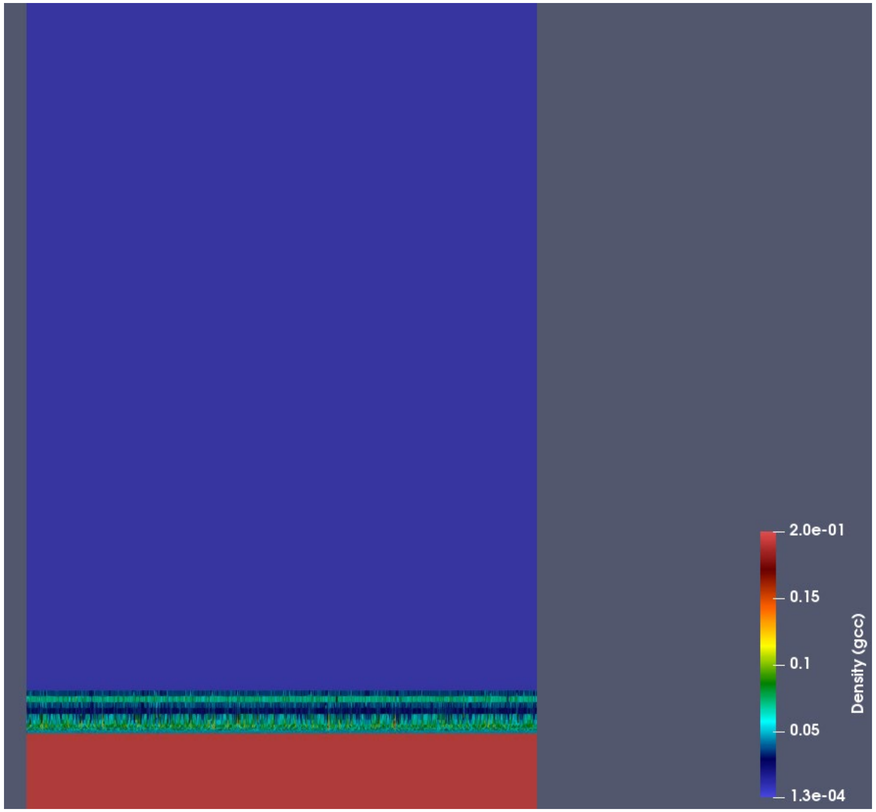
Simulation Contours – Case SN5

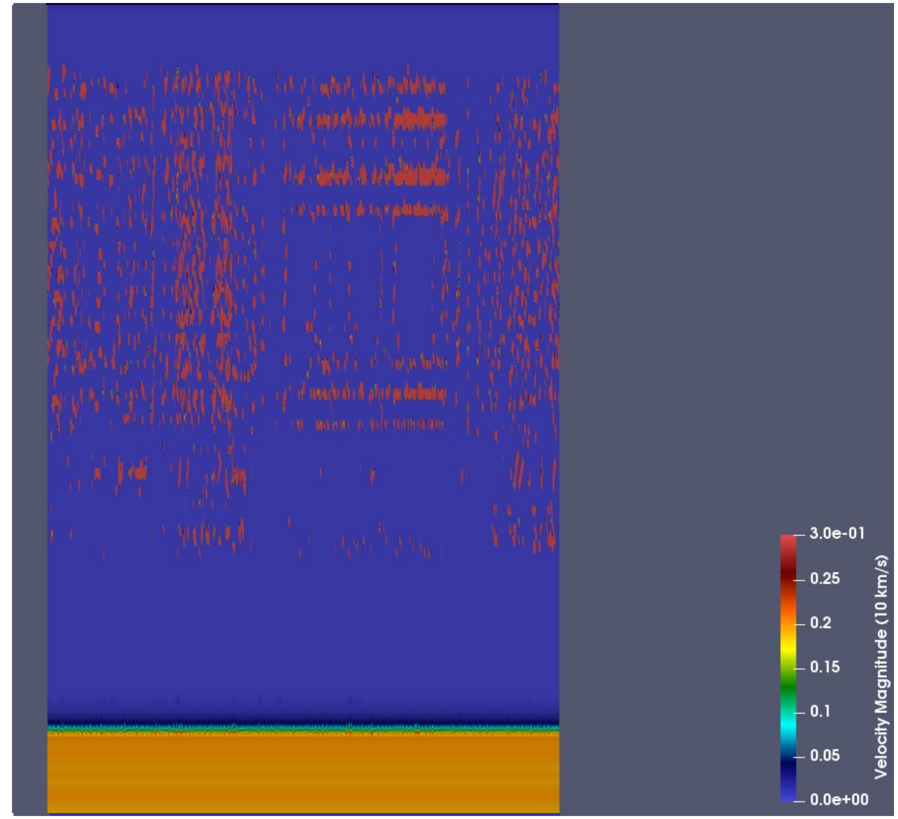




$t = 80\mu s$

Simulation Contours – Case SN6





$t = 0\ \mu s$

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Velocimetry Comparison

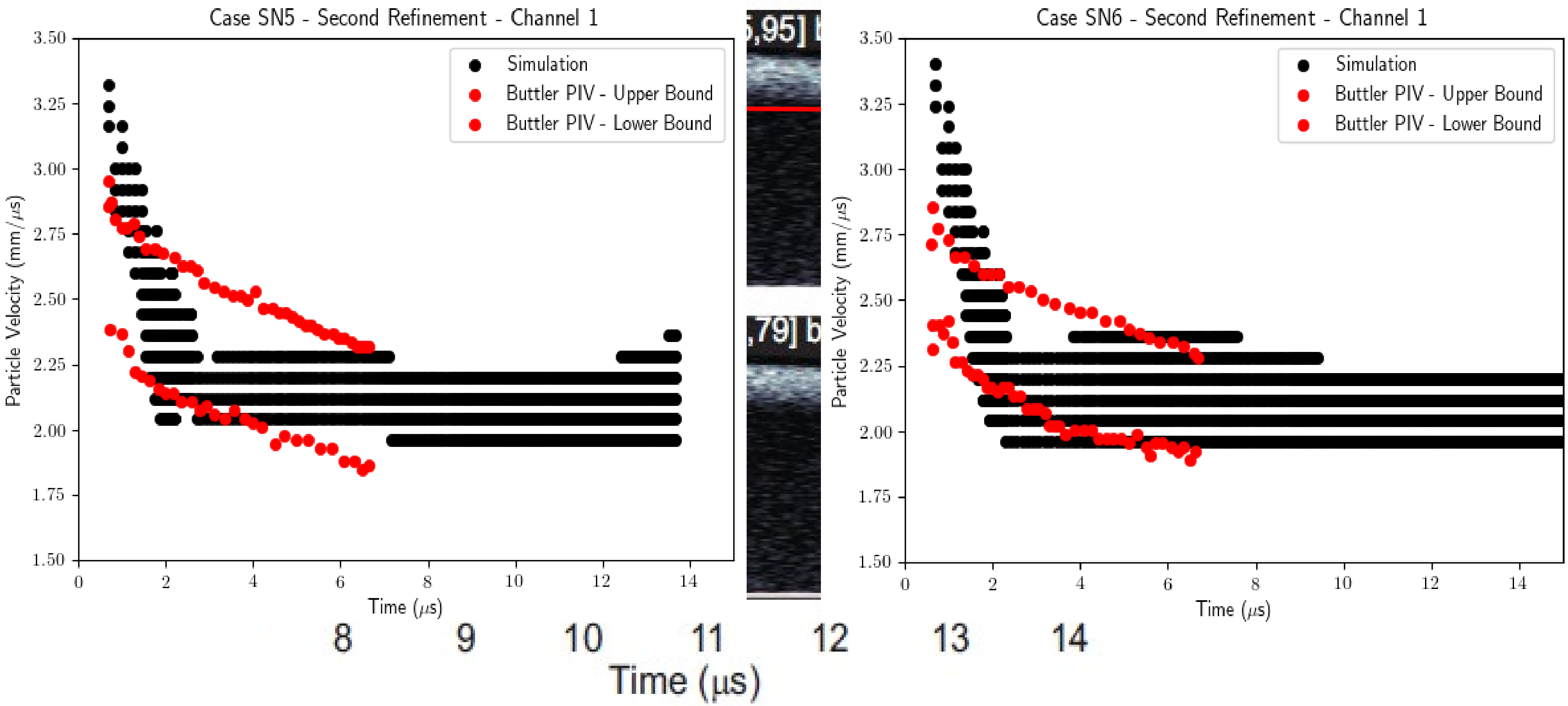


Figure 8: Velocimetry plots from [2] for Cases SN5 and SN6

- Simulation underpredicts particle velocity at early times
- Reasonable comparison for most of simulated time

[2] Buttler, W. T., Schulze, R. K., Charonko, J. J., et al. (2021). Understanding the transport and break up of reactive ejecta. *Physica D: Nonlinear Phenomena*, *415*, 132787.

Radiance Temperature Comparison

- Major issue with comparing the simulations to experiments is the emissivity to use to convert the experimental T_R to the simulation particle temperatures
- Current guidance is that using $\epsilon \approx 0.5$ is a good estimate for liquid tin

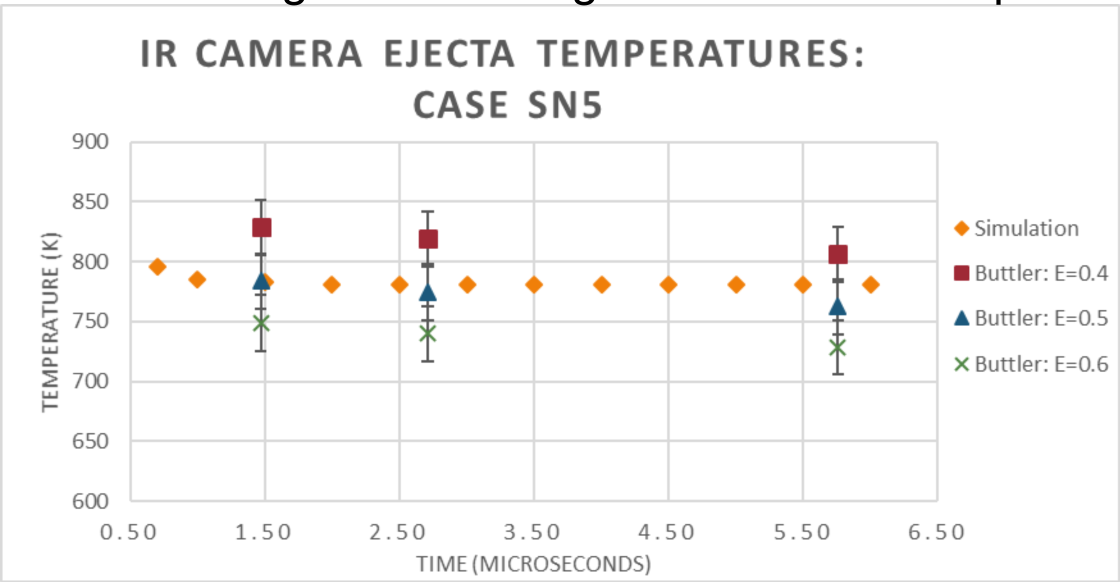


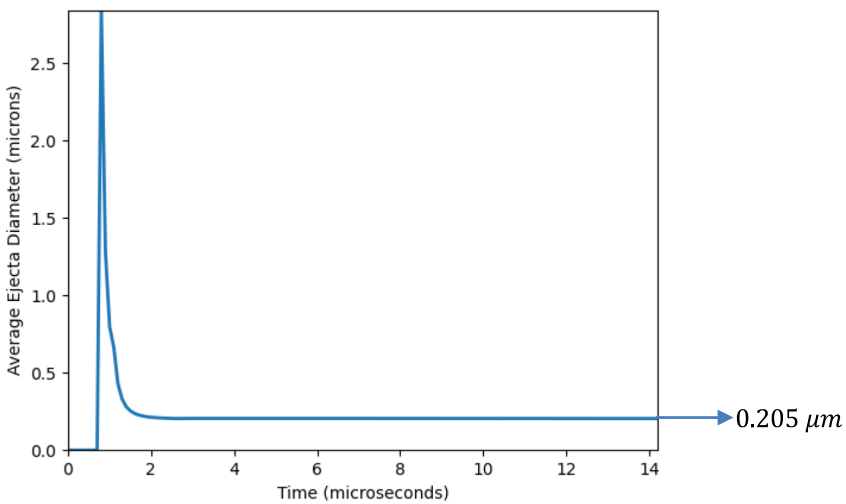
Figure 9: Particle temperature plot along with transformed radiance temperatures from [2] for for case SN5

- The simulation particle temperatures from SN5 agree well with radiance measurements under this assumption
- Case SN7 is currently post-processing and will be our second validation case

[2] Buttler, W. T., Schulze, R. K., Charonko, J. J., et al. (2021). Understanding the transport and break up of reactive ejecta. *Physica D: Nonlinear Phenomena*, *415*, 132787.

Ejected Mass and Size Comparisons

- We plan to compare simulation data to experimentally obtained ejecta size measurements to verify the ejecta sourcing model
- The comparison point for that will be simulation CE3, which is currently running
- Cloud averaged diameters are used for two of the finished runs (Fig. 10)
- Final comparison to experiments will be done at fixed heights corresponding to measurement locations



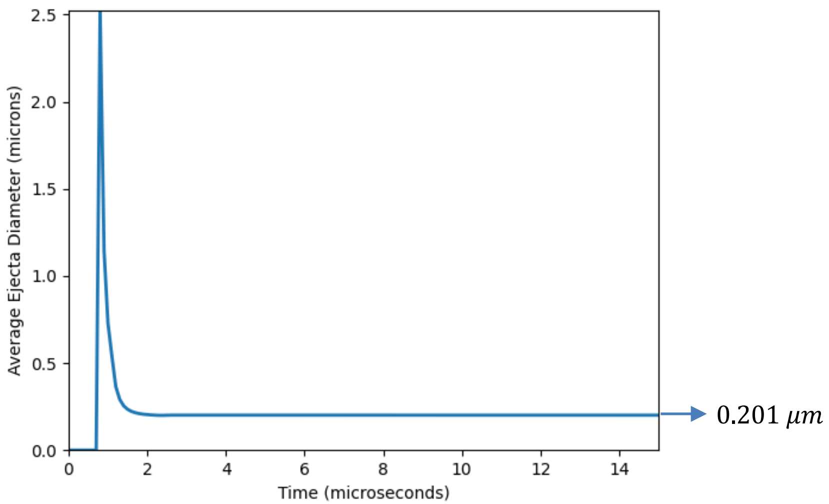


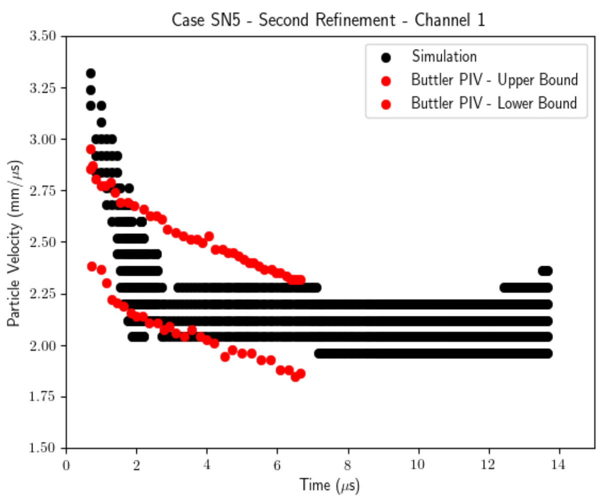
Figure 10: Average ejecta diameters over the entire cloud for simulations SN5 (left) and SN6 (right)

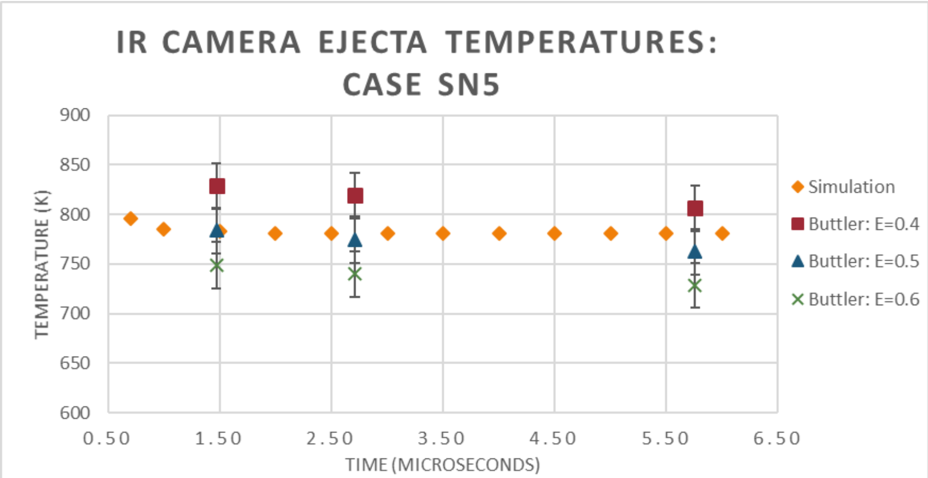
Conclusions

- Early project work focused on finding possible break-up mechanisms for the reactive ejecta and fixing some hydrocode stability issues
- Initial simulation work on replicating a subset of the experiments led to modifying the manner in which the thermodynamic properties of the ejecta were initialized in the code
- Preliminary comparisons of the simulated inert cases show ejecta velocities and temperatures with good agreement to reported experimental data
- Waiting for a few final simulations/comparisons before claiming that our simulation base is ready to proceed but current results are promising

Future Work

- Conclude verification of the inert simulations
  - Ejecta temperatures against radiance temperature measurements – SN7
  - Ejecta sizes against the experiments - CE3
  - This will confirm to us that the current simulation platform is ready to replicate the reactive experiments in a quantifiable manner
- Formulate melt-based break-up model for the transporting ejecta and implement the model into the hydrocode
- Run simulations of the reactive 2019 experiments and compare outputs to the reported diagnostics





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