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UCM/MMP cookoff models for explosives containing RDX

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Comp-B3

Comp-C4

Semtex 1H

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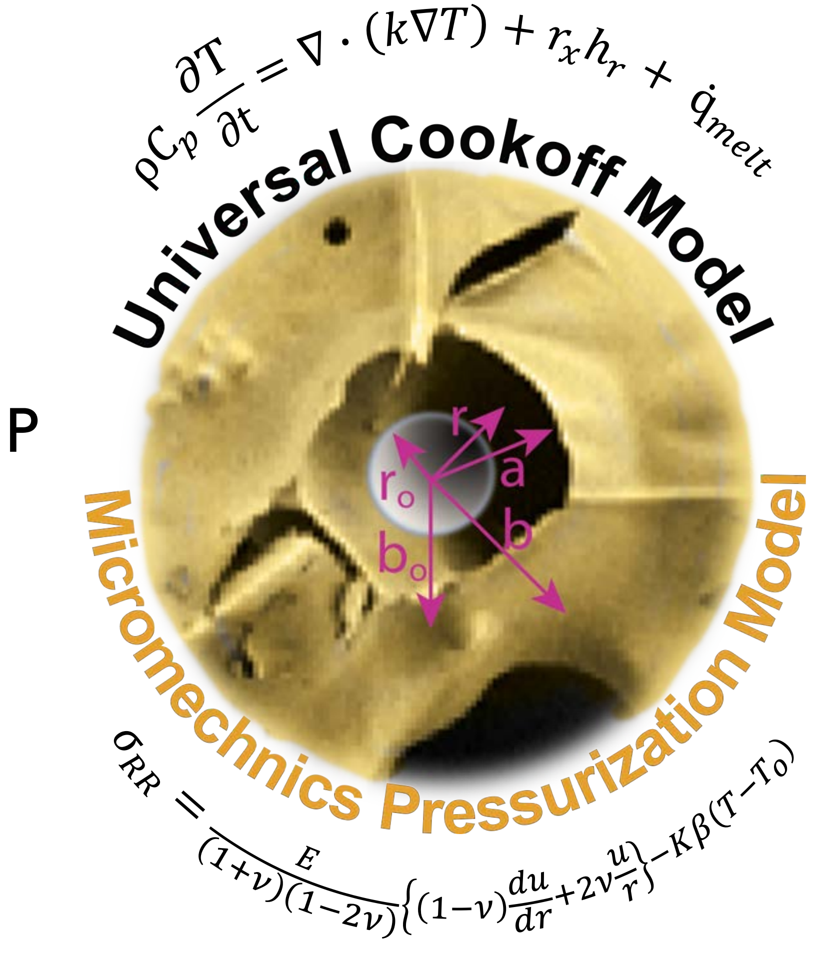
National Nuclear Security Administration

Introduction

(avoid high temperatures and confinement)

Name	Comp. (wt.%), formula	Mw_x g/mol	O_2 bal.	ρ_{co}, kg/m^3	h_f kJ/mol	D^b km/s	T_a K
Comp-B3	RDX/TNT (60/40) $C_{4.58}H_{5.6}N_{4.82}O_6$	224.2	-42.6	1742	16.9	7.81	2651
Comp-C4	RDX/DOA/PIB/Oil 91/5.3/2.1/1.6 $C_{3.83}H_{7.5}N_{5.2}O_{5.23}$	211.5	-46.1	1659	16.8	7.90	2471
PBX 9407	RDX/VCTFE (94/6) $C_{3.1}H_{5.9}N_{5.6}O_{5.6}Cl_{0.18}F_{0.18}$	221.8	-24.2	1799	18.4	8.37	2880
PBXN-109	RDX/AL/HTPB/DOA 64/20/8/8 $C_{1.61}H_{2.94}N_{1.44}O_{1.51}AL_{0.62}$	83.4	-78.7	1656	-4.7	7.24[c]	2033
RDX	RDX (100) $C_3H_6N_6O_6$	222.1	-21.6	1806	69	8.78	2930
Semtex 1H	RDX/PETN/Binder/Plastici. 65.5(max)/25(min)/2.5/11.6 or 43/43/2.5/11.5 $C_{4.8}H_{8.86}N_{3.8}O_{6.51}$	224.0	-53.7	1581	-226	7.45	2164
XTX-8004	RDX/Sylgard™ 182 (80/20) $C_{2.57}H_6N_{3.44}O_{3.86}Si_{0.43}$	158.9	-51.8	1579	-176	7.72	2260



Propell. Explos. Pyrotech., 47 (2022)

Single mechanism for 7 explosives

Product Hierarchy
(equilibrium at 400 K and 1 bar)

Comp-B3	$C_{4.58}H_{5.6}N_{4.82}O_6 \rightarrow 2.54\ H_2O + 2.41\ N_2 + 1.73\ CO_2 + 0.13\ CH_4 + 2.72\ C$ Comp-B3 $\rightarrow$ 6.81 Gas + 2.72 C
Comp-C4	$C_{3.83}H_{7.5}N_{5.2}O_{5.23} \rightarrow 3.14\ H_2O + 2.60\ N_2 + 1.09\ CO_2 + 0.3\ CH_4 + 0.01\ H_2 + 2.43\ C$ Comp-C4 $\rightarrow$ 7.14 Gas + 2.44 C
PBX 9407	$C_{3.1}H_{5.9}N_{5.6}O_{5.6}Cl_{0.18}F_{0.18} \rightarrow 2.51\ H_2O + 2.82\ N_2 + 1.57\ CO_2 + 0.18\ HCL + 0.18\ HF + 0.13\ CH_4 + 1.40\ C$ PBX 9407 $\rightarrow$ 7.37 Gas + 1.40 C
PBXN-109	$C_{1.61}H_{2.94}N_{1.44}O_{1.51}AL_{0.62} \rightarrow 1.08\ H_2O + 0.72\ N_2 + 0.215\ CO_2 + 0.195\ CH_4 + 0.62\ AL + 1.2\ C$ PBXN-109 $\rightarrow$ 2.21 Gas + 0.62 AL + 1.20 C
RDX	$C_3H_6N_6O_6 \rightarrow 2.7\ H_2O + 3\ N_2 + 1.65\ CO_2 + 0.15\ CH_4 + 1.2\ C$ RDX $\rightarrow$ 7.5 Gas + 1.2 C
Semtex 1H	$C_{4.8}H_{8.86}N_{3.8}O_{6.51} \rightarrow 3.75\ H_2O + 1.9\ N_2 + 1.38\ CO_2 + 0.34\ CH_4 + 3.08\ C$ Semtex 1H $\rightarrow$ 7.37 Gas + 3.08 C
XTX-8004	$C_{2.57}H_6N_{3.44}O_{3.86}Si_{0.43} \rightarrow 2.0\ H_2O + 1.72\ N_2 + 0.40\ CO_2 + 0.40\ CH_4 + 1.77\ C + 0.43\ SiO_2$ XTX-8004 $\rightarrow$ 1.77 Gas + 1.77 C + 0.43 SiO_2

Molar average properties

Kinetic Model
(Universal Cookoff Model/MicroMechanics Pressurization Model)

Energy equation

$$\rho_b C_p \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + h_r r_x + \dot{q}_{melt}$$

Mechanism

$$X \rightarrow \alpha G + \beta \mathrm{Al} + \gamma C + \delta SiO_2$$

Rate equation

$$r_x = A\left(\frac{P}{P_o}\right)^n \lambda T^m \exp\left[-\frac{(E + \xi\sigma)}{T}\right][\mathrm{X}]$$

First order decomposition

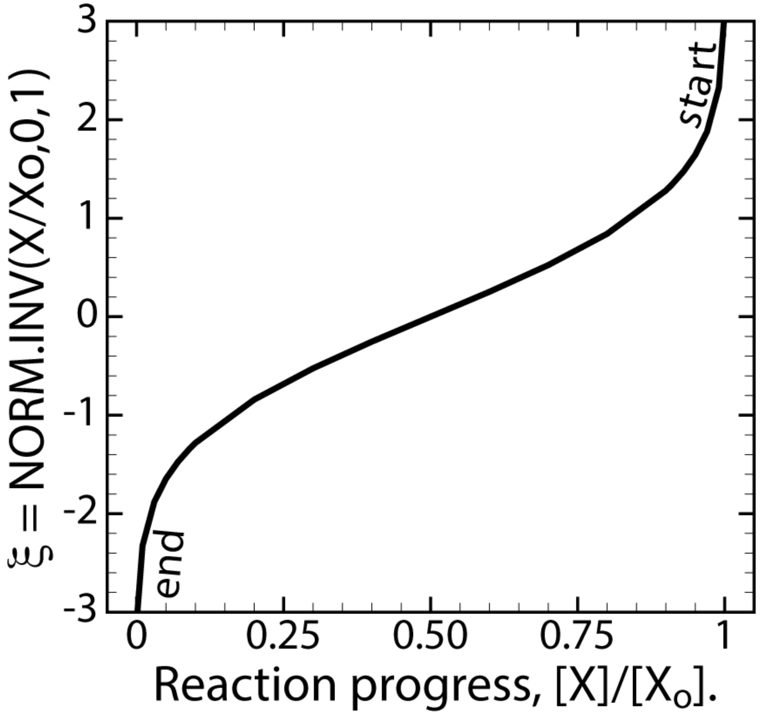
$\mathrm{Comp{-}B3} \rightarrow 6.81G + 2.72C$	RDX/TNT
$\mathrm{Comp{-}C4} \rightarrow 7.14G + 2.44C$	RDX/DOA/PIB/Oil
$\mathrm{PBX\ 9407} \rightarrow 7.37G + 1.40C$	RDX/VCTFE
$\mathrm{PBXN{-}109} \rightarrow 2.21G + 0.62Al + 1.20C$	RDX/Al/HTPB/DOA
$\mathrm{RDX} \rightarrow 7.5G + 1.2C$	RDX
$\mathrm{Semtex\ 1H} \rightarrow 7.37G + 3.08C$	RDX/PETN/Binder/Plastici.
$\mathrm{XTX{-}8004} \rightarrow 4.72G + 1.77C + 0.43SiO_2$	RDX/Sylgard

Explosive decomposes into gases and condensed species

Rate acceleration

Distributed activation energy

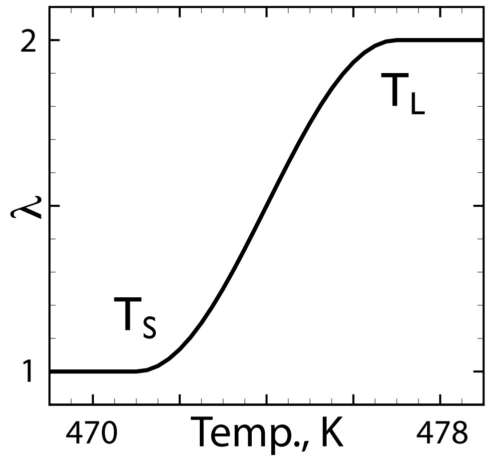
$$r_x = A\left(\frac{P}{P_o}\right)^n \lambda T^m \exp\left[-\frac{(E+\xi\sigma)}{T}\right][X]$$



$$r_x = A\left(\frac{P}{P_o}\right)^n \lambda T^m \exp\left[-\frac{(E+\xi\sigma)}{T}\right][X]$$

$$\lambda = \begin{cases} 1, & T \le T_S \\ 1 + 0.5\left(1 - [\lambda_m - 1]\cos\left[\pi\frac{(T-T_S)}{(T_S-T_L)}\right]\right) & T_S < T < T_L \\ \lambda_m & T \ge T_L \end{cases}$$

Phase change



Kinetic parameters

Name	n	m	E, K	σ, K	RDX: λ_m
Comp-B3	0.35	1.5	24500	-500	2
Comp-C4	0.16	2	25063	-1000	2
PBX 9407	0.23	0.5	22560	-400	10
PBXN-109	0.295	-1	17997	-400	2
RDX	0.295	3	29772	-400	4
Semtex1H	0[a]	-0.5	17200	-500	1
XTX-8004	0.15	3	28020	-1000	1

Temperature, reaction extent, and phase change accelerate rates

Effective capacitance method

$$\rho_b C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + h_{\mathrm{r}} r_{\mathrm{x}} + \dot{q}_{melt}$$

Details

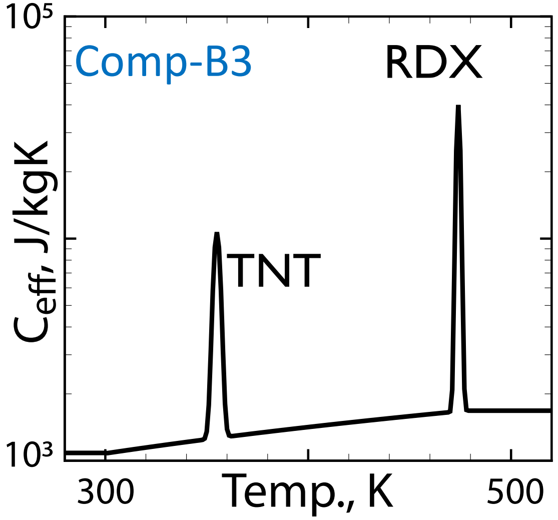
$$C_{eff} = C_p + \frac{\omega h_l}{\sigma\sqrt{2\pi}} e^{-\frac{z^2}{2}}$$

$$\sigma = \frac{(T_m - T_S)}{3}$$

$$z = \frac{(T - T_m)}{\sigma}$$

Thermophysical properties

Name	T, K	C_p, J/kgK	T, K	k, W/mK (ρ_b, kg/m^3)
Comp-B3	300	1084	300	0.2 (1710)
	350	1240	440	0.2 (1710)
	477	1680	477	0.8^b (1710)
Comp-C4	300	1004	300	0.16 (1500)
	600	1818	600	0.16 (1500)
PBX 9407	273	1008	400	0.20 (1625)
	482	1681	478	0.20 (1625)
PBXN-109	300	1500	300	0.4 (1650)
	600	1500	600	0.4 (1650)
RDX	300	1004	300	0.20 (1650)
	623	1760	600	0.20 (1650)
Semtex1H	300	1145	300	0.18 (1530)
	400	1470	500	0.24 (1530)
XTX-8004	298	1100	300	0.2 (1550)
	460	1520	600	0.2 (1550)



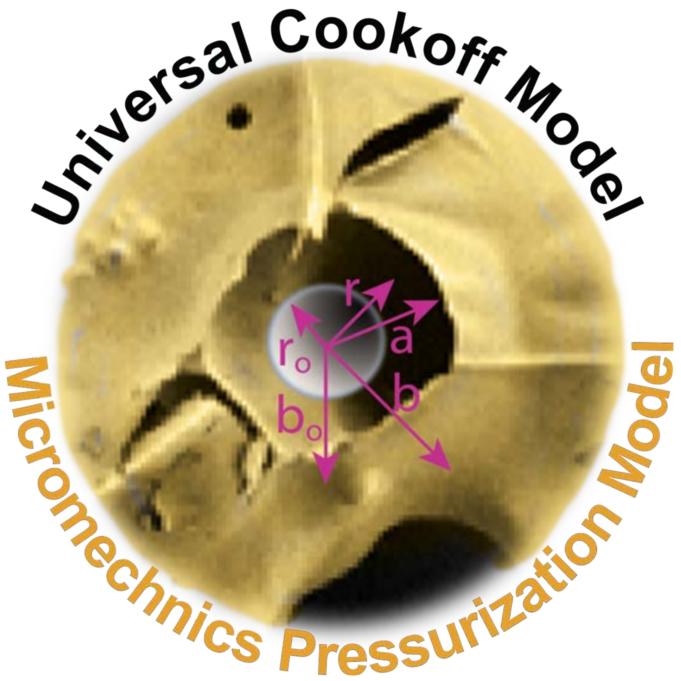
Melting components: RDX, TNT, PETN

Name	Melt: 471-477 K h_l: 160000 J/kg ω_{RDX}	350-360 K 98450 J/kg ω_{TNT}	413-415 K 177000 J/kg ω_{PETN}
Comp-B3	0.60	0.4	0
Comp-C4	0.91	0	0
PBX 9407	0.94	0	0
PBXN-109	0.64	0	0
RDX	1.00	0	0
Semtex1H	0.43	0	0.43
XTX-8004	0.80	0	0

Phase changes are modeled thermodynamically

Micromechanics pressurization (MMP) model

Initial explosive is impermeable to gases



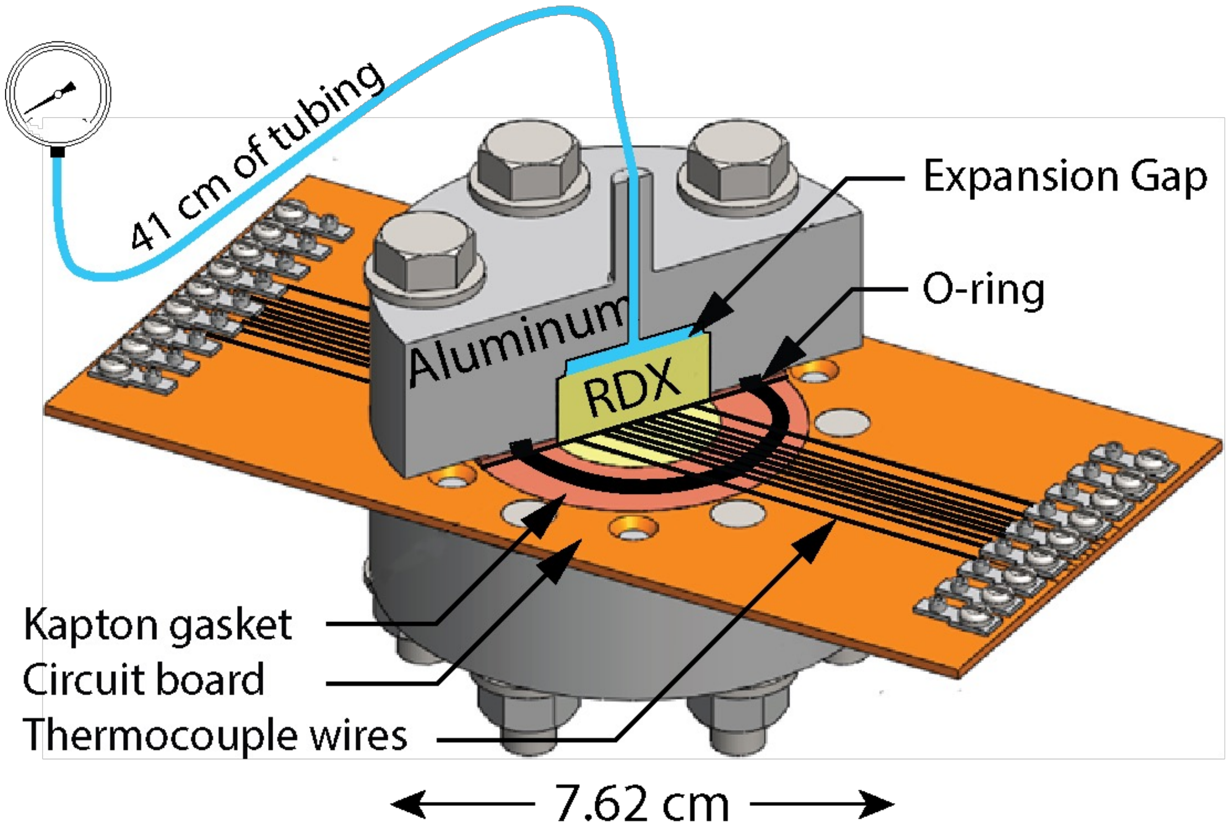
Basics

- Analytical solution of spherical elastic solid
- Tracks evolving defect radii
- Includes decomposition and thermal strain
- Includes mechanical strain and compressibility
- Damage based on maximum pore pressure
- Predicts evolution of permeability

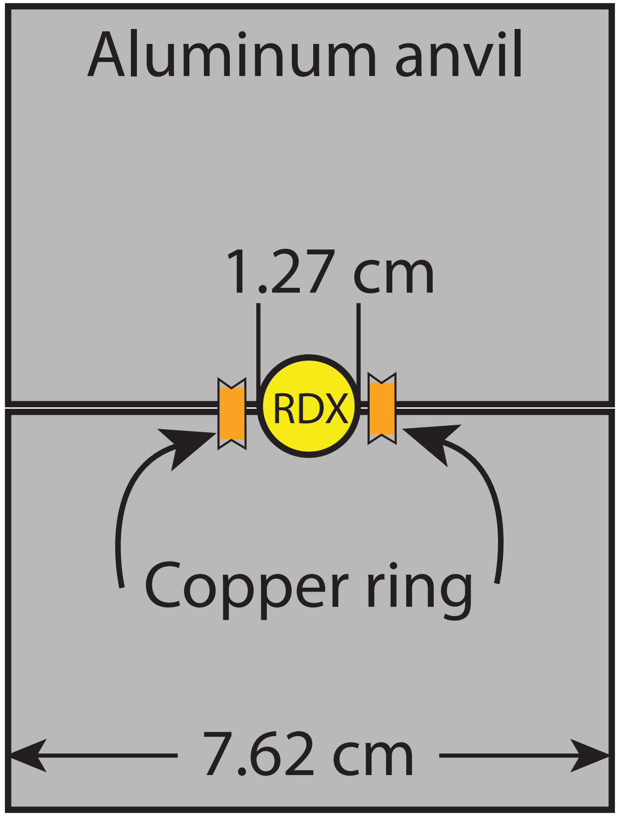
Thermal expansion, thermal damage, and abrupt gas release

SITI and ODTX
(time to thermal ignition)

Sandia Instrumented Thermal Ignition



One Dimensional Time-to-eXplosion



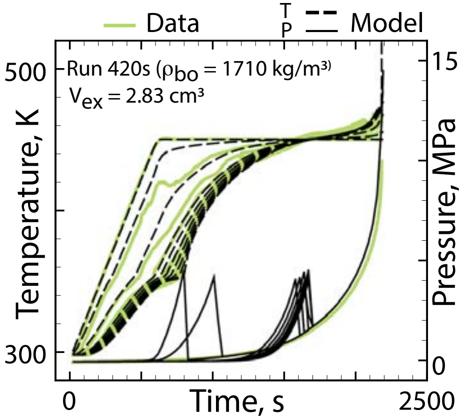
SITI is ramp and hold, ODTX is constant temperature

Measurements and Predictions

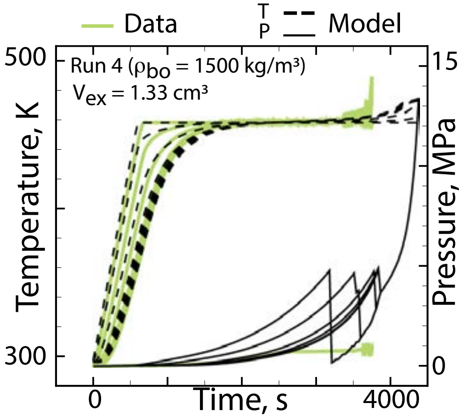
SITI run #420s

Individual

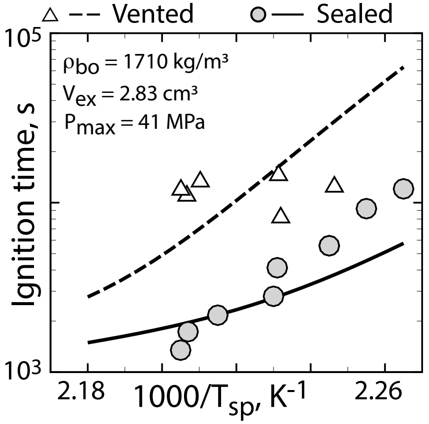
Comp-B3

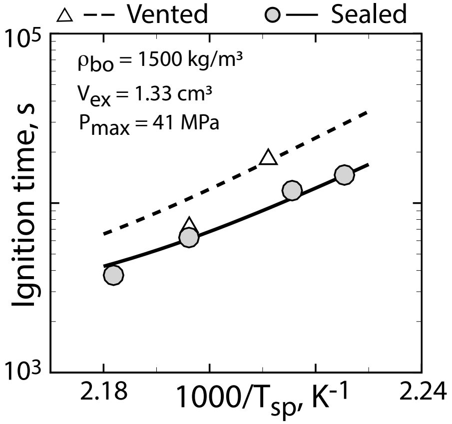


Comp-C4

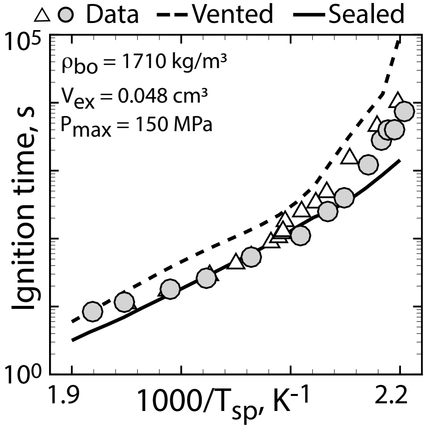


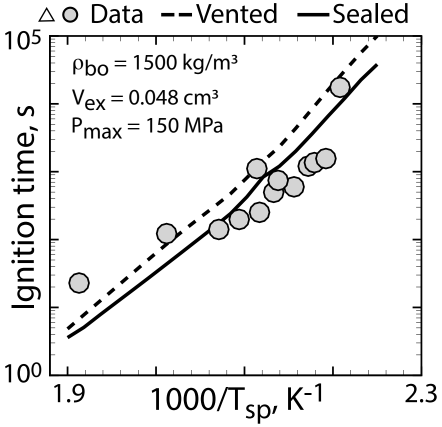
SITI





ODTX

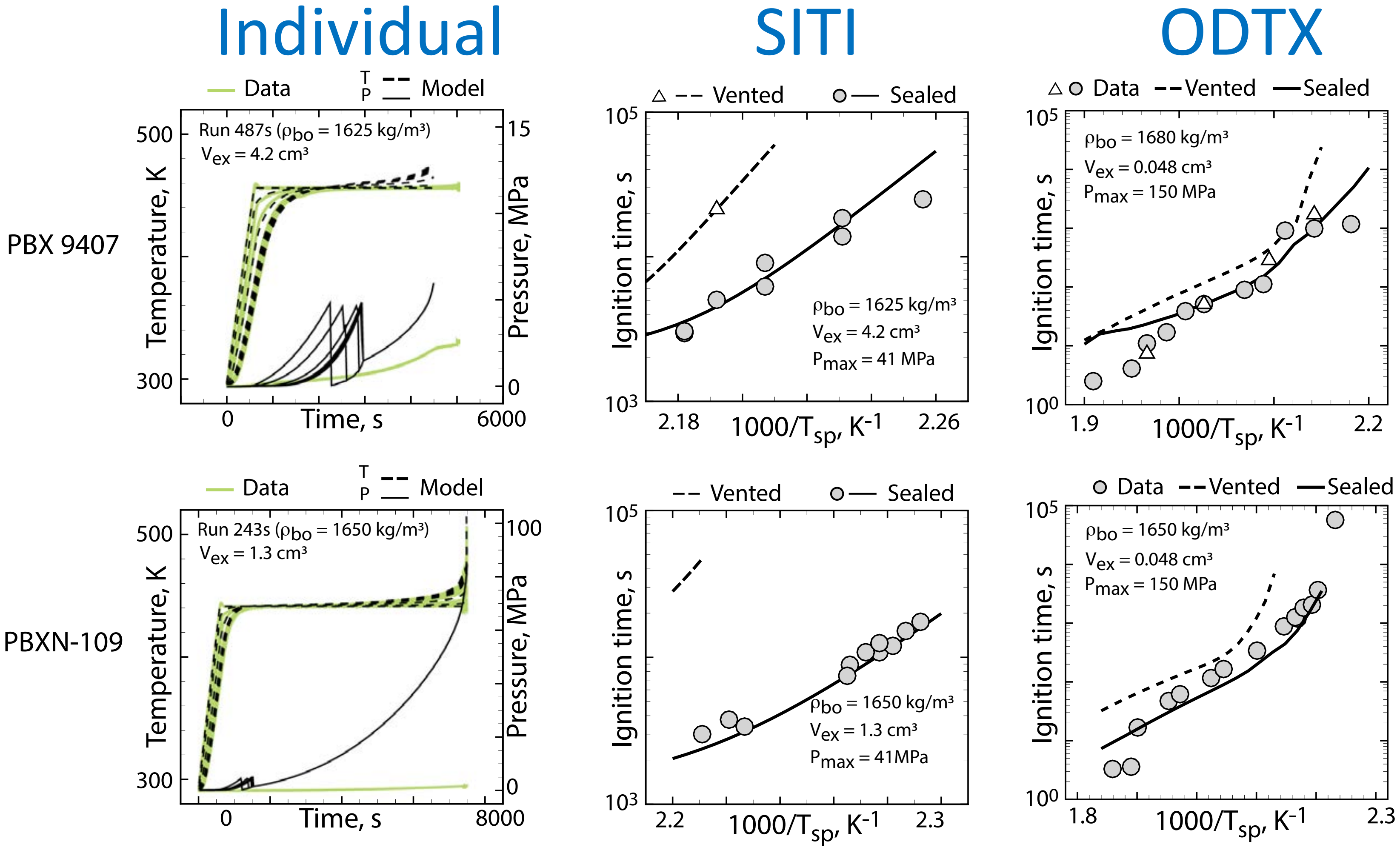




Temperature, pressure, ignition time

Measurements and Predictions

PBXN-109
SITI run #243s



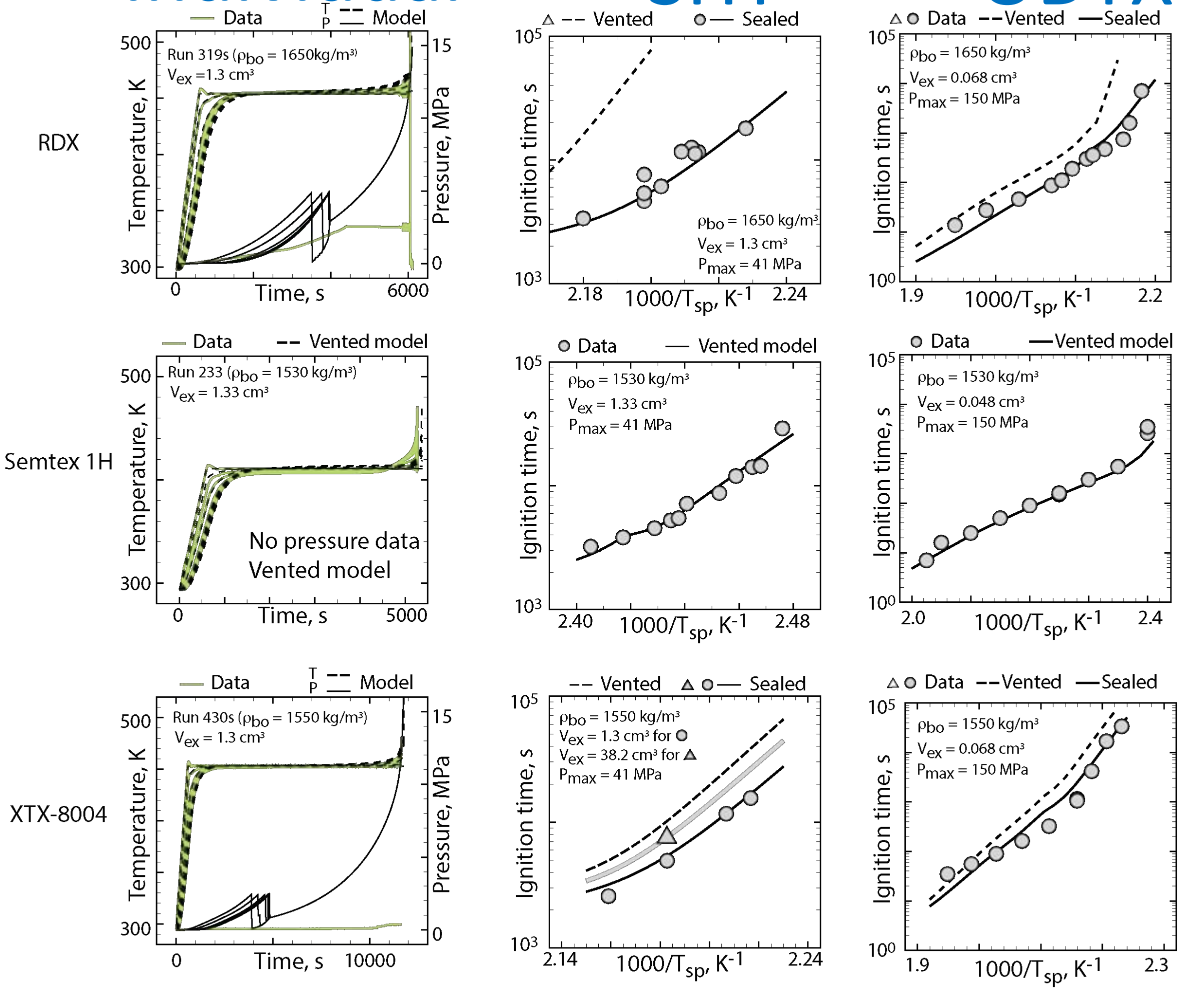
Temperature, pressure, ignition time

Measurements and Predictions

Semtex 1H #228

XTX-8004 #430

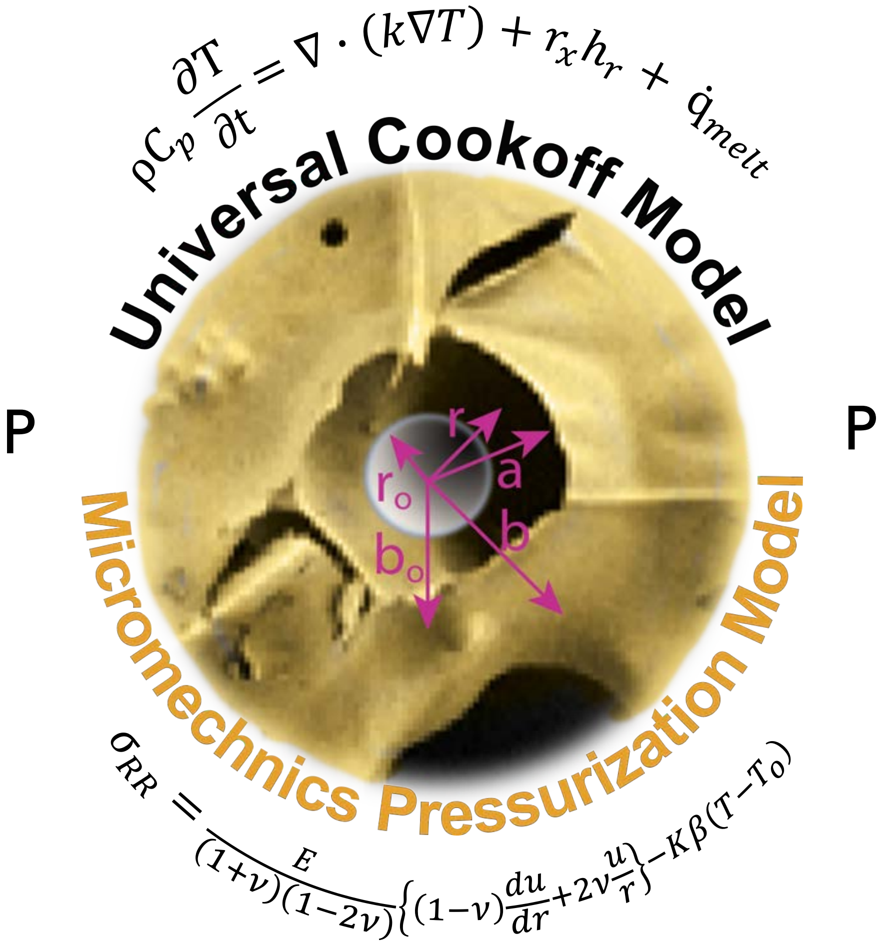
Individual SITI ODTX



Temperature, pressure, ignition time

Summary and conclusions

- UCM/MMP model simplified
- Single autocatalytic reaction
- Acceleration by phase change
- Effective capacitance
- Validated with SITI/ODTX data



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1-step UCM/MMP model for 7 HMX-based and 7 RDX-based explosives: Comp-B3, Comp-C4, EDC-37, HMX, LX-07, LX-10, LX-14, PBX 9407, PBX 9501, PBXN-109, PBXN-9, RDX, Semtex 1H, and XTX-8004