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Characterization of CL-20 for Shock Initiation Modeling and Simulation

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Characterization of CL-20

- Characterization of CL-20 for SDT modeling in novel next-generation devices
- Limited information available in open literature
- Single crystalline EOS data and compaction data missing in open literature
- Shock hugoniot estimated from NSWC DAC hydrostatic compression data
- SESAME tabular EOS built with CHEETAH and compared with cylinder expansion data
- Dynamic compaction of porous samples with Light Gas Gun Facility

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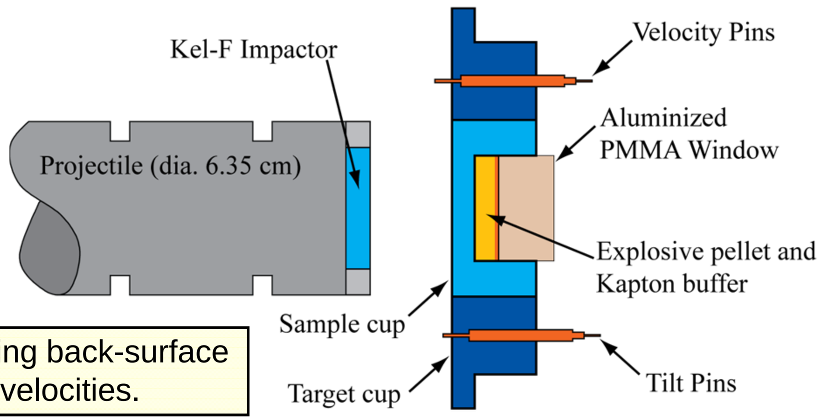
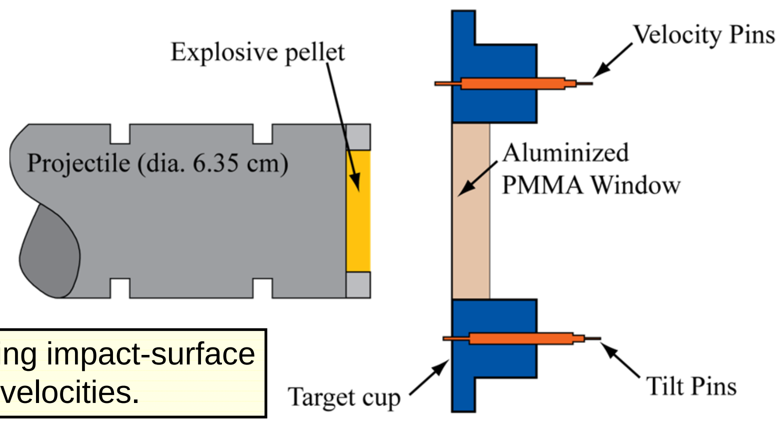
Gas Gun Experiments

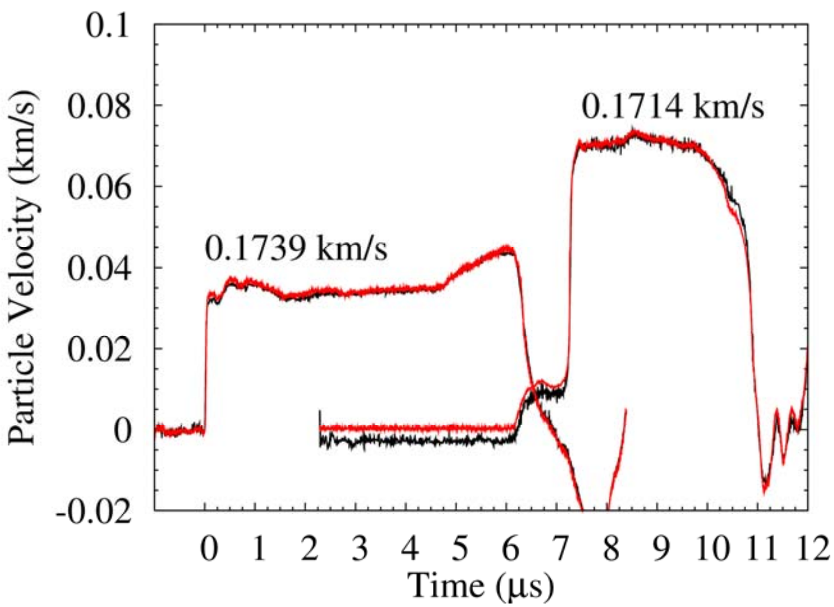
- Light Gas Gun facility used to study 70% TMD CL-20 (26-μm particle size) reaction due to planar impact. Impact velocities between 0.17 and 0.70 km/s.
- Experimentally measured particle velocities at back surface of sample or in reverse ballistic arrangement.



Measuring back-surface particle velocities.



Measuring impact-surface particle velocities.



Comparison of measured particle velocities using dual-delay-leg, "push-pull" VISAR.

CTH: A Shock Physics Analysis Package

- Eulerian shock wave physics computer code solving conservation equations of mass, momentum, & energy for multimaterials including gases, fluids, solids, & reactive mixtures
  - **Analytic & Tabular Equation-of-State representations**
  - **Advanced Strength & Fracture models**
  - **Adaptive Mesh Refinement**
  - **High Explosive models**
  - **Parallel and Serial platforms**
- Applications (CTH licensed to over 300 organizations including DOE, DoD, NASA and government contractors)
  - **large strain and/or high strain rate dynamics**
  - **multiphase interactions**
  - **examples include: high speed impact, blast-structural loads and deformations, armor/anti-armor, explosive detonation**

Slide courtesy of Mel Baer

Lagrangian Phase Conservation Eqns (dense to dilute limits)

$$\mathbf{V}_a = \mathbf{U}_a - \mathbf{U}$$

- Mass:

mass source — phase diffusion

$$\frac{d}{dt}\int_{\beta_t} \rho_a dV = \int_{\beta_t} c_a^+ dV - \oint_{\partial\beta_t} \rho_a \mathbf{V}_a \cdot \mathbf{n} dA$$

- Momentum:

i.e. drag effects — relative flow momentum effects — stress terms

$$\frac{d}{dt}\int_{\beta_t} \rho_a \mathbf{U}_a dV = \oint_{\partial\beta_t} \phi_a \mathbf{n}\cdot\mathbf{S}_a dA + \int_{\beta_t} \rho_a \mathbf{B}_a dV + \int_{\beta_t} \mathbf{m}_a^+ dV - \oint_{\partial\beta_t} \rho_a \mathbf{U}_a \mathbf{V}_a \cdot \mathbf{n} dA$$

- Energy:

energy source & heat transfer effects — work terms — energy phase diffusion

$$\frac{d}{dt}\int_{\beta_t} \rho_a E_a dV = \int_{\beta_t} \phi_a \mathbf{S}_a \cdot \nabla \mathbf{U}_a dV + \int_{\beta_t} \left(S_a + e_a^+\right) dV - \oint_{\partial\beta_t} \mathbf{n}\cdot\mathbf{V}_a \rho_a E_a dA$$

Shock Physics + CFD + Solid Mechanics with multi-material formalism

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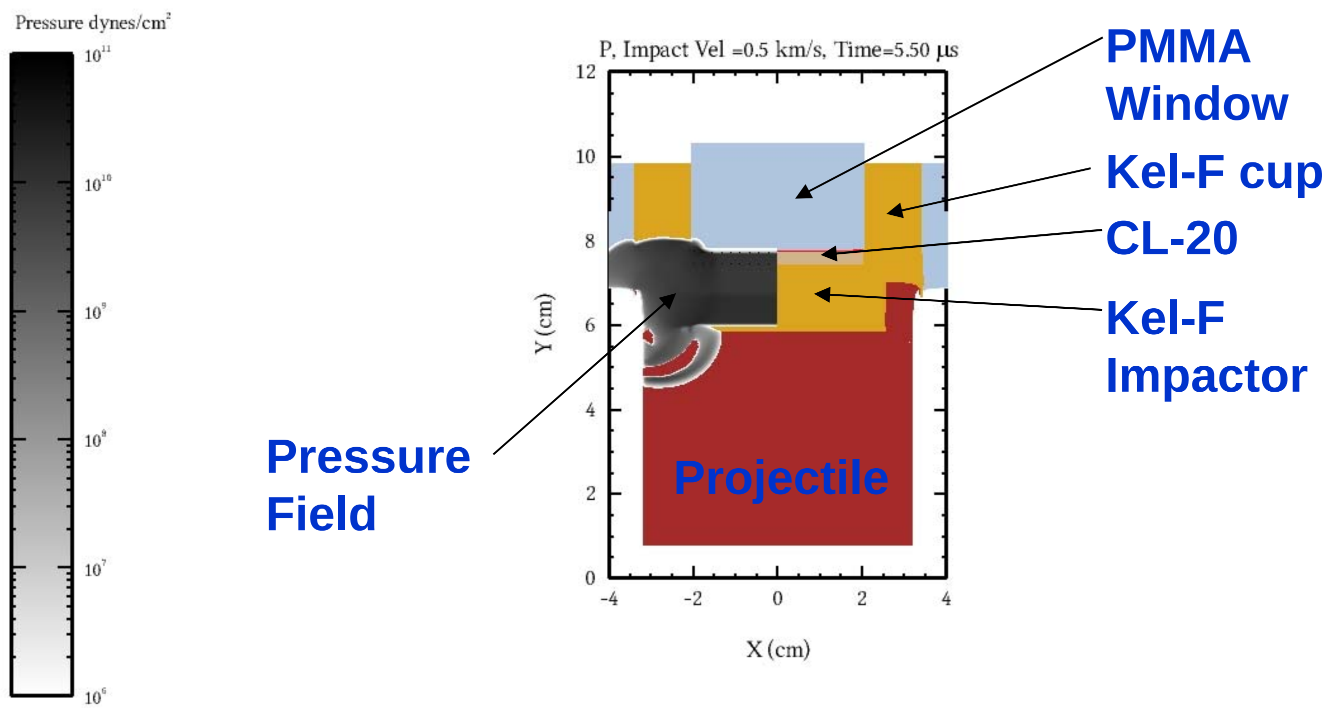
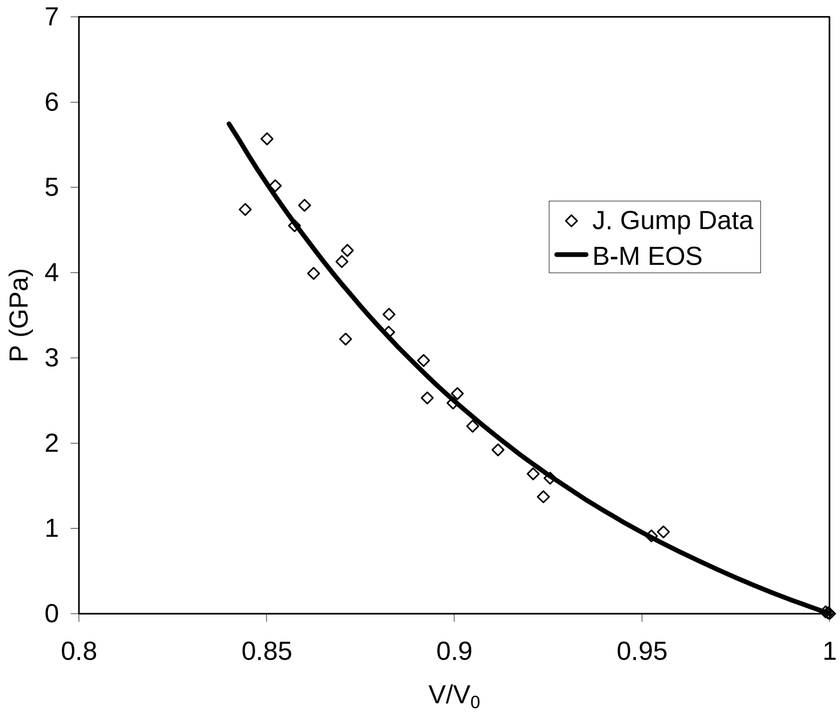
CTH Simulations

- Baer-Nunziato Multiphase model used to predict CL-20 response under shock loading



Crystalline EOS



- Diamond anvil cell data at temperature from J. Gump (NSWCIH)
  - Isothermal Bulk Modulus
  - Coefficient of thermal exp.
- Mie-Gruniesen EOS parameters from isothermal compression data

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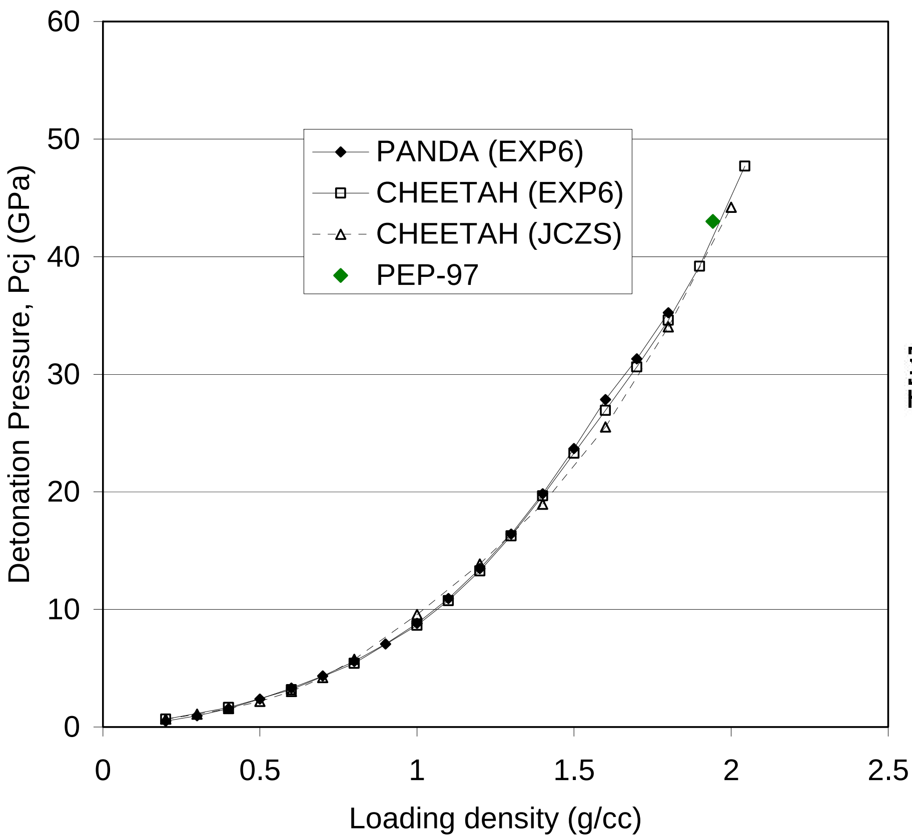
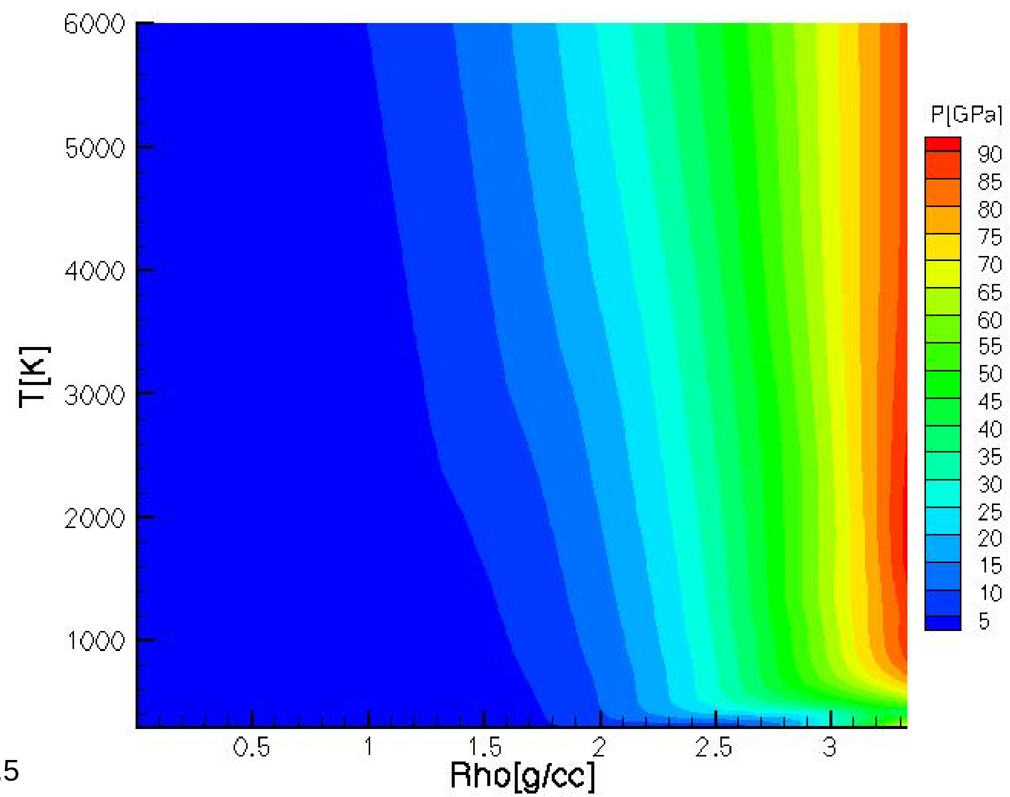
Detonation Product EOS





SESAME Tabular EOS (Detonation Products)

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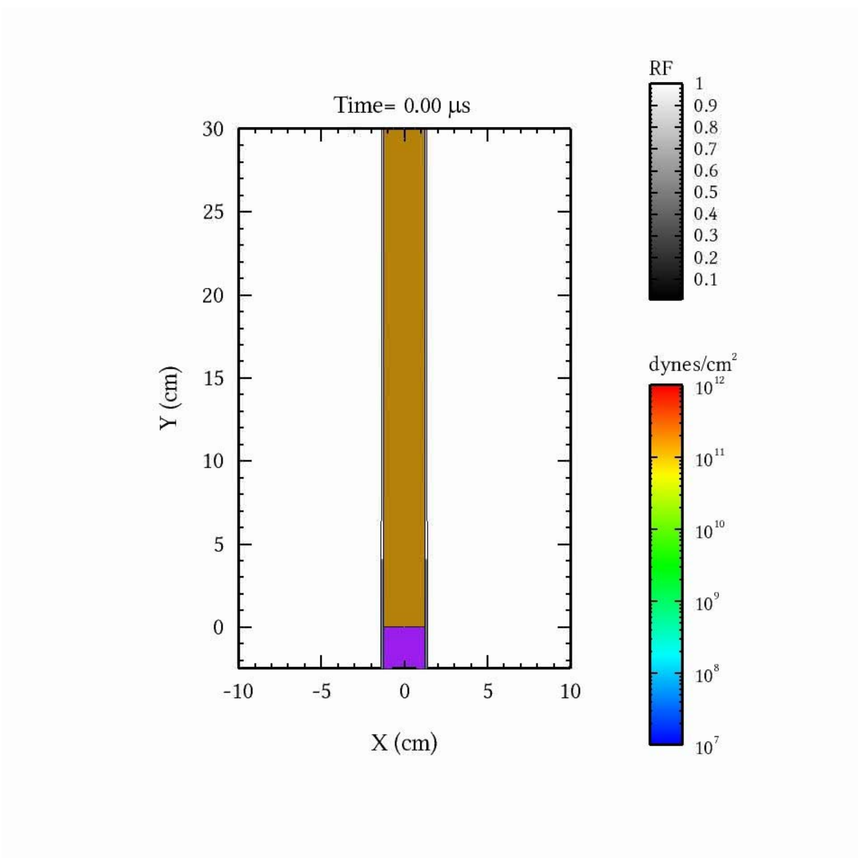
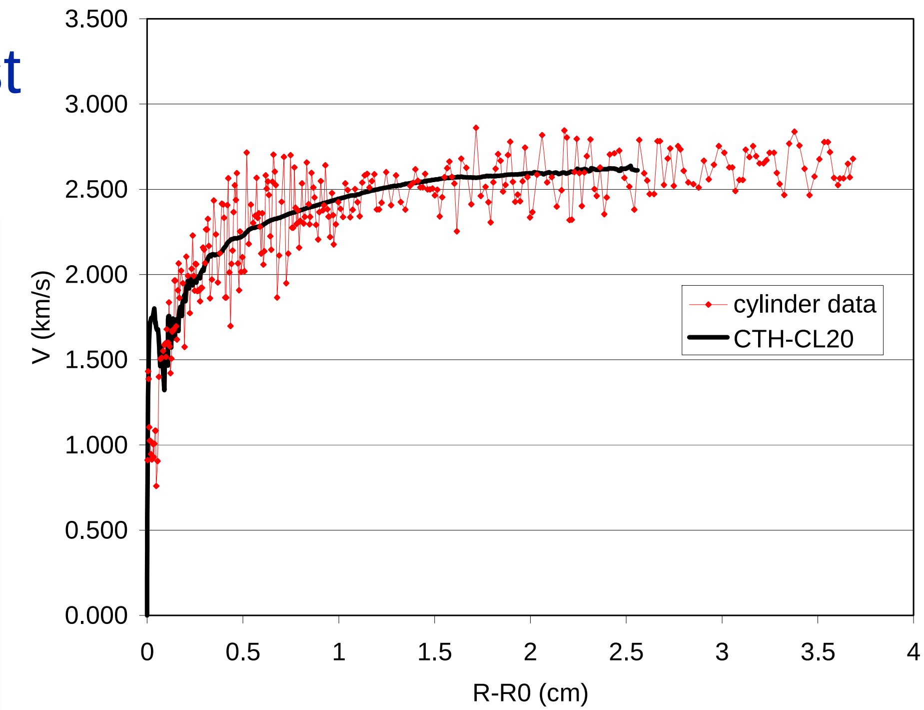
CL-20 Cylinder Expansion Data

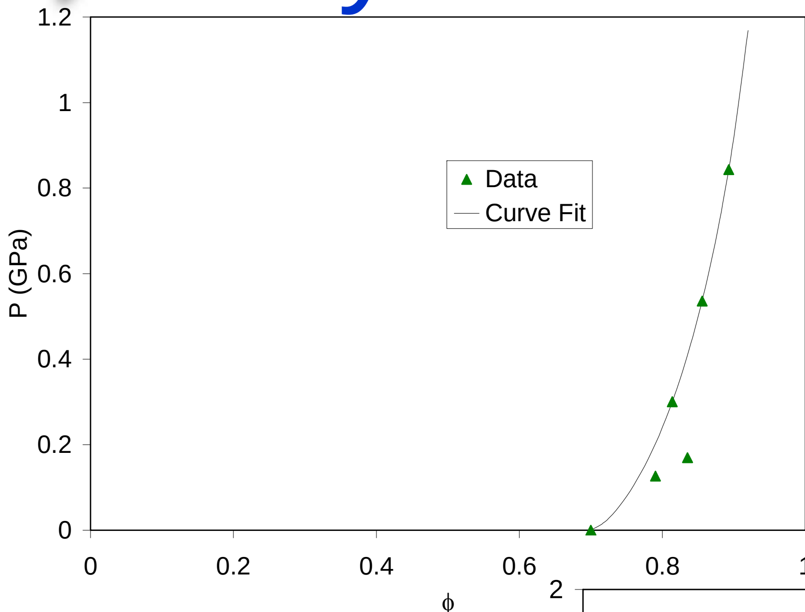
LLNL Cylinder Expansion Test (CTH simulation)

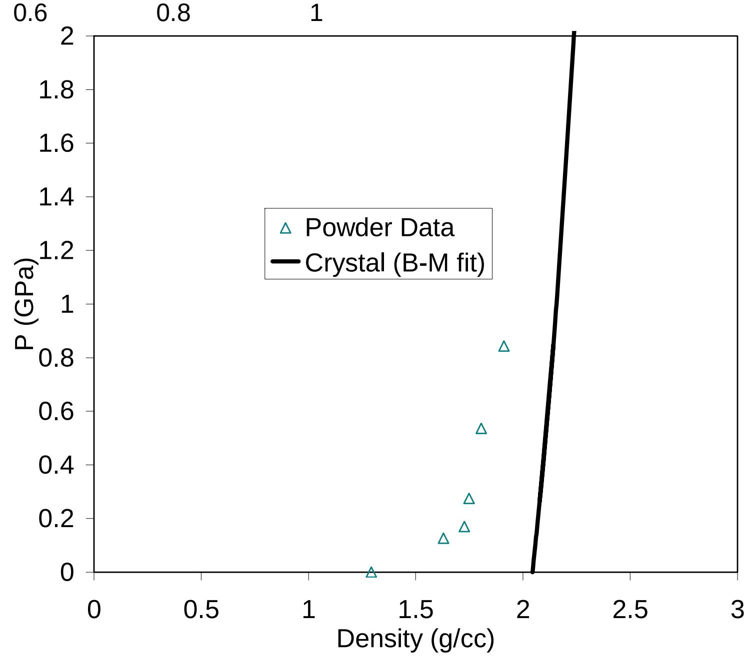


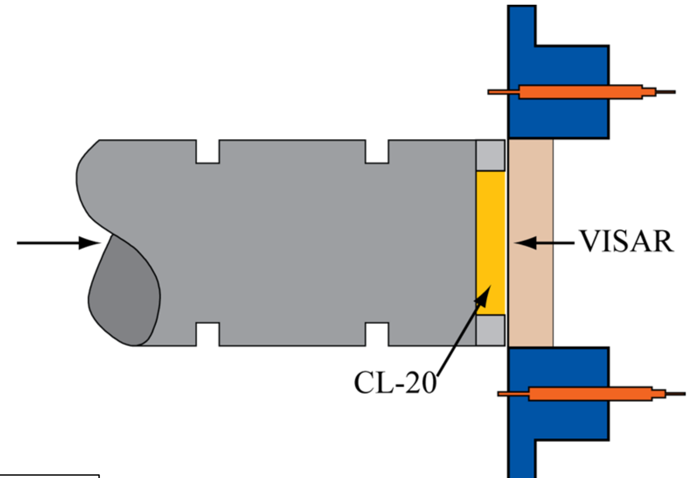


Excellent comparison to LLNL expansion data confirm adequacy of SESAME tabular EOS for detonation products

Dynamic Compaction Data







- Porous EOS needed for 63-70% TMD pellets
- Impact velocities measured in reverse ballistic gas gun shots

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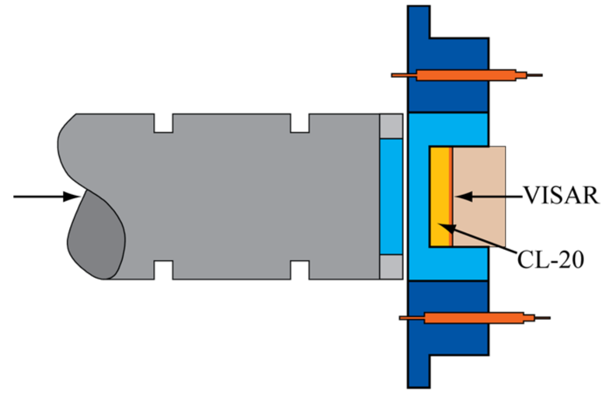
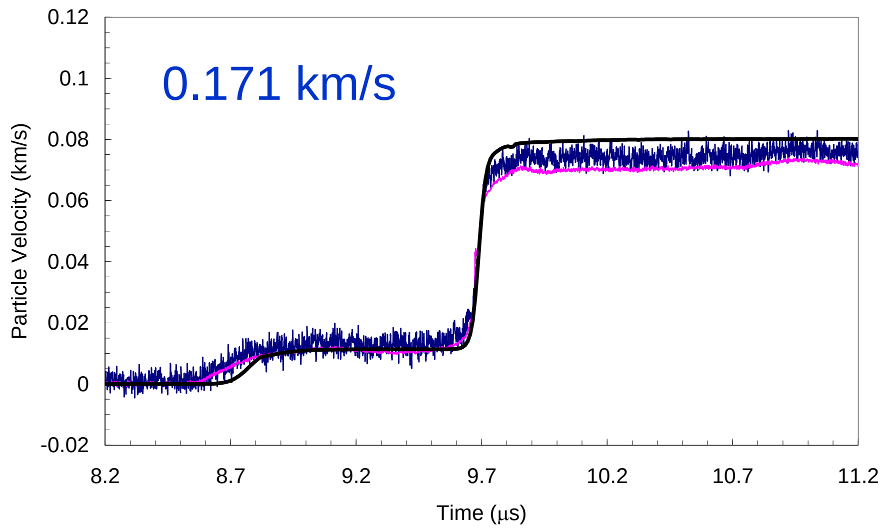
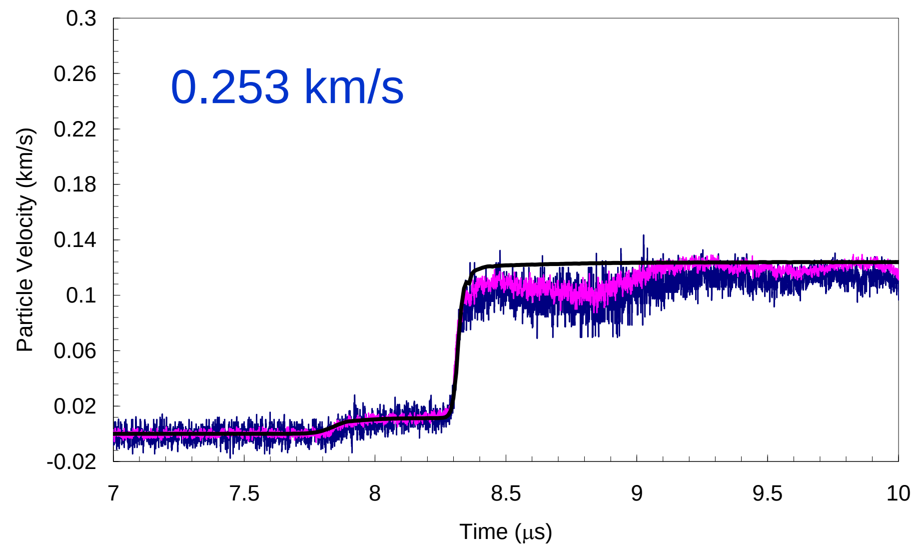
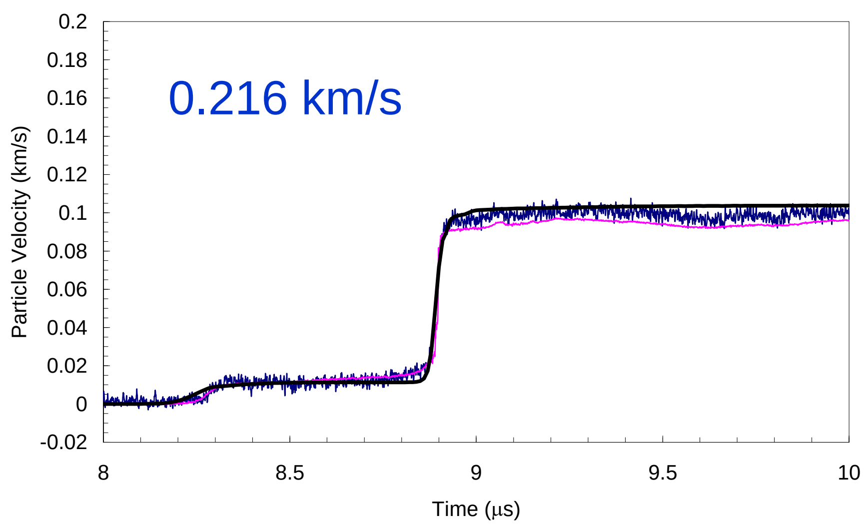
Low Velocity Data









Yield strength **Y= 80 MPa** (**ν = 0.37**) of 70% TMD pellets from low impact velocity experiments

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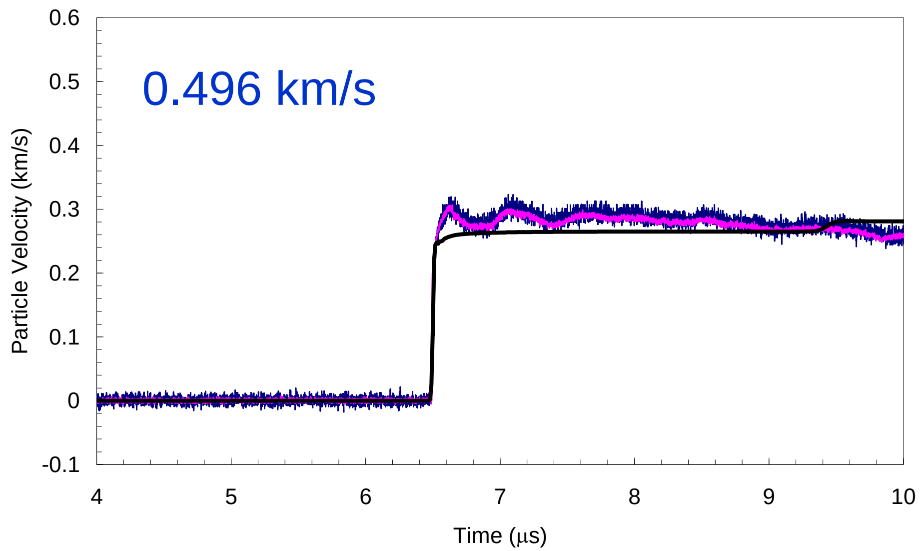
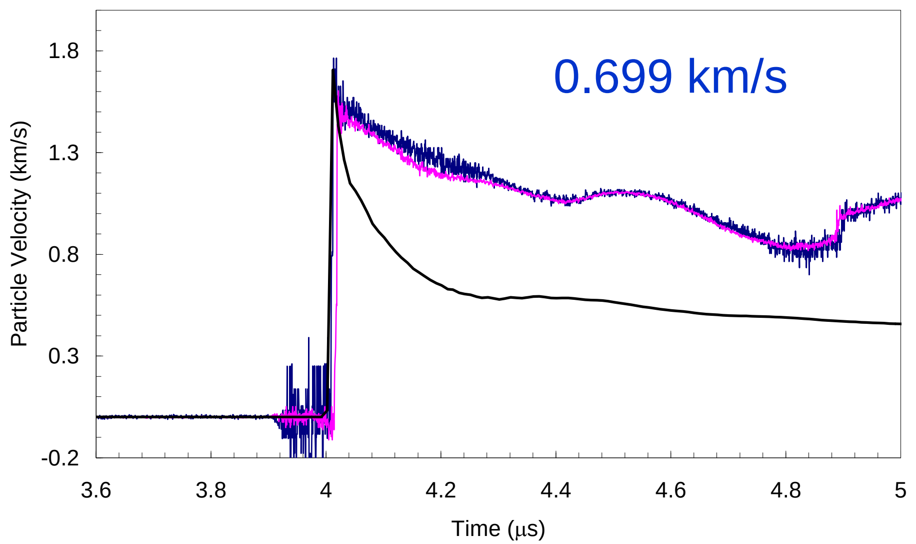
Gas Gun Studies, cont.





- Single wave structure at higher impact velocities
- Expansion along porous EOS not captured in model

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Conclusions

- Solid and reacted EOS determined for porous CL-20 from available published data and SNL gas gun experiments
- BN Multiphase model developed for prediction of shock initiation
- Gas Gun data used for SDT model validation
- Predictive capability extended for future device design with CL-20 initiation
- Future research needed to develop models to predict expansion along porous EOS