

Isentropic Compression Experiments (ICE) for Mesoscale Studies of Energetic Composites

Mel Baer, Clint Hall, Mike Hobbs

Sandia National Laboratories

Albuquerque, NM

Rick Gustavsen, Dan Hooks, Steve Sheffield

Los Alamos National Laboratory

Los Alamos, NM

Energetic Materials Review

Los Alamos National Laboratory

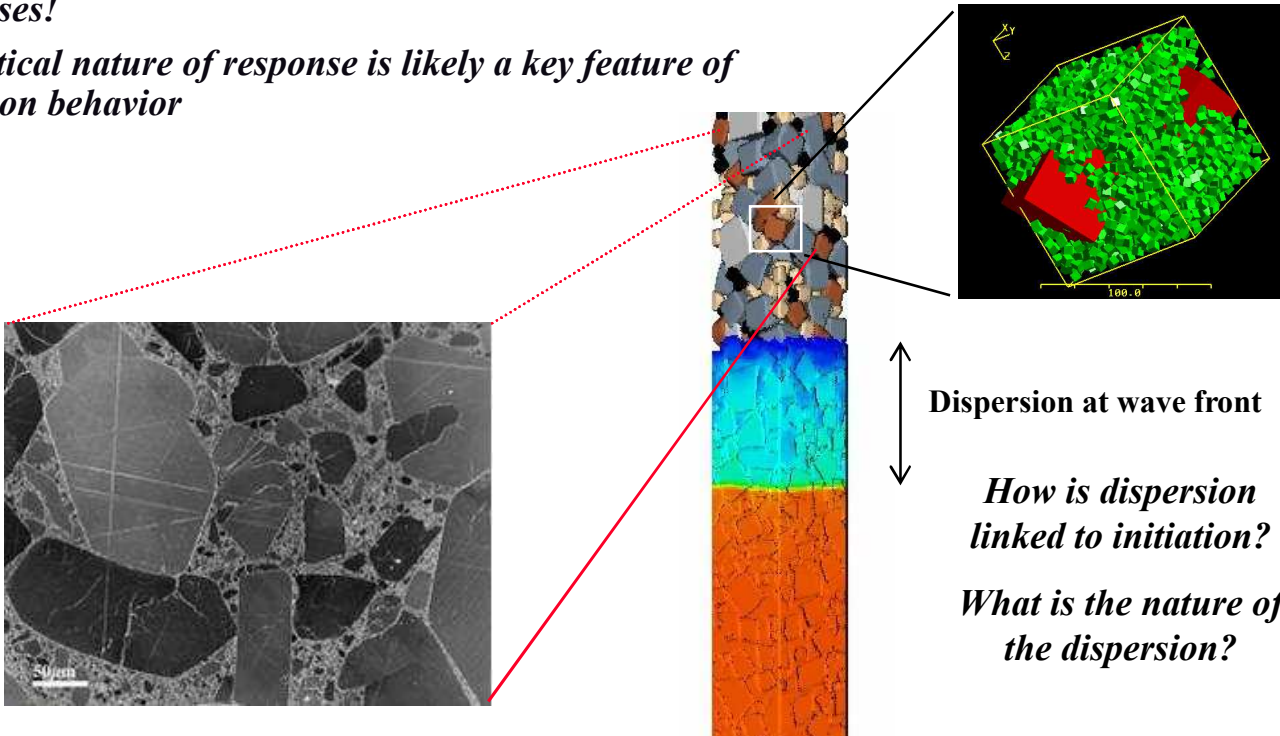
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Motivation

Reactive behavior dominated by mesoscale processes that have eluded continuum measurements and theory

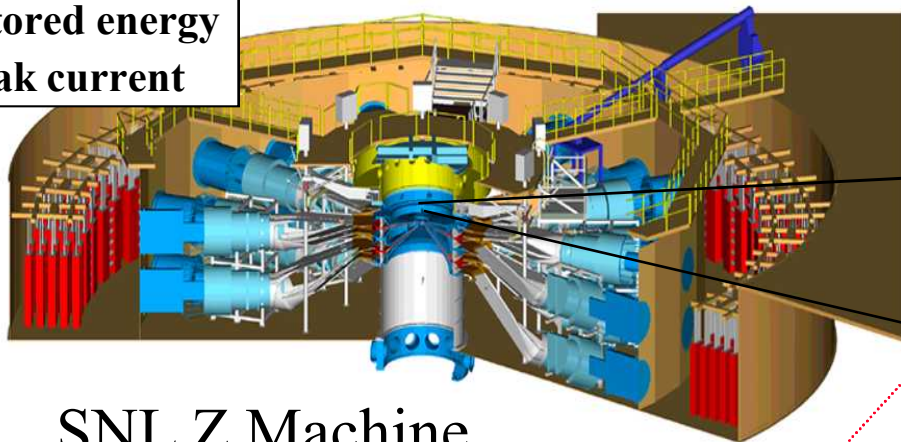
- *New energetic systems with manipulative response and reduced sensitivity requires understanding these processes!*
- *Statistical nature of response is likely a key feature of initiation behavior*

Do we have to model to this level?



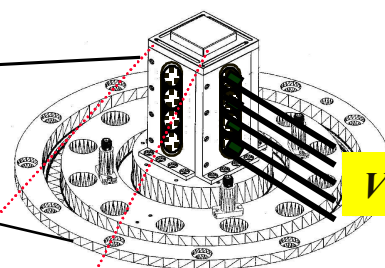
Experiments using Magnetic Field Driven Isentropic Compression

11.5 MJ stored energy
22 MA peak current

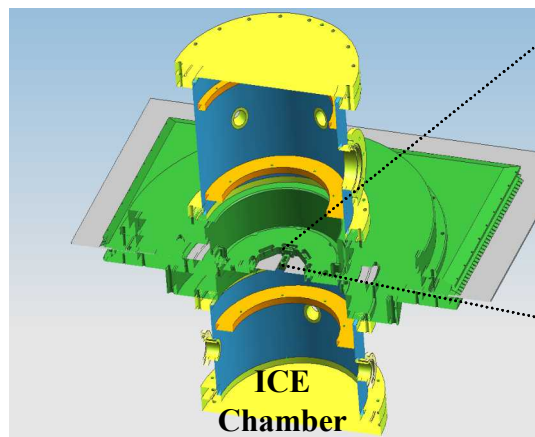


SNL Z Machine

Four Panel /Four Sample ICE Configuration



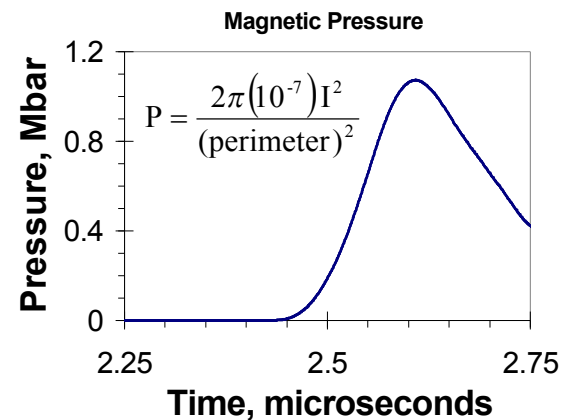
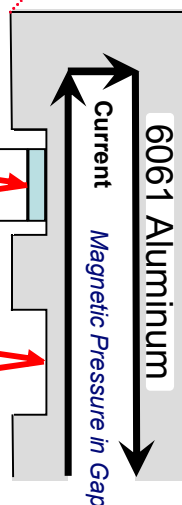
VISAR Probes



Small Pulser

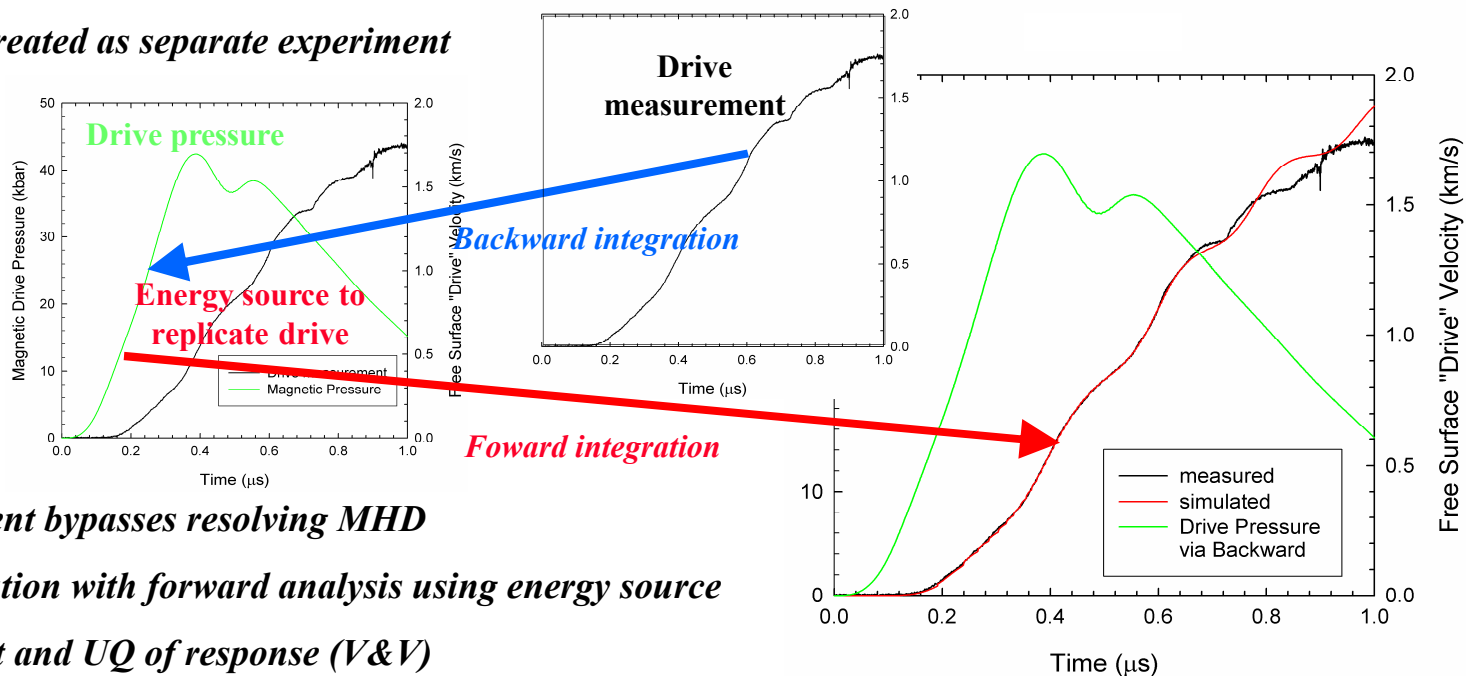
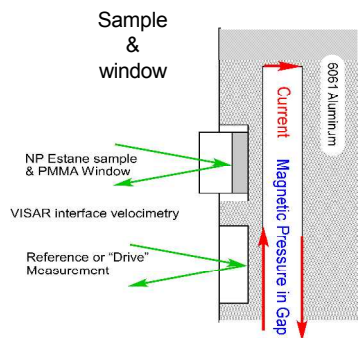


Window & Sample
VISAR Interface Velocimetry
Drive Measurement

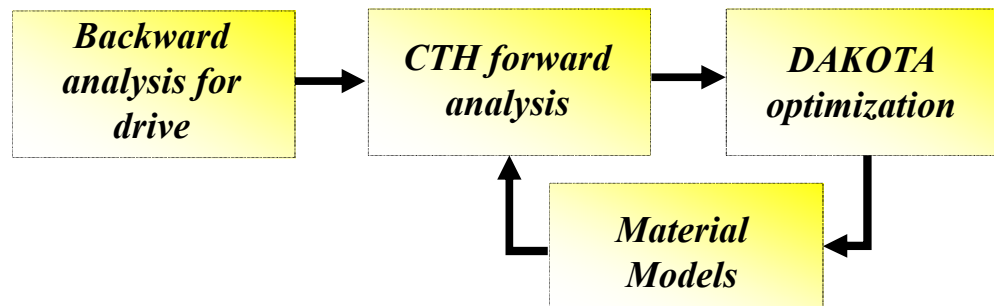


Data Analysis of VISAR Measurements

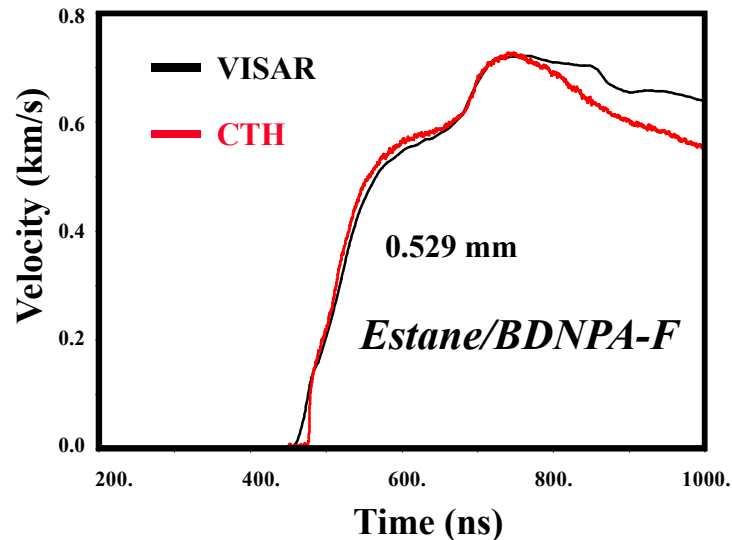
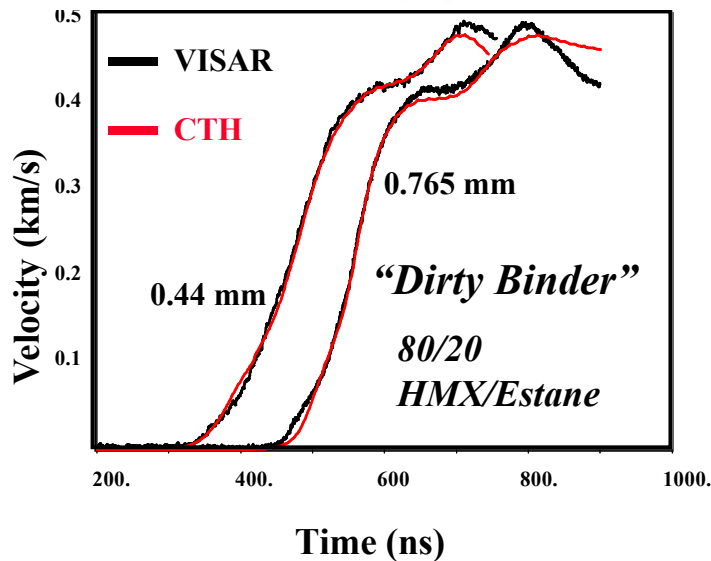
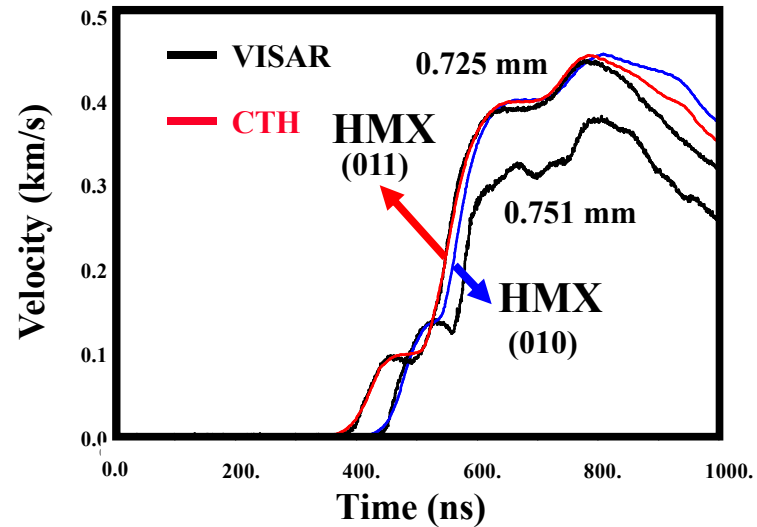
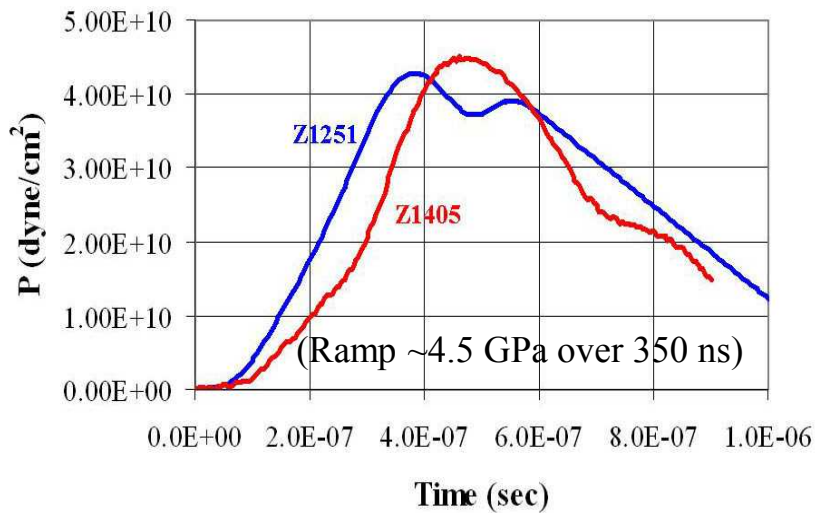
- Each panel treated as separate experiment



- Drive measurement bypasses resolving MHD
- Coupled optimization with forward analysis using energy source
- Assessment and UQ of response (V&V)
- Forward integration allows nonlinear and time-dependent constitutive response

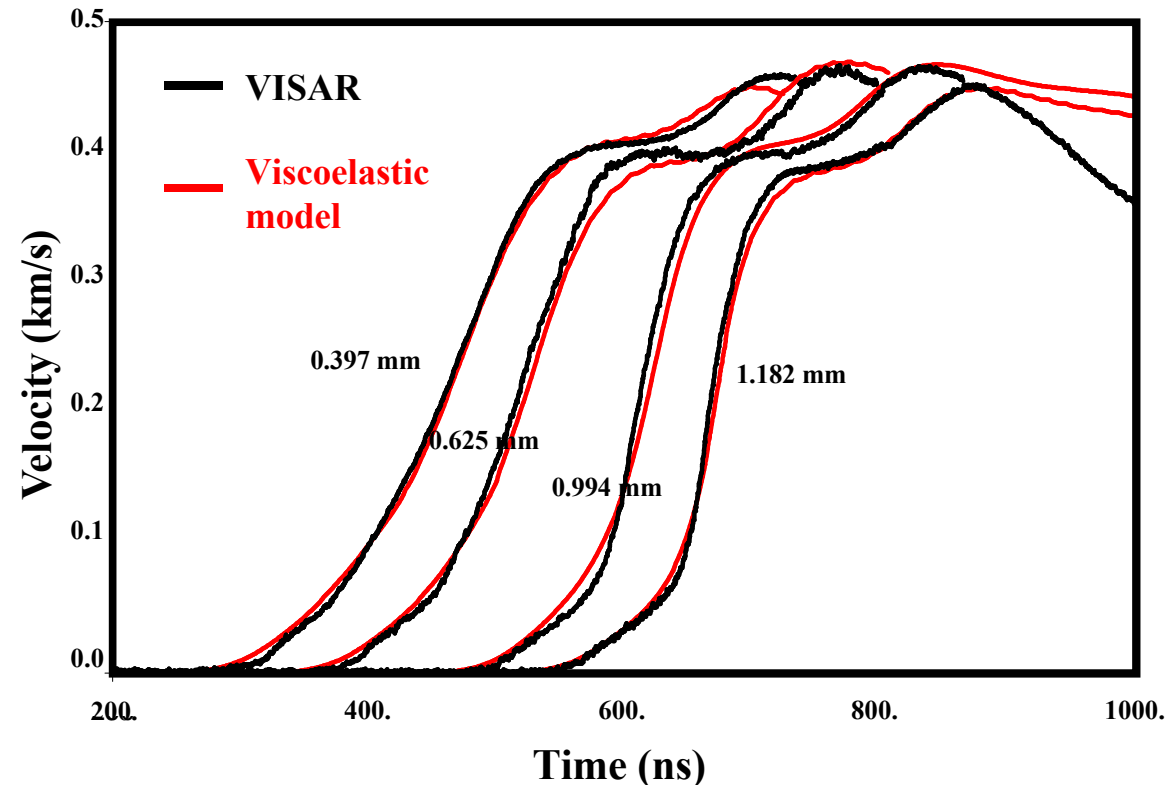


Z1251 – PBX9501 and Constituents



Viscoelastic Response of PBX9501

CTH Maxwell Viscoelastic Model



$$\dot{\sigma} = \frac{dp_I}{d\mu} \dot{\mu} + \frac{(\sigma - p_E)}{\tau}$$

where

$$\tau = \tau_0 \left(2 - \exp \left[-\frac{|\sigma - p_E|}{k} \right] \right); \sigma - p_E < 0$$

$p_E(\mu, e)$ & $p_I(\mu, e)$ EOS's

Mie-Grüneisen form using:

$$U_{s,E} = c_{0,E} + s_{1,E}u_p + s_{2,E}u_p^2 / c_{0,E}$$

$$U_{s,I} = c_{0,I} + s_{1,I}u_p + s_{2,I}u_p^2 / c_{0,I}$$

-Equilibrated states fixed as historical data

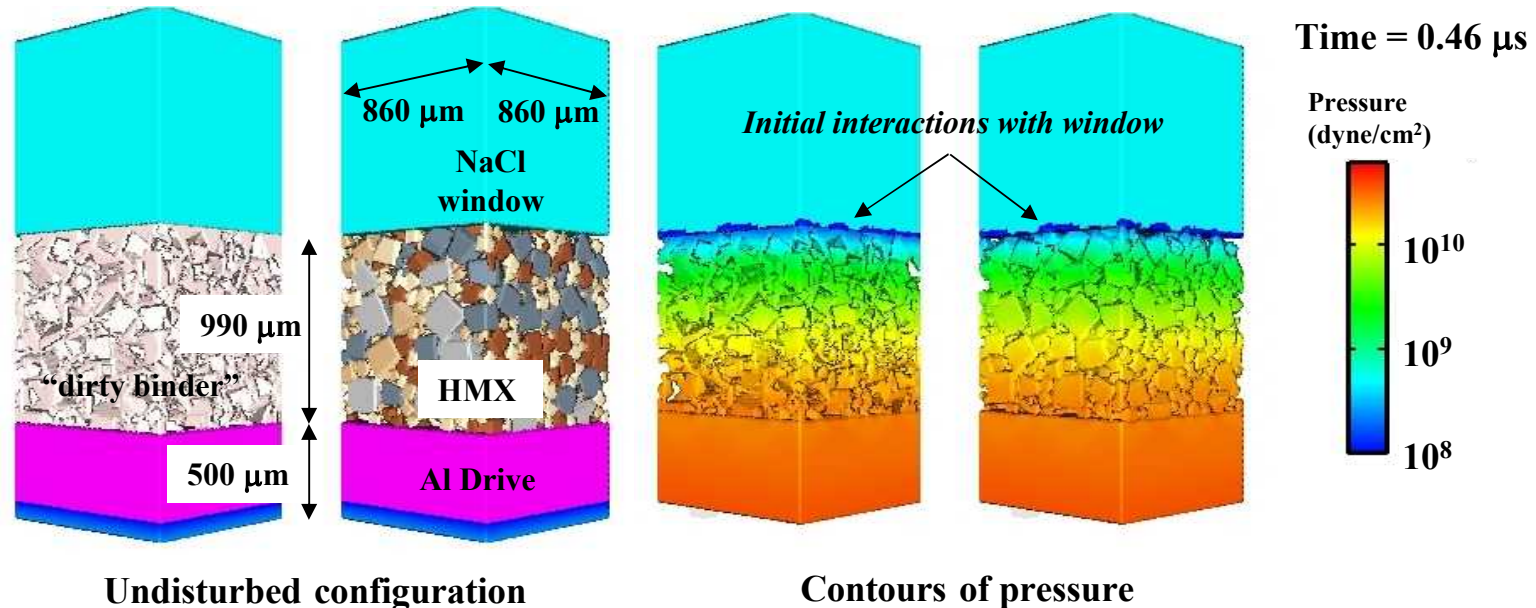
-Instantaneous $c_{0,I}$ determined by x-t of fronts

-parameters $s_{1,I}, \tau_0, k$ optimized by DAKOTA
($s_{2,I}$ & $s_{2,E} = 0.0$)

Optimized data fit for Maxwell Viscoelastic model

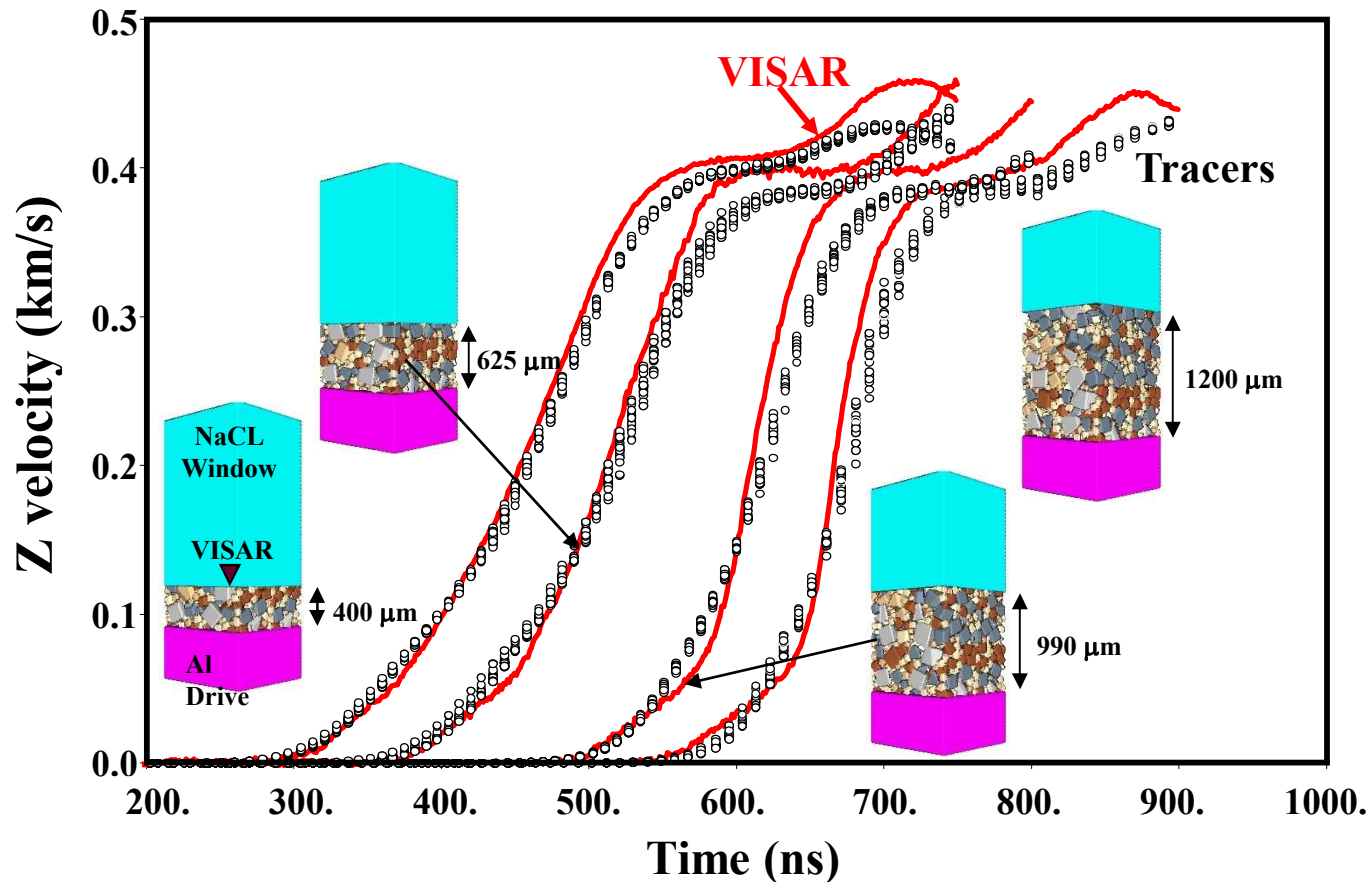
Precursor elastic effects, seen in large HMX crystals, are not observed!

Dynamic Response Suggested by Isentropic Compression Measurements



- Elastic wave initially associated with behavior of large HMX crystals
- Lockup of large crystallites – plastic deformation at contacts- localization effects
- Apparent rate effect as crystals undergo change in elastic response possibly due to anisotropy effects
- Large deformation associated with ‘dirty binder’
- Fine crystallite appear to not exhibit significant strength effects
- Localized plastic deformation at the contacts of the large crystals – this probably dominate initiation behavior

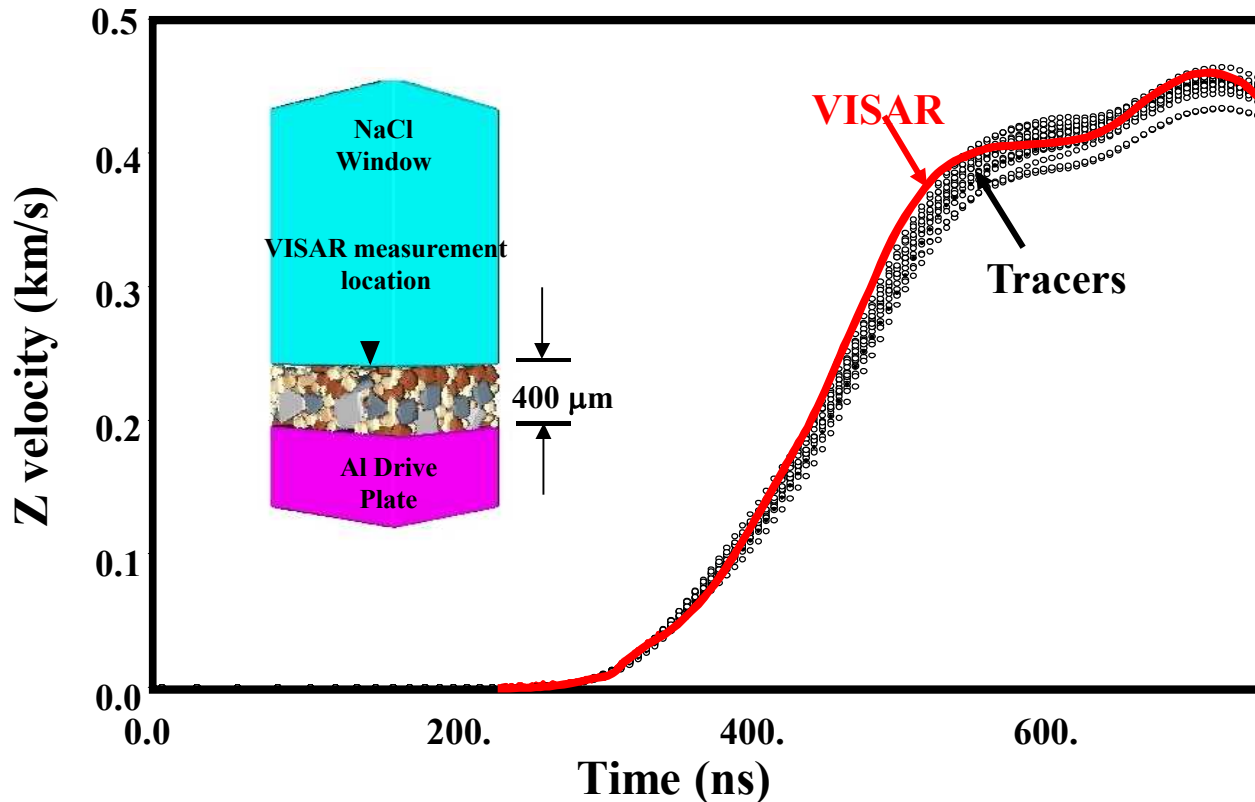
Variations due to sample thickness



Overlay of 10 uniform spaced tracers along the centerline of RVE

How do we related the observed fluctuations at the window interface to those actually occurring in the composite? - more statistics!

Statistical Variations in Mesoscale Simulation

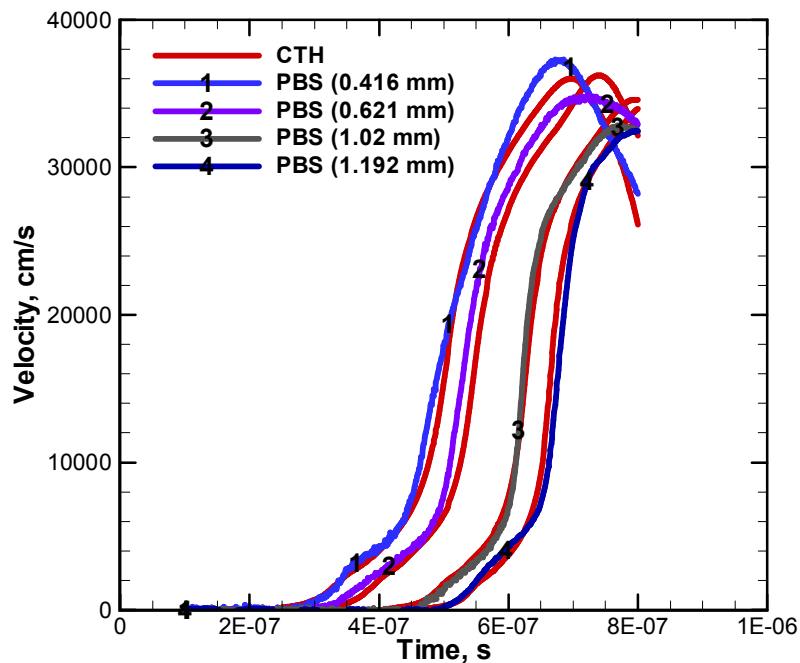


Overlay of 50 uniform spaced tracers – better statistics underway

Mesoscale particle velocity fluctuations $V_z' \sim \pm 0.1 \langle V_z \rangle$

No porosity in simulation – will enhance fluctuations

Z1444 – PBS and Al/Teflon Data Analysis



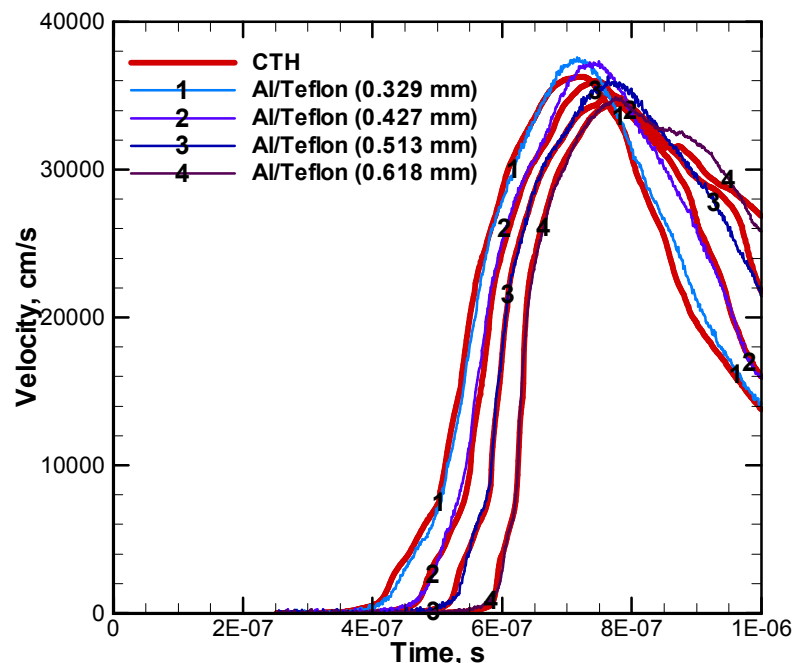
DAKOTA Maxwell VE:

$$\rho = 1.57 \text{ (g/cc)}$$

$$U_{SI} = 3.37 + 6.044 u_p \text{ (mm/}\mu\text{s)}$$

$$U_{SE} = 2.96 + 3.64 u_p \text{ (mm/}\mu\text{s)}$$

$$\tau_R = 0.137 \text{ (}\mu\text{s)} ; P_R = 0.8 \text{ (Kbar)}$$

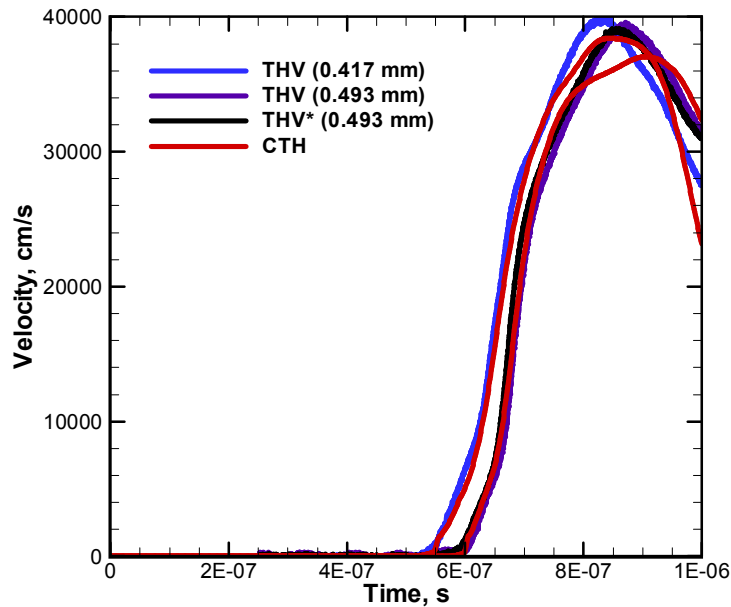


Homogenization model – quadratic
Mie-Grüneisen fit:

$$\rho = 1.57 \text{ (g/cc)}$$

$$U_{SI} = 1.536 + 3.172 u_p - 1.25 u_p^2 \text{ (mm/}\mu\text{s)}$$

Z1444 – THV 220 and “Filled VCE” Data Analysis



THV 220 (tetrafluorethylene, hexafluoropropylene, vinylidene fluoride plastic)

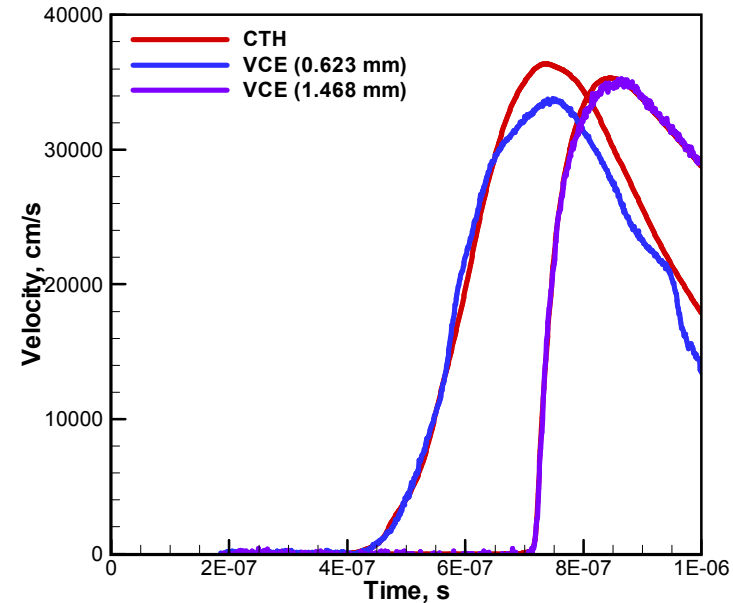
DAKOTA Maxwell VE:

$$\rho = 1.95 \text{ (g/cc)}$$

$$U_{SI} = 1.276 + 4.26 u_p \text{ (mm/}\mu\text{s)}$$

$$U_{SE} = 0.846 + 3.34 u_p \text{ (mm/}\mu\text{s)}$$

$$\tau_R = 0.176 \text{ (}\mu\text{s)} ; P_R = 0.132 \text{ (GPa)}$$



“filled VCE” (Vinyl-Chloride-Ethylene plastic filled with a high impedance metal additive)

DAKOTA Maxwell VE:

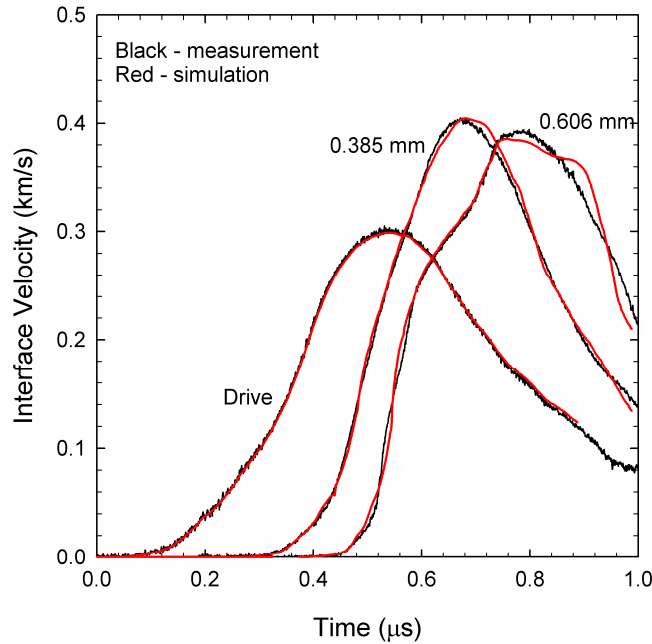
$$\rho = 1.71 \text{ (g/cc)}$$

$$U_{SI} = 2.89 + 8,786 u_p \text{ (mm/}\mu\text{s)}$$

$$U_{SE} = 2.815 + 5.968 u_p \text{ (mm/}\mu\text{s)}$$

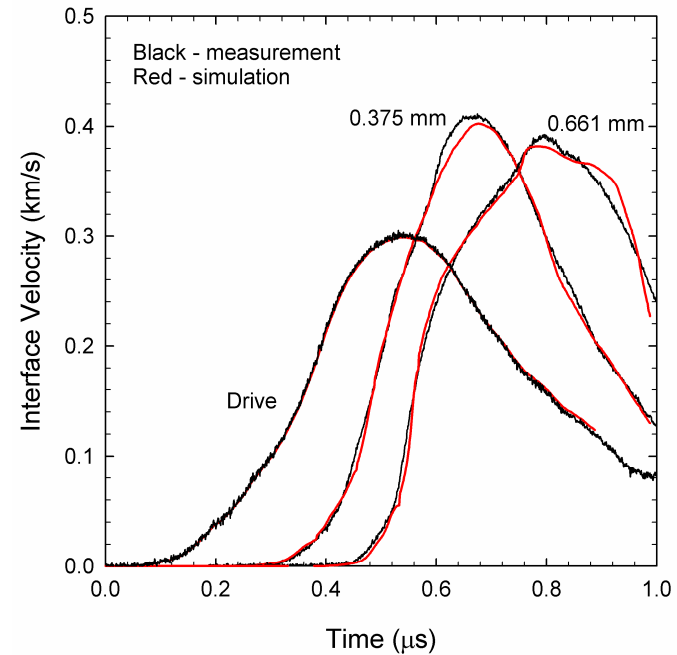
$$\tau_R = 0.012 \text{ (}\mu\text{s)} ; P_R = 0.08 \text{ (GPa)}$$

Z1444 – Estane and Hydrolyzed Estane Data Analysis



Estane Optimized M-G fit:

$$\begin{aligned}\rho_0 &= 1.191 \text{ (gm/cm}^3\text{)} \\ U_S &= 1.79 + 2.9u_P - 0.45 u_P^2 \text{ (mm/}\mu\text{s)} \\ \Gamma &= 1.34 \\ C_V &= 1.52 \text{ (J/gm}^\circ\text{K)}\end{aligned}$$

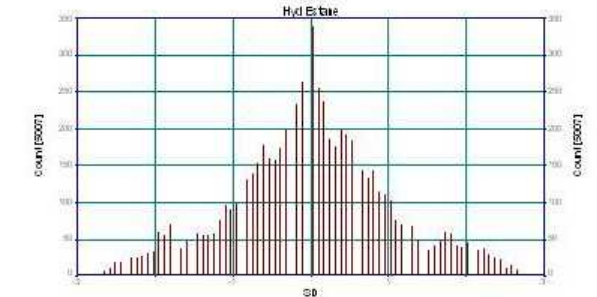
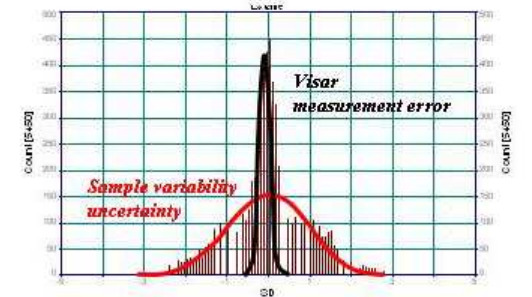
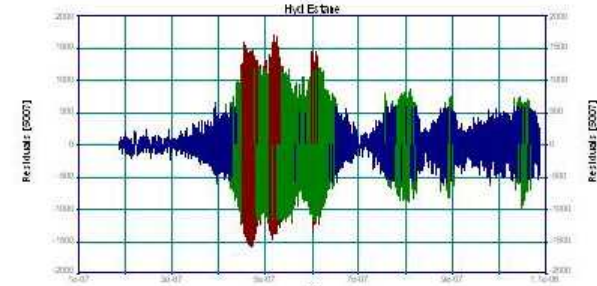
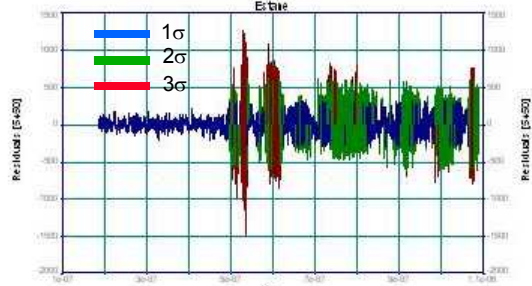
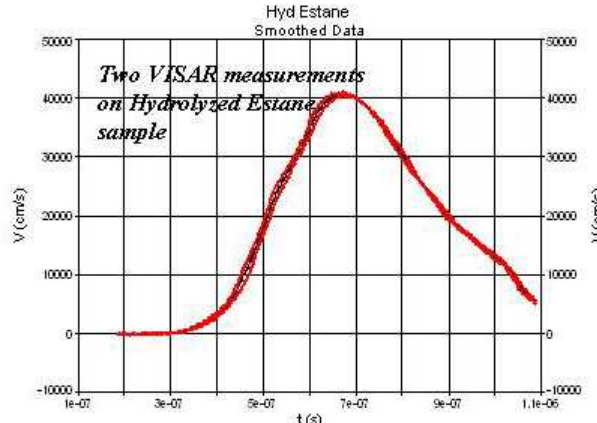
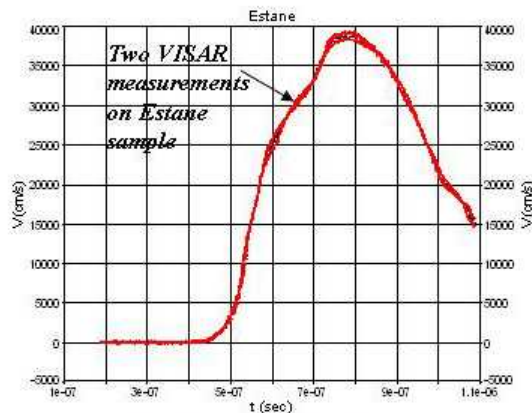


Hydro - Estane Optimized M-G fit:

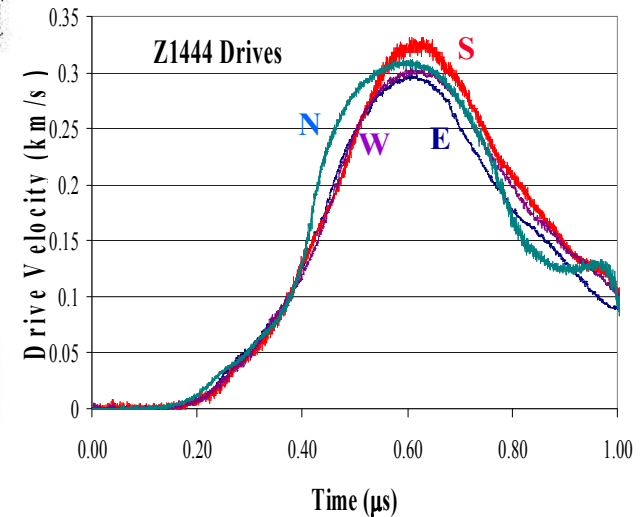
$$\begin{aligned}^*\rho_0 &= 1.191 \text{ (gm/cm}^3\text{)} \\ U_S &= 1.9 + 2.8u_P - 0.37 u_P^2 \text{ (mm/}\mu\text{s)} \\ ^*\Gamma &= 1.34 \\ ^*C_V &= 1.52 \text{ (J/gm}^\circ\text{K)}\end{aligned}$$

Analysis by R. Gustavsen (LANL)

Uncertainty Quantification (UQ) of Estane Analysis



Uncertainties in measurements



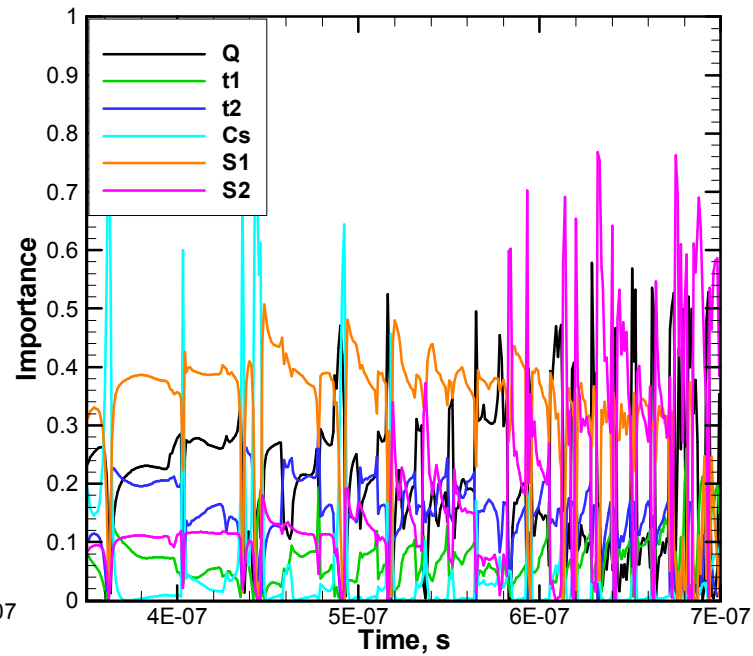
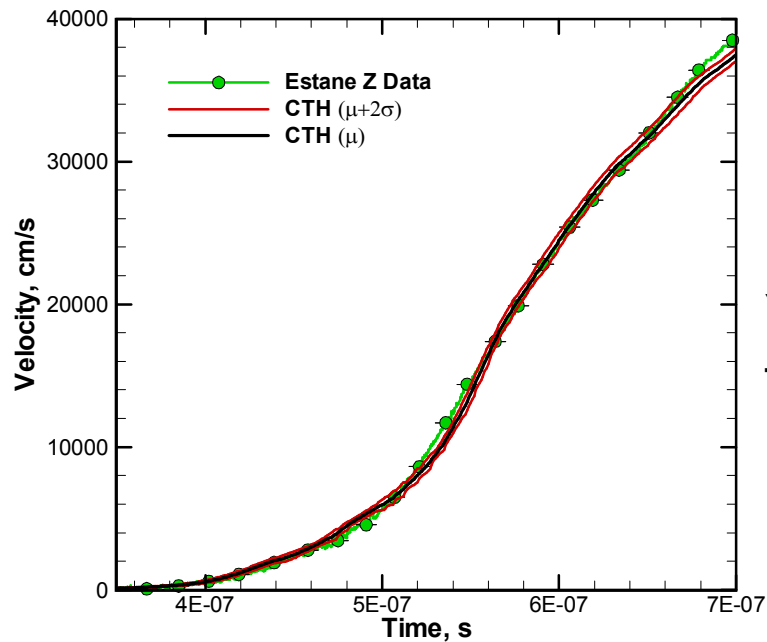
VISAR variations ~ 100 . (cm/s)

Panel to panel variations ~ 500 (cm/s)

Q source variations $\sim 1.e17$ (erg/gm-s)

Sample thickness variations ~ 5 (μ m)

Sensitivity Analysis of Estane (Latin Hypercube Method)



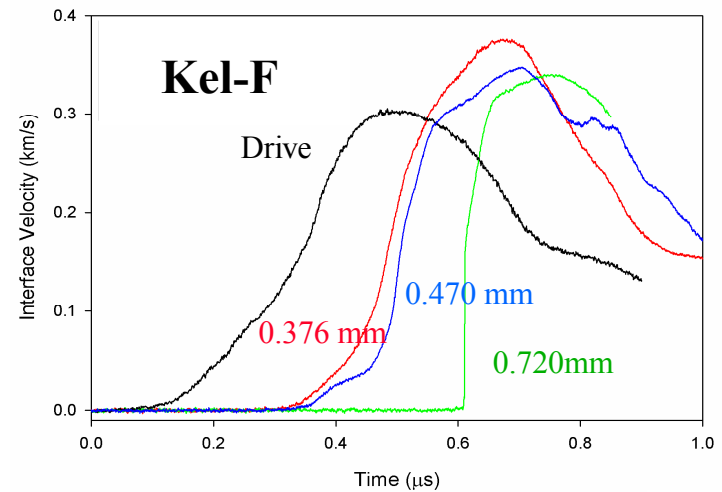
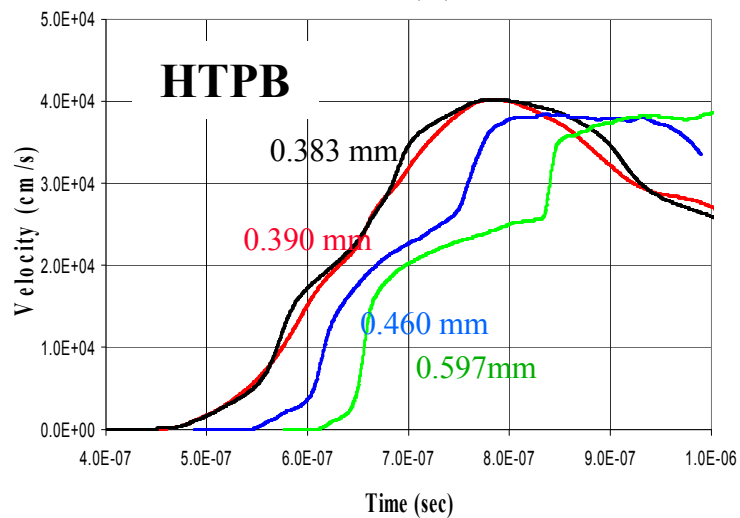
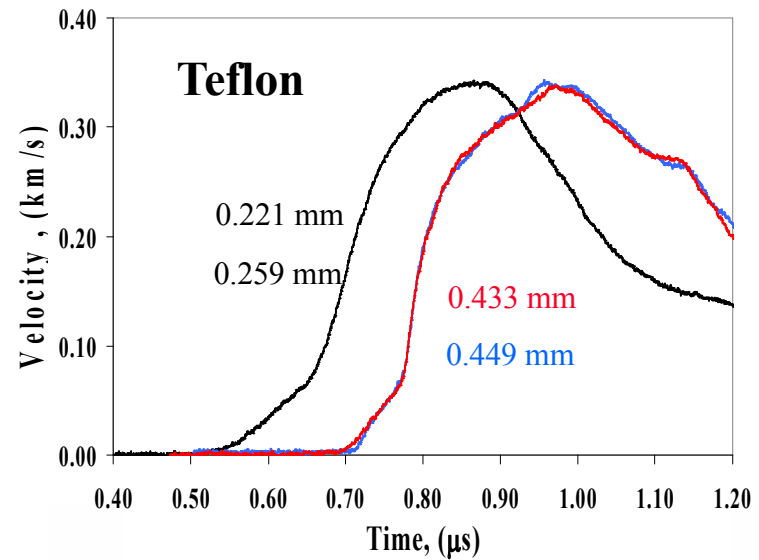
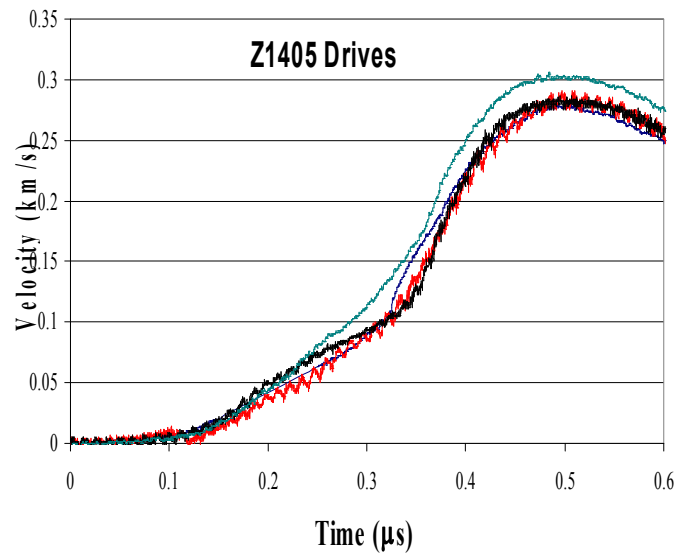
Mie-Grüneisen form : $U_s = c_s + s_1 u_p + s_2 u_p^2 / c_0$

$$c_s = 1.914 \pm 0.018 \text{ [mm}/\mu\text{s}]$$

$$s_1 = 2.889 \pm 0.015$$

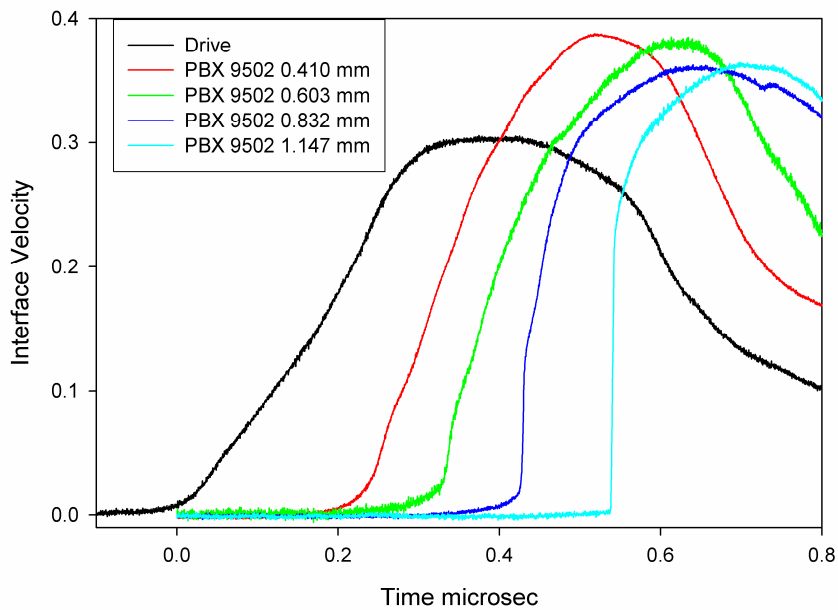
$$s_2 = -0.813 \pm 0.0445$$

Z1405 – Binders

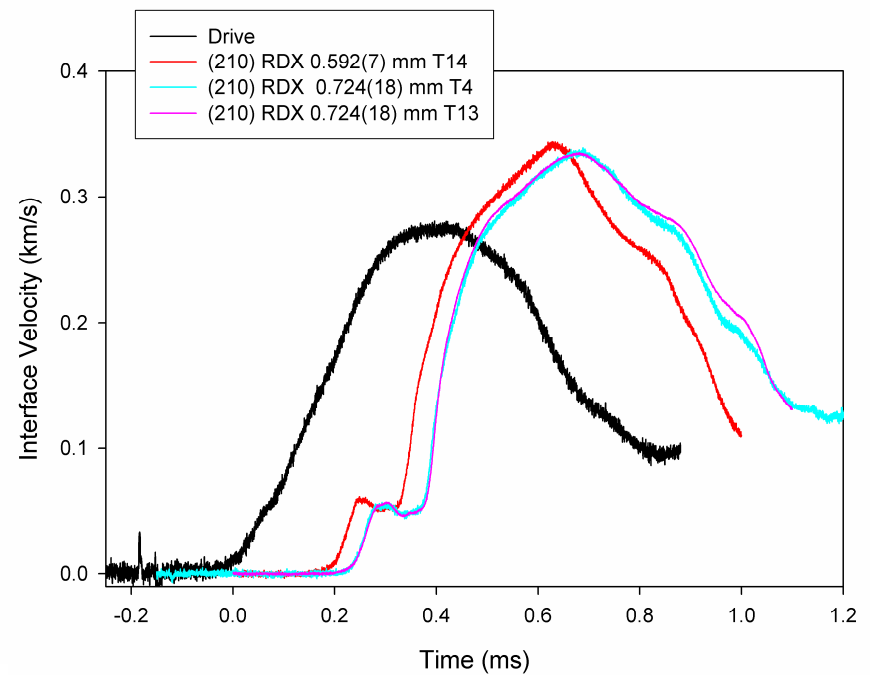


Z1483 – PBX9502 & RDX

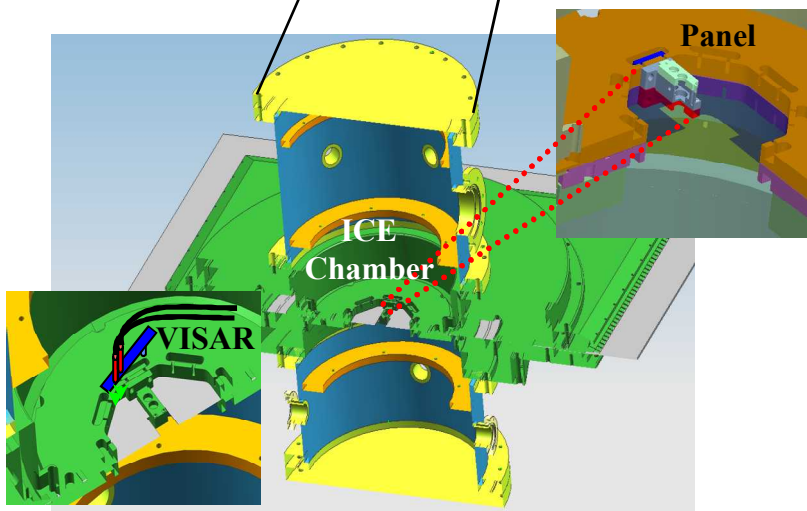
Z 1489 South Panel



Z 1489 East Panel



Small Pulser and Diagnostics



- Dedicated line-image ORVIS
- Flash x-ray
 - X-ray diffraction (in process)
- Pre-heating & cooling capabilities
 - Up to 400 C (in process)
- Multiple band pyrometry
- PDV (low velocity resolutions)



- Dual, Low VPF, high temporal resolution detectors
- VPF range 0.014 -10 km/s/fringe
 - 2X7 Channels
 - Detectors 90psec fwhm response
- Push/pull with quadrature recording
- 2 VALYN 4-Channel VISARs



New Material Studies

- *Acceleration studies on PBX9501 > 10.0 GPa to 50.0 GPa -requires Z (focus on interactions of materials at higher stress states) (ZR conversion begins FY06 Q3)*
- *Small pulser experiments*
 - *Repeat tests at 5.0 GPa/500 ns with ORVIS – PBX9501 (variation states)*
 - *Comparative studies of PBX9501 –ramp loaded gun vs. pulser in heated samples*
 - *Low stress studies in crystal HMX (all 3 directions) + RDX –investigate repeatability and more insight to the ‘visco-elastic’ like response*
 - *Crystals with defects – toward understanding pore collapse mechanisms*
 - *Reactive binders – NC*
 - *Other crystalline materials and composites – i.e. crystal AP, insensitive RDX*



Summary

- *Isentropic compression experiments can provide new information on energetic material behavior needed for mesoscale modeling*
- *A series of Z ramp loads have been successfully designed to study near-isentropic compression of a typical energetic composite + constituents (PBX9501), varied binders (Kel F, Estane, Teflon, HTPB) and composites with metal additives (B/polymer, Al/Teflon) - a wealth of new constitutive data has been produced*
 - *Comparative response has lead to new insights*
- *Data interrogation including coupling optimization and forward analysis techniques has been successfully used to determine material response*
- *Future studies will continue to explore energetic composite at isentropic loading conditions that should induce reaction behavior – localization effects during acceleration loading are fundamental to influencing initiation behavior*