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Numerical Simulation of Post-Detonation Processes with Detailed Chemical Kinetics

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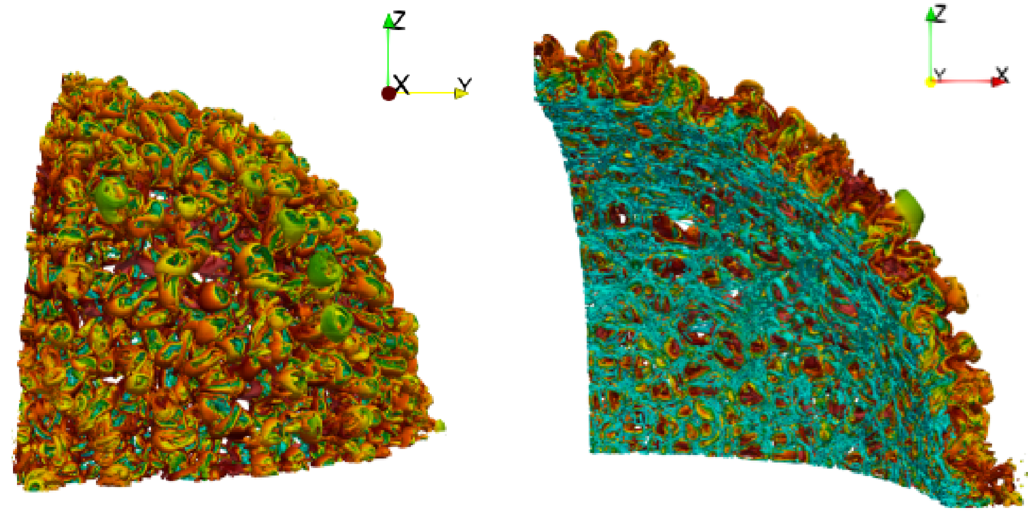

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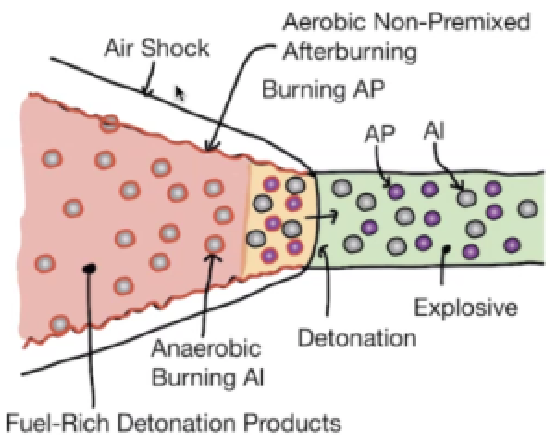
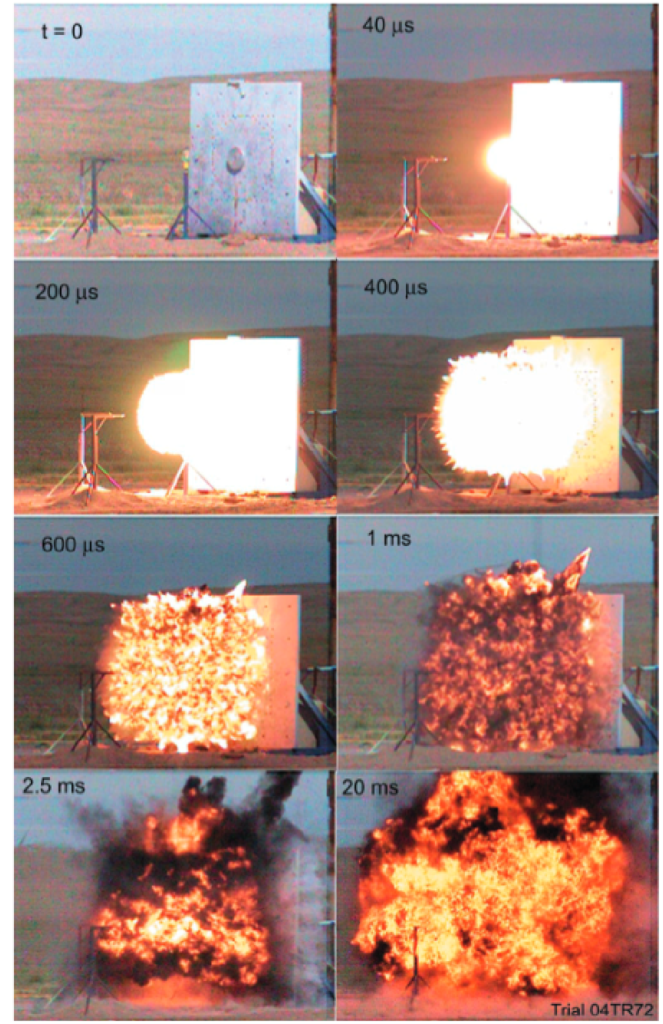
The detonation of explosive charges results in a powerful shock and fireball.

- The explosive charge is converted to hot, dense detonation product gases.
- Post-detonation afterburning of product gases can produce over half of the chemical energy released.
- Experiments observe that chemical reactions freeze.
- Our goal is to understand the chemical reaction processes in the post-detonation flow.





High-speed video record for the detonation of a 12.3 cm charge of 1,000 g of sensitized nitromethane*.

*Goroshin, Samuel, et al. An International Journal Dealing with Scientific and Technological Aspects of Energetic Materials 31.3 (2006): 169-181.

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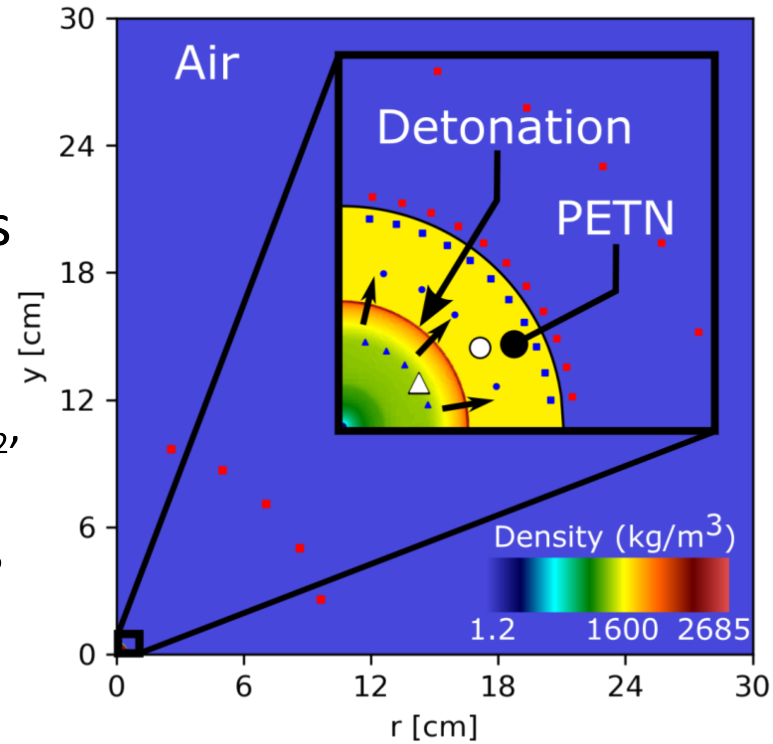
We use numerical simulations that fully couple an explosive detonation model to detailed gas phase chemical reactions in the expanding flow.

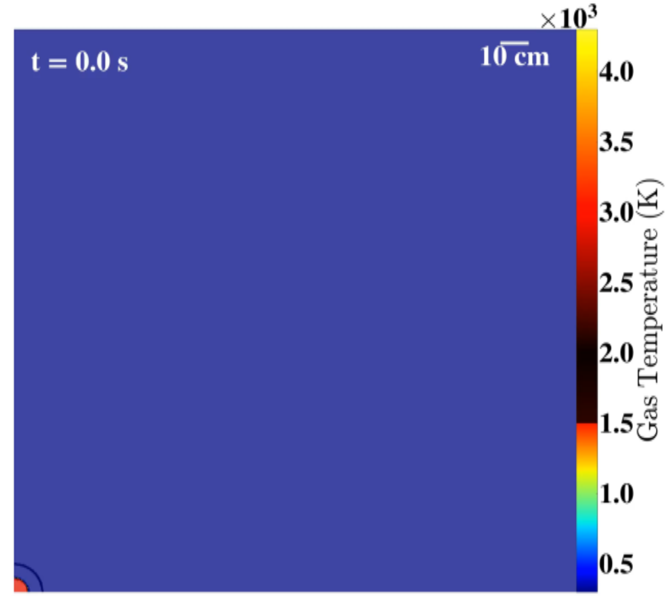
- A hemispherical $C_5H_8N_4O_{12}$ (PETN) charge is modeled in ambient air.
  - 12 mm diameter 1.6 g/cc
  - 2D axisymmetric coordinates
- A novel explosive burn algorithm is used to model the detonation
  - The detonation converts solid explosive into gaseous products that can react: CO_2, H_2O, CO, etc.
- Detailed chemistry with 59 species and 368 reactions captures:
  - Air dissociation by Mach 20+ shock
  - Equilibration in the fireball
  - Afterburning of the detonation products and air
- The BKW real-gas EoS is used



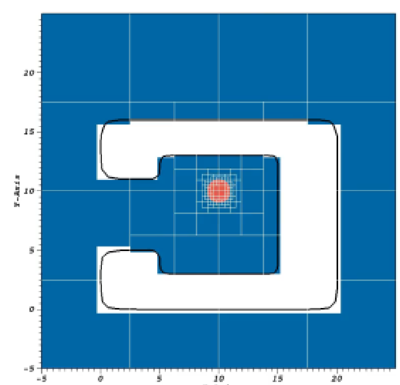
Geometrical setup in 2D.

We use an in-house code called HyBurn that has been verified for an extensive list of test problems.

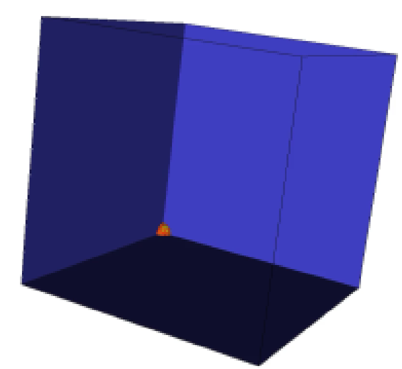
- Fully couples compressible reactive gases to granular flow
  - Eulerian and Lagrangian particles
- Combustion with **detailed** and simplified chemical kinetics
- Ideal and non-ideal (JWL, **BKW**) EoS models
- Massively parallel with adaptive meshing using the AMReX library
- High-order numerical methods – Up to 7th order
  - **5^{th} order MUSCL with HLLC is used here**
- Complex geometry using Immersed Boundary Methods
- Thermal radiation using filtered spherical harmonics



Combustion of TNT-dispersed Al particles.



Blast in an open room.



Explosive Al particle dispersal.

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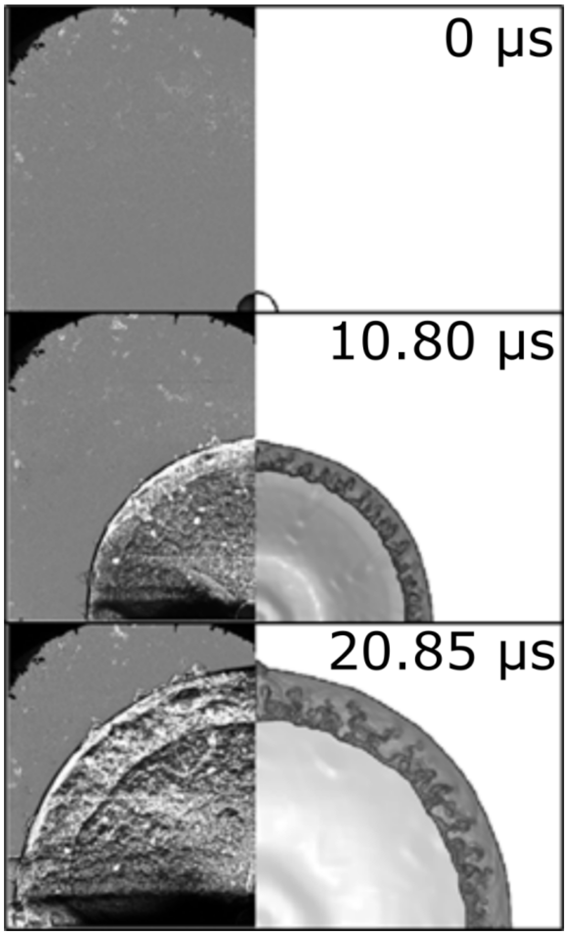
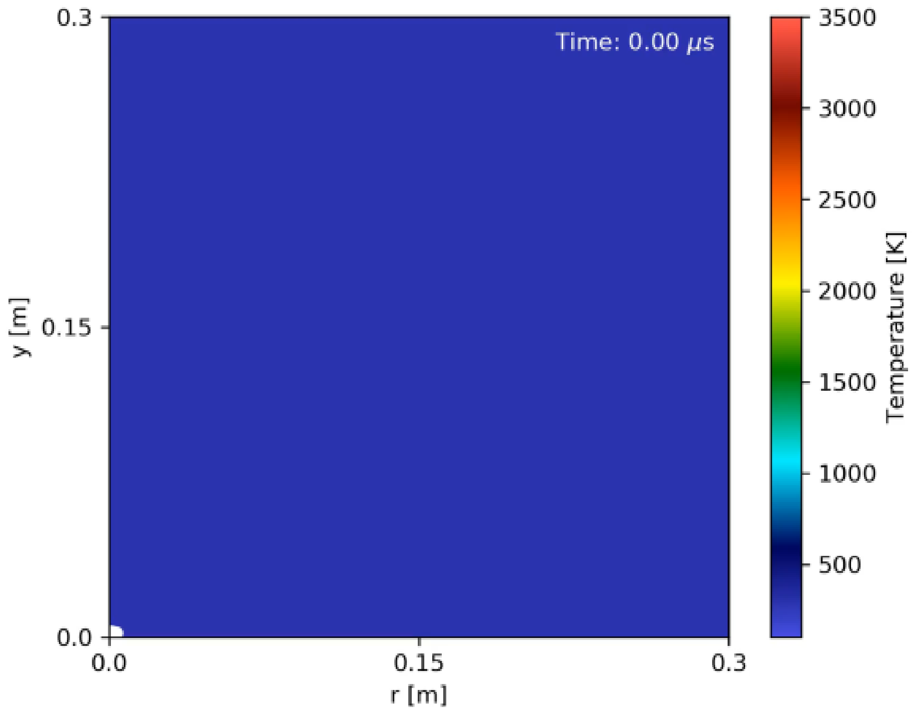
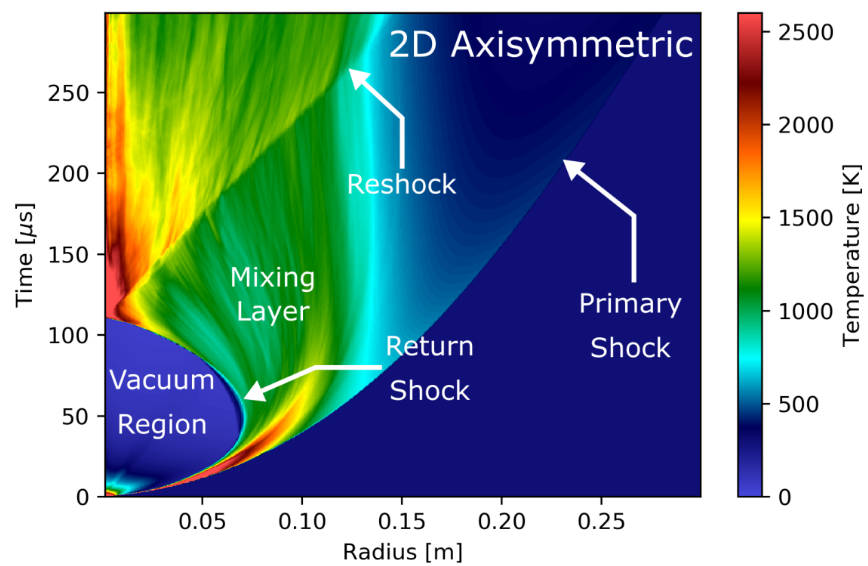
The numerical results compare well to experimental data and blast structures measured at Sandia.

Experiment Simulation



The blast structure shows regions where the flow is purely gas dynamic with no mixing and other regions where mixing is important due to RT and RM instabilities.





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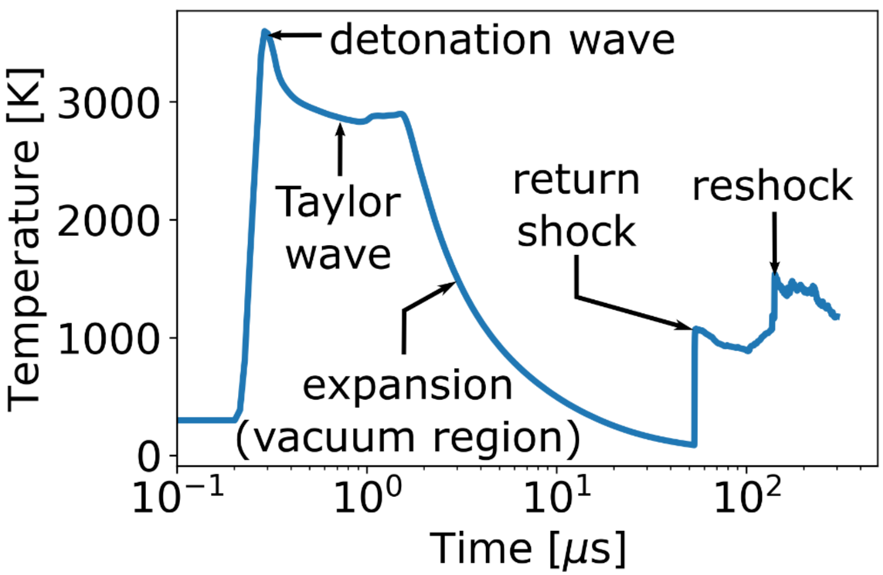
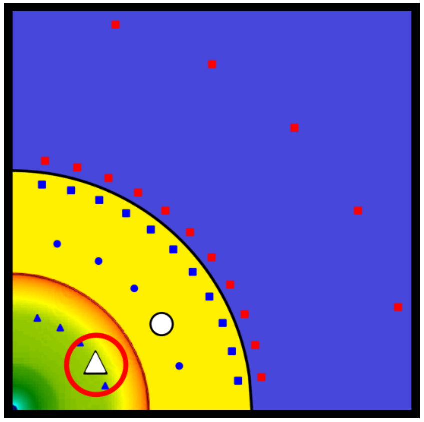
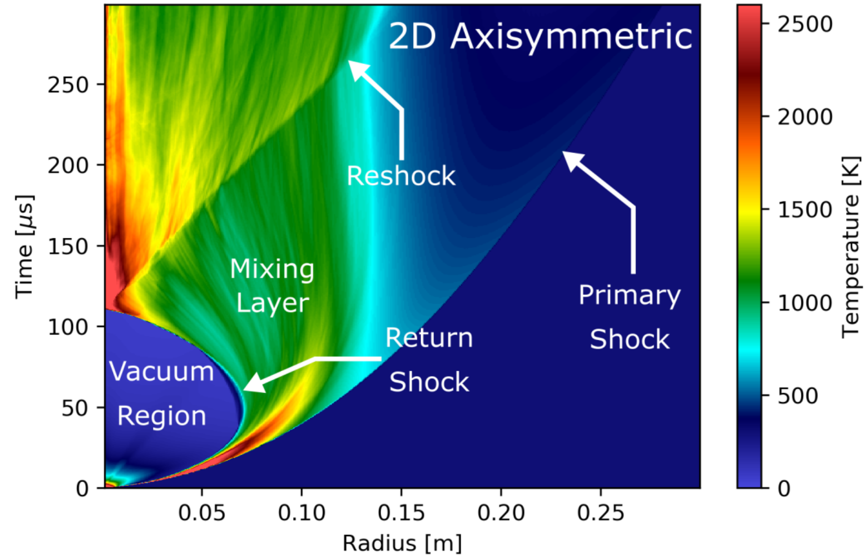
The tracer gauge results shows that the temperature inside the fireball decreases to ~100 K during the expansion.

Tracer gauge temperature inside of the fireball.





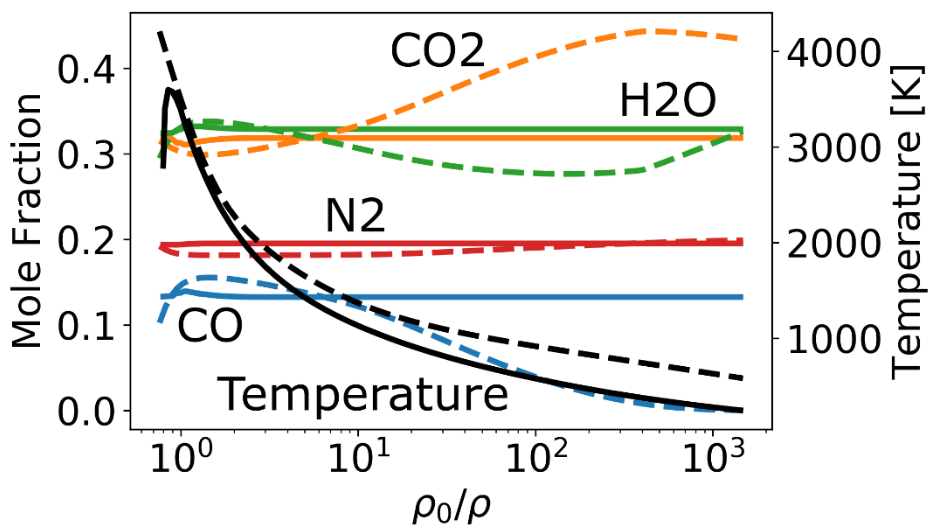


The tracer gauge results show the chemical composition inside the fireball is constant during expansion. Assuming full chemical equilibrium is highly inaccurate.

- Experimental results* have shown that the composition inside the fireball chemically "freezes out".
- The results show that assuming equilibrium (dashed lines) deviates significantly from full chemistry (solid lines) at large expansion ratios.

Table 1: Comparison of computed mole fractions inside the PETN detonation products to experimental measurements.

Species	Real γ_i	$\gamma_i = 1$	Measured
H_2O	0.309	0.329	0.313
CO_2	0.342	0.318	0.318
CO	0.110	0.133	0.142
N_2	0.195	0.195	0.181



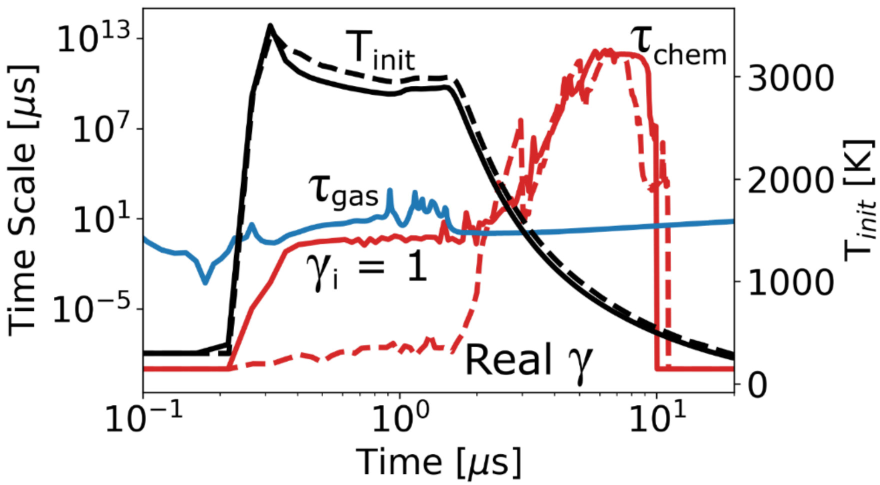
*D. L. Ornellas, J. H. Carpenter, S. R. Gunn, Rev. Sci. Instrum. 37 (7) (1966) 907–912.

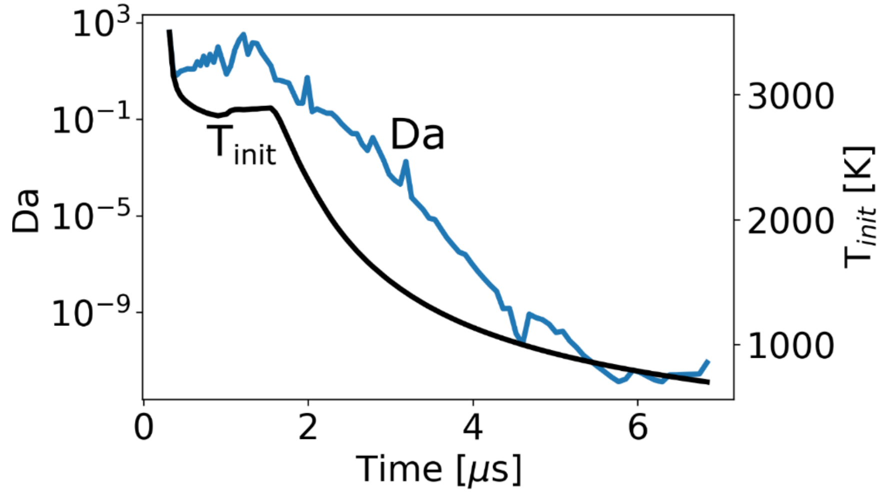
Analysis of gas dynamic and chemical time scales during expansion allows us to define a Damköhler number and determine if the chemistry is frozen or in equilibrium.

- The timescales are defined by:
  - $\tau_{gas} = \rho / |d\rho/dt|$
  - τ_{chem} is defined to be the time where $T(t) = 0.5\left(T_o + T_{eq}\right)$ in a constant volume reactor initialized from the local state.
- These time scales allow us to define a Damköhler number

$$Da \equiv \frac{\tau_{gas}}{\tau_{chem}}$$

- The Damköhler number gives us information on how the chemistry and flow interact:
  - $Da > 10$ implies chemical equilibrium
  - $Da < 0.1$ chemically frozen (inert)
  - $0.1 < Da < 10$ finite rate chemistry





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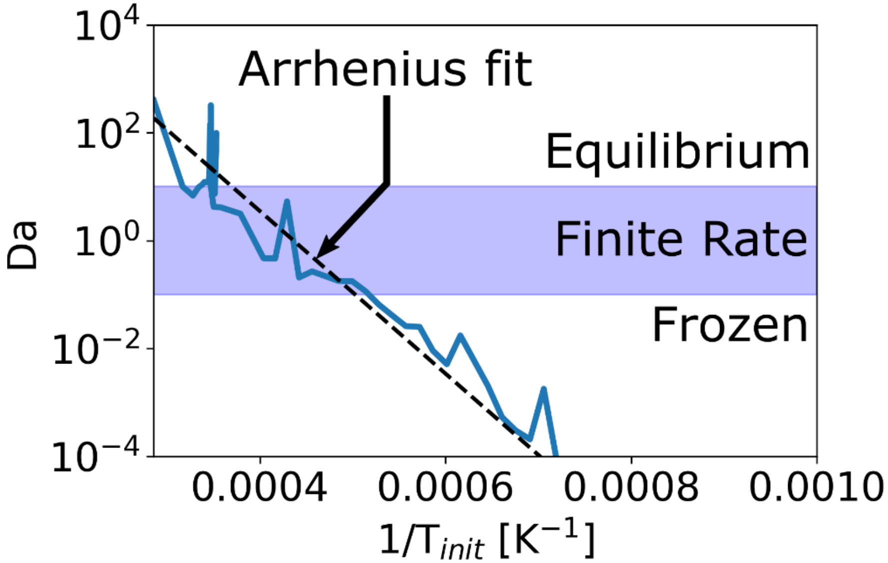
An Arrhenius fit of the data allows us to correlate the Damköhler number with local temperature in the fireball and to estimate the freeze-out temperature.

- A fit of the data gives A = 3.8 x 10^6 and T_a = 34,000 K $Da = Ae^{-T_a/T}$
- A freeze-out temperature can be found by defining a critical Da

$$Da = Da_c = 0.1$$

$$T_{freeze} = T_a ln\left(\frac{A}{Da_c}\frac{d_{PETN}}{12\ mm}\right)^{-1}$$

- For the 12 mm charge, **T_{freeze} = 1990 K**. This is close to accepted values in the literature.



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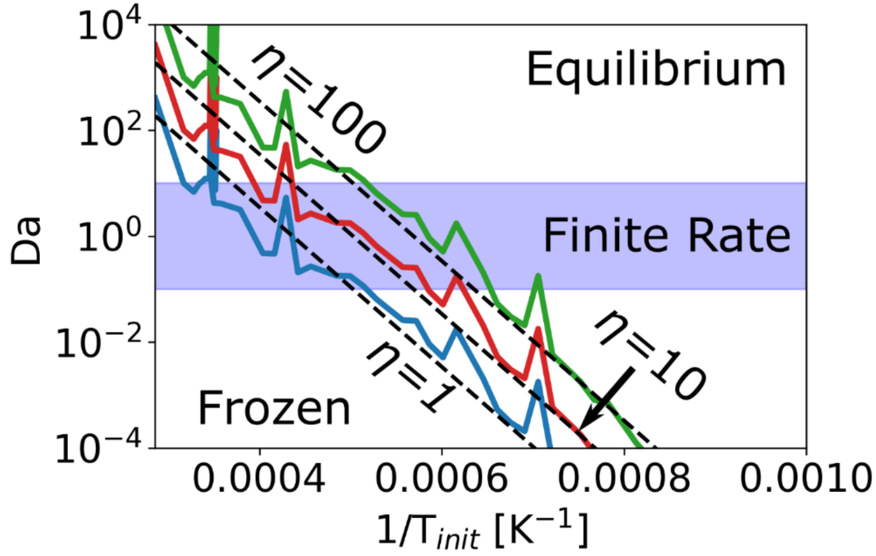
The chemical reaction time scales are many orders of magnitude higher than the gas-dynamic time scales, which are scale invariant with time and space. This allows us to estimate the effects of length scales.

- Estimated freeze-out temperatures for larger charges are:
  - **1757 K** for 120 mm
  - **1574 K** for 1200 mm
- We can now use the Lagrangian tracer gauges on larger simulations to validate this influence of scaling.

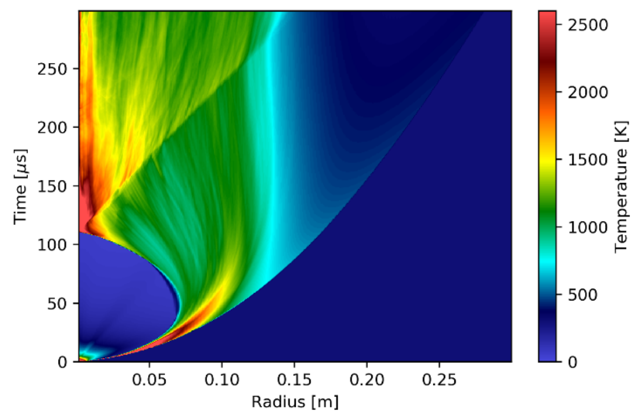


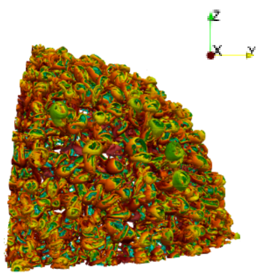
In conclusion, the close agreement of the blast structures, freeze-out composition, and freeze-out temperature with literature values validates our proposed modeling approach for explosive afterburning.

- On going work is exploring 3D simulations with realistic turbulence
    - The bulk structures are nearly identical between 2D and 3D
- We are analyzing mixing layer thicknesses of species and temperature
- We are developing a simplified approach to incorporate soot chemistry and radiation

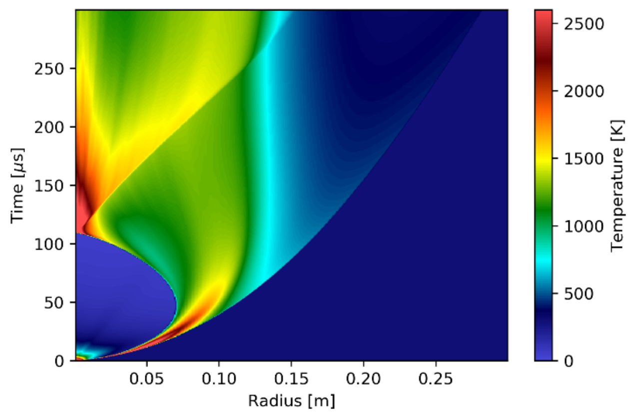
Questions???

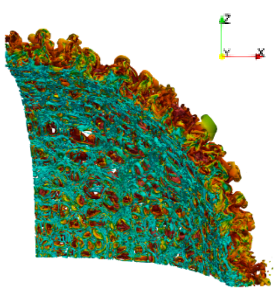
2D





3D

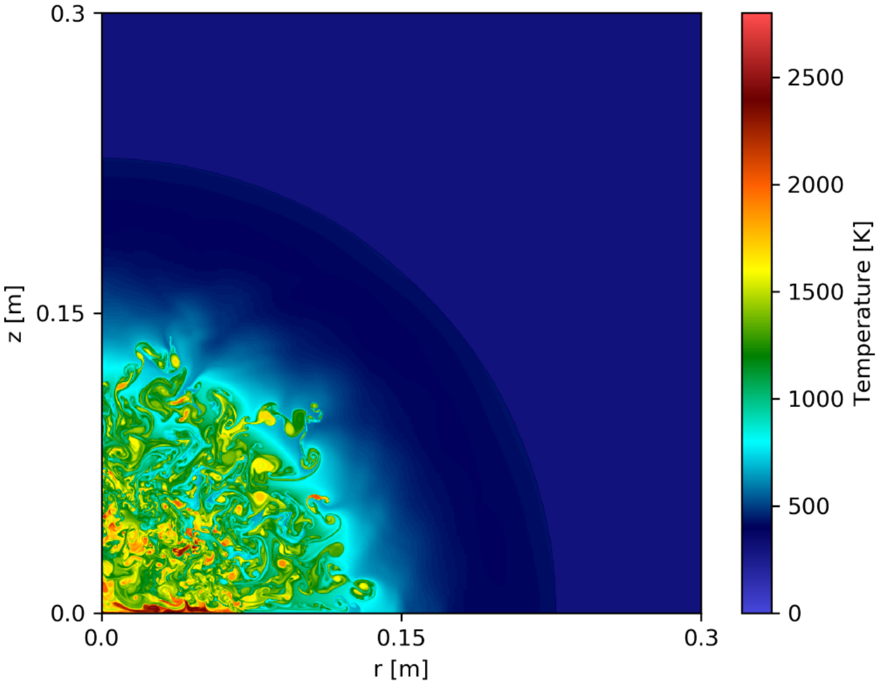




Spare

Slice plots in 3D show a substantial increase in mixing compared to 2D.

2D



3D