Exceptional service in the national interest

SAND2016-2872PE

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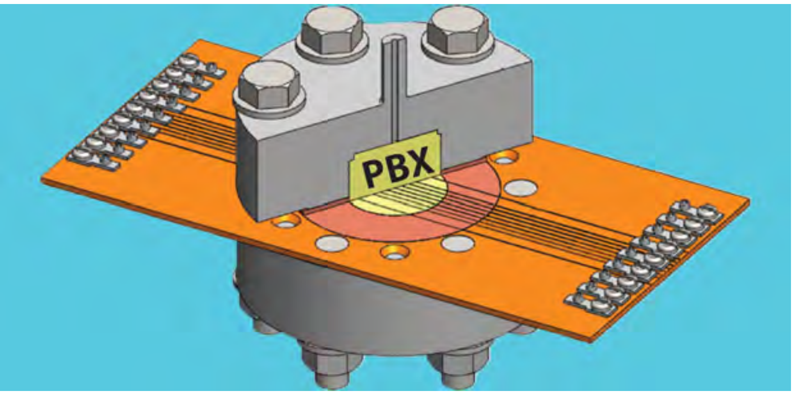
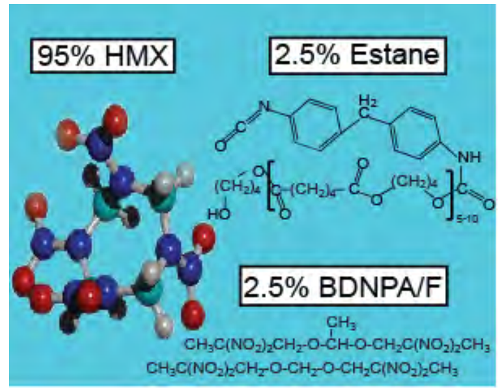
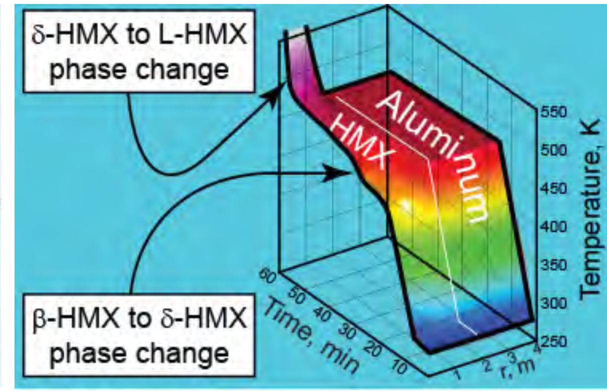
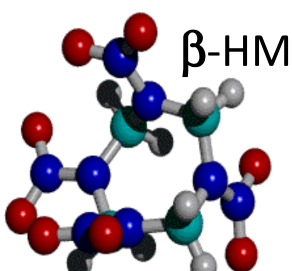




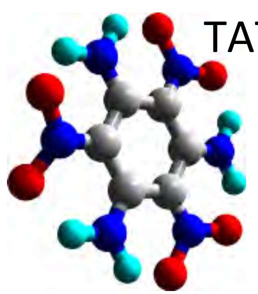


Modeling Ignition and Failure of Explosives

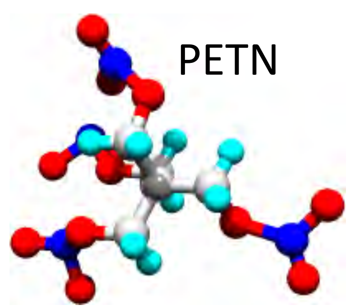
Michael L. Hobbs



β-HMX

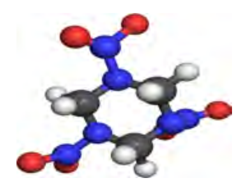


TATB

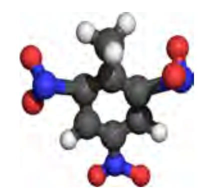


PETN

RDX



TNT



U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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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!

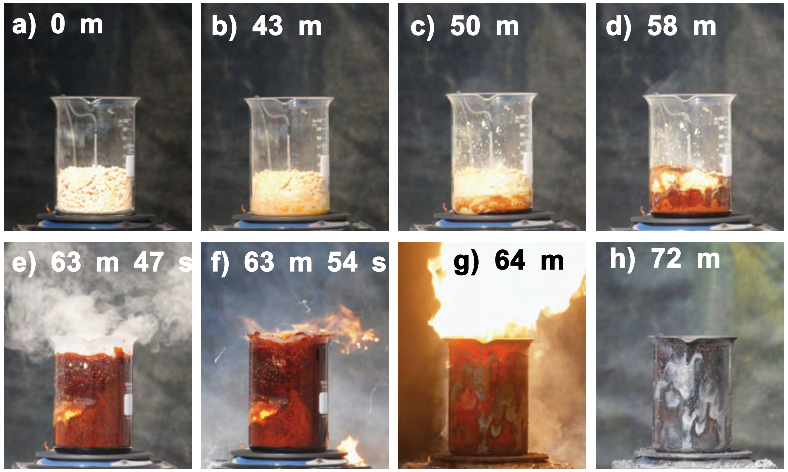
What does PBX 9501 and PBX 9502 look like?
(There are no dyes in these explosives.)

Pressed PBX 9501

99.7% TMD, 1.84 g/cc, φ= 1.3%

PETN

Comp-B3 (60% RDX, 40% TNT)



PBX 9502

Pressed

98.2% TMD, 1.906 g/cc, φ = 1.8%

PBX 9502

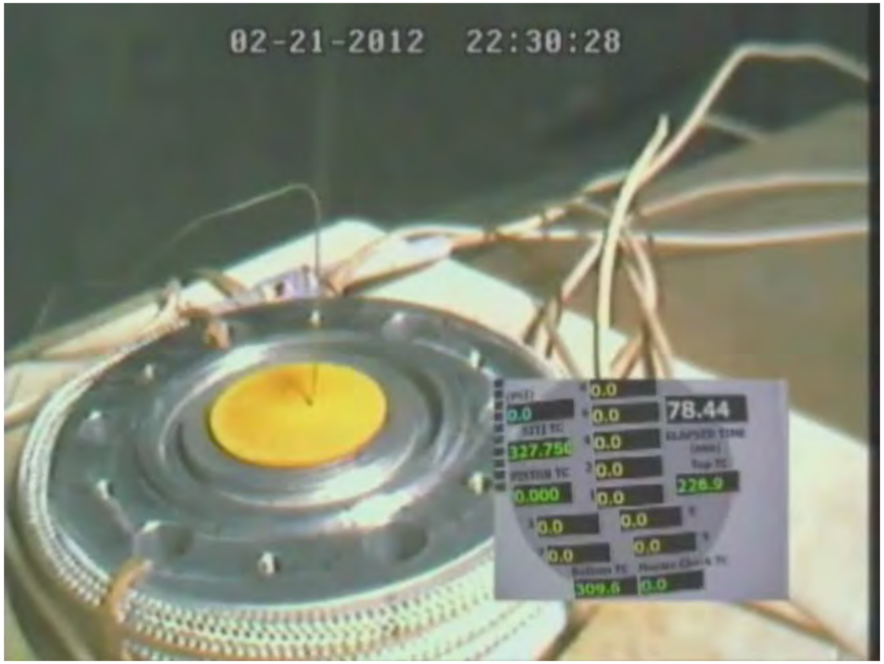
Molding powder

38.6% TMD, 0.749 g/cc, φ = 61.4%

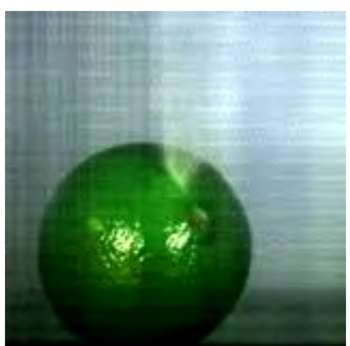
Degraded PBX 9502

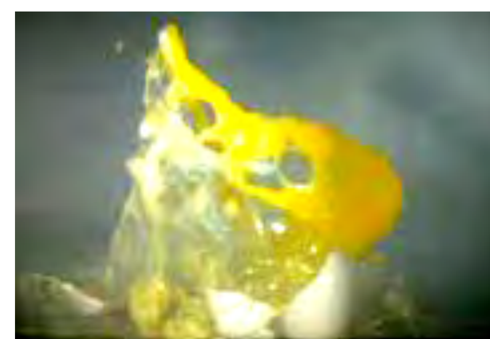
If porosity is less than about 5%, the pores are not connected.

Burning PBX 9502



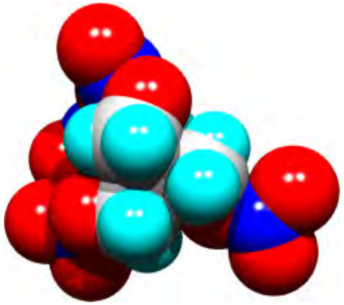
Internal gas generation in closed pore system leads to failure.





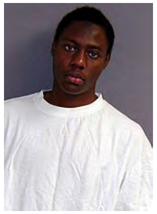
What causes inoperability?

- 50 g PETN gained notoriety for the shoe bomber Richard Reed (2002)



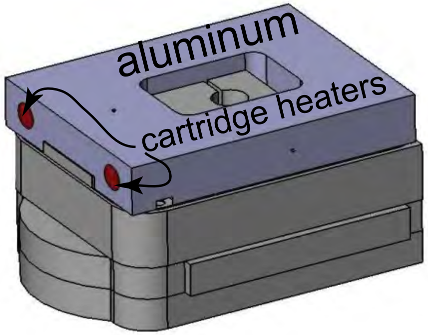
Detonater was likely, triacetonetriperoxide (TATP) or the “mother of Satan”

- **80 g PETN gained notoriety for the underwear bomber Umar Abdulmutallab (2009**



YouTube video of 20 g of PETN cutting down tree

today's discussion:



Mechanism for Decomposition

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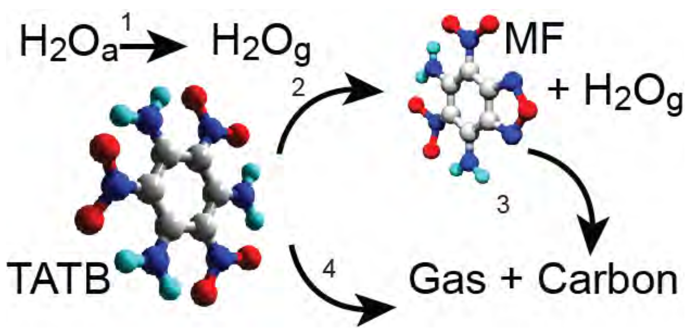
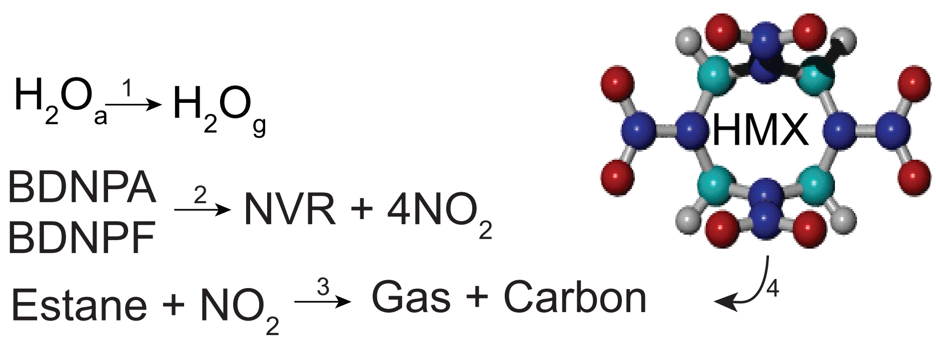
PBX 9502 (95% TATB 5% Kel-F)



Hobbs ML and Kaneshige MJ, *J. Chem. Phy.* **140**, 124204 (2014).

PBX 9501 (95% HMX 2.5% Estane 2.5% BDNPAF)



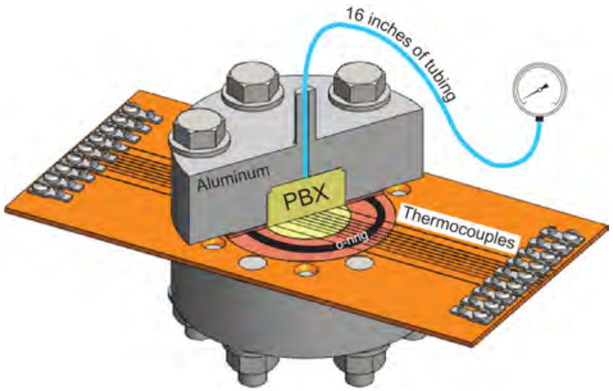
Highlights

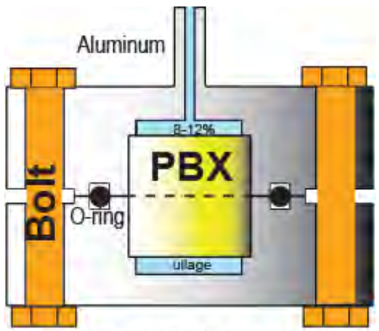
- Reactions occur in gas, solid, and molten phases and depend on physical and morphological changes in the PBX.
- Phase transitions create grain structure and promote cracking and nucleation sites.
- Nucleation sites fill with decomposition gases and NVR.
- Controlling mechanisms include unimolecular decomposition and gas phase reactions occurring within a closed pore network.

Binder: 9502 (Kel-F is assumed inert) 9501 (BDNPAF is a major reactant)

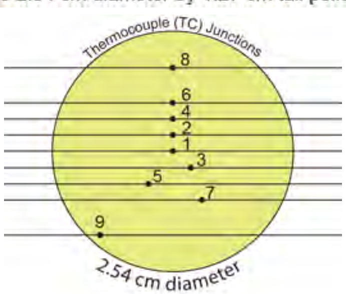
Sandia's Instrumented Thermal Ignition (SITI)

Sandia National Laboratories

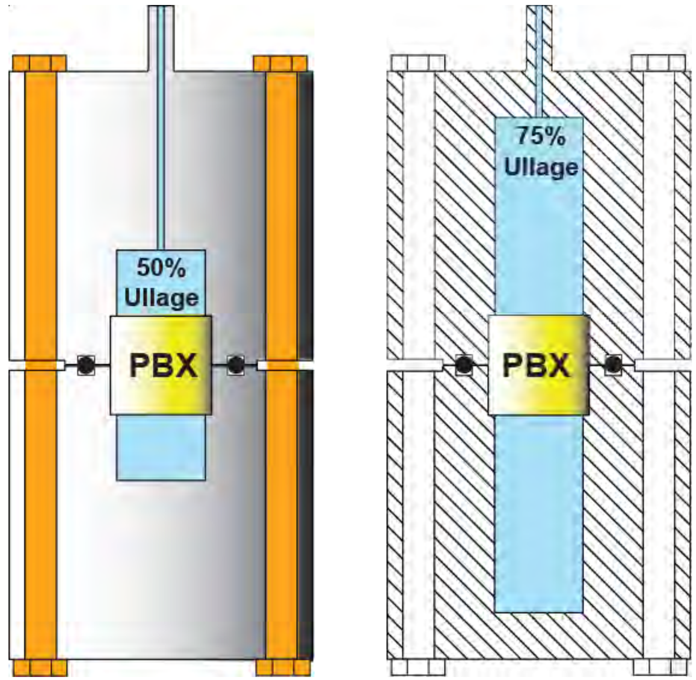




two 2.54 cm diameter by 1.27 cm tall pellets



Large ullage SITI



SITI:

ρ = 1.84 g/cc

453 K ≤ T_{sp} ≤ 473 K

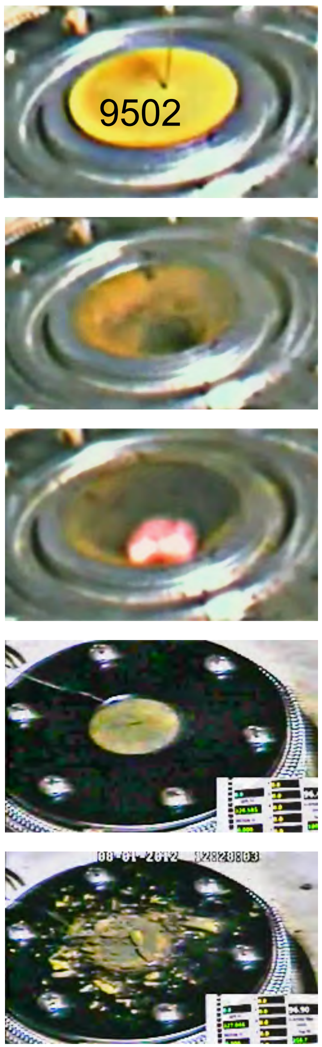
28 sealed, 1 vented

8, 12, 18% ullage (excess gas volume)

Measures: Ignition time, temperature, pressure

Damage example

onset
crater
burn
washer
spall



Incremental bursts heard as audible noises (pop, thud, etc.)

"Couple of popping noises in the video, but no visible smoke." (lab notes)

My Favorite SITI Experiment (#277 9502)

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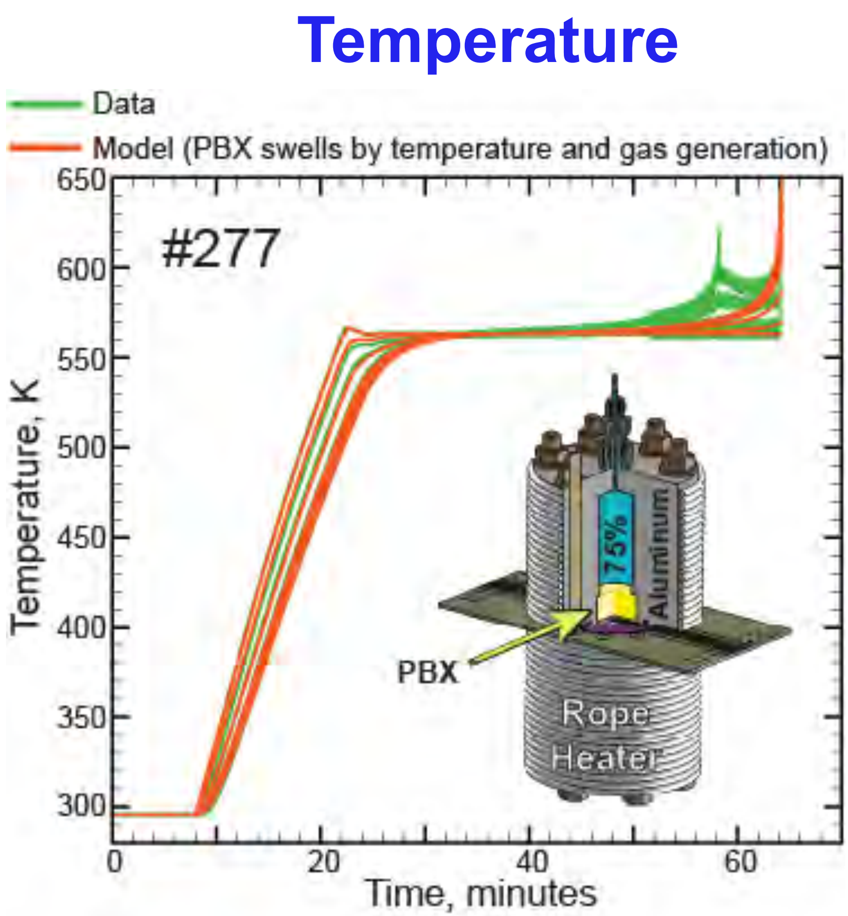
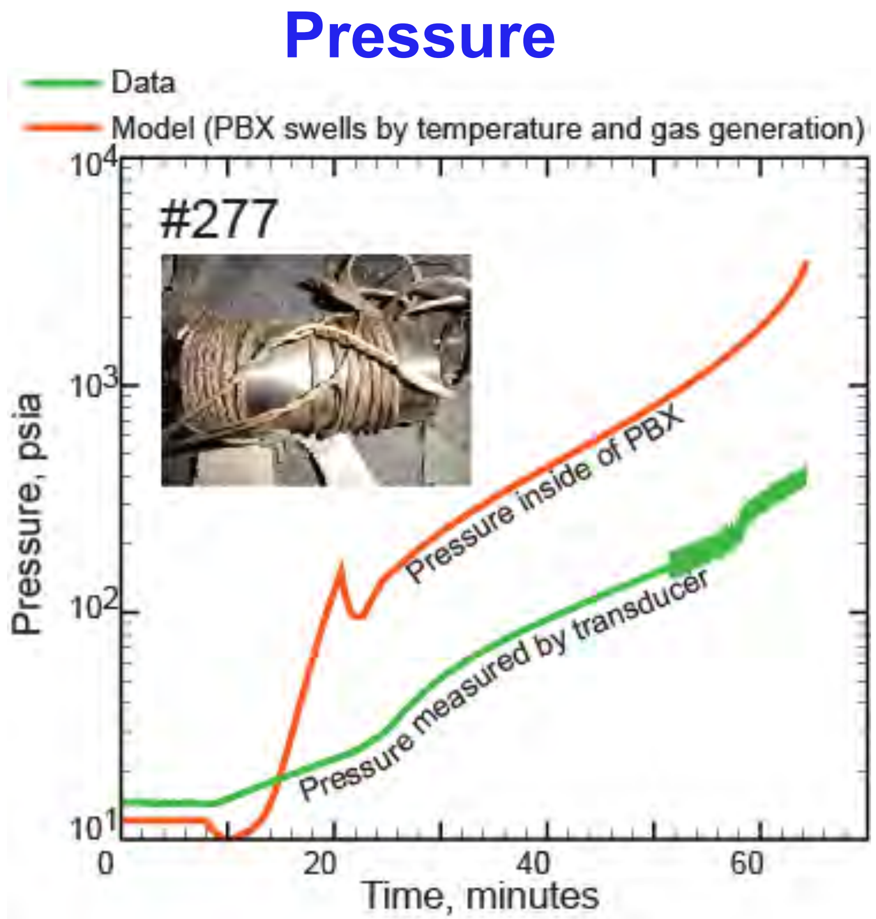
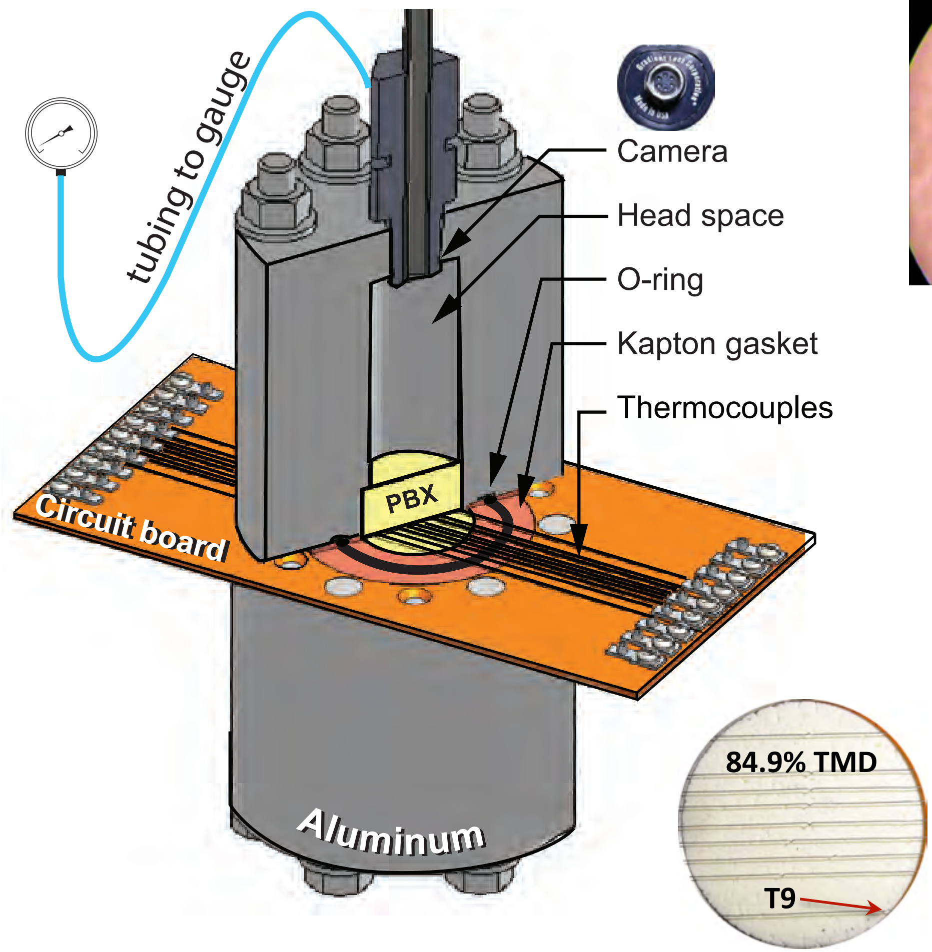




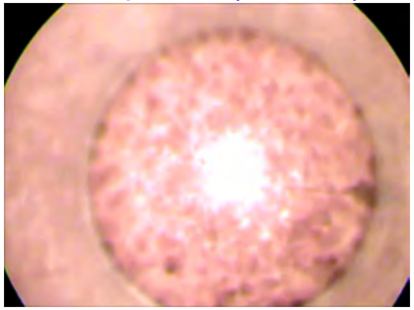
Hobbs ML and Kaneshige MJ, "Ignition experiments and models of a plastic bonded explosive (PBX 9502)," *J. Chem. Phys.*, **140**, 124203 (2014).

Anomalies may not be anomalies.

Boroscope in SITI with PBX 9501

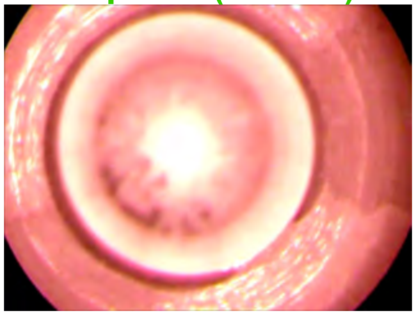


Exp 445 (sealed)

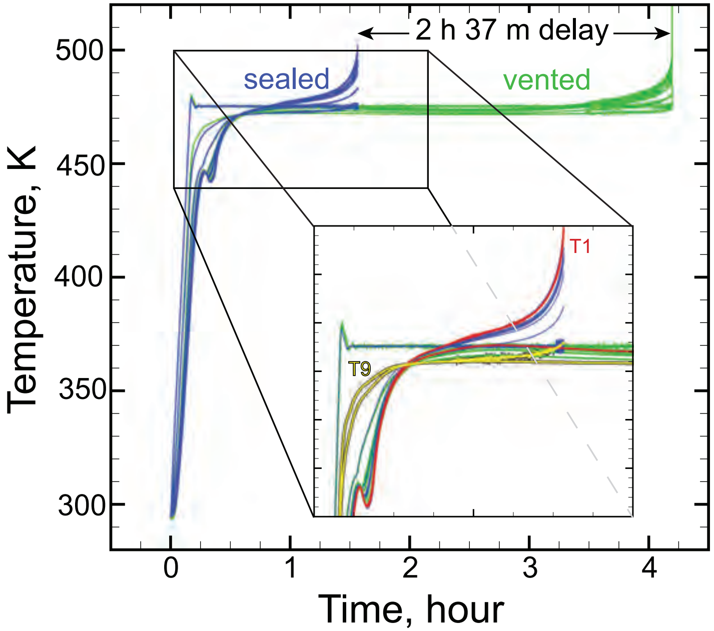


Minimal binder flow

Exp 444 (vented)

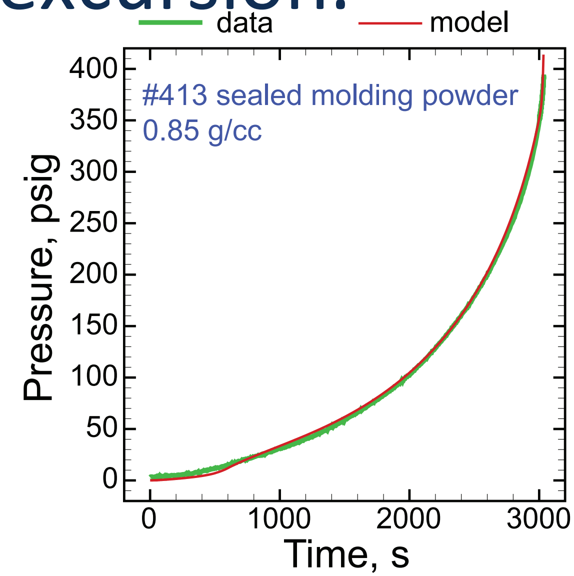


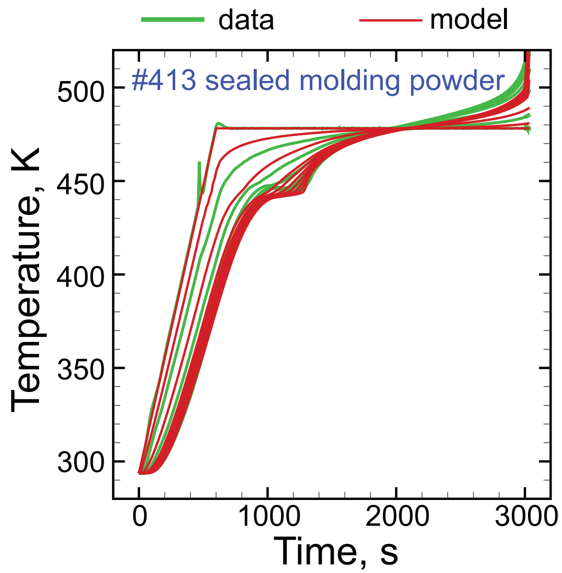
Binder flows to edges

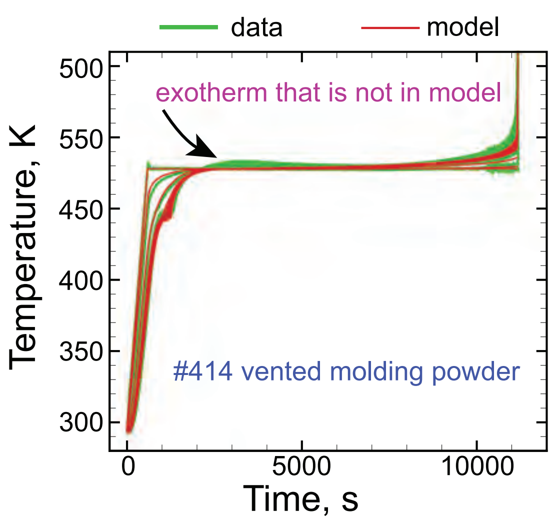


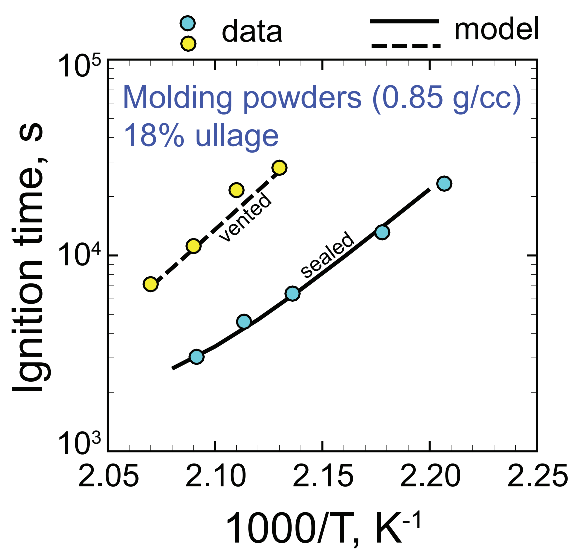
For unconfined decomposition, binder migrates to the edge. A wetted surface provides better heat transfer for the vented case.

Mechanism from 15th Det. Symp does not match excursion.







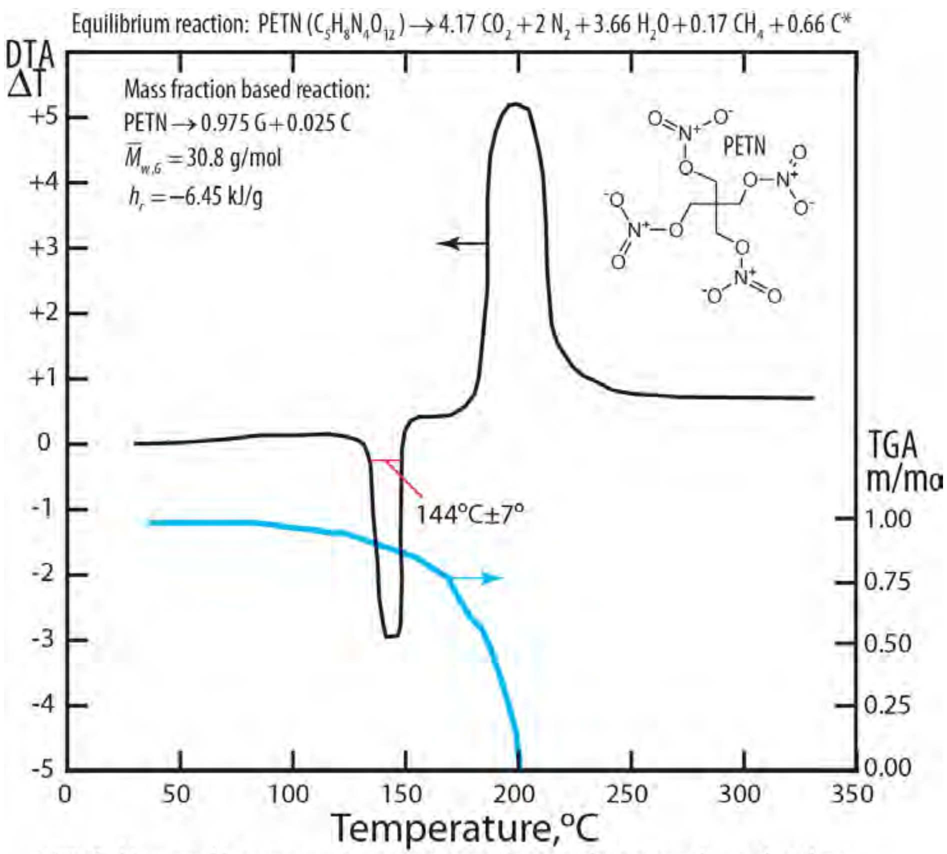


Observations

- Distributed activation energy model can be used to match curvature in pressure.
- Steric factor can be used to match slope of ignition curve.
- Poor agreement with T9 for sealed SITI may be due to contact resistance.
- Better agreement with T9 for vented SITI may be related to binder extruding preferentially along Al/EM interface causing better contact at this surface.
- Temperature excursion may be caused by a limiting reactant such as the binder.

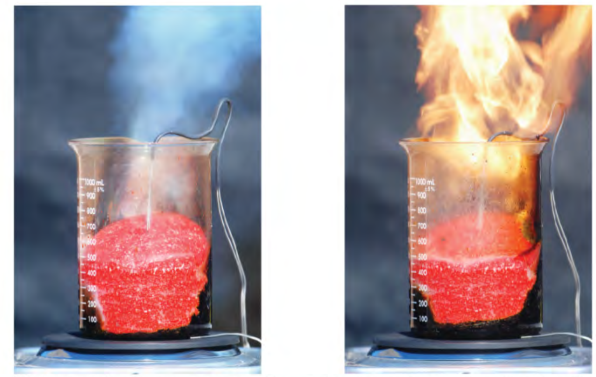
PETN inoperability

(Some observations)



*G, C, $M_{w,G}$, and h_r represent gaseous reaction products, condensed carbon, average gas product molecular weight, and reaction enthalpy, respectively.

A) Semtex 1A (87% PETN with dye, antioxidant, plasticizer, and binder)



Does not slump as melting occurs, gases ignite in air.

B) Semtex 10 (82% PETN with dye, antioxidant, plasticizer, and binder)

Decomposes and ignites before melting completes.

Violence increase with fast rates and confinement.

Violence prediction is of interest

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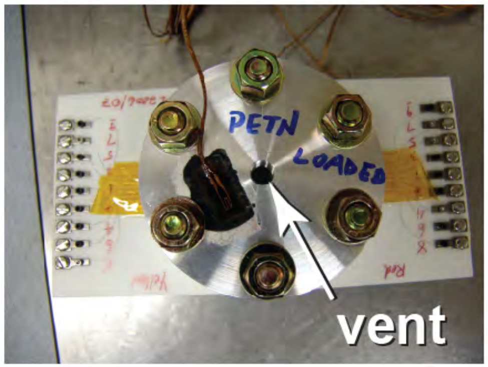
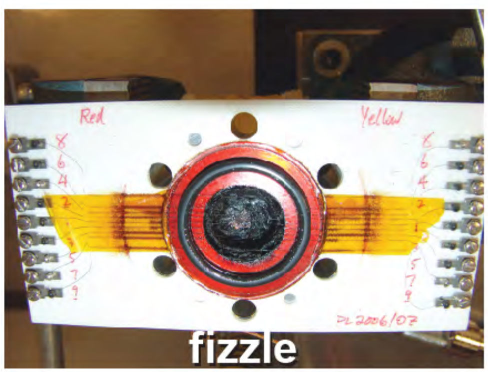
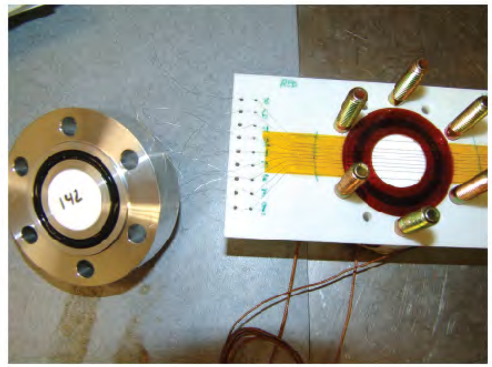
Run #102
(unconfined powder)

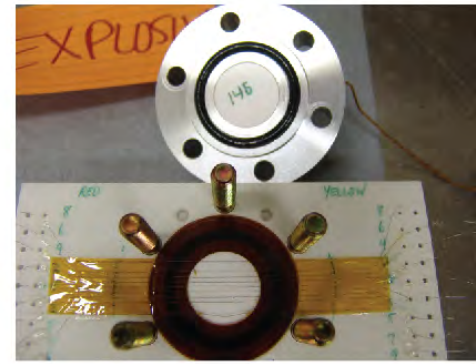




Run #103
(confined pressed solid)

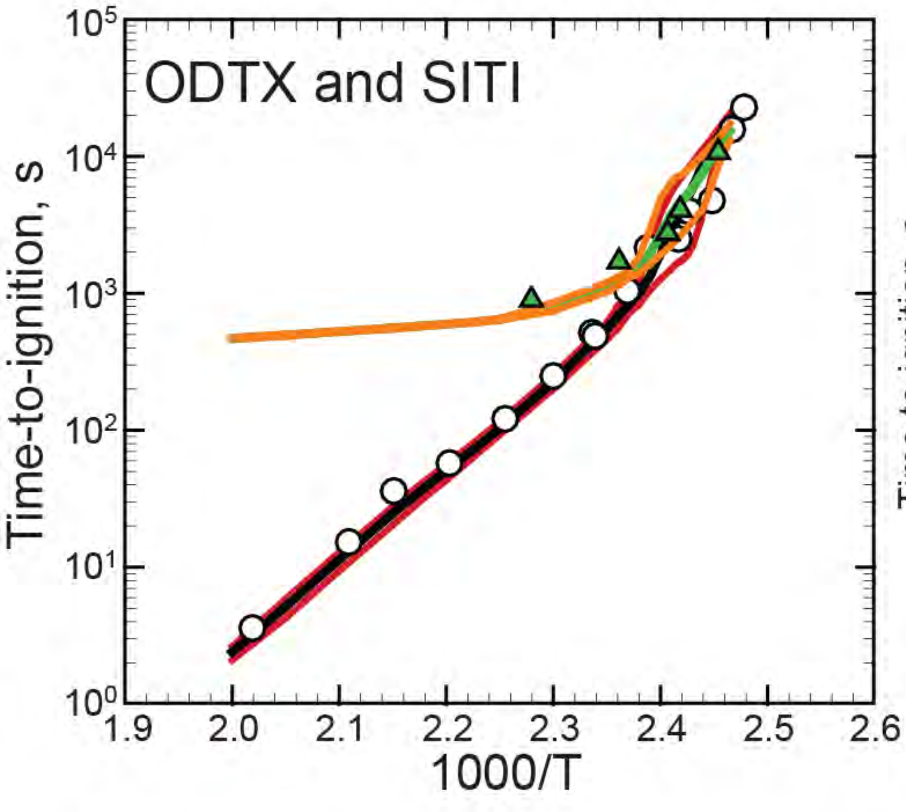


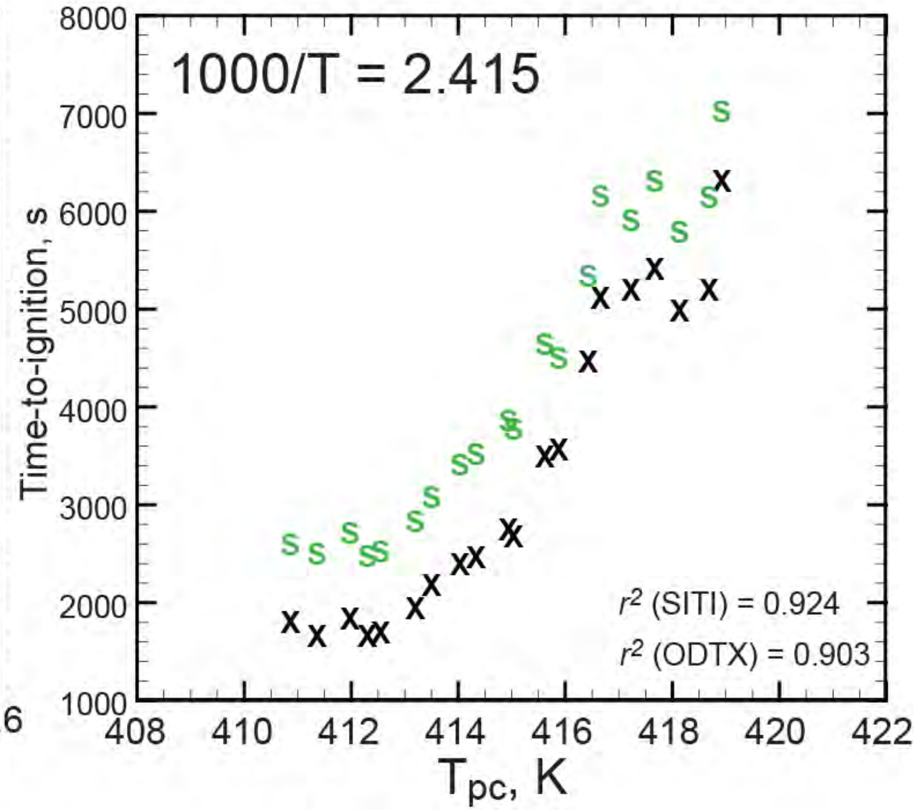
Run #105
(confined pressed solid)



Does it go pop, bang, or kablooey?

Model predicts ignition time





Uncertainty calculated with 20 LHS samples

Model predicts temperatures/pressures

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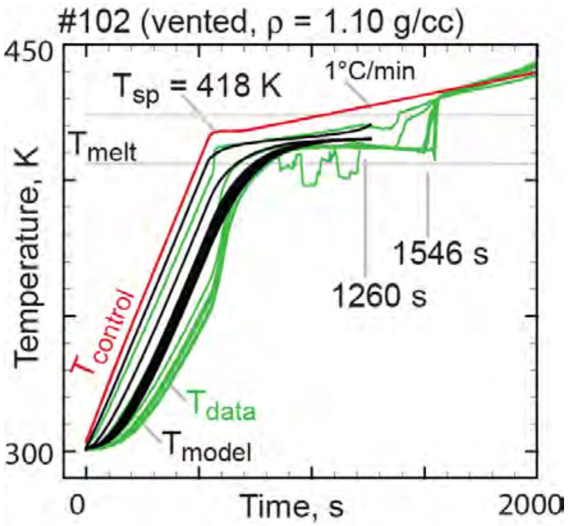
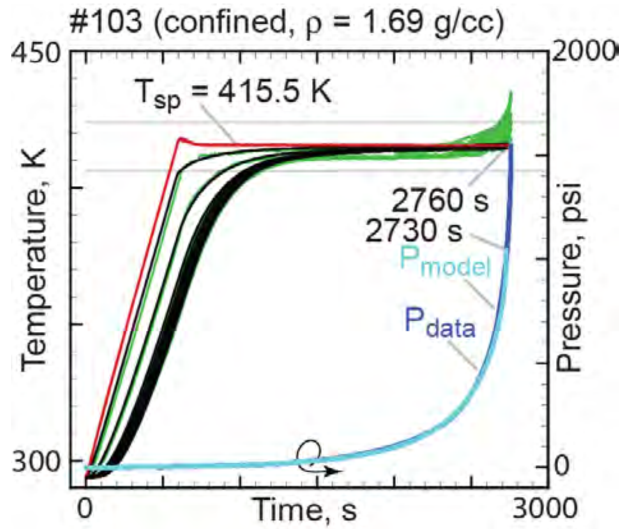
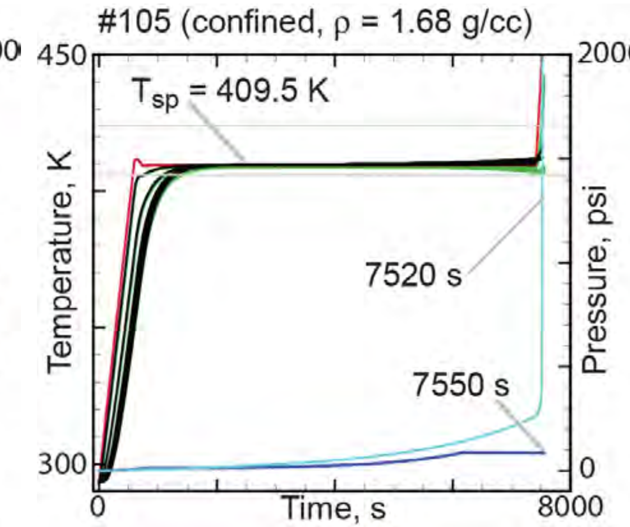
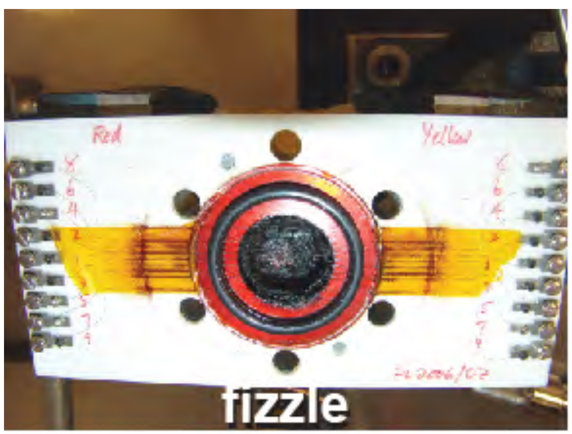






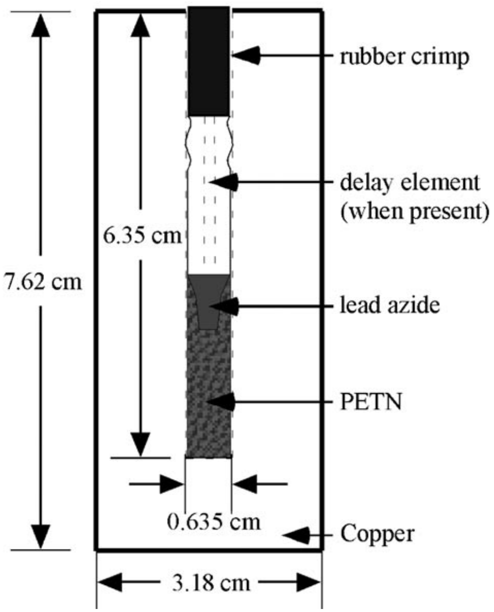


Model does not calculate violence

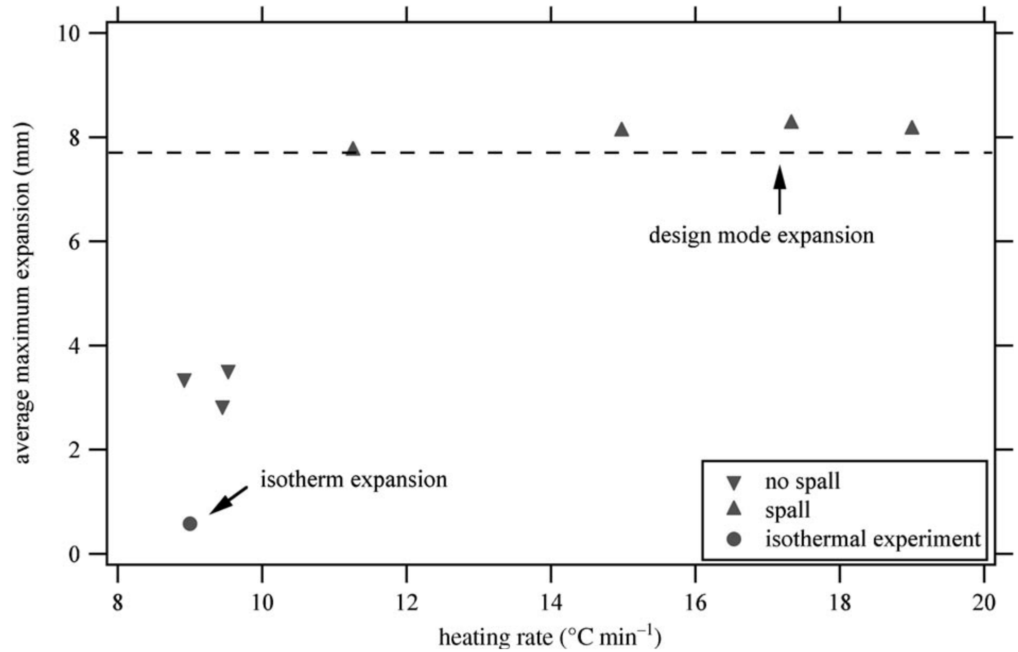
Does ignition guarantee failure?

Not always, here's an example of failure for fast cookoff!

Cookoff of detonator



Expansion of copper



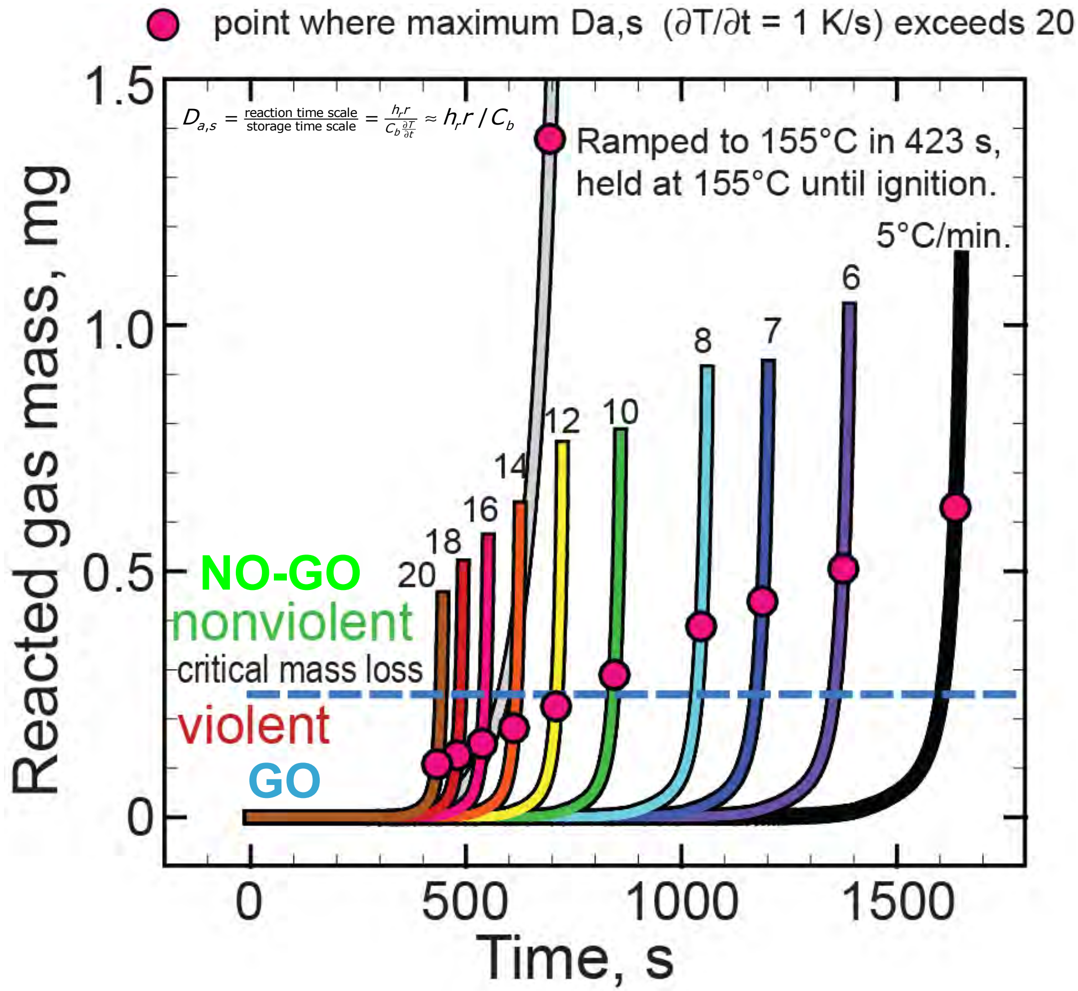
*J.M. Zucker, P. Dickson, V.E. Sanders, *Propellants Explos. Pyrotech.*, **34**, 142 (2009).

†Without PbN_3, all tests would be duds, supporting violence correlation with extent of reaction.

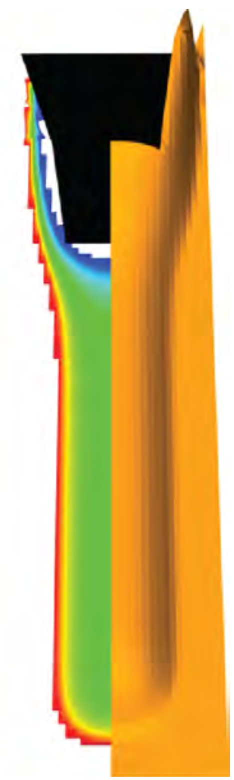
Hypothesis: Violence can be correlated to conditions at the onset of ignition, whether initiated by cookoff or intentionally.

Failure correlates with extent of reaction

20°C/min
GO

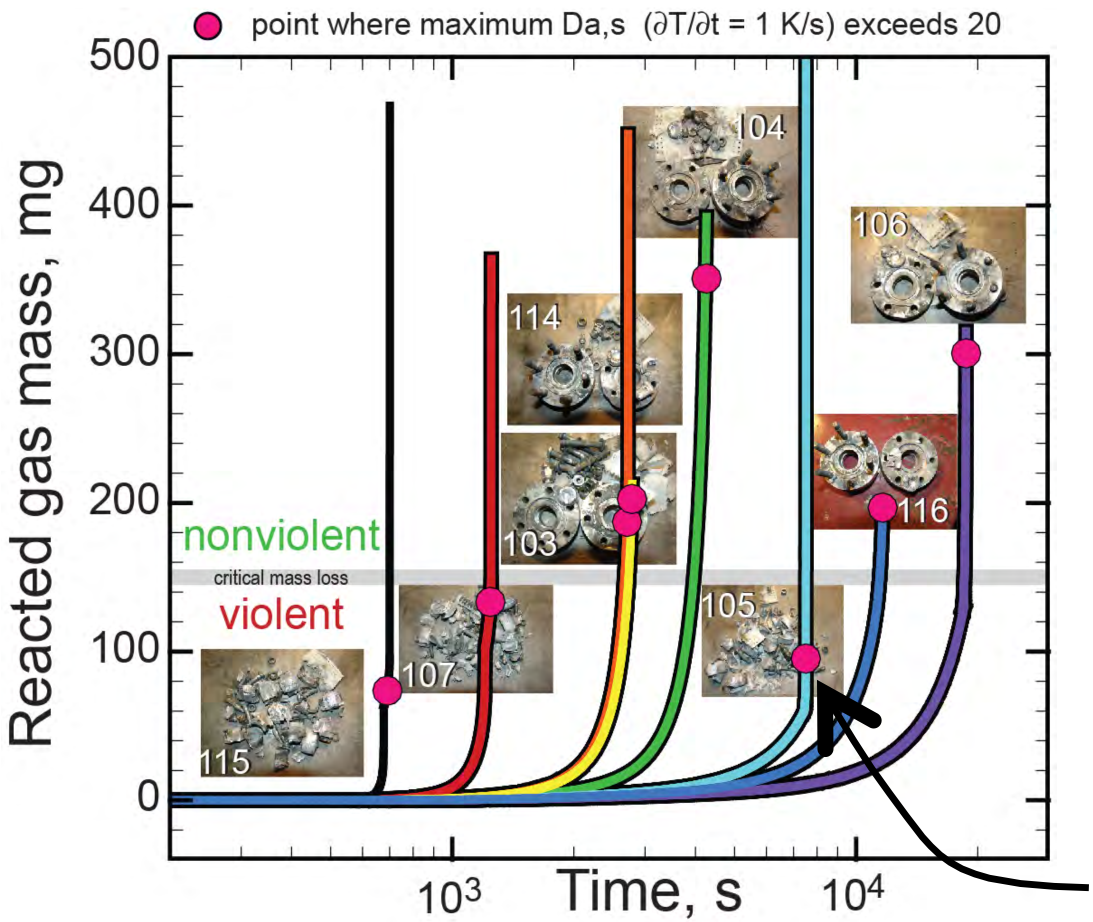


Ramped to 155°C
NO-GO



What about failure of firing set initiated intentionally after some thermal damage rather than via cookoff?

SITI cookoff violence correlates with extent of reaction



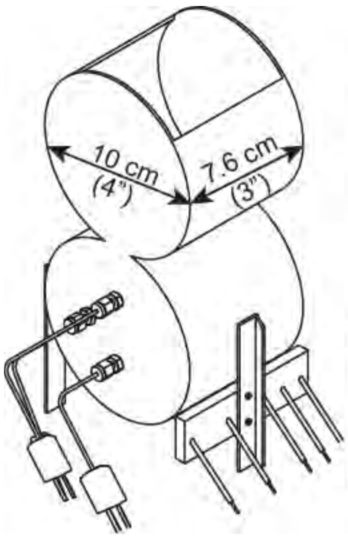
T_{sp} = 413.5 K (self ignited after 1 h 12 s)

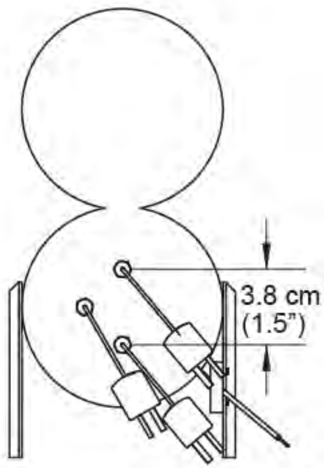
T_{sp} = 409.5 K (intentionally ignited after 2 h)

What about failure of a reactive firing set that is initiated intentionally after some thermal damage rather than via cookoff?

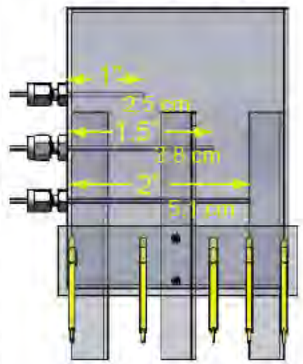
Cookoff of a melt-castable explosive

Oven test (a.k.a snowman)

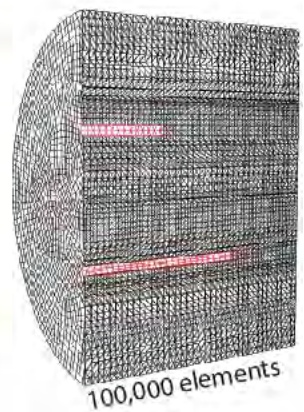


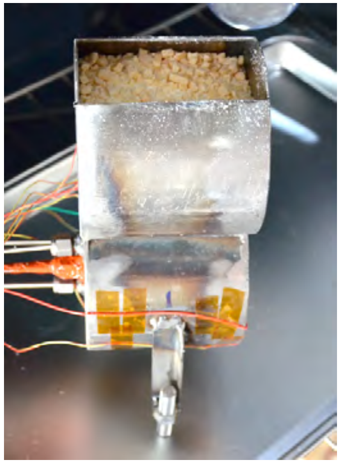


Lower cylinder fills with liquid



Mesh





45 minutes

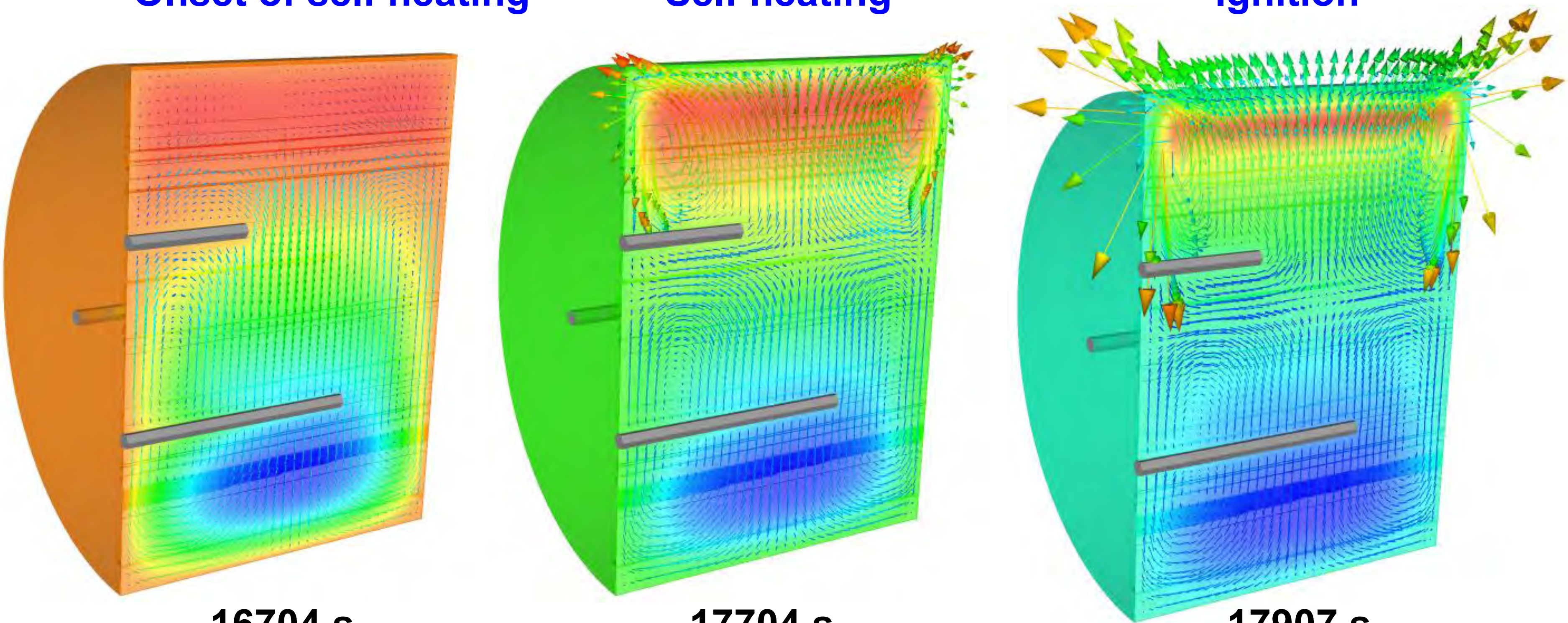
135 minutes

270 minutes

Post test oven

3D Modeling of Snowman Test #3

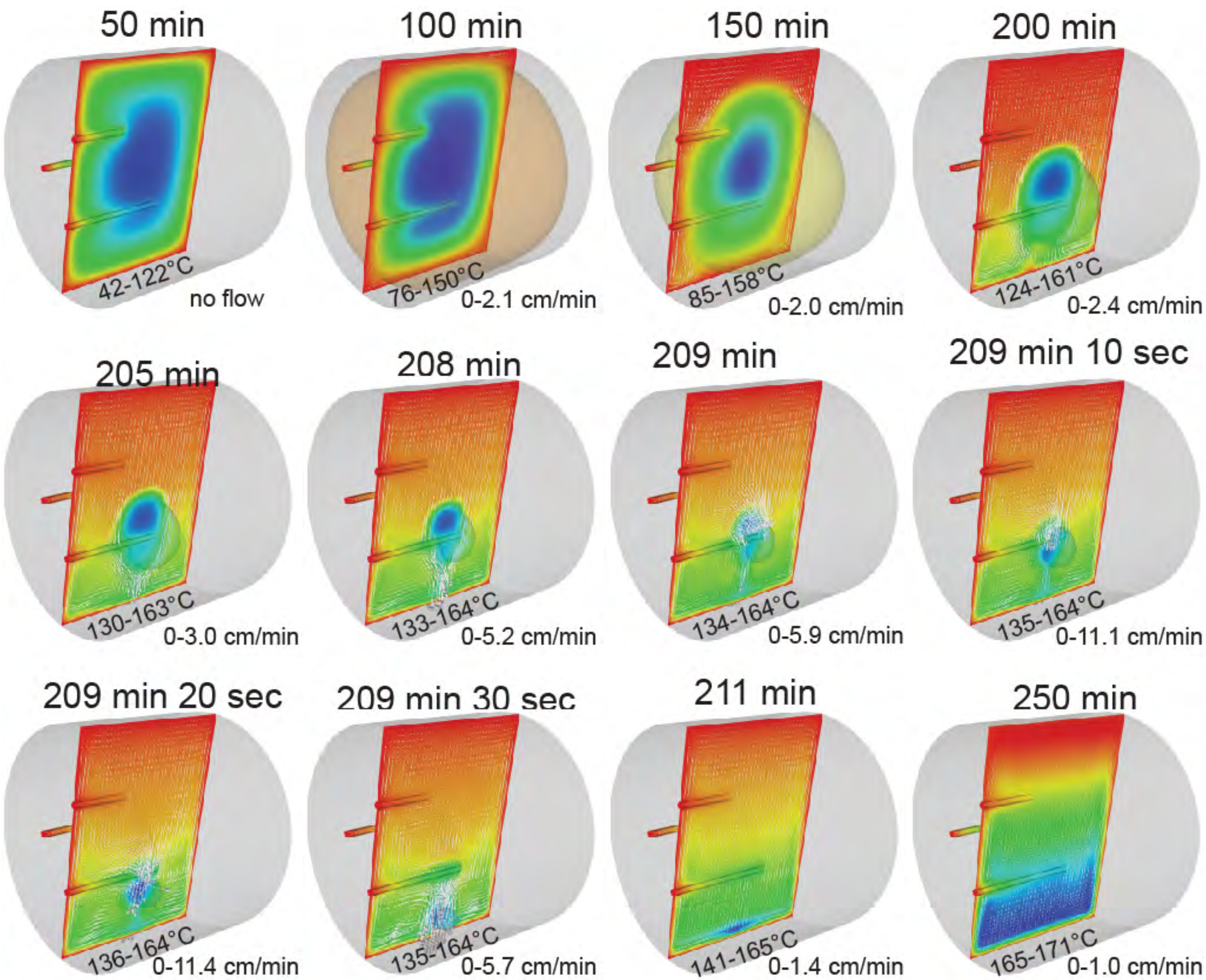
Onset of self heating | **Self heating** | **Ignition**



16704 s | **17704 s** | **17907 s**

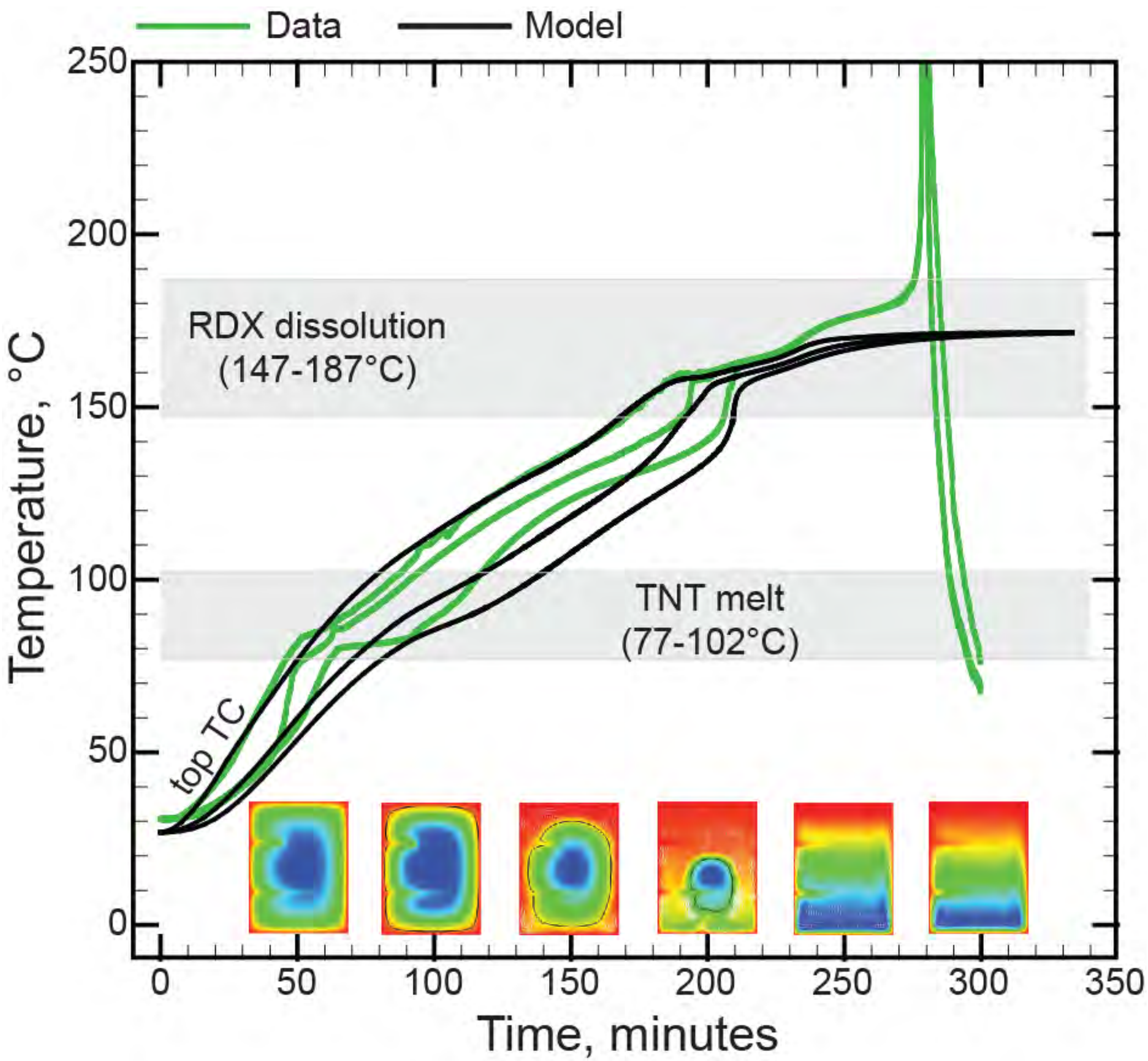
Slice through center of 3D simulation

Oven test results



- Melts from outside to the inside.
- Solid plug gets smaller and starts to fall toward the bottom of the can.
- Liquid heats up and eventually self-heats and ignites at the top of the can.

Oven test results



- Temperature pinch occurs in middle of RDX dissolution range.
- Model predicts slightly longer ignition times.
- Discrepancy in ignition time could be related to the method of melting the Comp-B flakes.
- In the experiment, the flakes were melted in the combined system.

Summary and Conclusions

- Models used for safety assessments to predict ignition time, ignition location, and pressurization, but typically not component failure.
- Models can correlate material state at ignition to device failure.
- Reaction extent correlates commercial detonators, but alone, does not correlate failure of our reactive firing sets.
- Failure of our firing sets correlates with the extent of reaction multiplied by an activation temperature.
- For high density pressed PBX, the decomposition gases are retained within the explosive. Periodically the high pressure gases vent from the PBX by cracking, spalling, or some other damage mechanism. The release of the trapped gases is associated with temperature excursions and acoustic noise.
- Modeling cookoff of melt-castable explosives is complicated.