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SAND2019-3766C

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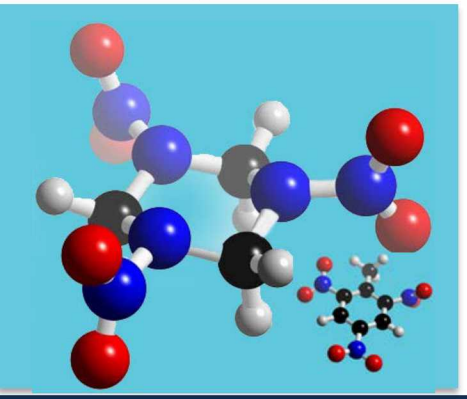
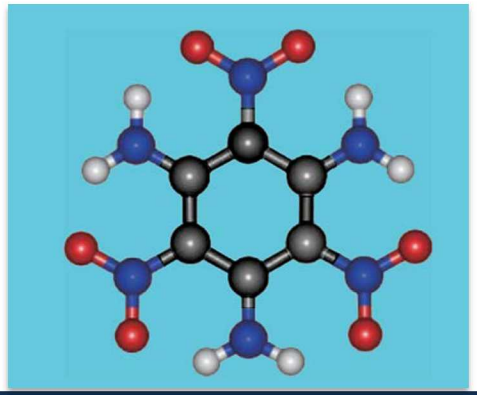
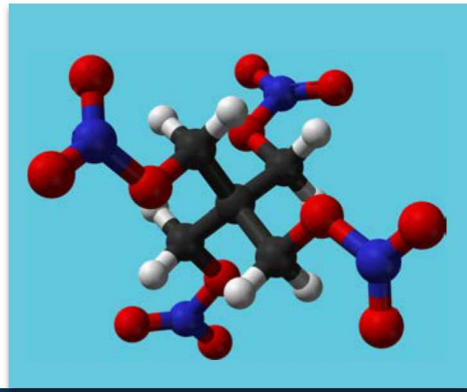
RDX (Comp-B) TATB (PBX 9502) HMX (PBX 9501) PETN







The reaction mechanism is assumed to be universal with rates specific for each explosive.

A "UNIVERSAL" Cookoff Model for Explosives

134 deaths

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Is a "UNIVERSAL" cookoff model (UCM) feasible?

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- Model similarities are amenable to a universal model.
- Model based on the conductive energy equation with a volumetric energy source for decomposition chemistry.
- Model uses material specific properties (k_T, C_p, T_{mp}, H_{lat}, etc.)
- Model uses a "UNIVERSAL" mechanism with rates determined by the Sandia Instrumented Thermal Ignition experiment
- Model predicts spatial temperatures, pressurization rates, and ignition time.
- Model utility is demonstrated by applying the model to four diverse explosives that contain RDX (Comp-B), HMX (PBX 9501), TATB (PBX 9502), and PETN.

UCM simplifies cookoff modeling and scales!

UCM demonstrated with 4 diverse EMs

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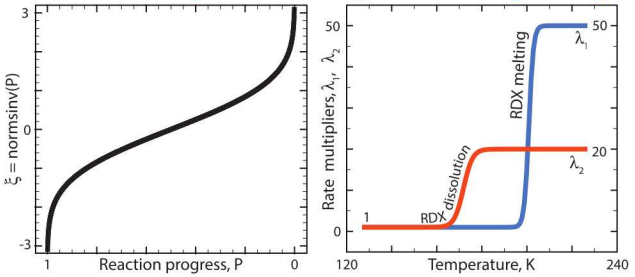
"UNIVERSAL" Cookoff Model

Energy	$\rho_b C_b \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \sum_{i=1,4} r_i h_{r,i} Mw_i$
Mechanism	$S \xrightarrow{1} S_g$, adsorbed gases (e.g. moisture) $E \xrightarrow{2} \alpha G_E + \beta C_E$, Condensed-phase dominant ($r_2 \neq f[P]$) $E \xrightarrow{3} \alpha G_E + \beta C_E$, Gas-phase dominant ($r_3 = f[P]$) $B \xrightarrow{4} \gamma G_B + \delta C_B$, Binder
Rates	$r_1 = A_1 T^{m_1} exp\left(\frac{-E_1+\xi_1\sigma_1}{RT}\right)[S]$ $r_2 = A_2 \lambda_2 T^{m_2} exp\left(\frac{-E_2+\xi_2\sigma_2}{RT}\right)[E]$ $r_3 = A_3 \lambda_3 T^{m_3} \left(\frac{P}{P_o}\right)^{n_3} exp\left(\frac{-E_3+\xi_3\sigma_3}{RT}\right)[E]$ $r_4 = A_4 T^{m_4} exp\left(\frac{-E_4+\xi_4\sigma_4}{RT}\right)[B]$
Species	$\frac{d[S]}{dt} = -r_1; \frac{d[S_g]}{dt} = r_1 ; \frac{d[E]}{dt} = -r_1 - r_2; \frac{d[G_E]}{dt} = \alpha(r_2 + r_3);$ $\frac{d[C_E]}{dt} = \beta(r_2 + r_3) ; \frac{d[B]}{dt} = -r_3; \frac{d[G_B]}{dt} = \gamma r_3; \frac{d[C_B]}{dt} = \delta r_3$
Distribution	$\xi_1 = \text{invnorm}\left(\frac{[S]}{[S_o]}\right); \xi_2 = \xi_3 = \text{invnorm}\left(\frac{[E]}{[E_o]}\right); \xi_4 = \text{invnorm}\left(\frac{[B]}{[B_o]}\right)$

4 EMs

Acronym	Composition
Comp-B3	60|40 wt% RDX|TNT
PBX 9501	95|2.5|2.5 wt% HMX|Estane|NP
PBX 9502	95|5 wt% TATB|Kel-F
PETN	100 wt% PETN

Multipliers (example)



Key: 1) distributed activation energies and 2) pressure dependency.

Material specific properties
(thermal conductivity and specific heat)

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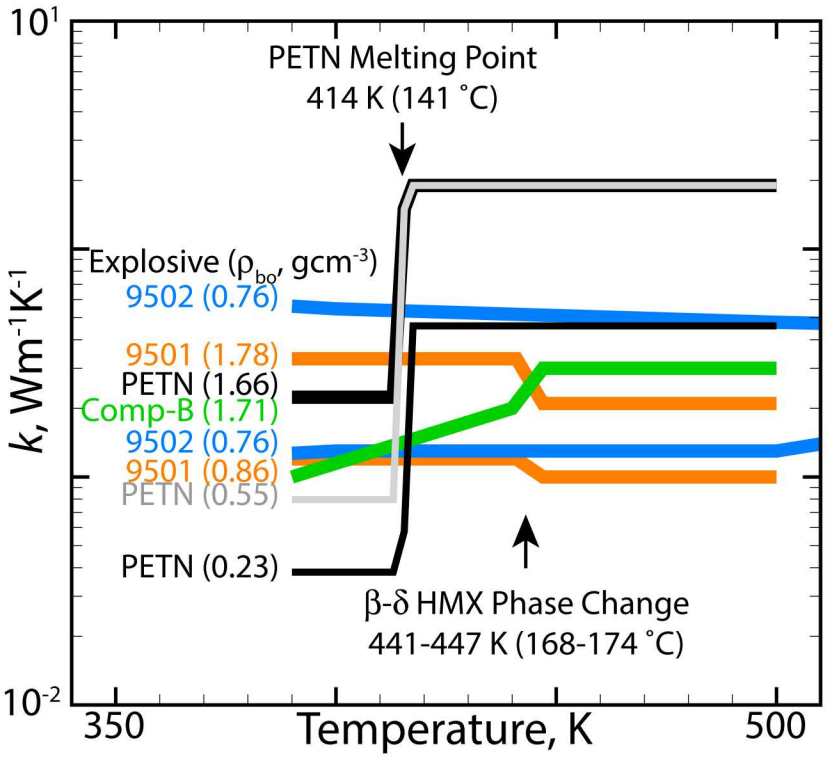
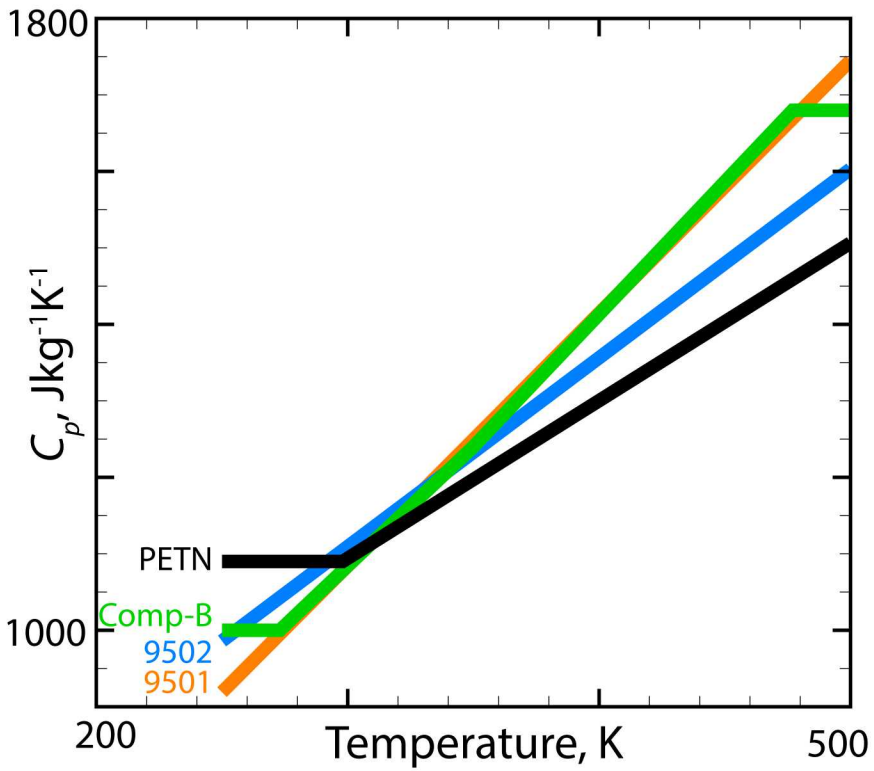
Thermal Conductivity



Specific Heat



Obtained from data (SITI and DSC) or from the literature.

Material specific properties
(Phase changes and dissolution)

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Explosive	Phase Change	T_S, K (°C)	T_L, K (°C)	Enthalpy,* Jkg^{-1}
Comp-B	TNT melt	350 (77)	360 (87)	$(1-\omega_{RDX})\times 98{,}450$
	RDX dissolution	419 (146)	471 (198)	$\omega_{diss}\times\omega_{RDX}\times 100{,}000$
	RDX melt	471 (198)	477 (204)	$(1-\omega_{diss})\times\omega_{RDX}\times 160{,}000$
PBX 9501	$\beta-\delta$	441 (168)	447 (174)	$\omega_{HMX}\times 33{,}000$
	HMX melt	529 (256)	531 (258)	$\omega_{HMX}\times 236{,}000$
PBX 9502	Not Applicable (NA)	NA	NA	NA
PETN	PETN melt	413 (140)	415.5 (142.5)	$\omega_{PETN}\times 177{,}000$

*ω is mass fraction, ω_{diss} = 0.5 (based on DSC data)

Phase changes are modeled as an energy sink using a normal distribution spread over a temperature range defined by T_s and T_L. The distribution is sized so that 99% of the energy release occurs between T_s and T_L.

"UNIVERSAL" mechanism

(Rates determined for each individual explosive)

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$S \xrightarrow{1} S_g$, adsorbed gases (e.g. moisture)

$E \xrightarrow{2} \alpha G_E + \beta C_E$, Condensed-phase dominant ($r_2 \neq f[P]$)

$E \xrightarrow{3} \alpha G_E + \beta C_E$, Gas-phase dominant ($r_3 = f[P]$)

$B \xrightarrow{4} \gamma G_B + \delta C_B$, Binder

Comp-B

$RDX \xrightarrow{2} 7.51G + 10.97C$

$RDX \xrightarrow{3} 7.51G + 10.97C$

PBX 9501

$S \xrightarrow{1} S_g$

$HMX \xrightarrow{2} 10G_X + 1.6C$

$HMX \xrightarrow{3} 10G_X + 1.6C$

$BDNPAF \xrightarrow{4} 4G_b + NVR$

PBX 9502

$S \xrightarrow{1} S_g$

$TATB \xrightarrow{2} 7.5G_X + 3.9C$

$TATB \xrightarrow{3} 7.5G_X + 3.9C$

PETN

$PETN \xrightarrow{2} 10G + 0.76C$

$PETN \xrightarrow{3} 10G + 0.76C$

We found that 400 K and 1 atm is a reasonable cookoff condition to obtain most product hierarchy and reaction energies using TIGER.

The form of the rate expression is key

(Comp-B mechanism used as example)

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Mechanism

$RDX \xrightarrow{1} 7.51G + 0.97C$

$RDX \xrightarrow{2} 7.51G + 0.97C$

Rates

$$r_1 = A_1 \lambda_1 T^{m_1} \exp\left(\frac{-E_1 + \xi\sigma_1}{RT}\right)[\mathrm{RDX}]$$

$$r_2 = A_2 \lambda_2 T^{m_2} \left(\frac{P}{P_o}\right)^{n_2} \exp\left(\frac{-E_2 + \xi\sigma_2}{RT}\right)[\mathrm{RDX}]$$

Accelerations

$$\lambda_1 = 1 + 0.5\left[1 + \tanh\left(\frac{T - 474}{2}\right)\right] \times 49$$

$$\lambda_2 = 1 + 0.5\left[1 + \tanh\left(\frac{T - 445}{4}\right)\right] \times 19$$

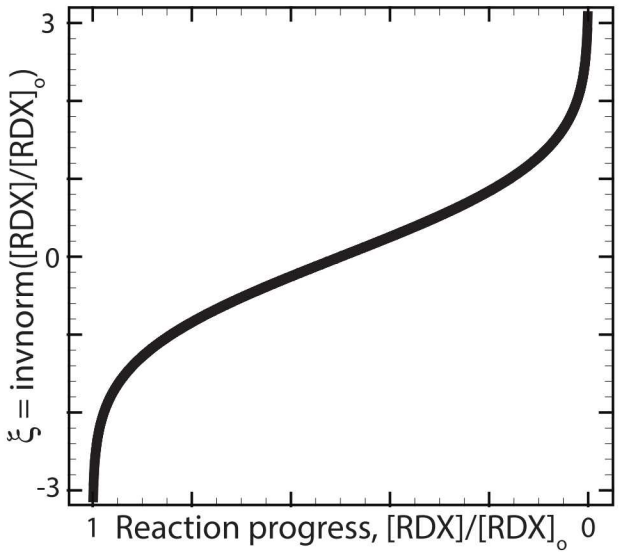
Flexibility

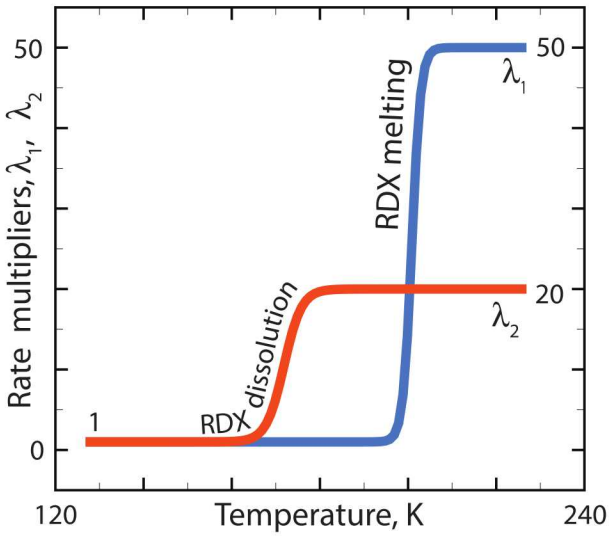
Negative σ_1 and σ_2 autocatalytic

Positive σ (desorption) diffusion limited

σ helps with accurate pressure match $\left(\frac{P}{P_o}\right)^{n_2}$ fit to vented and sealed systems

Works for explosives with variable density





Combining several phenomena into a single rate expression makes parameterizing the model simple and accurate.

Experiments used to calibrate and validate

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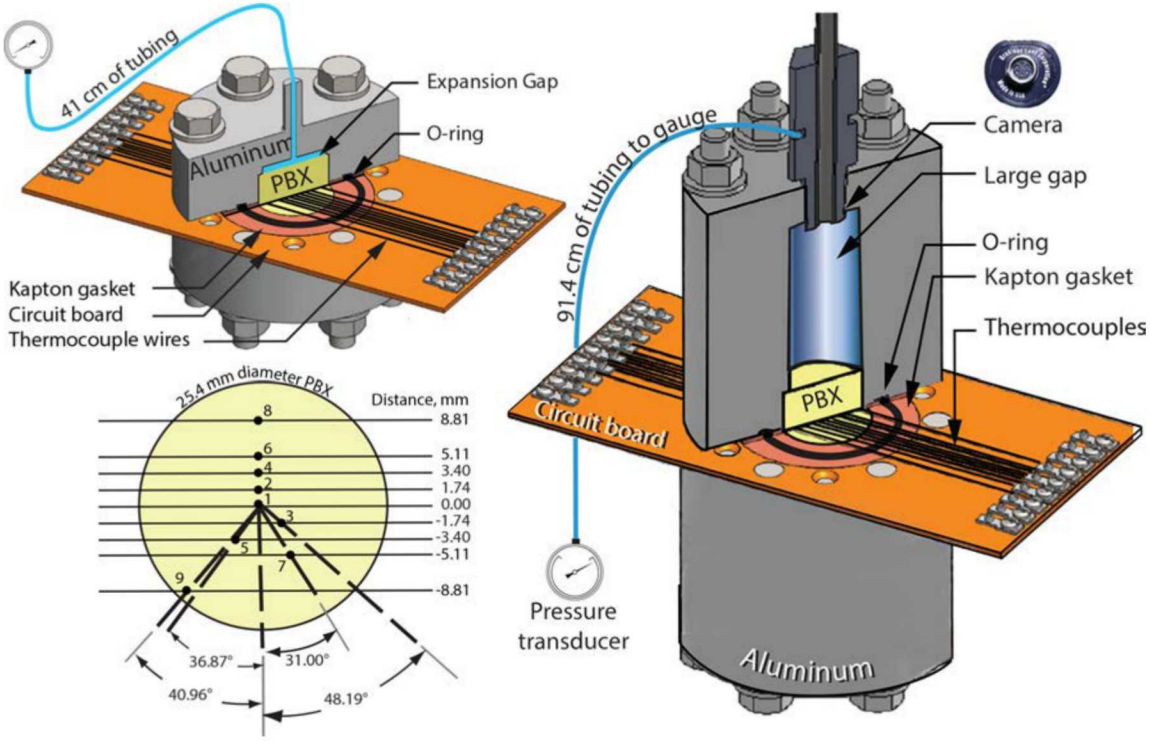
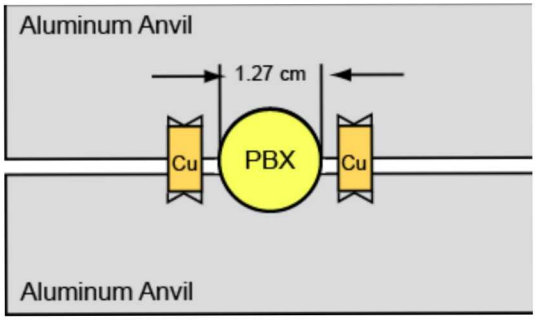
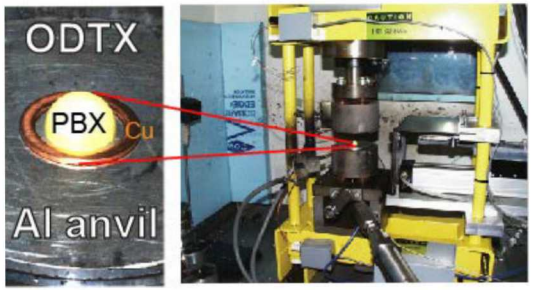
SNL's SITI experiment



LLNL's ODTX experiment





Typically, we obtain thermal conductivity and the reaction rate coefficients with vented and sealed SITI experiments. Either DSC or literature values are used for specific heat. We use TIGER for product hierarchy.

Predicts temperature, pressure, ignition time

(**Comp-B**: SITI and ODTX predictions)

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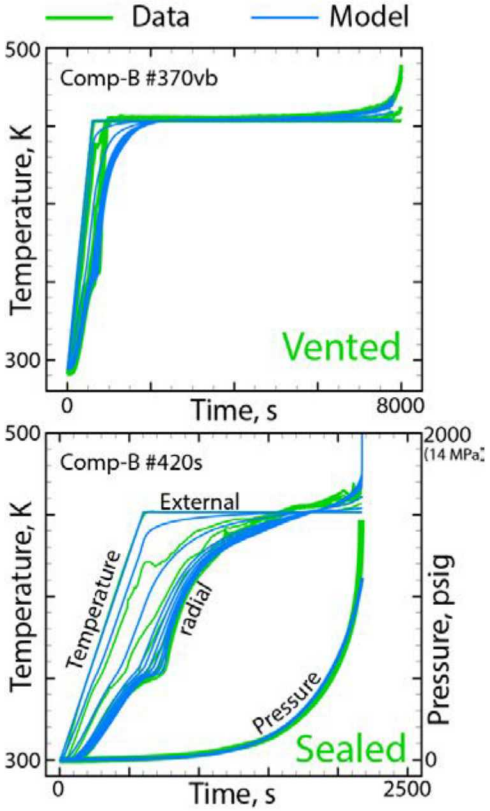
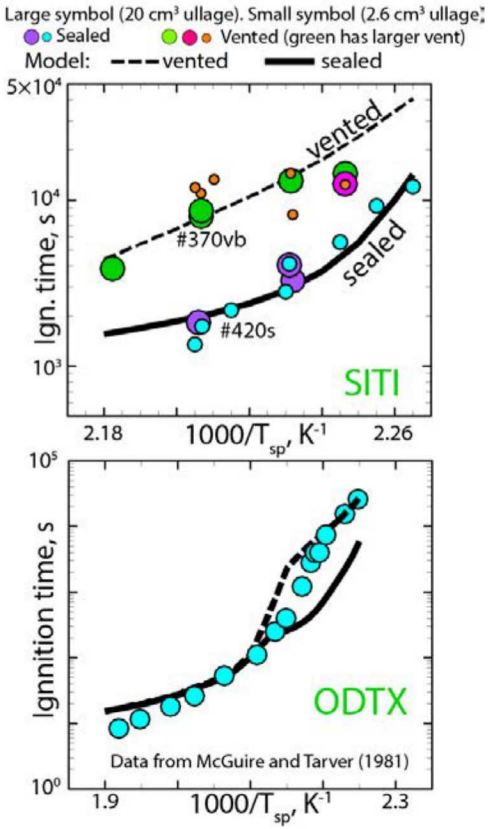
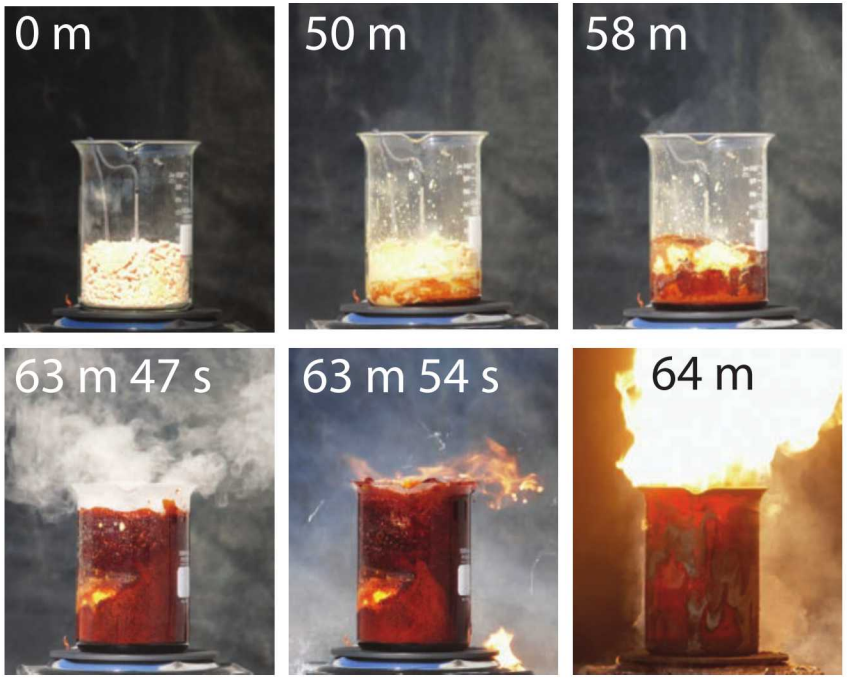
Temperature and pressure



Ignition times



TNT melts, but RDX suspension inhibits flow



The RDX suspension inhibits flow making the "UNIVERSAL" Cookoff Model (UCM) an ideal framework for Comp-B

Predicts temperature, pressure, ignition time

(**PBX 9501**: SITI and ODTX predictions)

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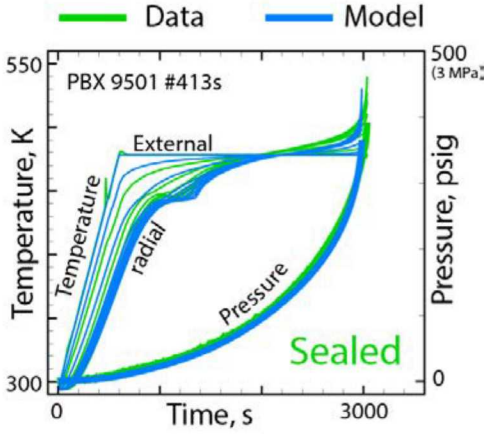
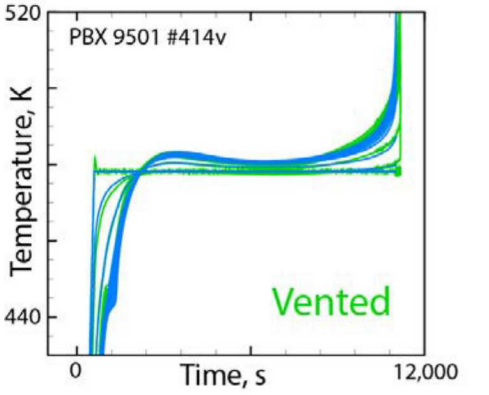
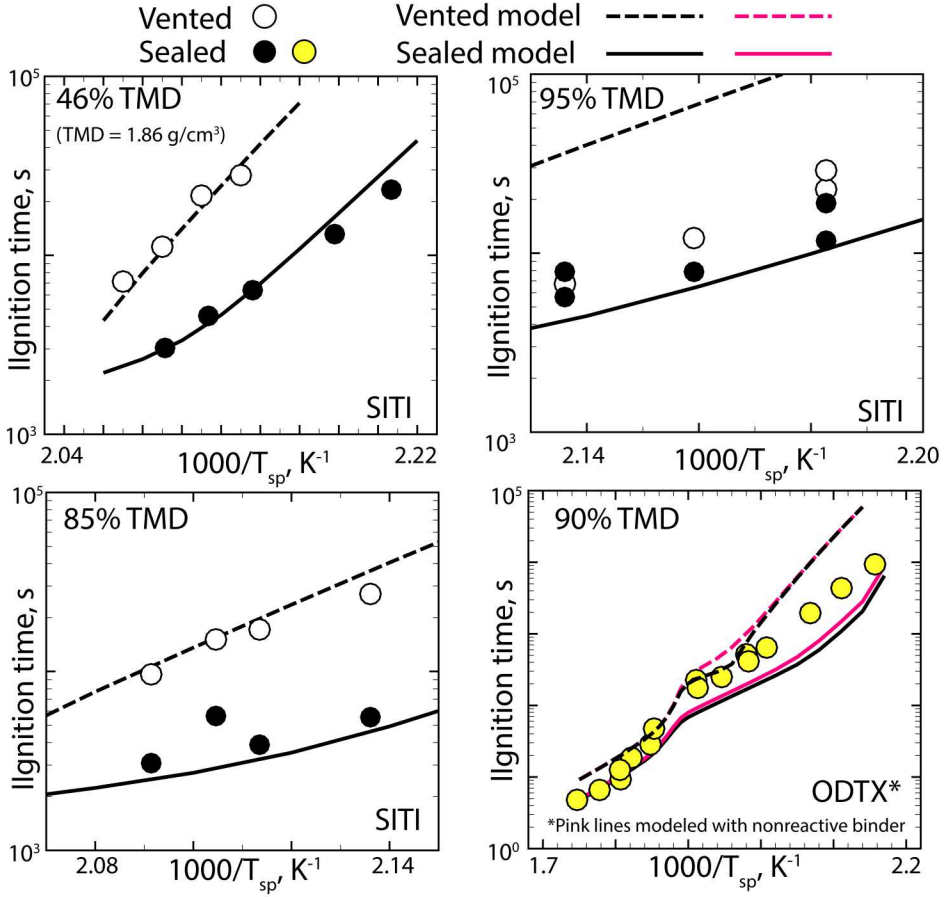
Temperature and pressure



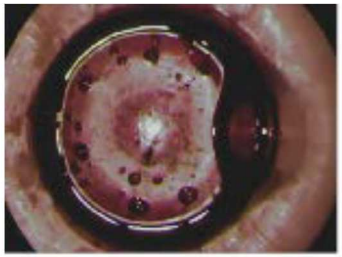


SITI and ODTX ignition times



96% TMD

96% TMD



Gases are retained within the high density PBX and have high reaction rates since the internal pressures are high

Predicts temperature, pressure, ignition time

(**PBX 9502**: SITI and ODTX predictions)

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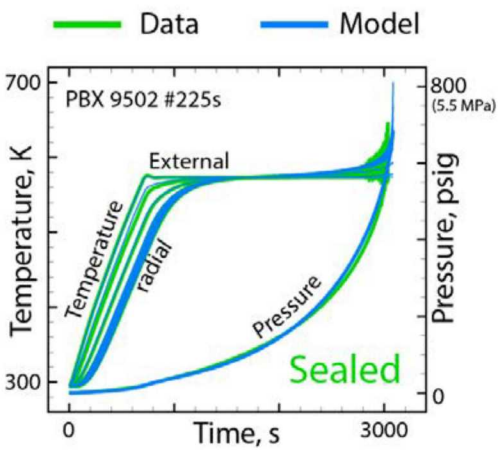
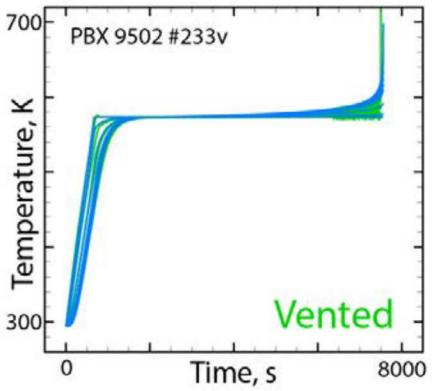
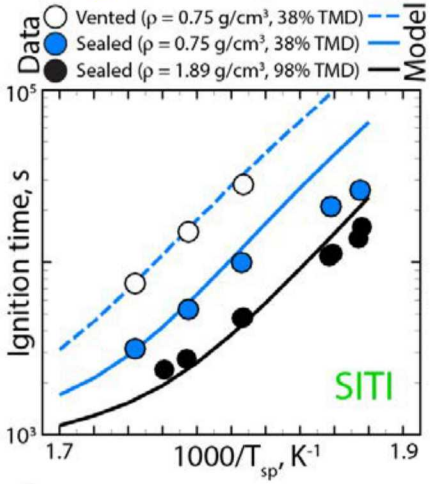
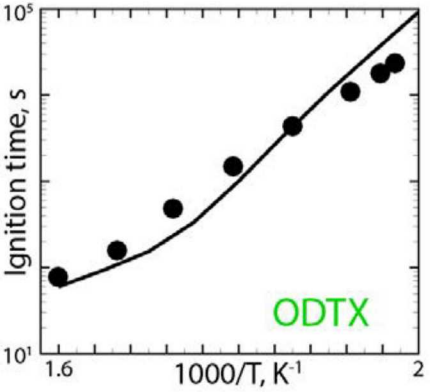
Temp. and Press.



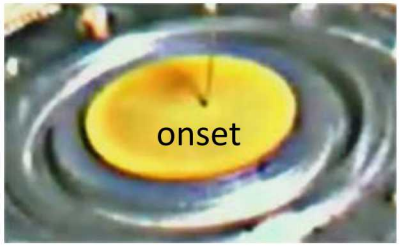


Ignition time

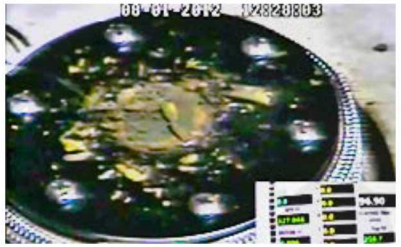




Open SITI half shell



Washer added to prevent crater



Ignition time depends on density and the degree of confinement.

Predicts temperature, pressure, ignition time

(**PETN**: SITI and ODTX predictions)

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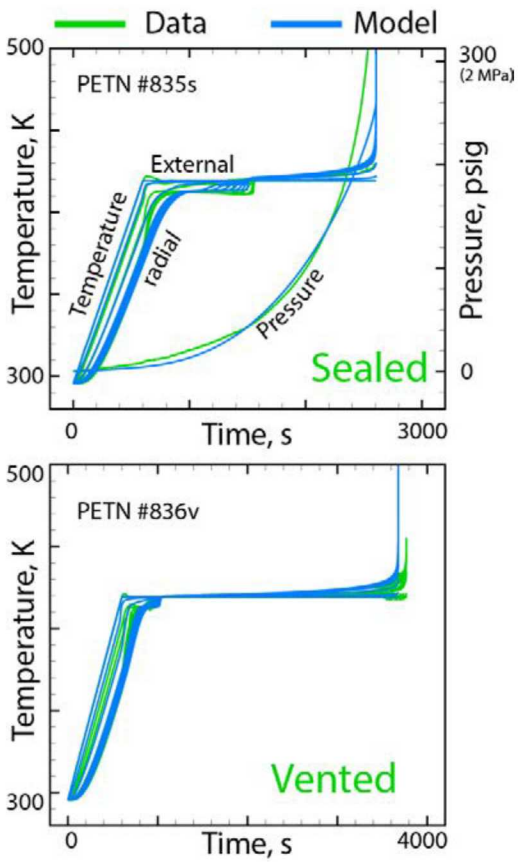
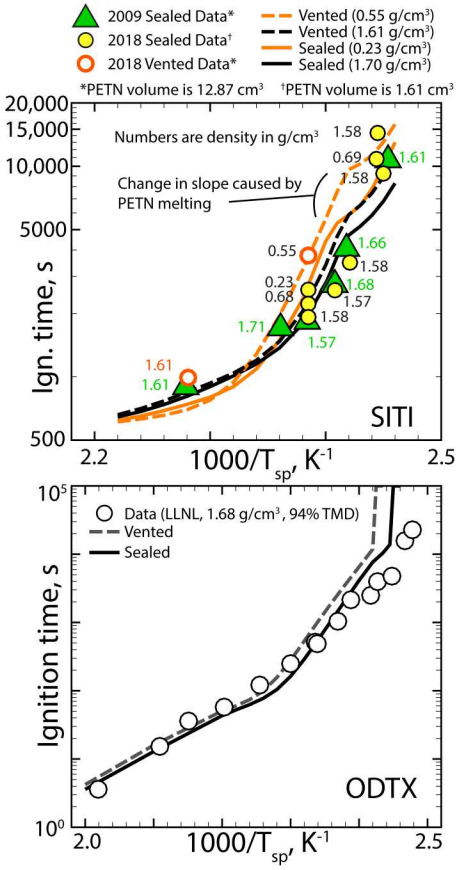
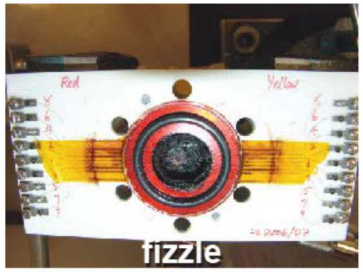
Temp. and Press.



Ignition time



Does it go pop, bang, or kablooey?



Our <u>limited</u> data implies the PETN is slightly pressure dependent.

Summary and Conclusions

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- Over the past decade, we have been developing cookoff models for various explosives based on the SITI experiment that scale from g to kg.
- We have observed similarities that are amenable to a universal cookoff model.
- All thermophysical properties are obtained from data. However, the reaction mechanism is assume to be universal with rates specific for each explosive.
- Universal cookoff mechanism is based on four reactions:
  - Desorption reaction
  - gas-phase dominated reaction
  - condensed-phase dominated reaction
  - Binder reaction
- Utility of the universal cookoff model was demonstrated by applying the model to diverse explosives.
- Success attributed to good thermophysical properties, use of modified Arrhenius rate expressions using distributed activation energies, and pressure dependent reaction rates.