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SAND2017-4134C

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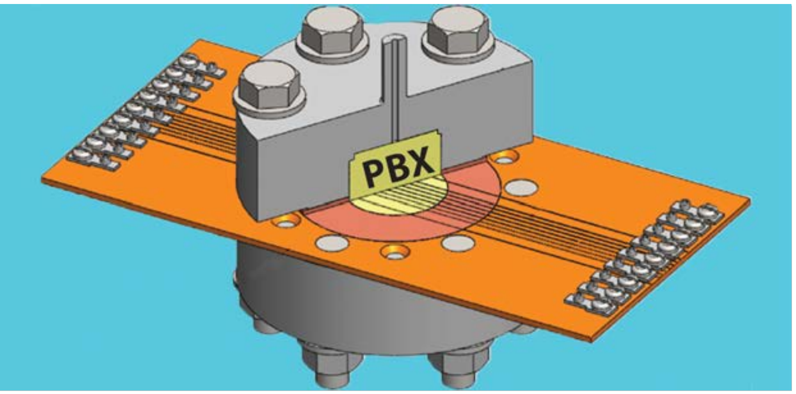
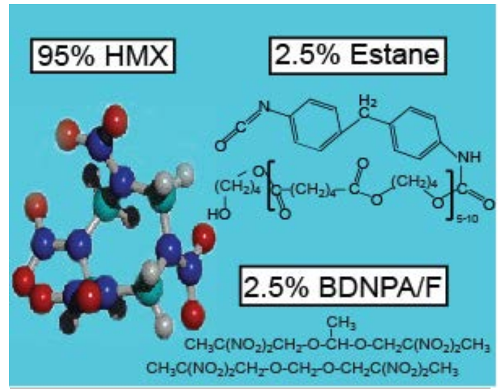
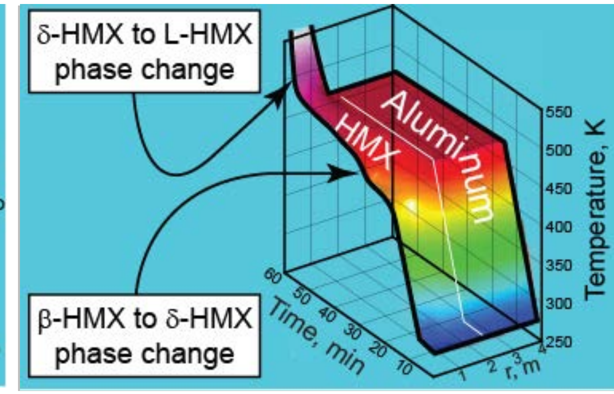
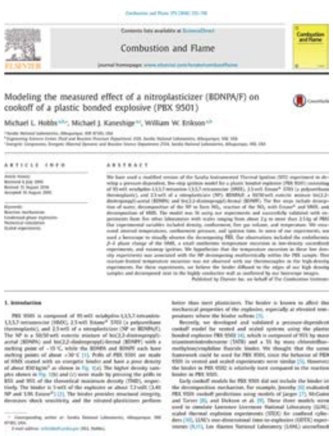






Model on PBX 9501 (Combustion and Flame 173, 2016) applied to other HMX based PBXs



Binder Effects During Cookoff of HMX

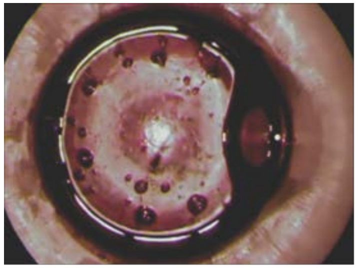
$$H_2O_a \xrightarrow{1} H_2O_g$$

$$\text{BDNPA/F} \xrightarrow{2} \text{NVR} + 4NO_2$$

$$\text{Estane} + NO_2 \xrightarrow{3} \text{Gas} + C$$

$$\text{HMX} + NO_2 \xrightarrow{4} \text{Gas} + C$$

$$\text{HMX} \xrightarrow{5} \text{Gas} + C$$



Michael L. Hobbs

Michael J. Kaneshige

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Why model cookoff?

- Need to know behavior in **accidental fires** to assess safety.
- Need to know the **time-to-ignition** for safety timing studies.
- Need to know the **amount of gas produced** to determine if confinement will rupture before ignition.
- Need to know how the damaged state of the material affects the subsequent **burn behavior**.
- Ignition time, gas production, burn behavior are **all affected by confinement** variables such as venting, density, permeability, and ullage.

Carrier	Deaths	Injured	Cost
Oriskany, 1966	44	156	$63.6M
Forestal, 1967	134	162	$758M
Enterprise, 1969	28	343	$554M
Nimitz, 1981	14	48	$150M
	220	**709**	**$1525M**

Atwood et al, "Experimental Support of a Slow Cookoff Model Validation effort," 2004 Insensitive Munitions & Energetic materials Technology Symposium (2004).

Tremendous cost considering none were under attack!

Applying PBX 9501 model to other PBXs

Single model

Energy	$\rho_b C_b \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \sum_{i=1,4} r_i h_{ri} M_{w,i}$
Mechanism	$H_2O_a \xrightarrow{1} H_2O_g$
	$\text{BDNPA/F} \xrightarrow{2} \text{NVR} + 4NO_2$
	$\text{Estane} + NO_2 \xrightarrow{3} 7.1\ \text{Gas}_E + 8.1\ \text{Carbon}$
	$\text{HMX} + NO_2 \xrightarrow{4} 11.5\ \text{Gas}_{x1} + \text{Carbon}$
	$\text{HMX} \xrightarrow{5} 10\ \text{Gas}_{x2} + 1.6\ \text{Carbon}$
Rates	$r_1 = A_1 \exp\left(\frac{-E_1+\zeta\sigma_1}{RT}\right)[H_2O]$
	$r_2 = A_2 \exp\left(\frac{-E_2+\zeta\sigma_2}{RT}\right)[\text{BDNPA/F}]$
	$r_3 = A_3 \left(\frac{P}{P_o}\right)^{n_3} T^{m_3} \exp\left(\frac{-E_3+\zeta\sigma_3}{RT}\right)[\text{Estane}][NO_2]$
	$r_4 = A_3 \left(\frac{P}{P_o}\right)^{n_4} T^{m_4} \exp\left(\frac{-E_4+\zeta\sigma_4}{RT}\right)[\text{HMX}][NO_2]$
	$r_5 = A_5 \left(\frac{P}{P_o}\right)^{n_5} T^{m_5} \exp\left(\frac{-E_5+\zeta\sigma_5}{RT}\right)[\text{HMX}]$
Species	$\frac{d[H_2O_a]}{dt} = -r_1;\ \frac{d[H_2O_g]}{dt} = r_1;\ \frac{d[\text{BDNPA/F}]}{dt} = -r_2;\ \frac{d[\text{NVR}]}{dt} = r_2;\ \frac{d[NO_2]}{dt} = 4r_2 - r_3 - r_4$
	$\frac{d[\text{Estane}]}{dt} = -r_3;\ \frac{d[\text{Gas}_E]}{dt} = 7.1r_3;\ \frac{d[\text{Carbon}]}{dt} = 8.1r_3 + r_4 + 1.6r_5$
	$\frac{d[\text{HMX}]}{dt} = -r_4 - r_5;\ \frac{d[\text{Gas}_{X1}]}{dt} = 11.5r_4;\ \frac{d[\text{Gas}_{X2}]}{dt} = 10r_5$
Progress	$P_1 = \frac{[H_2O]}{\omega_{H_2O_a}\rho_{b,o}/Mw_{H_2O_a}};\ P_2 = \frac{[\text{BDNPA/F}]}{\omega_{\text{BDNPA/F}}\rho_{b,o}/Mw_{\text{BDNPA/F}}};\ P_2 = \frac{[\text{Estane}]}{\omega_{\text{Estane}}\rho_{b,o}/Mw_{\text{Estane}}}$
	$P_4 = P_5 = \frac{[\text{HMX}]}{\omega_{\text{HMX}}\rho_{b,o}/Mw_{\text{HMX}}}$

12 explosives

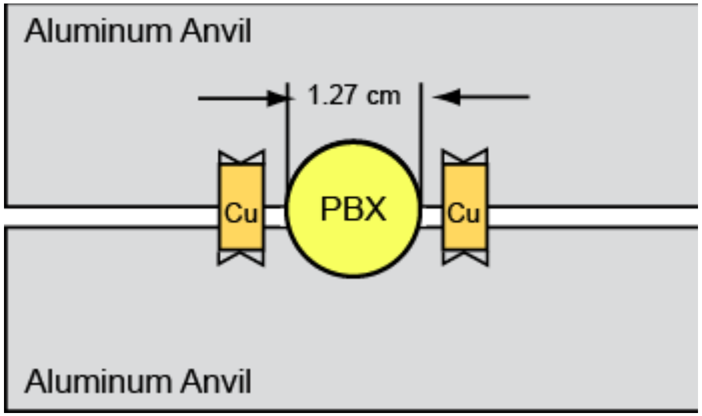
Acronym*	Composition
BDNPA/F	bis(2,2-dinitropropyl)acetal/formal (50/50)
CEF	tris-β-chloroethylphosphate
EDC-29	95 wt% HMX, and 5 wt% polyurethane
EDC-37	91 wt% HMX, 9 wt% oil and nitrocellulose
Estane®	a polyurethane thermoplastic
FEFO	1,1'-[methylenebis(oxy)]bis[2-fluoro-2,2-dinitroethane]
HMX	octahydro-1,2,5,7-tetranitro-1,3,5,7-tetrazocine
LX-04	85 wt% HMX and 15 wt% Viton A
LX-07	90 wt% HMX and 10 wt% Viton A
LX-09	93% HMX, 4.6% pDNPA, and 2.4 wt% FEFO
LX-10-0	95 wt% HMX and 5 wt% Viton A
LX-14	95.5 wt% HMX and 4.5 wt% Estane®
NC	Nitrocellulose
PBX 9011	90 wt% HMX and 10 wt% Estane®
PBX 9404	94% HMX, 3% CEF, 3% nitrocellulose
PBX 9501	95 wt% HMX, 2.5 wt% Estane®, 2.5 wt% BDNPA/F
pDNPA	2,2- dinitropropyl acrylate
Viton A	vinylidine fluoride/hexafluoropropylene copolymer
X-0298	97.5% HMX and 2.5 wt% Kraton oil

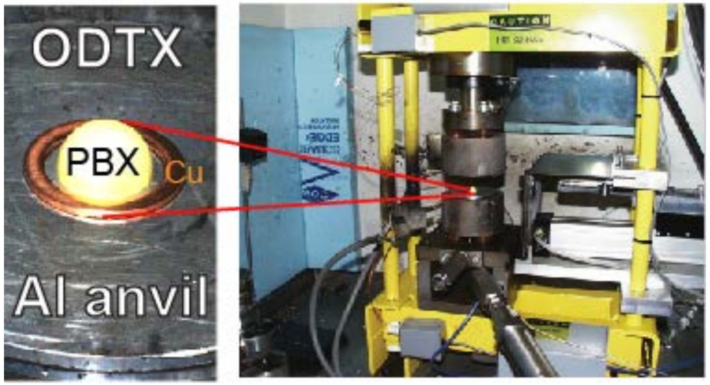
* Green (endothermic binder), Yellow (exothermic binder)

Need to account for HMX molar volume and binder reactivity

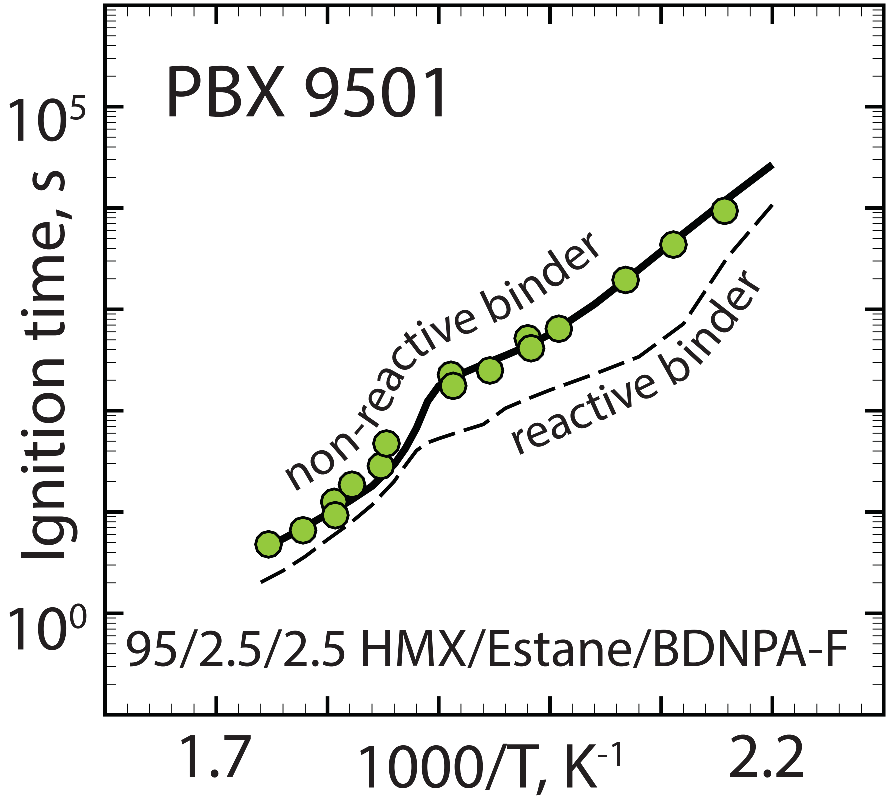
One-dimensional time-to-explosion (ODTX)

LLNL's ODTX experiment





Measured/Predicted Ignition time



The thermal expansion is about 14 time greater for the binder than HMX. As the PBX 9501 gets hot, the binder is extruded to the edge, where the binder energy is dissipated by the conductive aluminum.

Sandia Instrument Thermal Ignition (SITI)

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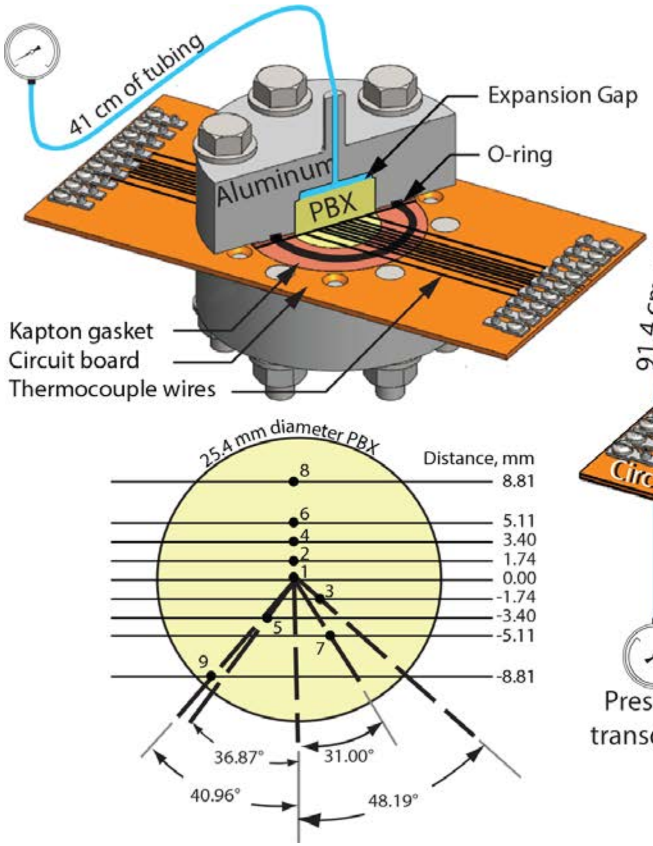
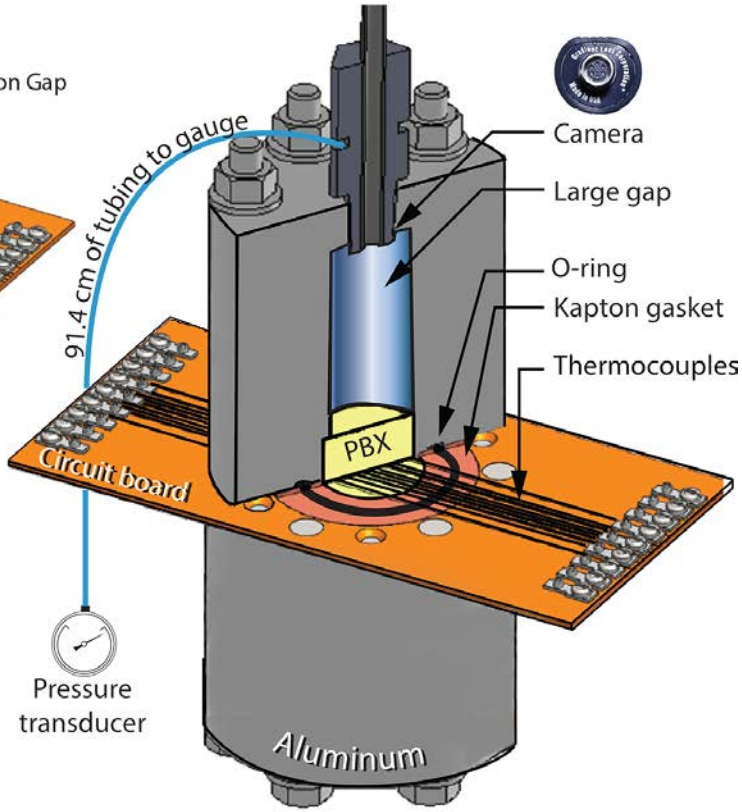
Small ullage

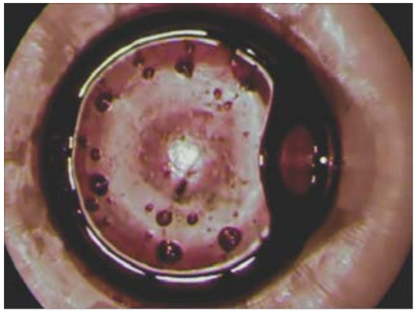


Large ullage with borescope

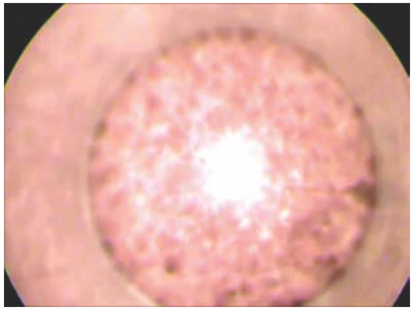


Binder extrusion

1.78 g/cc (96% TMD)

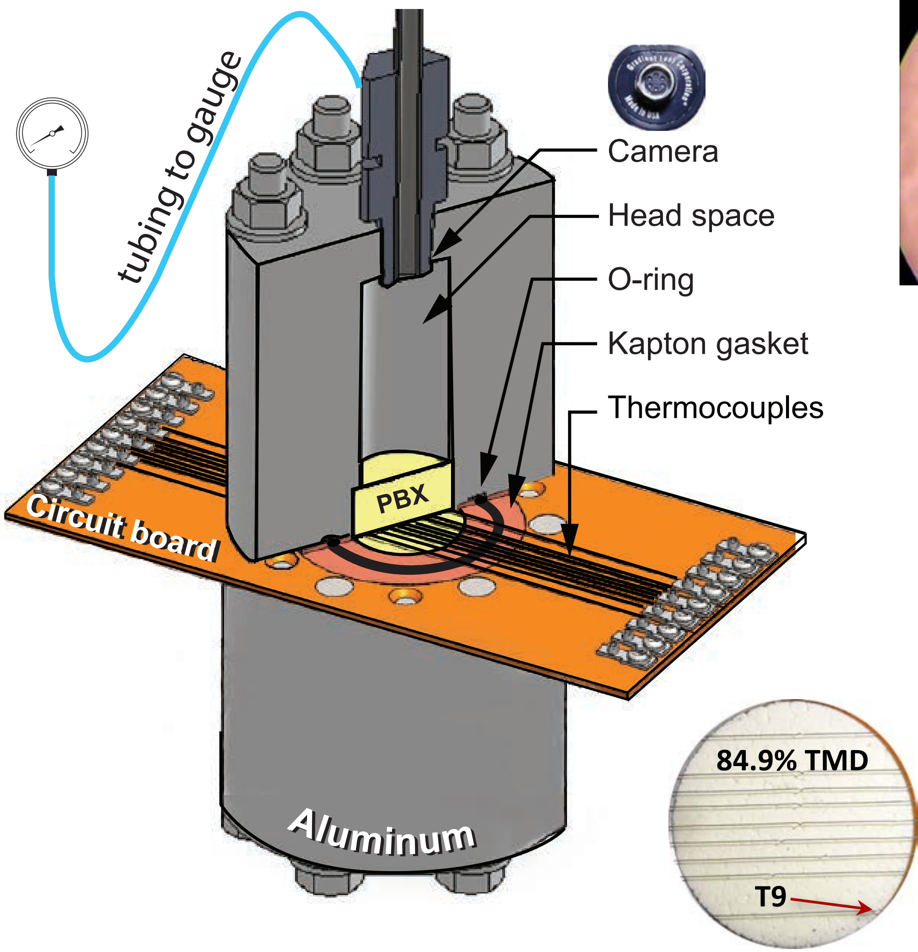


1.58 g/cc (85% TMD)

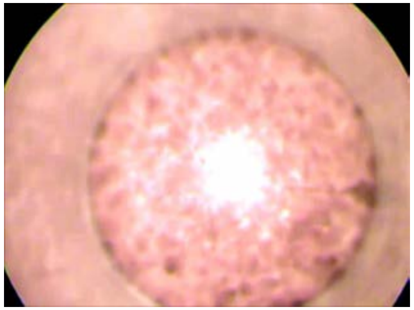


Binder leaves high density explosive and decomposes on heated boundary

Boroscope in SITI with PBX 9501

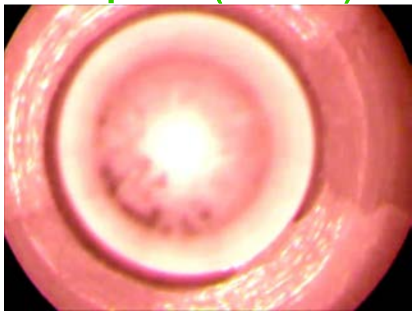


Exp 445 (sealed)

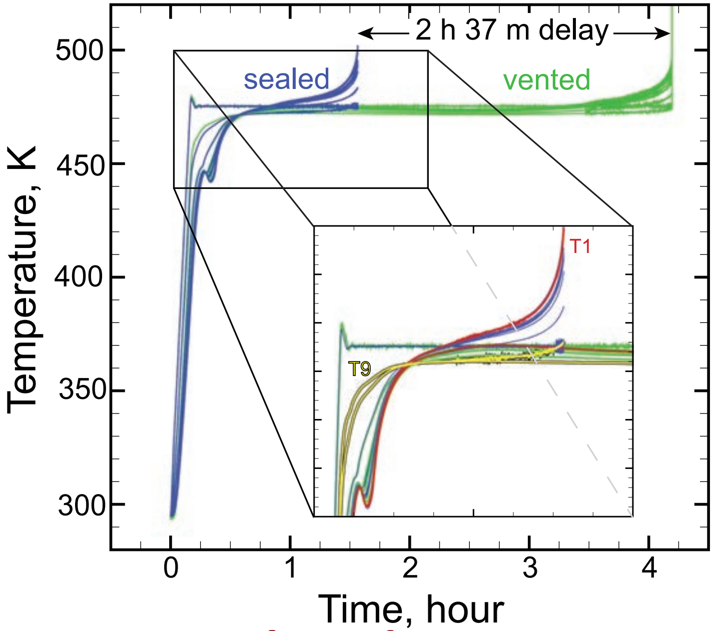


Minimal binder flow

Exp 444 (vented)



Binder flows to edges



For unconfined decomposition, binder migrates to the edge. A wetted surface provides better heat transfer for the vented case.

PBX 9501 molding powder (46% TMD)

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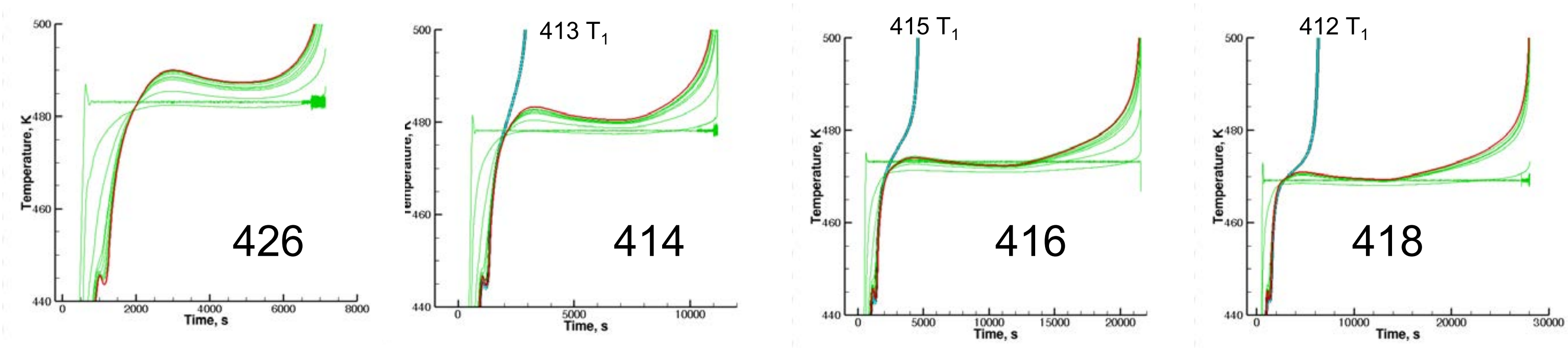
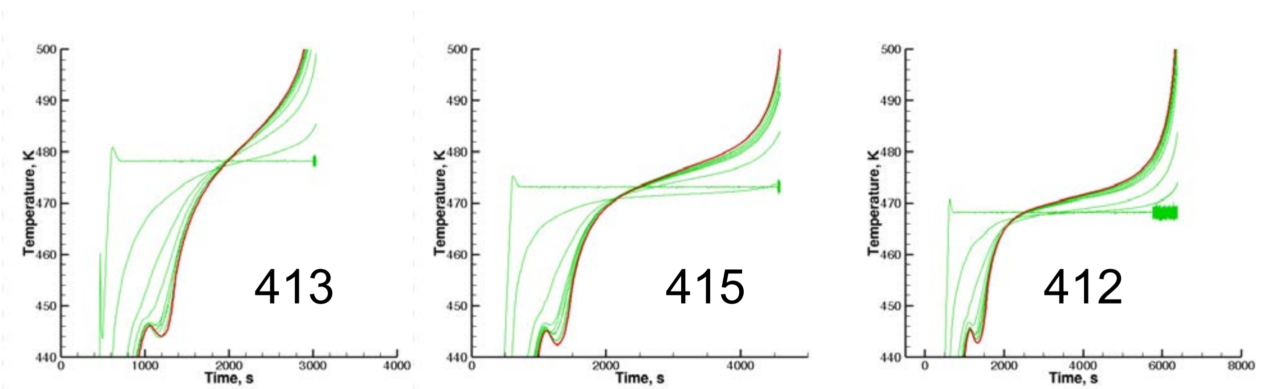
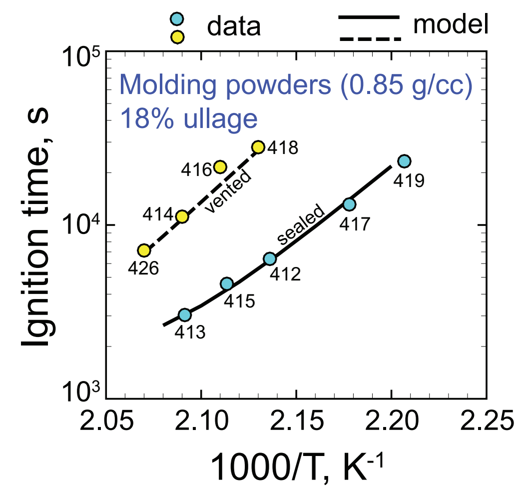
Vented



Sealed





Similar trend shown with 85% TMD SITI experiments. The binder is a major player in cookoff of PBX 9501 for some systems but not all systems.

PBX 9501 pressed pellets (95% TMD)

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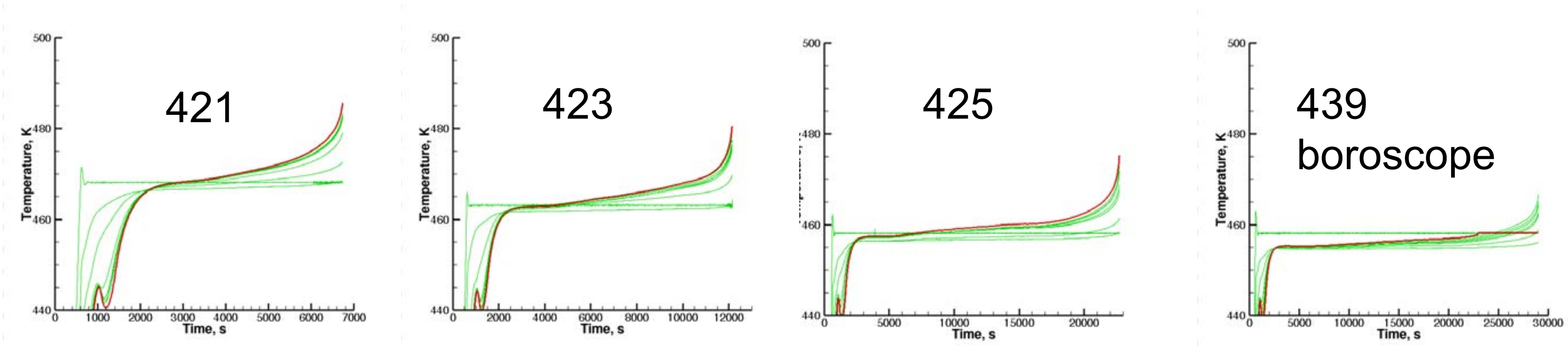
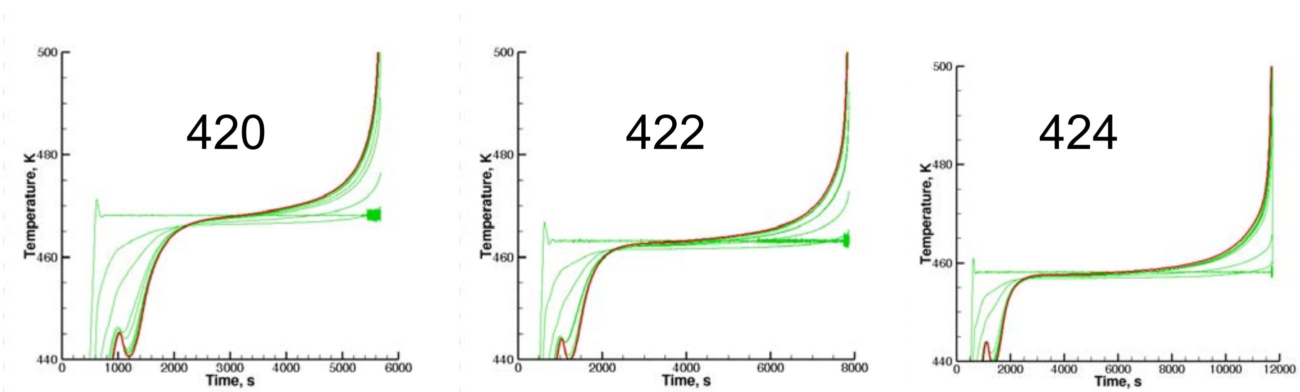
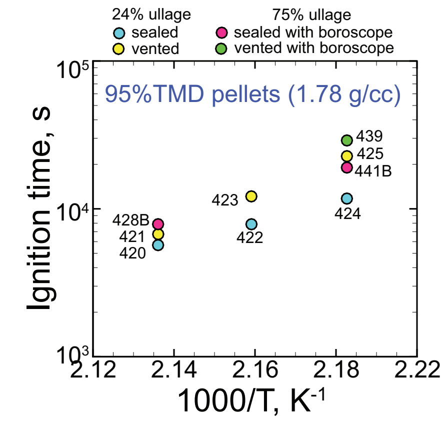
Vented



Sealed



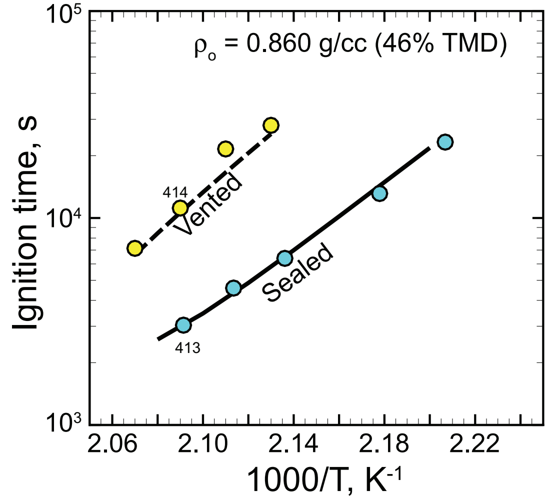


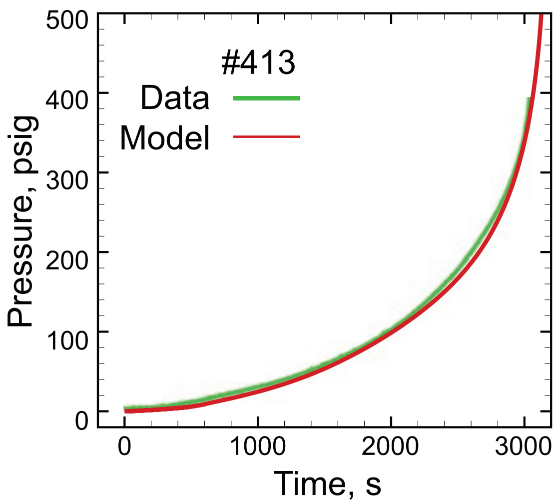
Is this evidence of binder extrusion?

SITI Predicted vs. Measured Ignition Times

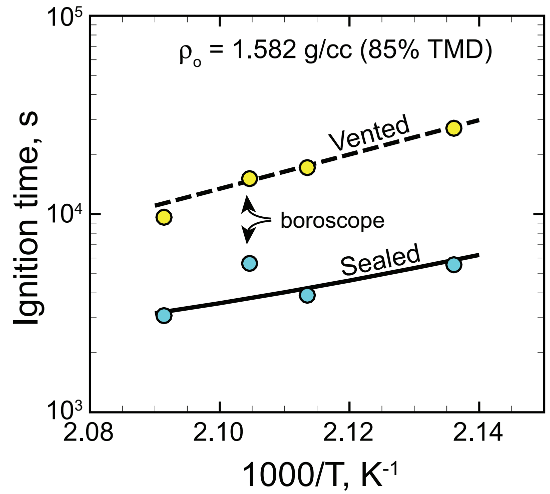
(Symbols are data and lines are model)

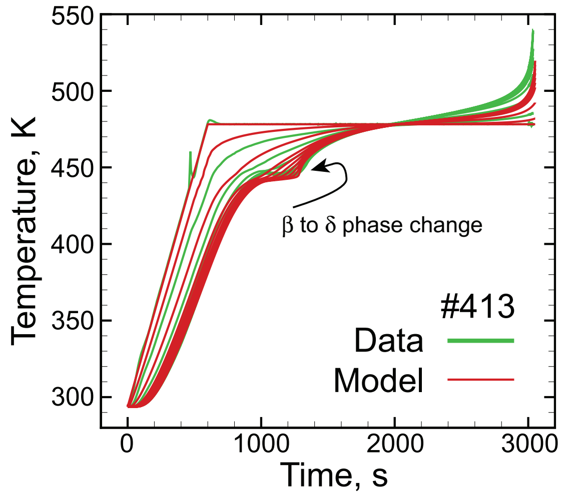
Molding powders



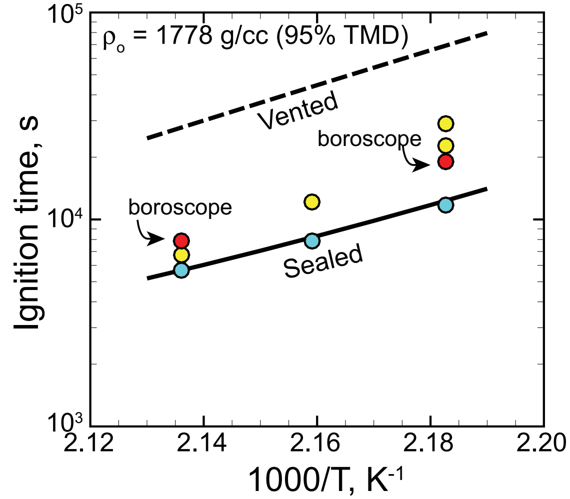


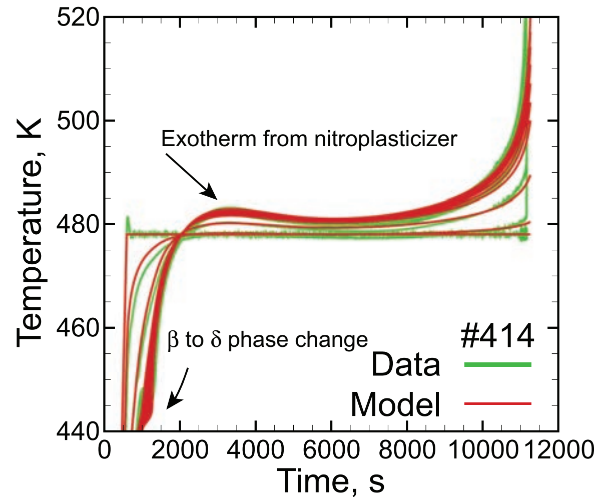
Lightly pressed





Fully pressed





Nitroplasticizer migrates to explosive exterior for high density PBX

Validation with experiments from other labs

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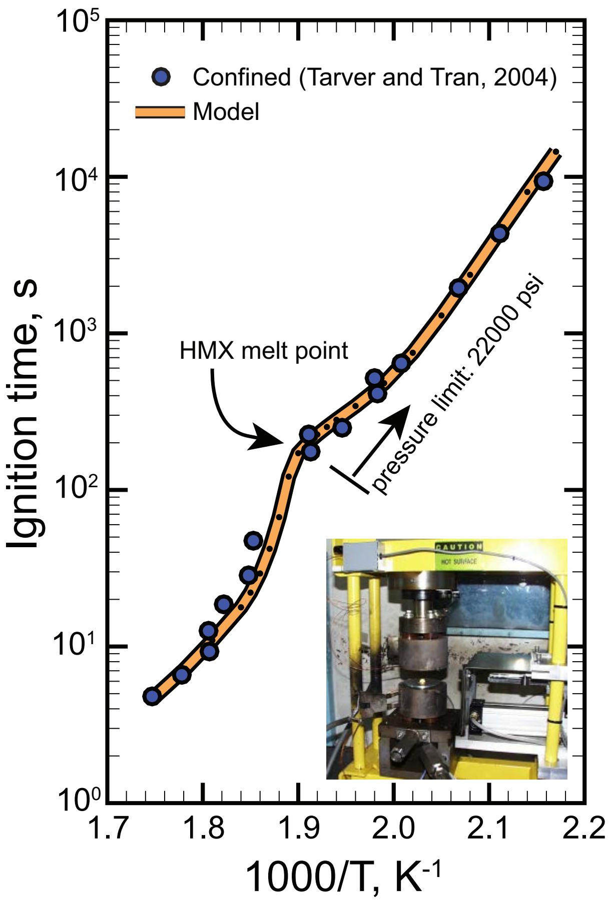
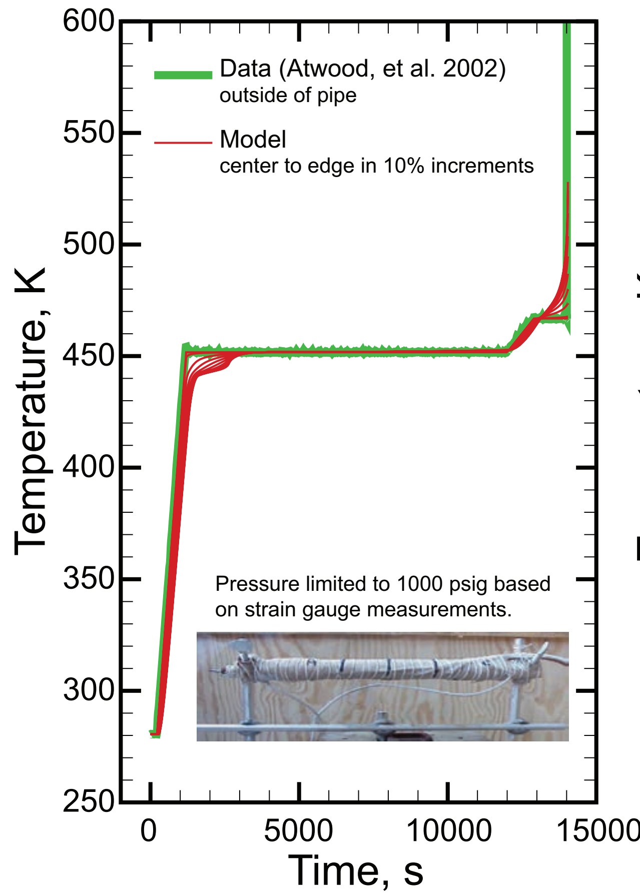
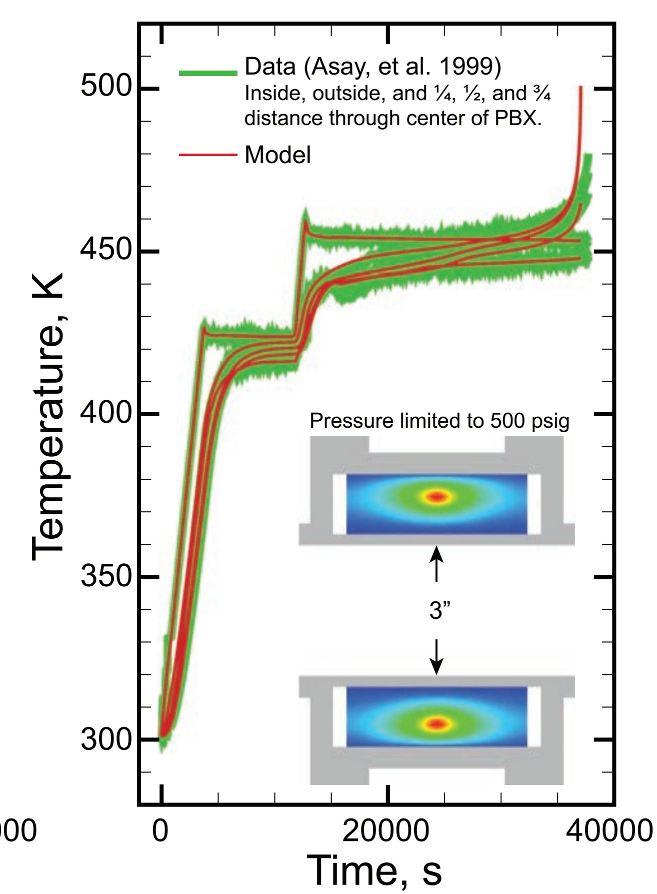
LLNL ODTX



NAWC pipe



LANL LASC



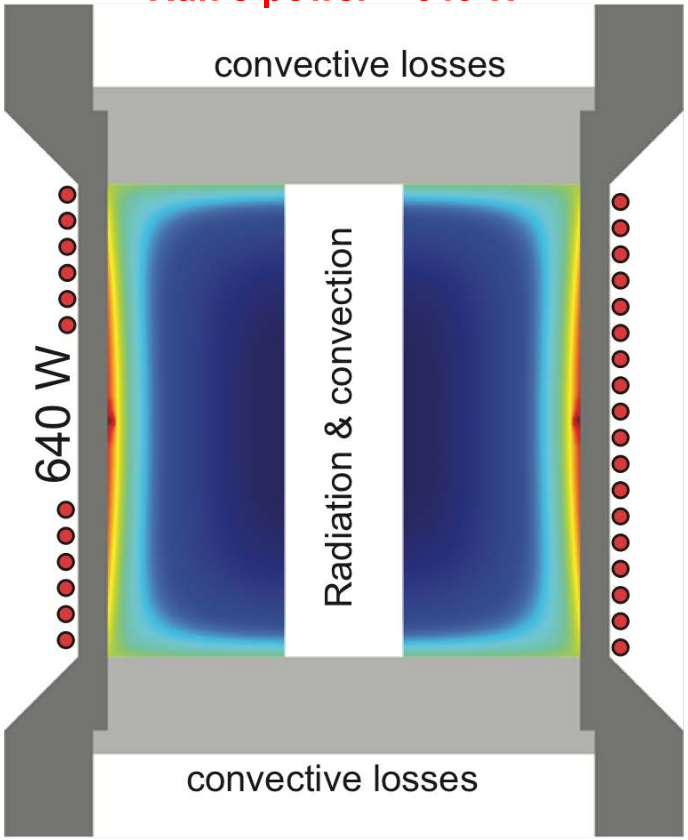
Model predicts scales from 2 g → 36 g → 2540 g. However, we need to know volumes and working pressures accurately!

Other simulations

Fast

CSAFE (1.42 kg PBX)

Run 8 power = 640 W

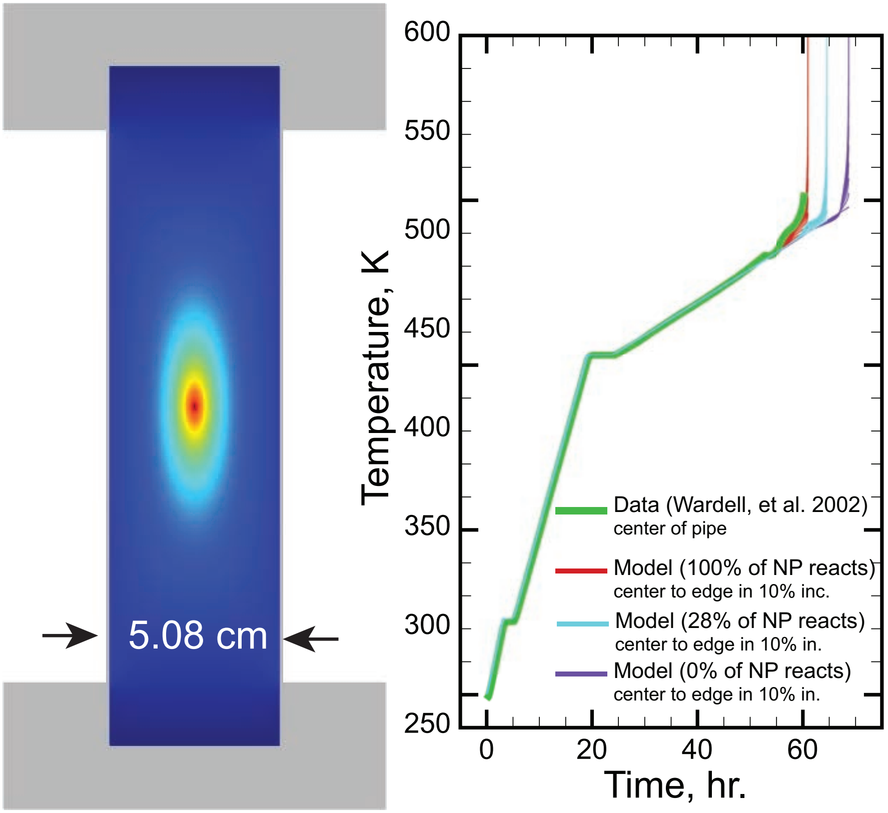


Ignition in 1545 s (model predicts 1500 s)

Slow

STEX (705 g PBX)

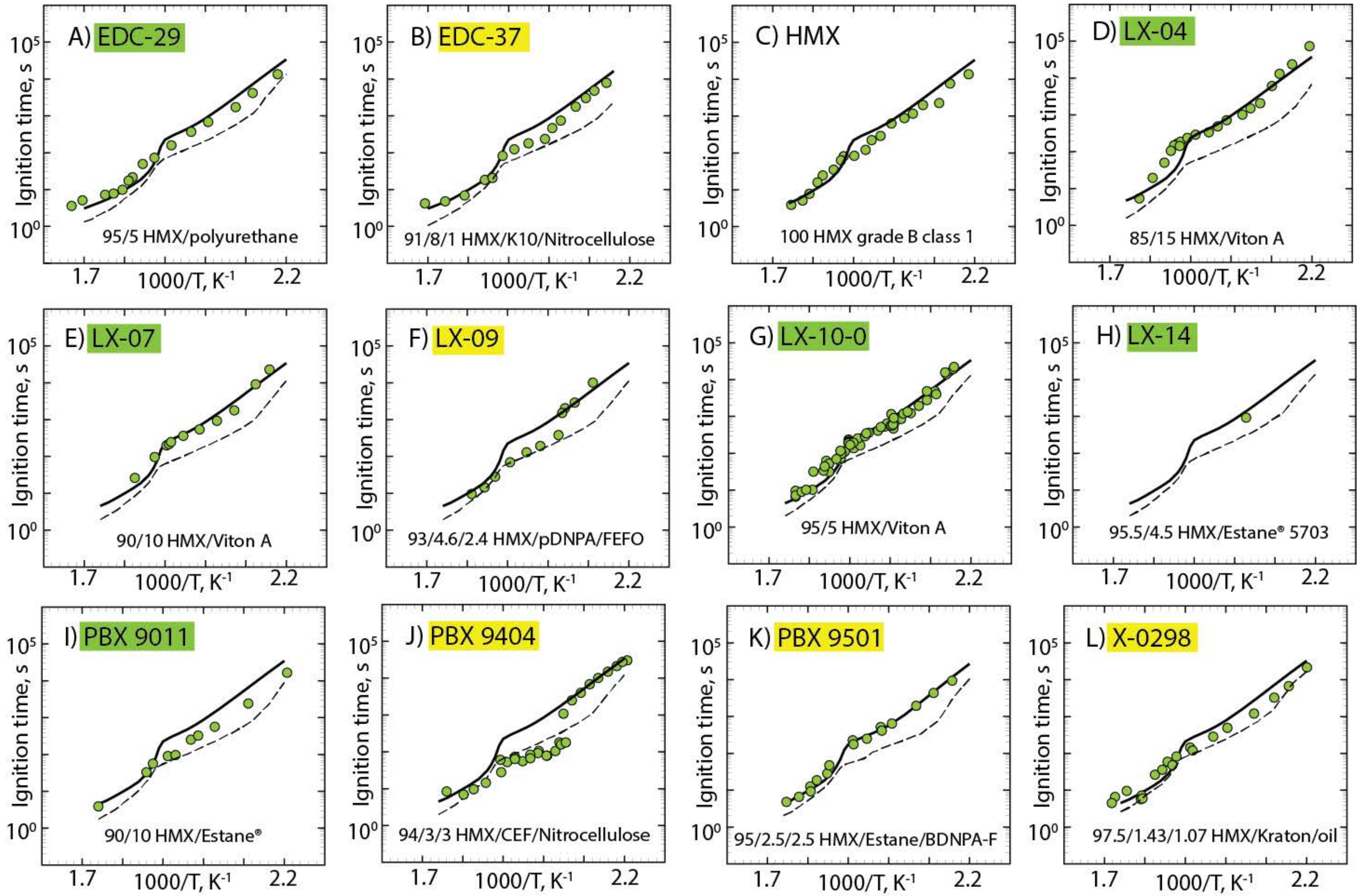
Run 27 with thin walls



Need accurate boundary conditions, ullage, vessel working pressure.

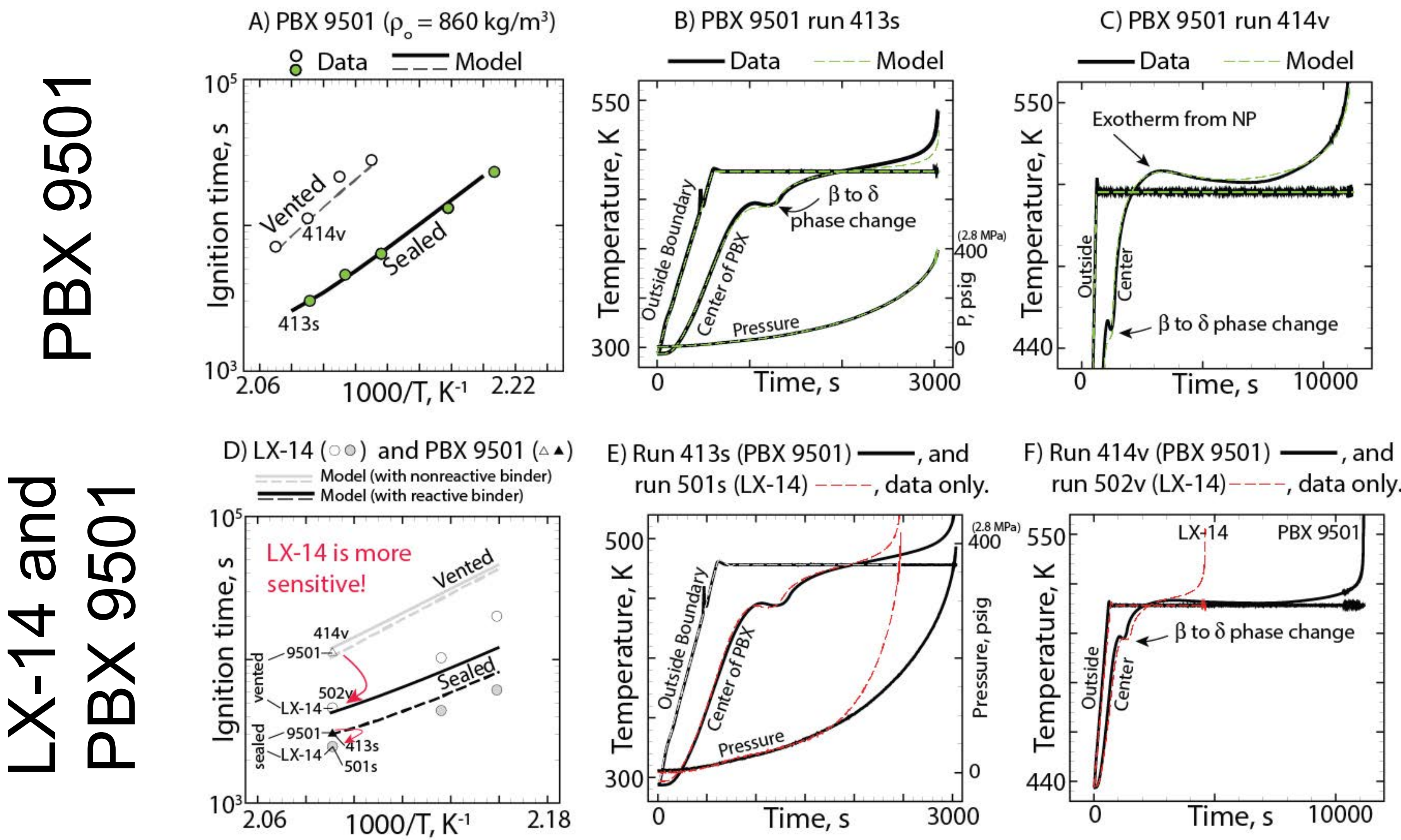
PBX 9501 model applied to explosives in ODTX

Nonreactive binder assumption works best in ODTX, possible due to extruding binders. SITI experiments should give more insight.



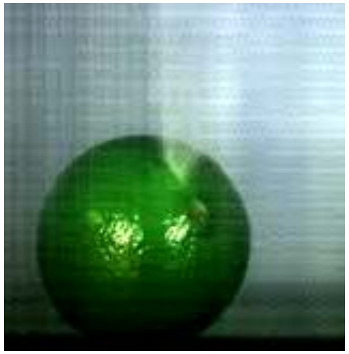
LX-14 has higher reactivity than PBX 9501

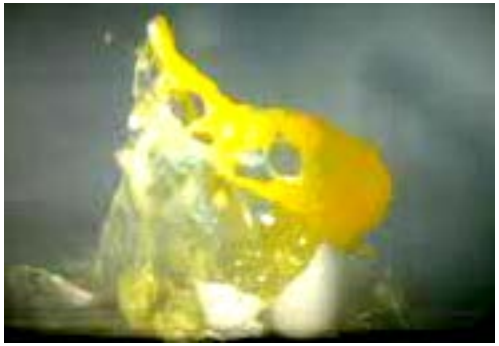
Tough urethane binder in LX-14 retains gases better than the soft binder in PBX 9501 causing increased gas phase rates that are pressure dependent.



Summary and Conclusions

- A model developed for cookoff of PBX 9501 has been applied to neat HMX and 11 PBXs containing HMX (EDC-29, EDC-37, LX-04, LX-07, LX-09, LX-10-0, LX-14, PBX 9011, PBX 9404, PBX 9501, and X-0298) by accounting for the molar volume of HMX and the reactivity of the binder.
- The model with an inert binder matched ODTX data best.
- Borescope images in SITI show that the binder extrudes to the outer explosive edge where the binder energy is quickly dissipated by the conductive Aluminum.
- We initially *suspected that PBX 9501 would be more reactive than LX-14* due to the energetic binder. *Our experiments show the opposite trend*. We believe the brittle polyurethane binder in LX-14 retains reactive gases better than the softer binder in PBX 9501 resulting in faster ignition times.
- Binder mechanics may be more important than thermicity of the binder.



Internal gas generation in closed pore system leads to failure.