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A Universal Cookoff Model (UCM) coupled to a MicroMechanics Pressurization (MMP) model

Michael L. Hobbs

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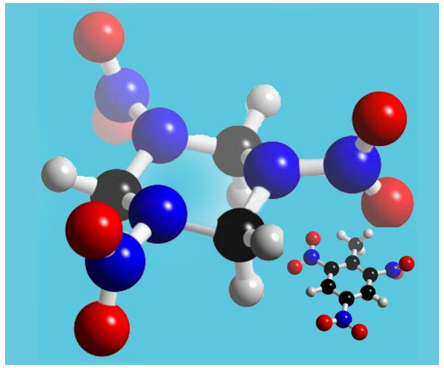
U.S. DEPARTMENT OF ENERGY

NNSA

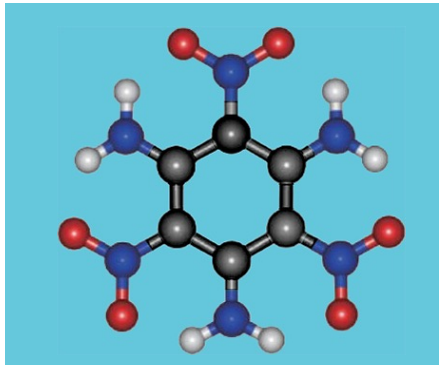
Universal Cookoff Model (UCM)

USS Forrestal 134 deaths

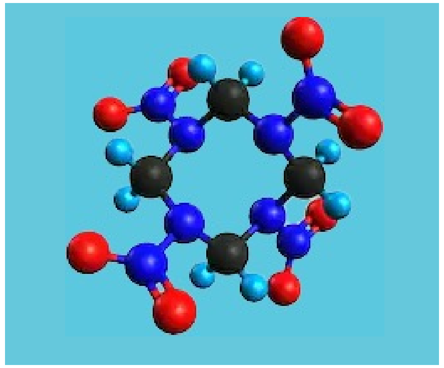
RDX (Comp-B)



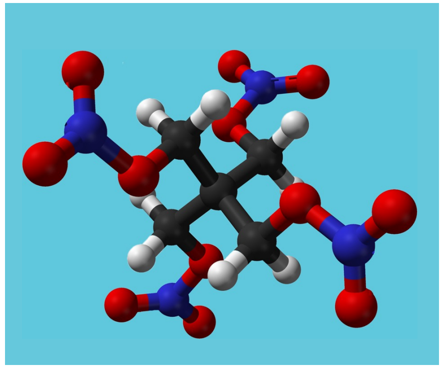
TATB (PBX 9502)



HMX (PBX 9501)



PETN



Original

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	$S \overset{1}{\rightarrow} S_g$, adsorbed gases (e.g. moisture) $E \overset{2}{\rightarrow} \alpha G_E + \beta C_E$, Condensed-phase dominant ($r_2 \neq f[P]$) $E \overset{3}{\rightarrow} \alpha G_E + \beta C_E$, Gas-phase dominant ($r_3 = f[P]$) $B \overset{4}{\rightarrow} \gamma G_B + \delta C_B$, 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	$\xi_1 = \mathrm{invnorm}\left(\frac{[S]}{[S_o]}\right); \xi_2 = \xi_3 = \mathrm{invnorm}\left(\frac{[E]}{[E_o]}\right); \xi_4 = \mathrm{invnorm}\left(\frac{[B]}{[B_o]}\right)$

Current

Use the following modified Arrhenius rate expression for each reactive component:

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

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

The form of the rate expression is key

(Comp-B mechanism used as example)

Cosine ramps are currently used for the acceleration terms to permit precise specification of the temperature where the rates change.

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

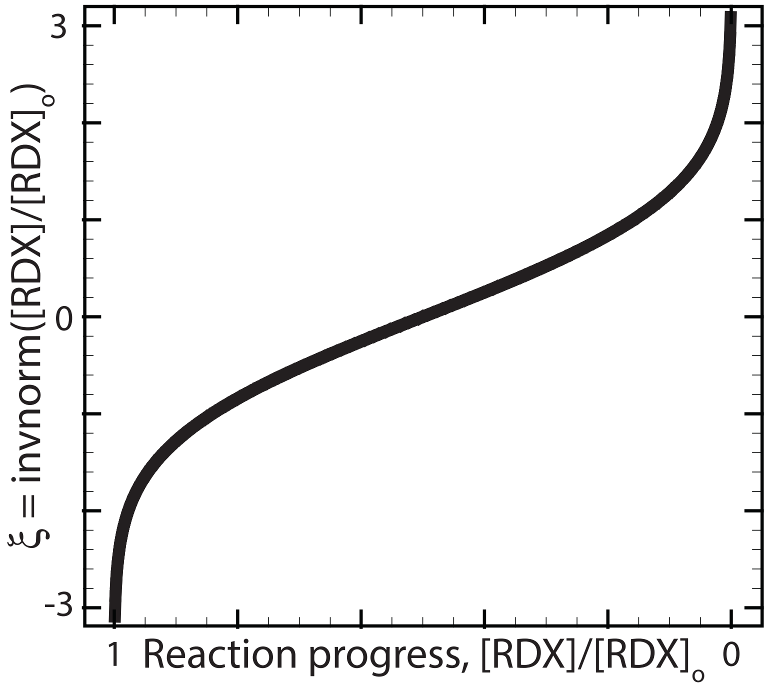
$$\lambda_1 = 1 + 0.5\left[1 + \tanh\left(\frac{T - 474}{2}\right)\right]\times 49$$

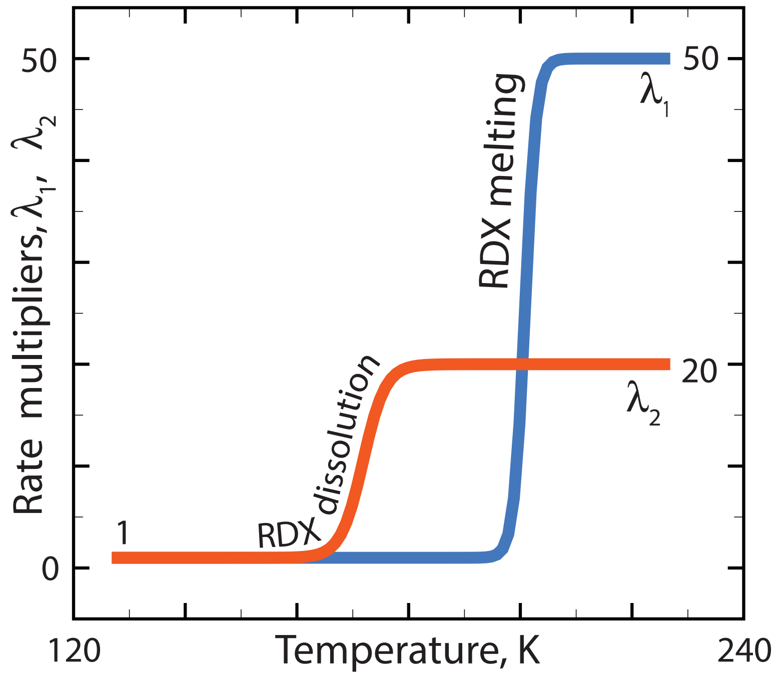
$$\lambda_2 = 1 + 0.5\left[1 + \tanh\left(\frac{T - 445}{4}\right)\right]\times 19$$

Flexibility

Negative σ autocatalytic
Positive σ diffusion limited
σ Fit with pressure profile data
E fit with vented data
n fit with sealed data
m fit with ignition data
λ fit with ignition data

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

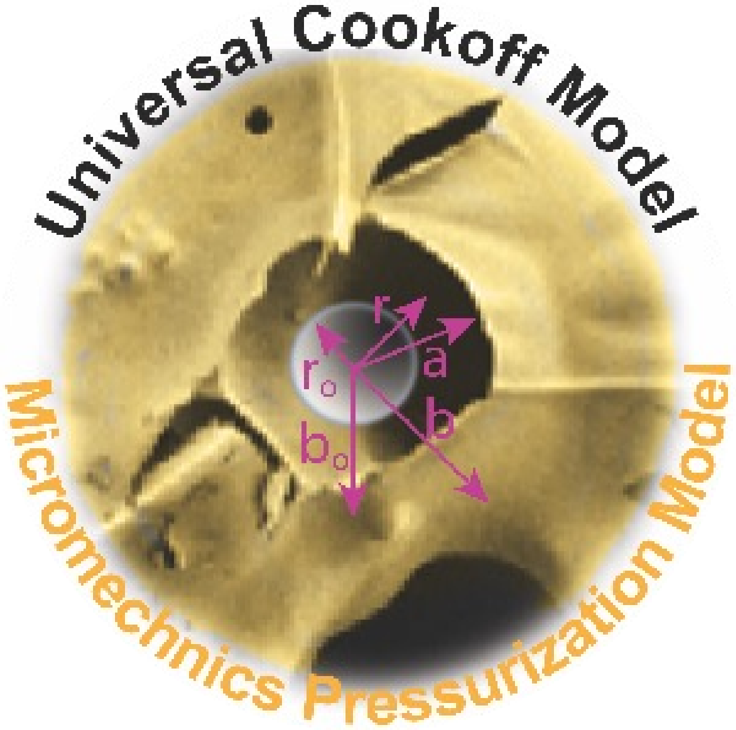


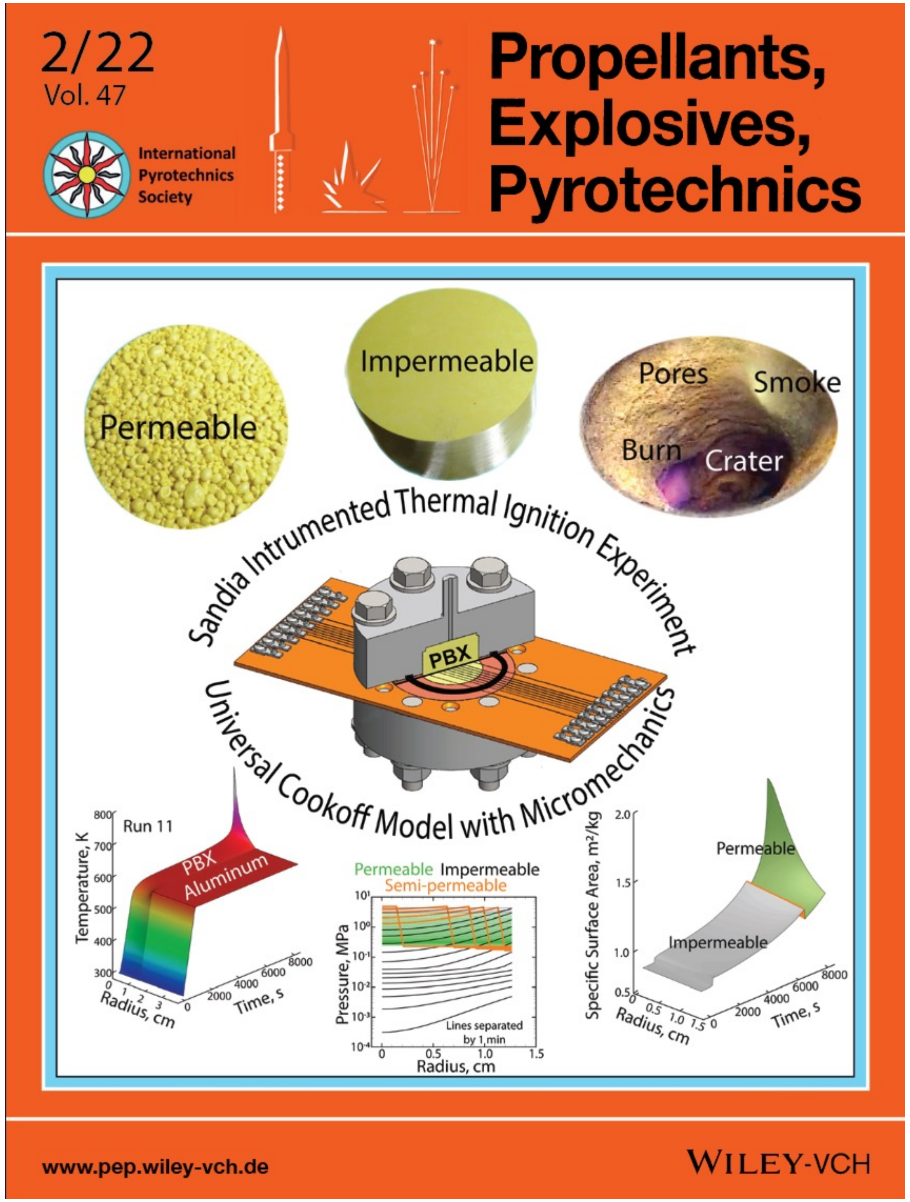


A single modified Arrhenius rate expression can fit data as good or better than multiple Arrhenius rate expressions.

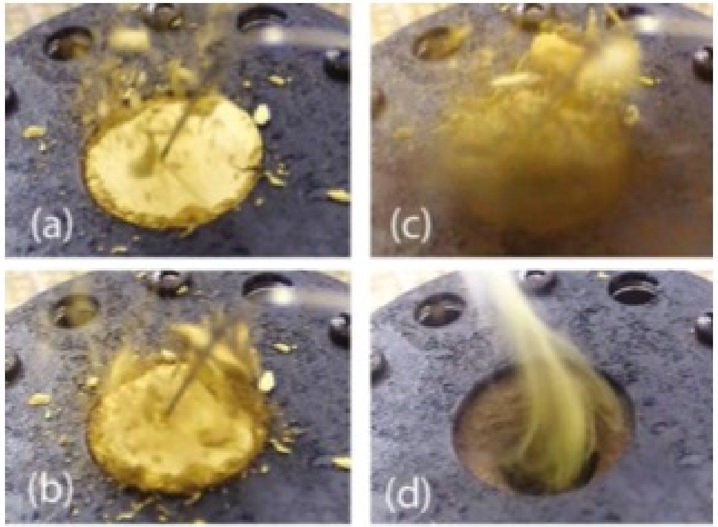
Micromechanics Pressurization model

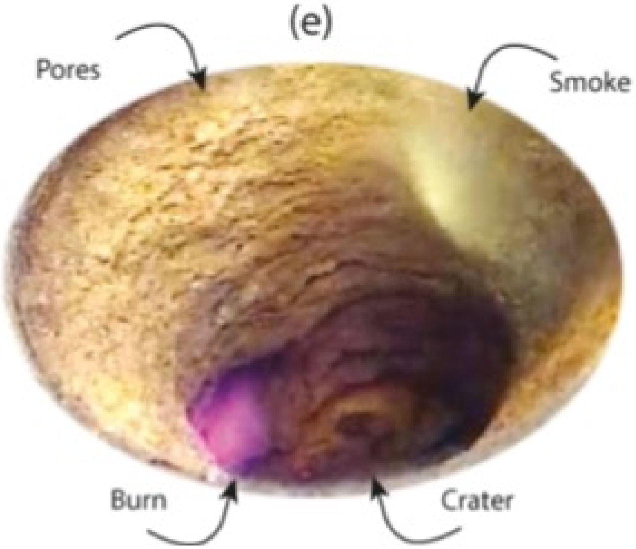
MicroMechanics Pressurization (MMP) model developed for high density explosives where the decomposition gases are initially impermeable to decomposition gases

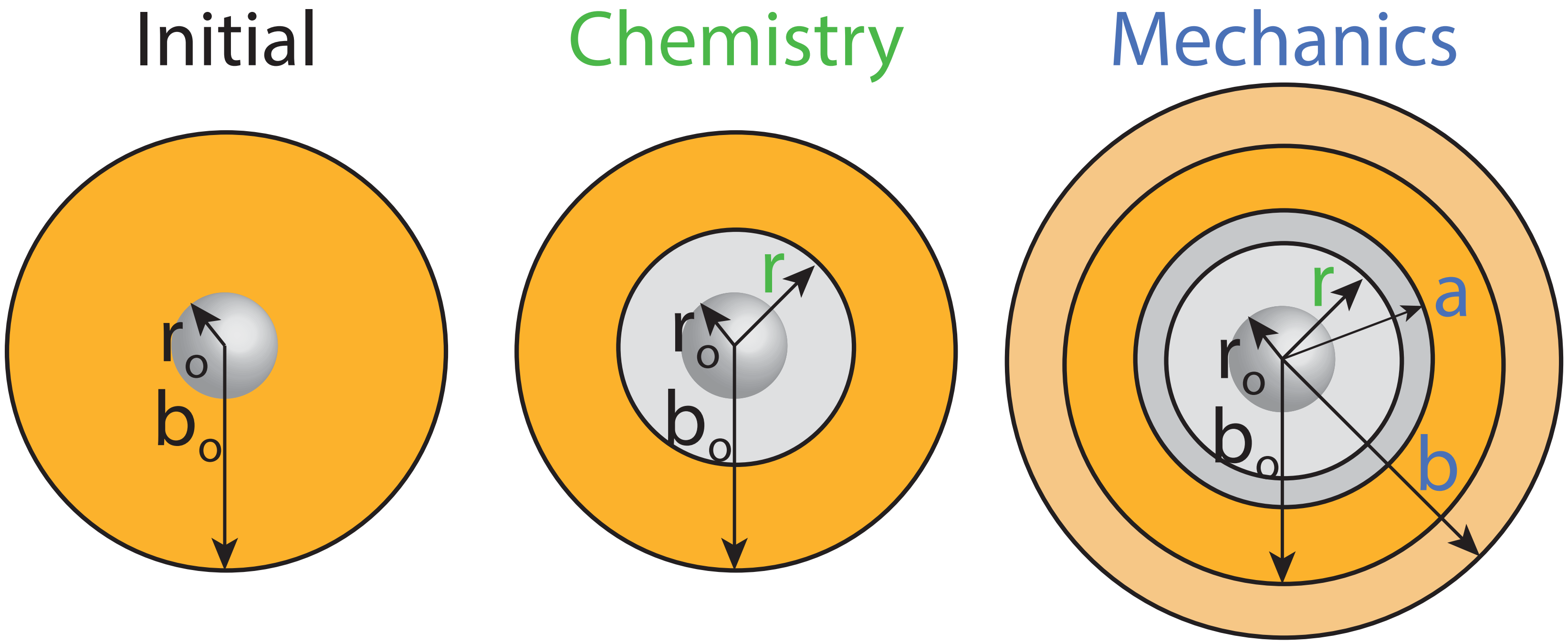




Micromechanics Pressurization model







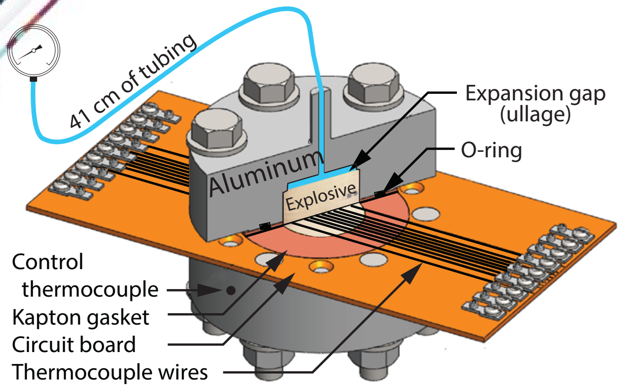
r_o Initial defect radius.
b_o Half the initial distance between defects.

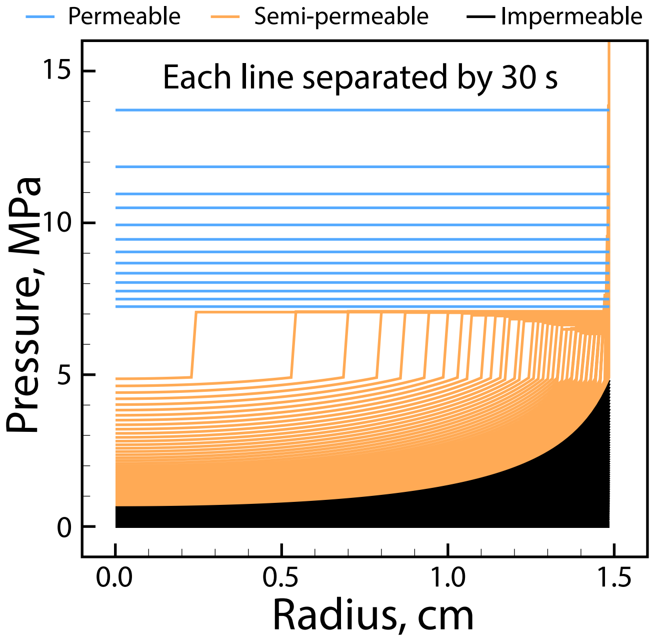
r Initial radius plus radial increase due to decomposition.

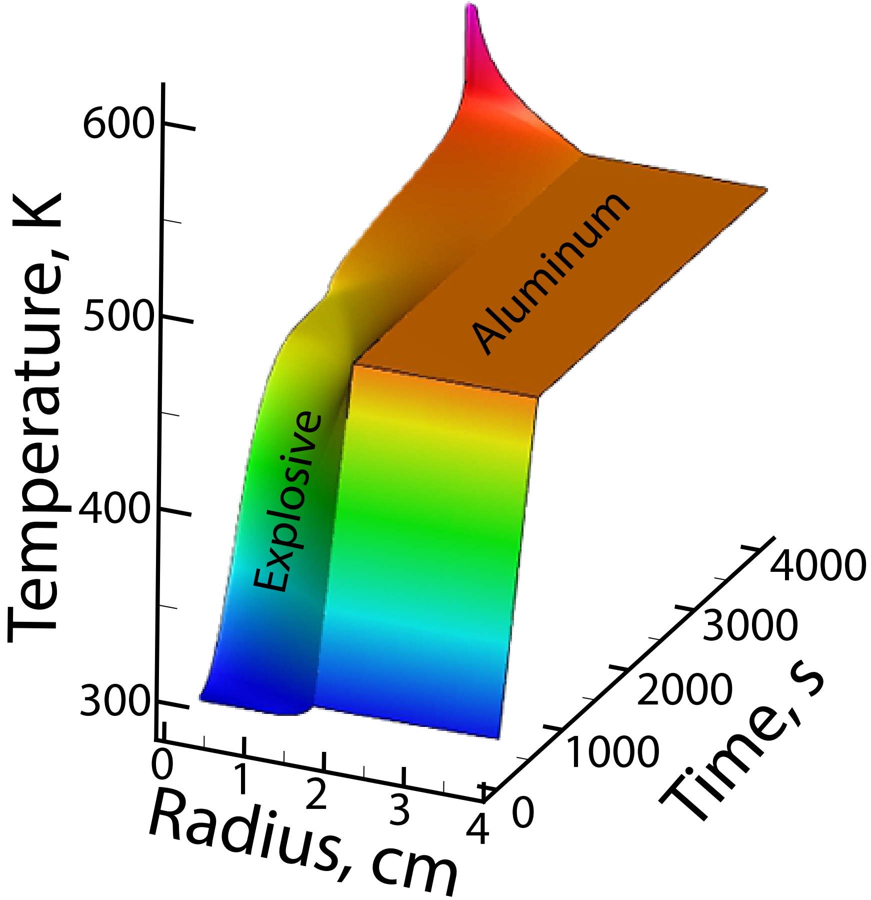
a Defect radius resulting from chemistry and mechanical deformation.
b Half the distance between defects.

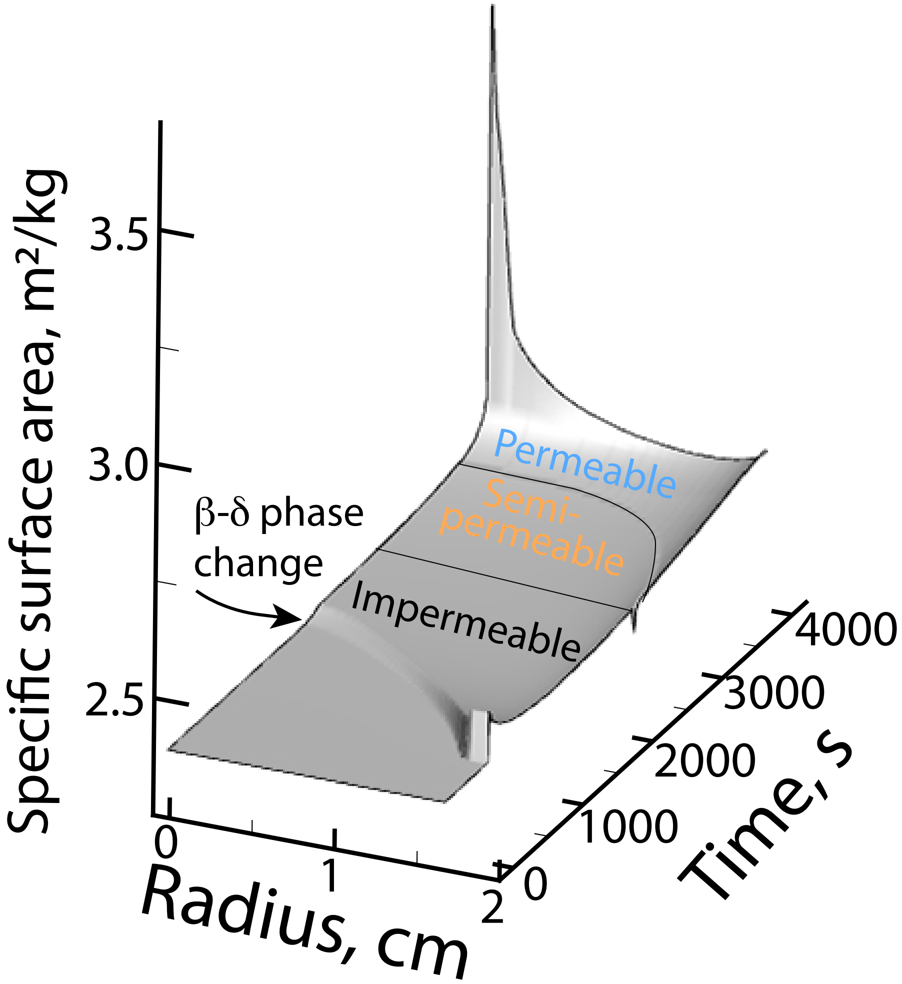
MMP model gives better pressure for high-density pressed explosives (e.g., PBX 9501, PBX 9502, etc.)

MMP predicts thermal damage in HMX based explosive







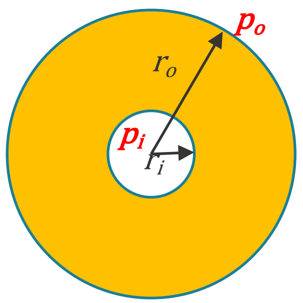


Combined UCM/MMP model predicts transient evolution of permeability.

Micromechanics pressurization MMP model

Micromechanical Pressurization (MMP) model

- Based on simple analytic expressions for deformation in a spherical pressure vessel



radial stress at inner surface:

$$\sigma_{rr} = \frac{p_o r_o^3}{r^3}\frac{r^3 - r_i^3}{r_i^3 - r_o^3} + \frac{p_i r_i^3}{r^3}\frac{r_o^3 - r^3}{r_i^3 - r_o^3}$$

displacement at inner surface:

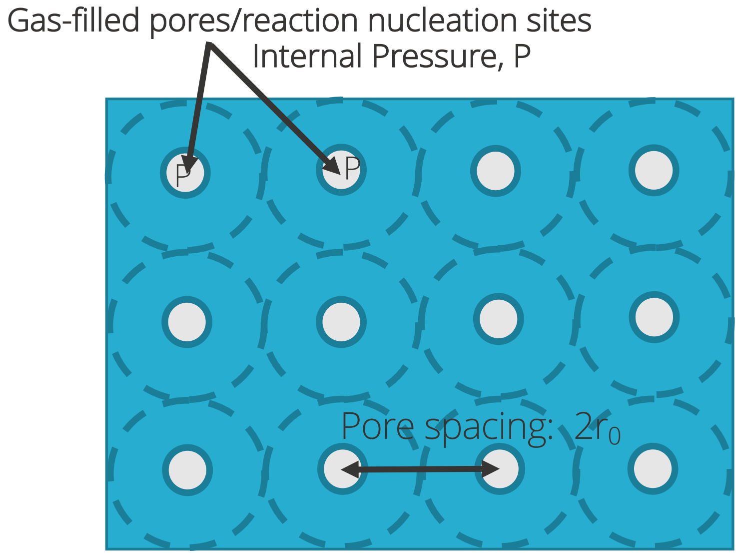
$$u_{r=r_i} = \frac{3(p_i - p_o) r_i r_o^3}{4E\left(r_i^3 - r_o^3\right)}$$

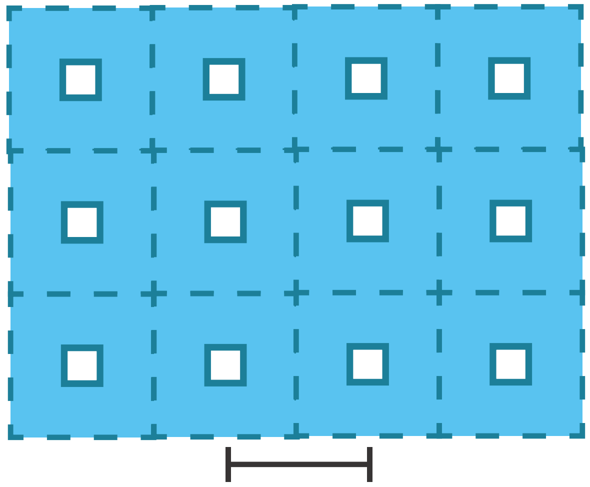
The idea is that one can:

1. determine the effective pore size and internal pressure by balancing the internal gas with material strength properties;
2. use internal pressure in chemical reaction models;
3. start to address permeability prediction (so far used in a gross sense, either "non permeable" or "fully permeable") by using percolation limits of pore density and size;
4. do this without having to resort to an expensive full poromechanics formulation & code (i.e. it is still tractable).

Use mesoscale FE modeling to investigate some key assumptions of MMP model:

- How reasonable is the assumption that pores remain isolated from each other as they grow from chemical reaction producing gases?
- At what conditions would interactions of pores produce "connectedness" which would allow permeation of gases?
- Are there aspects from a group (rather than single pore) analysis which would help improve MMP model?
- Etc.
- Status: work in progress, plan to continue through FY22



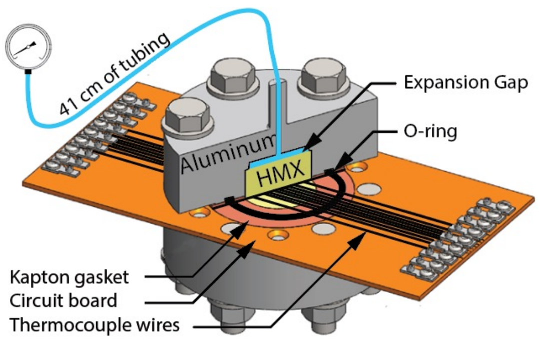


Pore spacing is $\sim 2b_o$

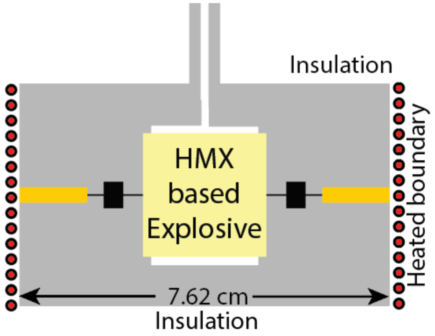
Model couples chemistry and mechanics.

UCM/MMP ARIA implementation of HMX/NC/K10 of SITI

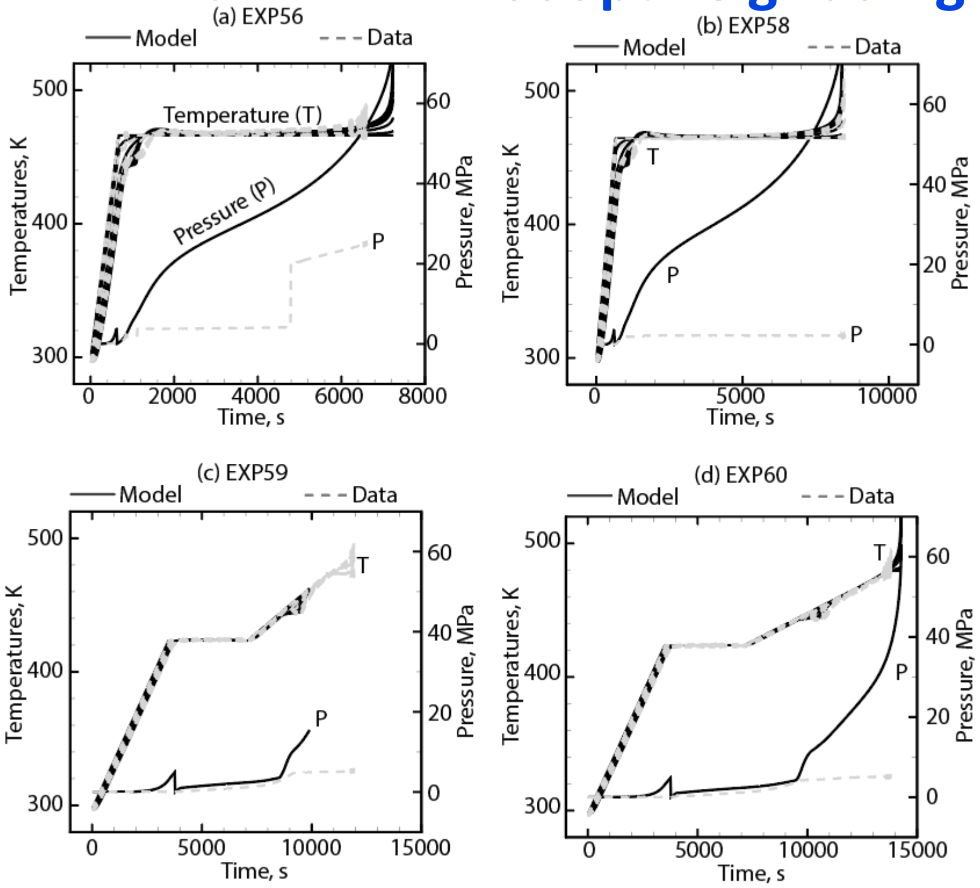
SITI configuration



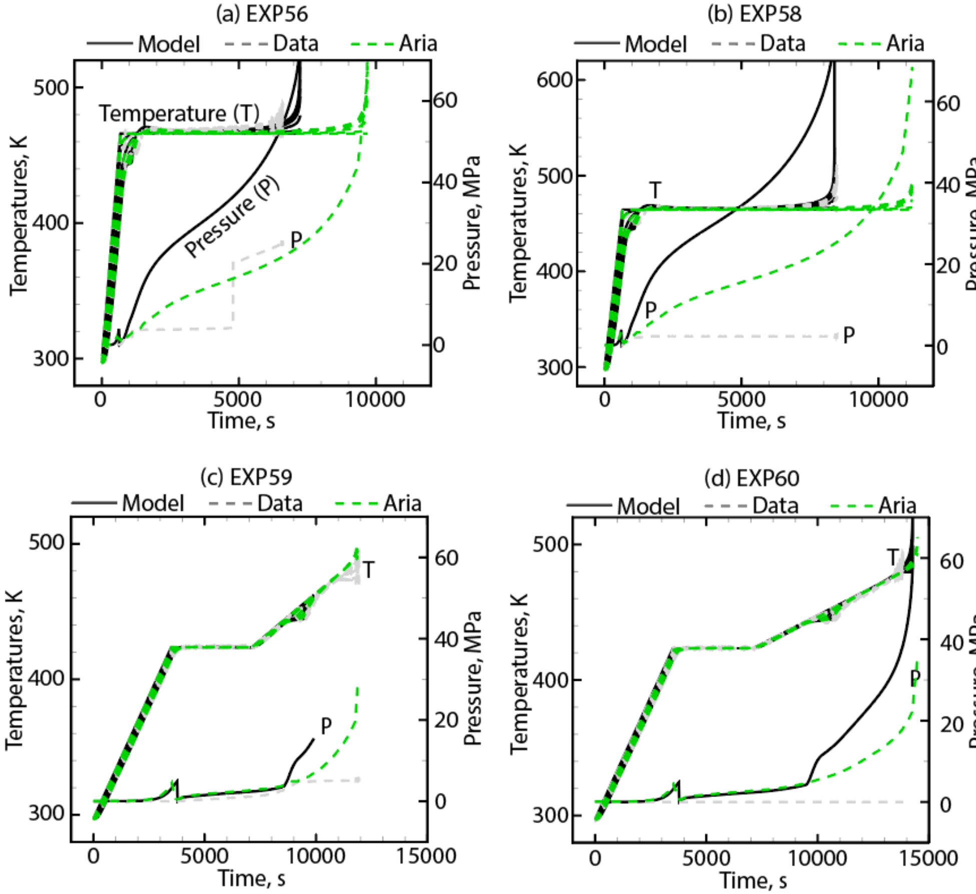
SITI schematic



XCHEM—1D adaptive gridding



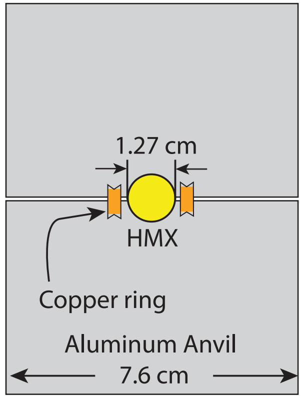
ARIA—2D axisymmetric



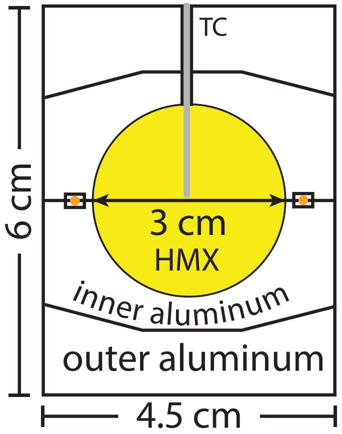
ARIA model lacks volume change associated with β–δ polymorph

UCM/MMP ARIA implementation of HMX/NC/K10 of ODTX and ODTV

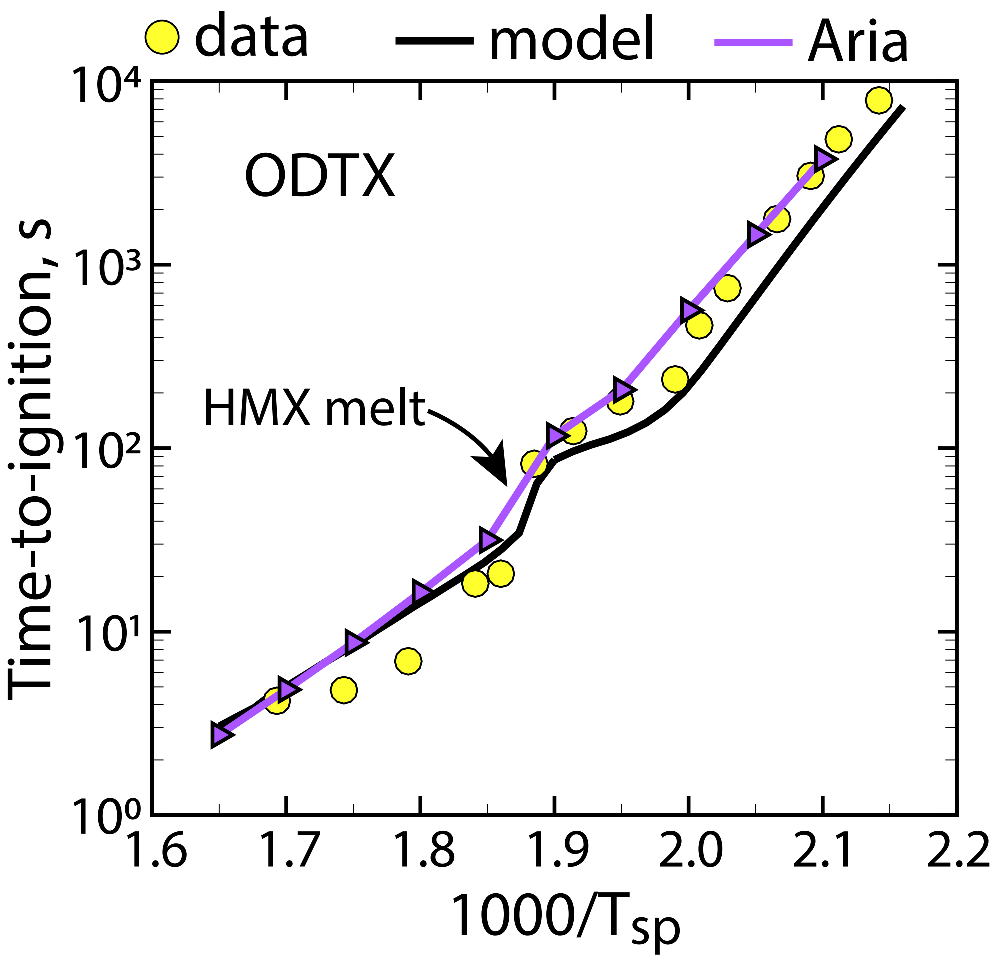
ODTX schematic



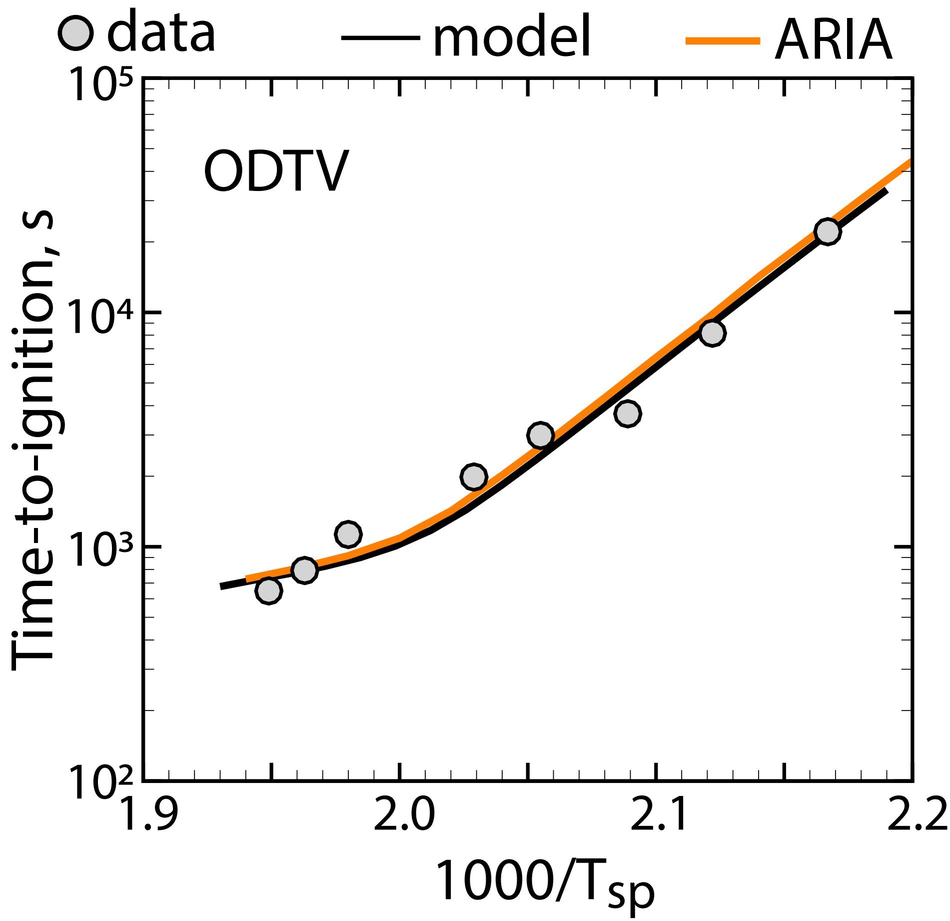
PDTV schematic



ODTX simulations

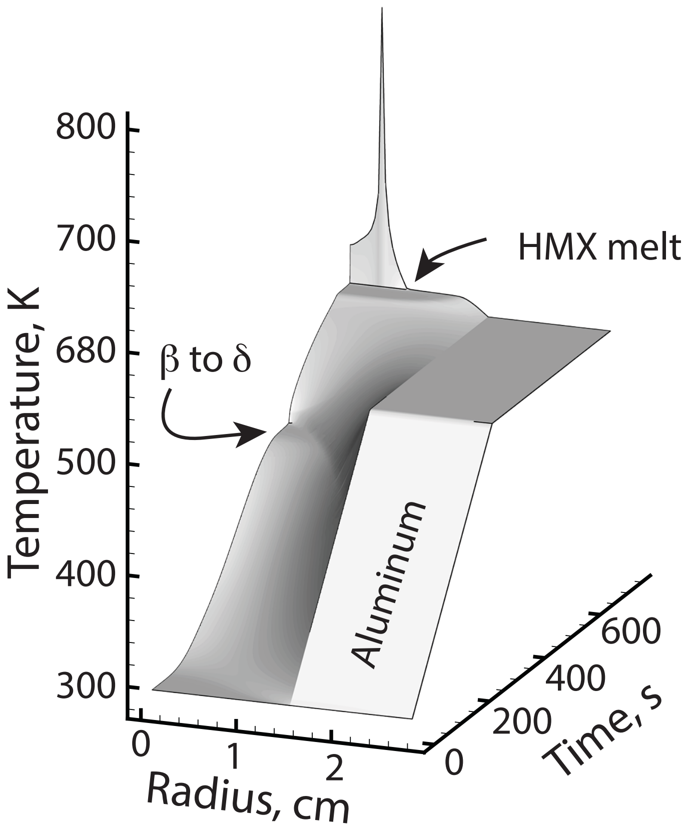


ODTV simulations

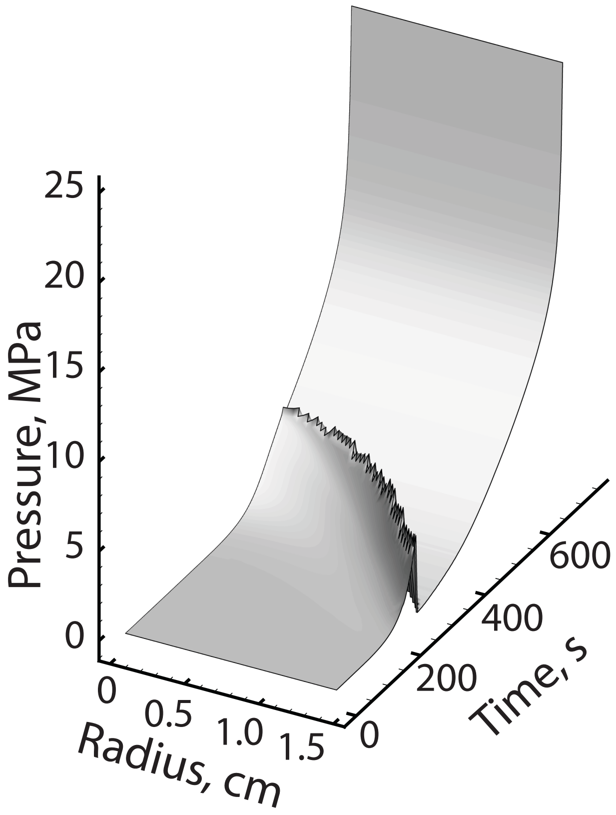


UCM/MMP Predictions of Thermal Damage in ODTV

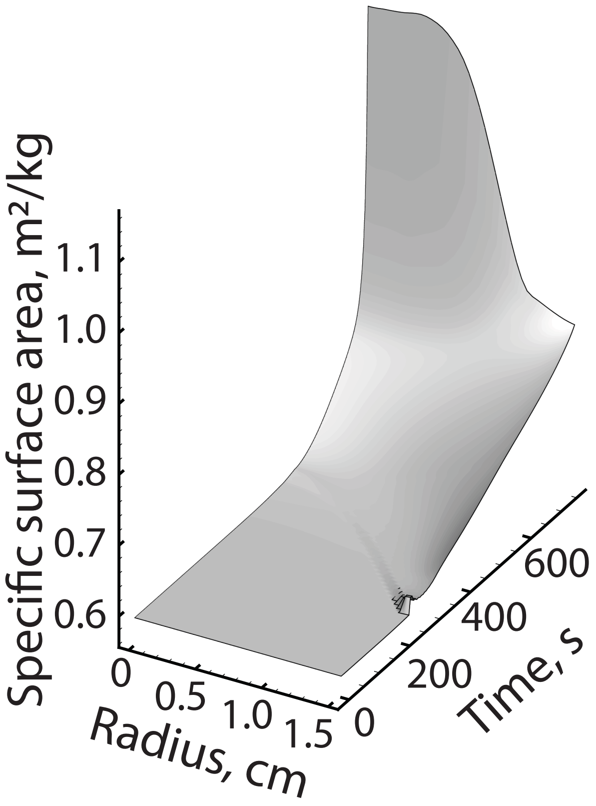
Temperature



Pressure

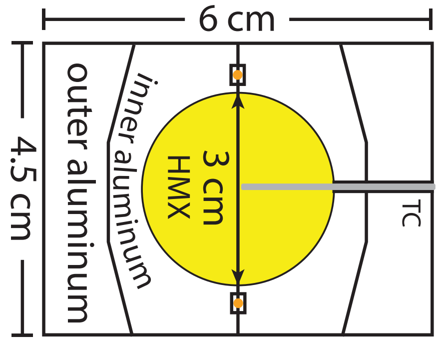


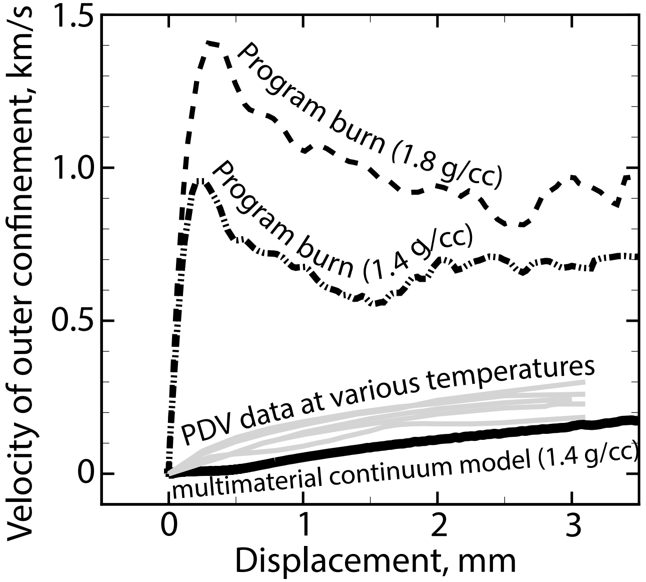
Surface Area

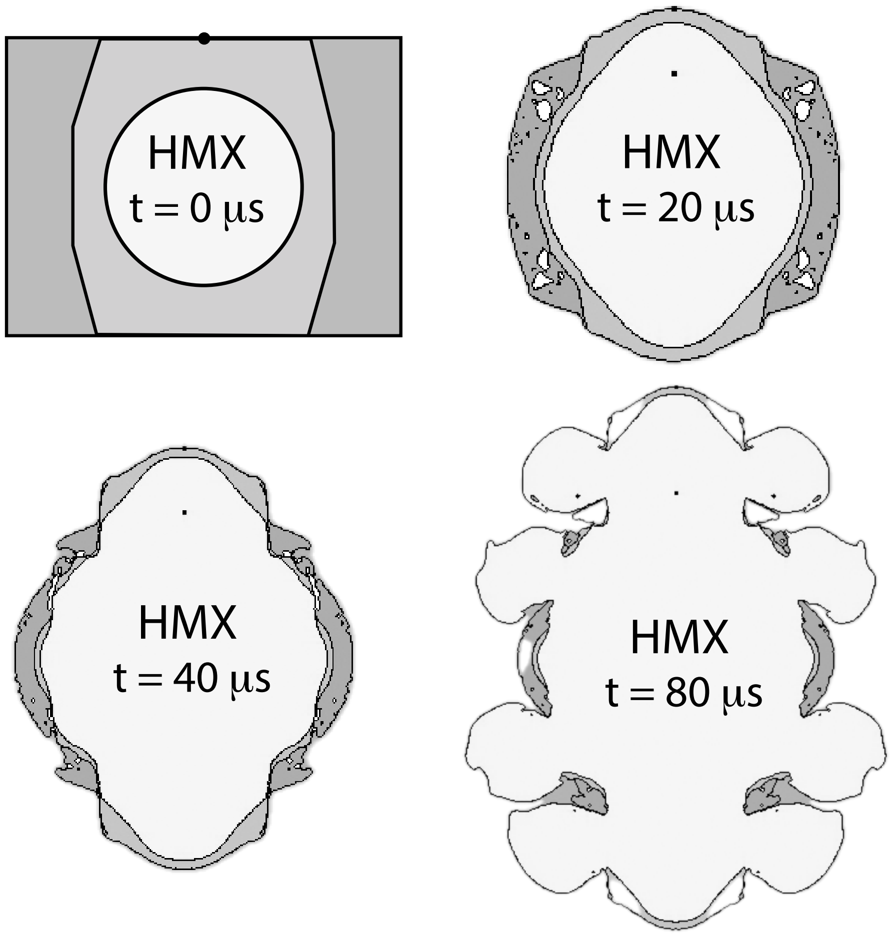


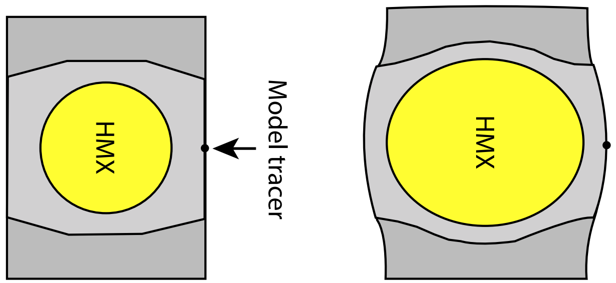
Challenge is to incorporate these results into violence predictions.

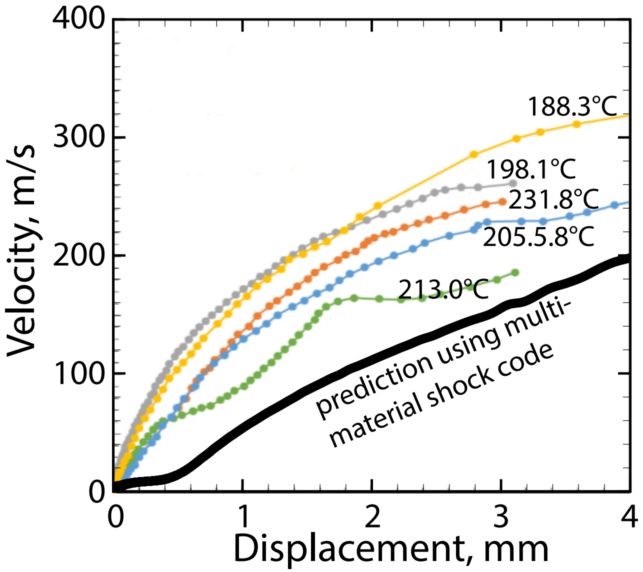
Programmed burn vs multimaterial DDT







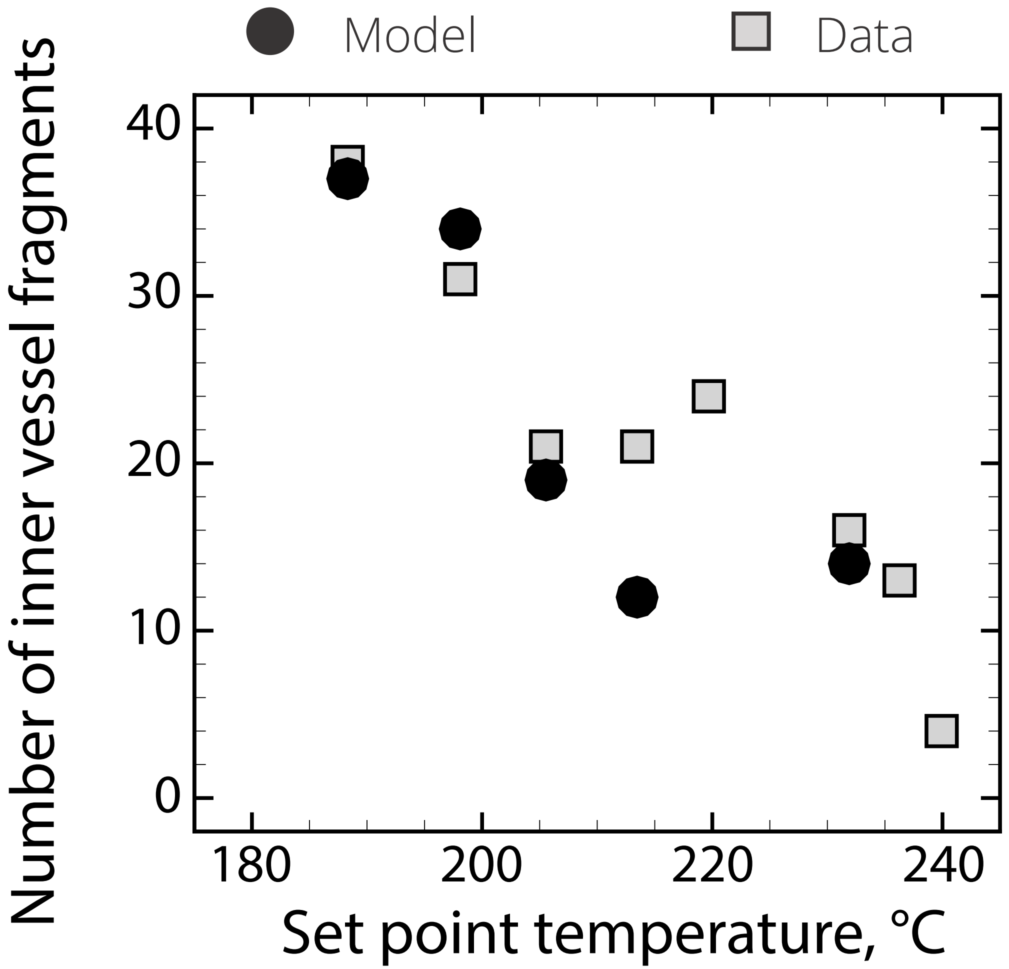




Programmed burn is not close. However, DDT models are promising even though the density used was only 1.4 g/cc and the VCCT was 1.8 g/cc

Fragmentation based on fracture toughness

$$s = \left(\frac{\sqrt{24}K\left(1 - \frac{T}{T_m}\right)^n}{\rho c \dot{\varepsilon}} \right)$$



M. E. Kipp, D. E. Grady and J. W. Swegle, *International Journal of Impact* Engineering, 1993, **14**, 427.

The agreement was obtained by judicious selection of the temperature exponent n (-3.5) in the equation and usage of the experimentally measured velocities rather than the predicted velocities.

Summary and conclusions

- UCM model uses 1 modified Arrhenius rate for each reactive ingredient.
- UCM reaction rate is a function of temperature, pressure, phase
- MMP model determines effective pore size by balancing internal gas generation with mechanical strength.
- UCM/MMP models can be calibrated with two experiments, but cannot model aging without additional experimetns.
- UCM/MMP model has been validated with several materials and is native in SIERRA/ARIA
- Model is sensitive to both temperature and pressure.
- Post-ignition violence was estimated based on DDT simulations