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UCM/MMP cookoff models for explosives containing HMX

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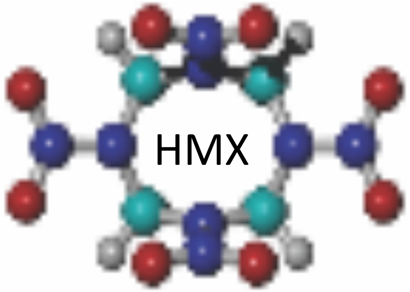

Single-step reactions

$\rightarrow$ 4 N_2 + 3.6 H_2O + 2.2 CO_2 + 0.2 CH_4 + 1.6 C

Simpler and more accurate

Fraunhofer ICT

53rd International Annual Conference of the Fraunhofer ICT: Energetic Materials—Structure and Properties
June 27-June 30, 2023 Convention Center, Gartenhalle, Karlsruhe, Germany

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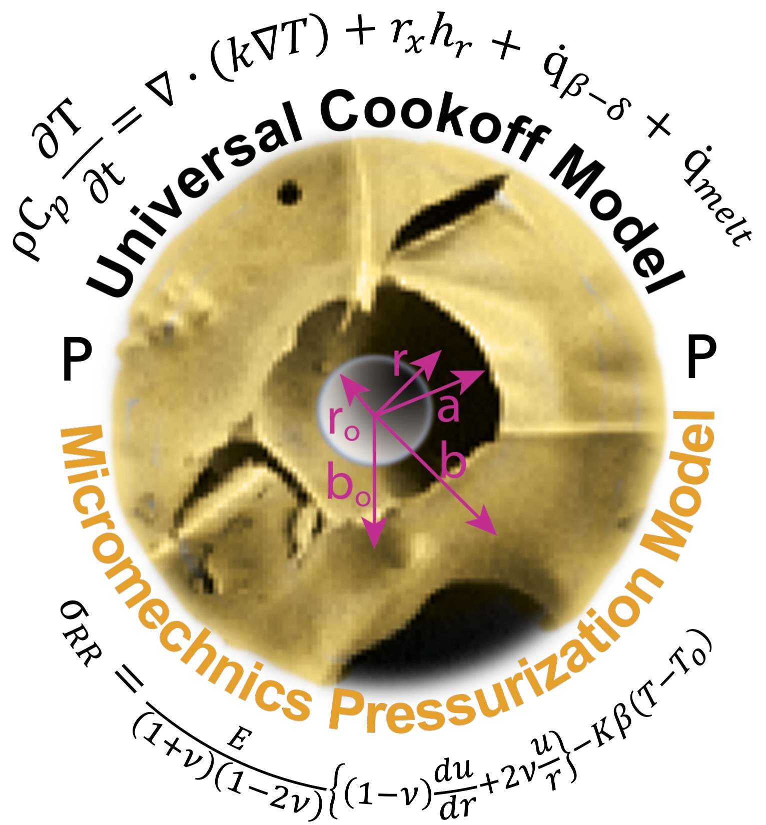
NNSA National Nuclear Security Administration

Introduction

(Composite explosive treated as single material)

Name	Comp. (wt.%), formula	Mw_x g/mol	O_2 bal.	ρ_{co}, kg/m³	h_f kJ/mol	D^b km/s	T_a K
EDC-37	HMX/NC/K10 (91/1/8) $C_{4.46}H_{7.96}N_{7.3}O_{7.66}$	286.7	-29.2	1858	50.6	8.82	2845
HMX	HMX (100) $C_4H_8N_8O_8$	296.2	-21.6	1905	75.0	9.18	2920
LX-07	HMX/Viton-A® (90/10) $C_{4.48}H_{7.89}N_{7.36}O_{7.34}F_{1.05}$	302.2	-26.7	1899	-156.1	8.72	2827
LX-10	HMX/Viton-A® (95/5) $C_{4.25}H_{7.98}N_{7.68}O_{7.69}F_{0.52}$	299.6	-24.2	1902	-39.4	8.94	2882
LX-14	HMX/Estane® (95.5/4.5) $C_{4.4}H_{8.44}N_{7.48}O_{7.7}$	289.3	-29.5	1854	18.3	8.84	2809
PBX 9501	HMX/Estane®/NP (95/2.5/2.5) $C_{4.3}H_{8.34}N_{7.62}O_{7.87}$	292.7	-26.9	1859	27.2	8.75	2850
PBXN-9	HMX/PB/DOA (92/2/6) $C_{4.8}H_{9.32}N_{6.84}O_7$	274.8	-42.2	1755	11.1	8.18	2550



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Single mechanism for 7 explosives

Product Hierarchy
(equilibrium at 400 K and 1 bar)

EDC-37	$C_{4.46}H_{7.96}N_{7.32}O_{7.66}$ (EDC-37) $\rightarrow$ 3.66 N_2 + 3.54 H_2O + 2.06 CO_2 + 0.22 CH_4 + 2.18 C EDC-37 $\rightarrow$ 9.48 G + 2.18 C
HMX	$C_4H_8N_8O_8$ (HMX) $\rightarrow$ 4 N_2 + 3.6 H_2O + 2.2 CO_2 + 0.2 CH_4 + 1.6 C HMX $\rightarrow$ 10 G + 1.6 C
LX-07	$C_{4.48}H_{7.89}N_{7.36}O_{7.34}F_{1.05}$ (LX-07) $\rightarrow$ 3.68 N_2 + 3.10 H_2O + 2.12 CO_2 + 0.16 CH_4 + 1.05 HF + 2.2 C LX-07 $\rightarrow$ 10.11 G + 2.2 C
LX-10	$C_{4.25}H_{7.98}N_{7.68}O_{7.69}F_{0.52}$ (LX-10) $\rightarrow$ 3.84 N_2 + 3.35 H_2O + 2.17 CO_2 + 0.15 CH_4 + 0.52 HF + 1.89 C LX-10 $\rightarrow$ 10.07 G + 1.89 C
LX-14	$C_{4.4}H_{8.44}N_{7.48}O_{7.7}$ $\rightarrow$ 3.74 N_2 + 3.72 H_2O + 1.99 CO_2 + 0.25 CH_4 + 2.16 C LX-14 $\rightarrow$ 9.83 G + 2.16 C
PBX 9501	$C_{4.3}H_{8.34}N_{7.62}O_{7.87}$ (PBX 9501) $\rightarrow$ 3.81 N_2 + 3.73 H_2O + 2.07 CO_2 + 0.22 CH_4 + 2.01 C PBX 9501 $\rightarrow$ 9.83 G + 2.01 C
PBXN-9	$C_{4.8}H_{9.32}N_{6.84}O_7$ (PBXN-9) $\rightarrow$ 3.42 N_2 + 3.96 H_2O + 1.52 CO_2 + 0.35 CH_4 + 2.93 C PBXN-9 $\rightarrow$ 9.25 G + 2.93 C

Molar average properties (*e.g.*, M_{wg}, h_f)

Kinetic Model

(Universal Cookoff Model/MicroMechanics Pressurization Model)

Energy equation

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

Mechanism

$$X \rightarrow \alpha G + \beta C$$

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

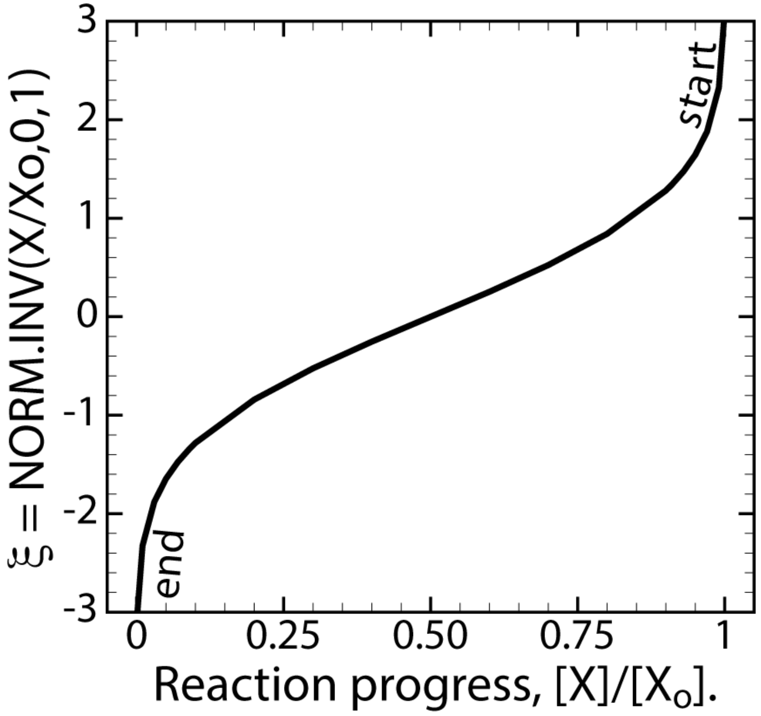
EDC–37 ⍰ 9.48 G + 2.18 C	HMX/NC/K10
HMX ⍰ 10 G + 1.6 C	HMX
LX–07 ⍰ 10.11 G + 2.2 C	HMX/Viton-A®
LX-10 → 10.07 G + 1.89 C	HMX/Viton-A®
LX–14 ⍰ 9.83 G + 2.16 C	HMX/Estane®
PBX 9501 ⍰ 9.83 G + 2.01 C	HMX/Estane®/NP
PBXN-9 → 9.25 G + 2.93 C	HMX/PB/DOA

Composite decomposes into gases and condensed species

Rate acceleration

Distributed activation energy

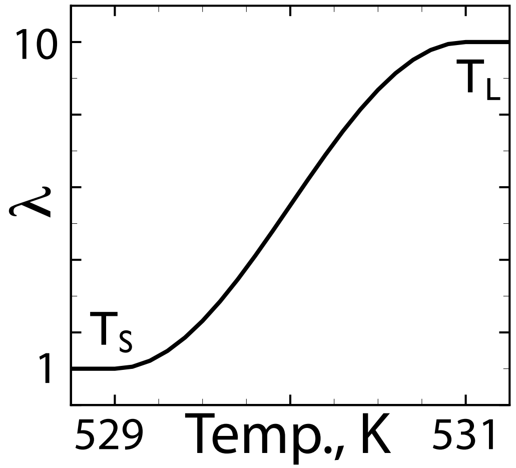
$$r_x = A\left(\frac{P}{P_o}\right)^n \lambda T^m \exp\left[-\frac{(E+\xi\sigma)}{T}\right][\mathrm{X}]$$



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

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

Phase change



Kinetic parameters

Name	n	m	E, K	σ, K	HMX: λ_m
EDC-37	0.5	-2	15030	-1000	10
HMX	0.33	-2.5	14265	-500	10
LX-07	0.33[c]	0	21715	-750	2
LX-10	0.29 [c]	0	21886	-500	2
LX-14	0.42	-2	14985	-700	2
PBX 9501	0.3	-2	15348	-700	20
PBXN-9	0.3[c]	-2	14838	-900	20

Temperature, reaction extent, and phase change accelerate rates

Effective capacitance method

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

Details

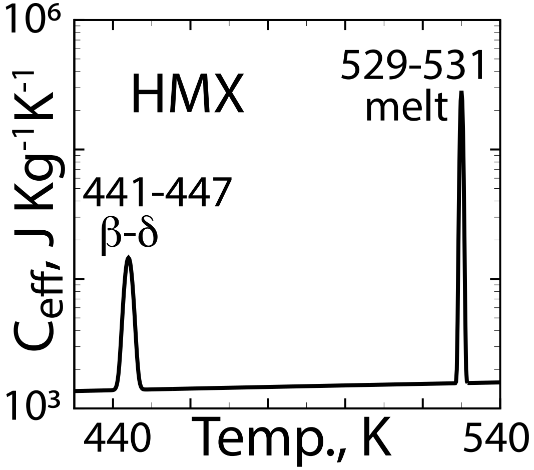
$$C_{eff} = C_p + \frac{\omega h_l}{\sigma\sqrt{2\pi}} e^{-\frac{z^2}{2}}$$

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

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

Thermophysical properties

Name	T, K	C_p, J/kgK	k, W/mK
EDC-37 1834 kg/m³	300	990	0.31
	320	1082	0.37
	349	1216	0.37
HMX 1630 kg/m³	300	1094	0.25
	623	1760	0.25
LX-07 1864 kg/m³	300	1206	0.35
	441	1735	0.35
	447	1758	0.24
	700	2706	0.24
LX-10 1844 kg/m³	300	1206	0.50
	441	1735	0.50
	447	1758	0.30
	700	2706	0.30
LX-14 1780 kg/m³	300	1084	0.32
	441	1550	0.32
	447	1570	0.27
	700	2406	0.27
PBX 9501 1778 kg/m³	300	1084	0.33
	441	1550	0.33
	447	1570	0.21
	700	2406	0.21
PBXN-9 1753 kg/m³	300	1084	0.33
	441	1550	0.33
	447	1570	0.21
	700	2406	0.21



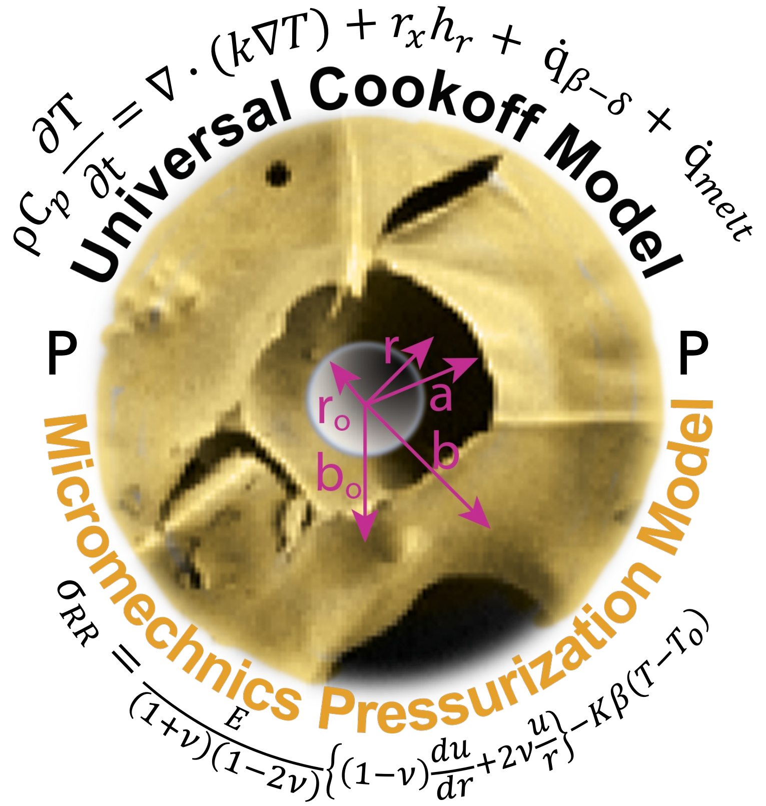
β-δ phase change & melting enthalpies

Name	ω_{HMX}	441-447 K $h_{\beta-\delta}$ = 33000 J/kg $\omega_{HMX}\,h_{\beta-\delta}$	529-531 K 236000 J/kg $\omega_{HMX}\,h_{melt}$
EDC-37	0.91	30030	214760
HMX	1.00	33000	236000
LX-07	0.90	29700	212400
LX-10	0.95	31350	224200
LX-14	0.955	31515	225380
PBX 9501	0.95	31350	224200
PBXN-9	0.92	30360	217120

Phase changes are modeled thermodynamically

Micromechanics pressurization (MMP) model

Initial explosive is impermeable to gases



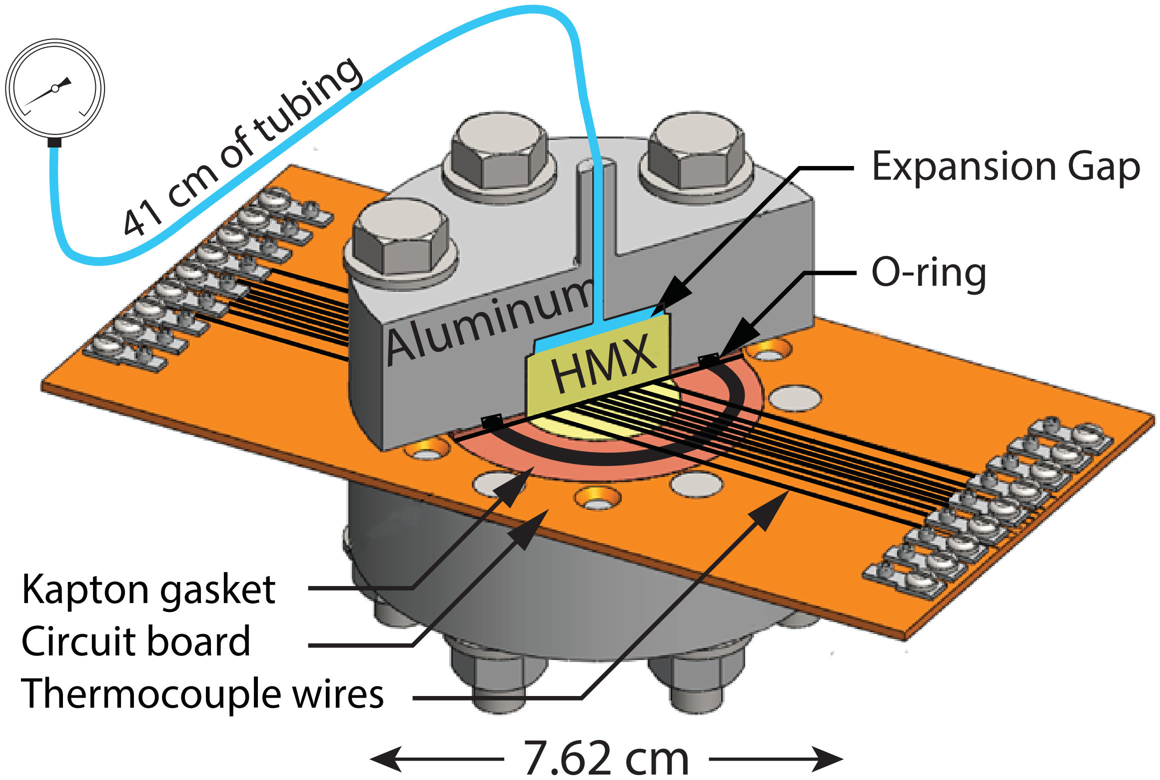
Basics

- 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

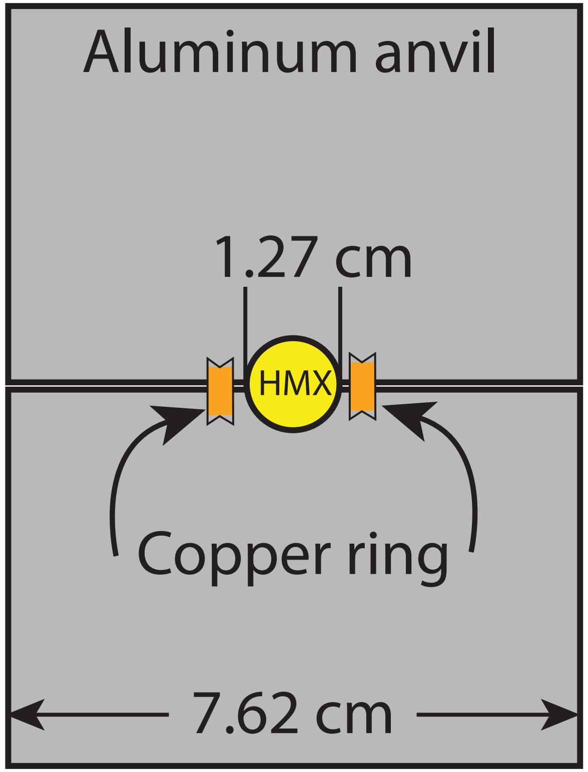
Thermal expansion, thermal damage, and abrupt gas release

SITI and ODTX
(time to thermal ignition)

Sandia Instrumented Thermal Ignition



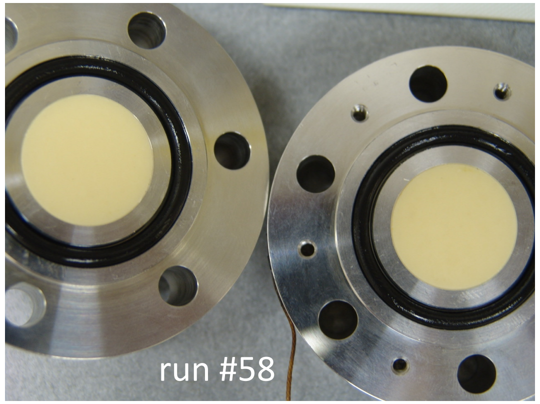
One Dimensional Time-to-eXplosion



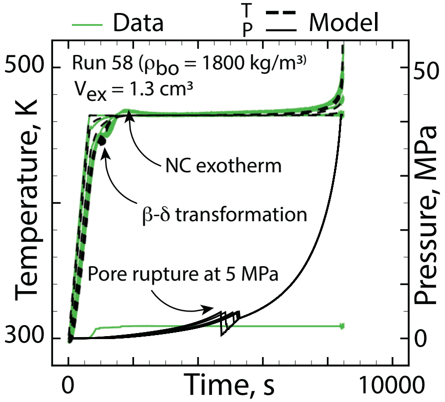
SITI is ramp and hold, ODTX is constant temperature

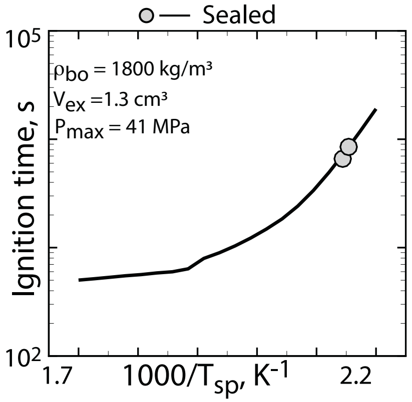
Measurements and Predictions

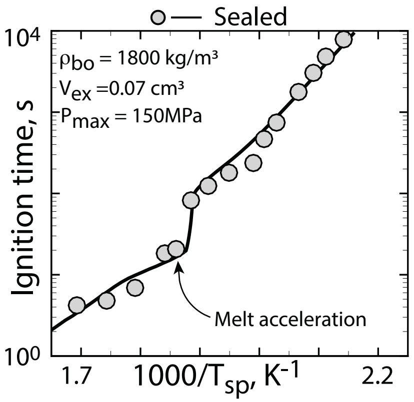
Individual | SITI | ODTX



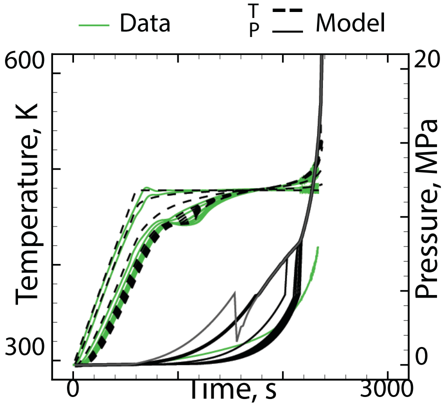
EDC-37

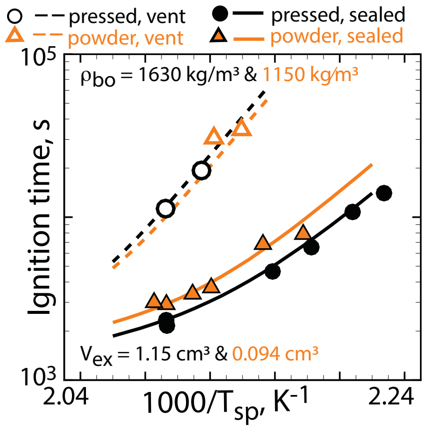


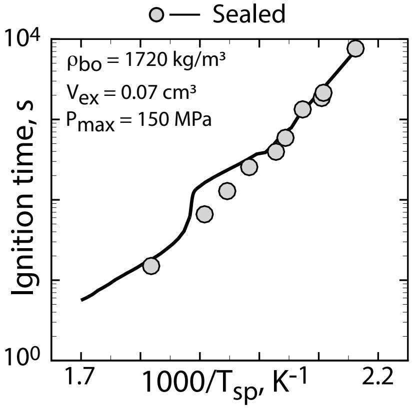




HMX





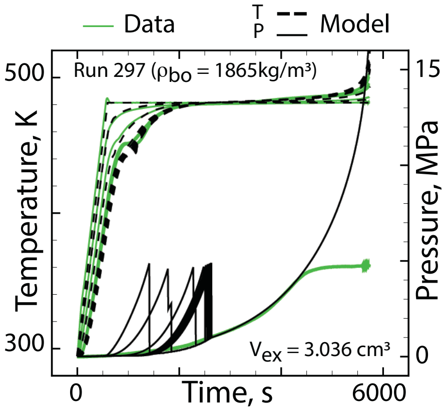


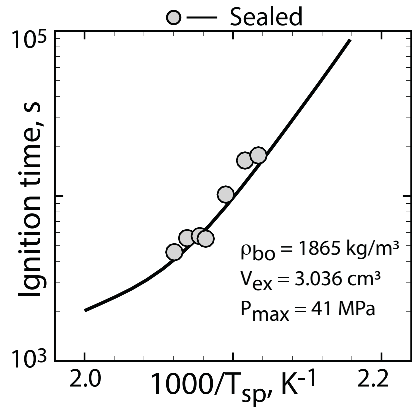
Temperature, pressure, ignition time

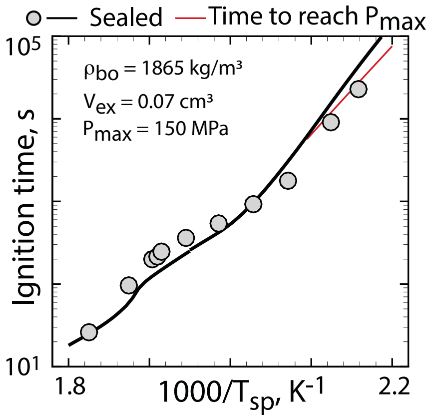
Measurements and Predictions

Individual SITI ODTX

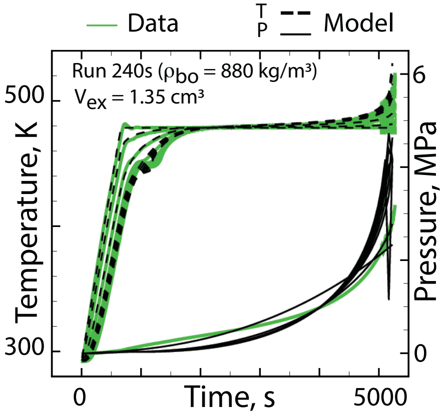
LX-07

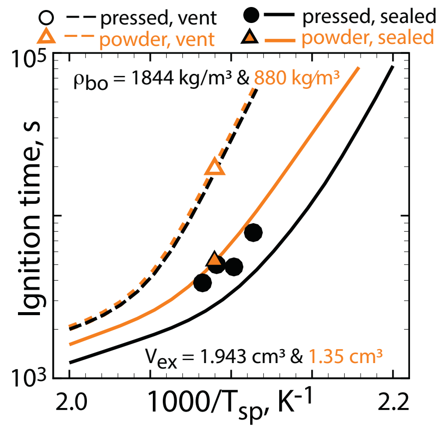


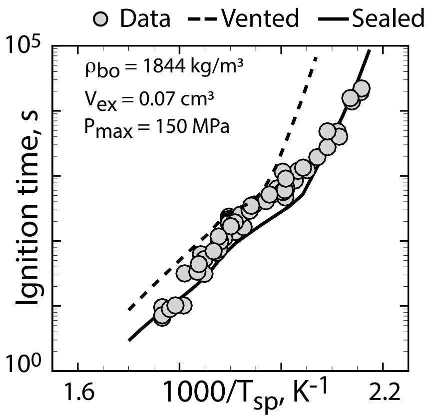




LX-10







Temperature, pressure, ignition time

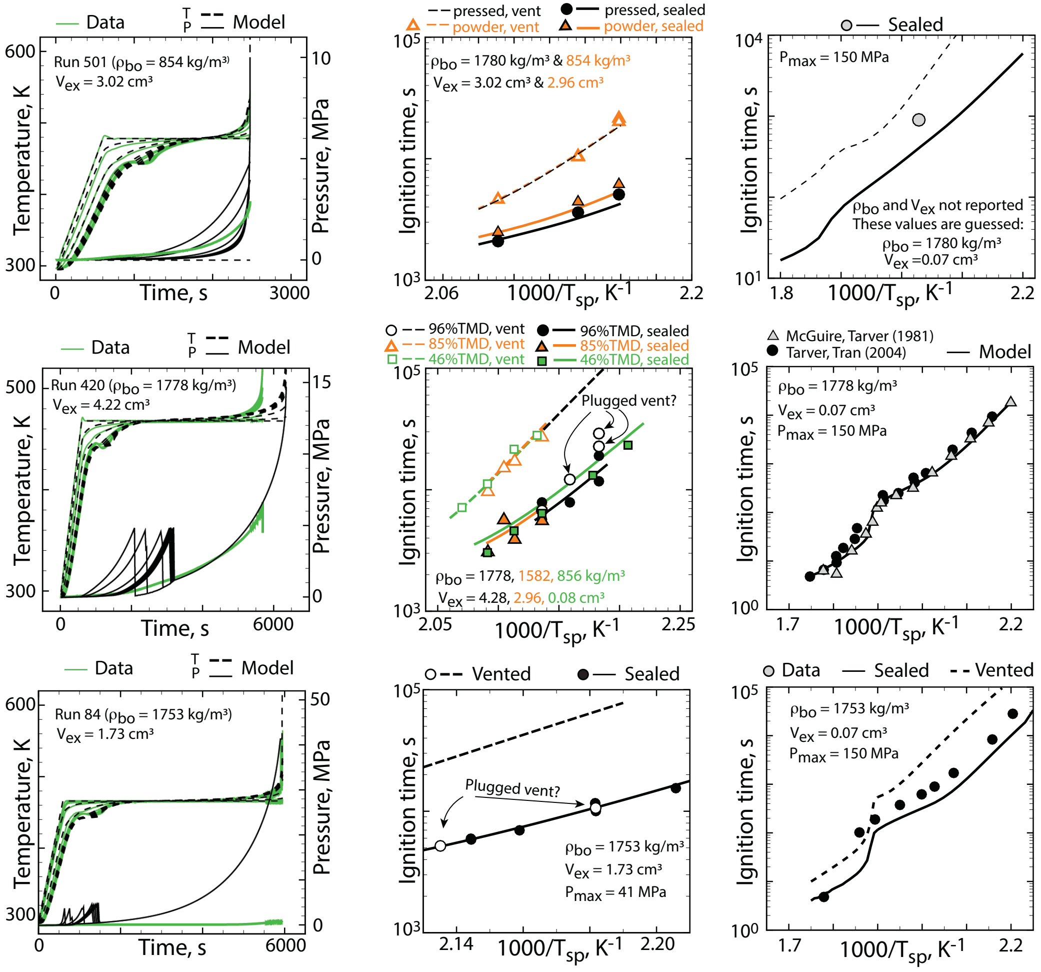
Measurements and Predictions

Individual | SITI | ODTX

LX-14

PBX 9501

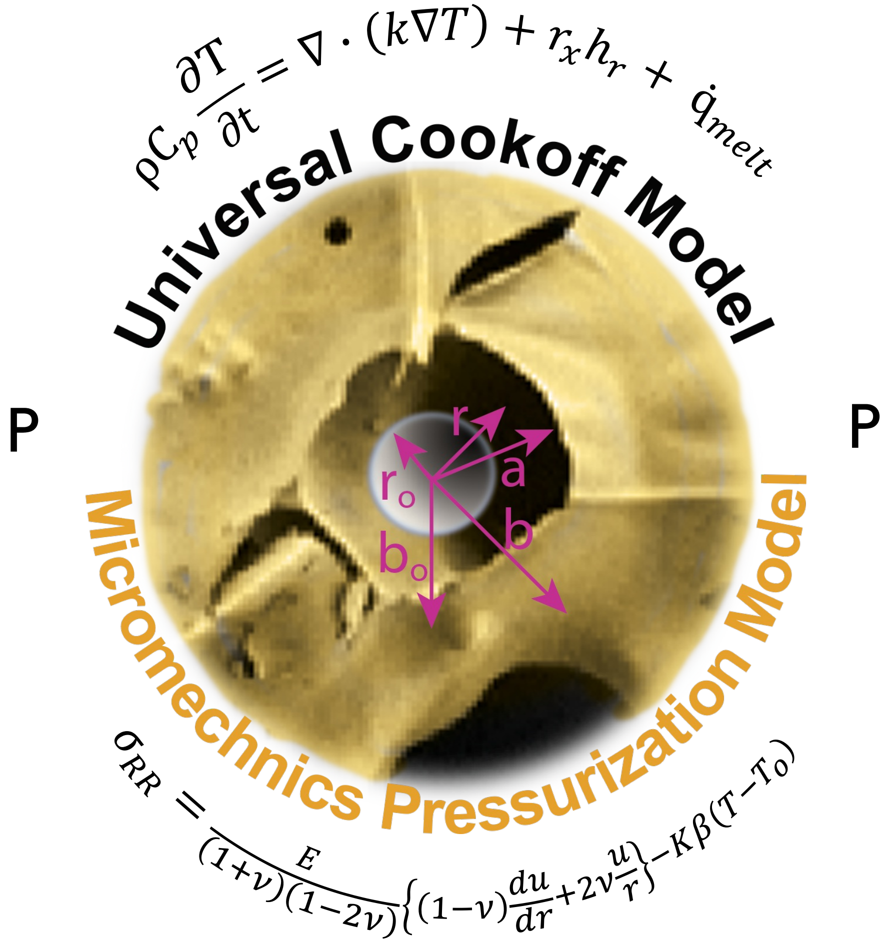
PBXN-9



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



Propell. Explos. Pyrotech., 47 (2022)

1-step UCM/MMP model completed 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