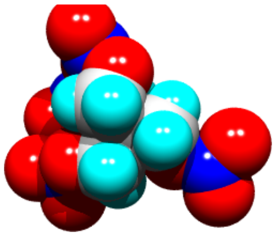
SAND2009-7672C

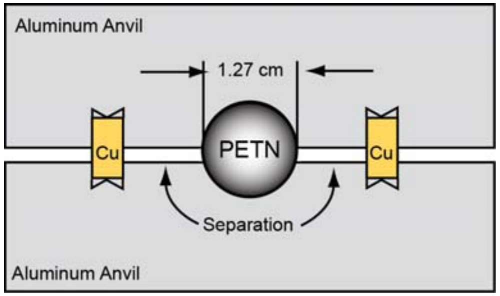


MODELING PETN IGNITION

Michael L. Hobbs

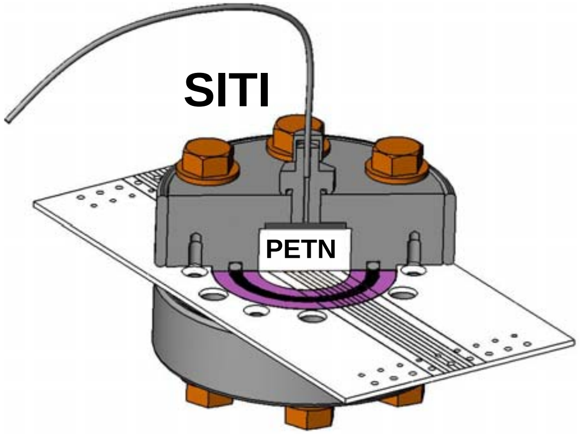
Sandia National Laboratories
Albuquerque, New Mexico

ODTX



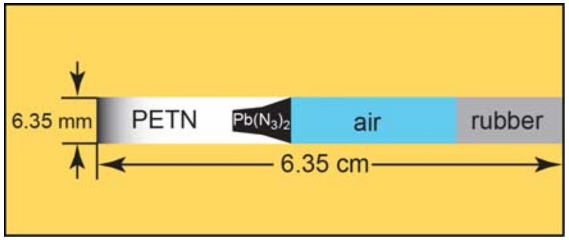
1.8 grams in ~1 cc

SITI



21.7 grams in ~13 cc

Detonator



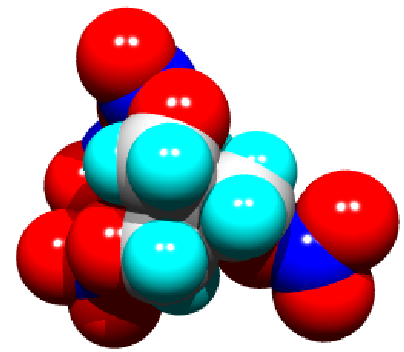
0.5 grams in ~0.7 cc

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

Why study PETN ignition?

- **Used extensively in military and civilian applications**

- **Used in numerous explosives**
  - **LX-02 (73.5% PETN, 17.6% butyl rubber, 6.9% acetyltributyl citrate, 2% Cab-O-Sil)**
  - **LX-08 (63.7% PETN, 34.3% Sylgard, 2% Cab-O-Sil)**
  - **LX-16 (98% PETN, 4% FPC 461)**
  - **Pentolite (50% PETN, 50% TNT)**
  - **PEP-3 (86% PETN, 14% plasticizing oil)**
  - **PTX-2 (43.2%RDX, 28% PETN, 28.8% TNT)**
  - **Semtex 1A (87% PETN, dye, antioxidants, plasticizer, binder)**
  - **Semtex 10 (82% PETN, dye, etc.)**



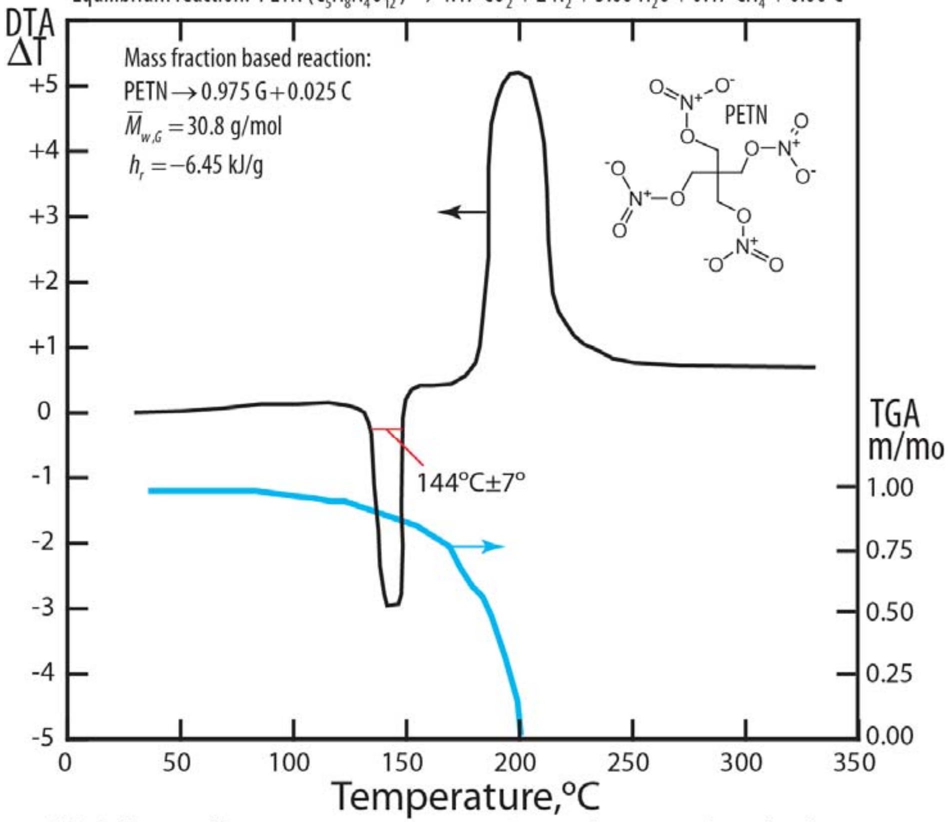
- **Standard booster and bursting charge**
  - **Small caliber ammunition**
  - **Detonators**
  - **Explosive core of detonation cord**

- **Explosive chosen by Richard Reid (shoe bomber)**

YouTube video of 20 g of PETN cutting down tree

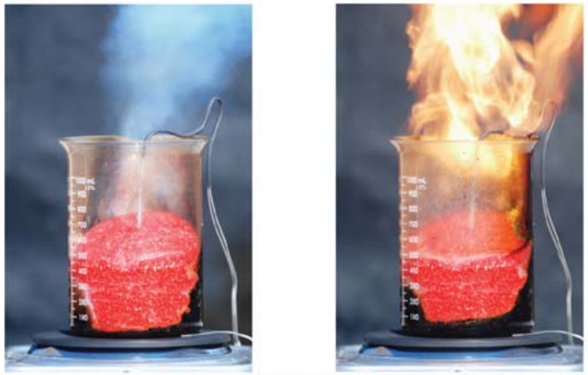
Some observations

Equilibrium reaction: PETN ($C_5H_8N_4O_{12}$) $\rightarrow$ 4.17 CO_2 + 2 N_2 + 3.66 H_2O + 0.17 CH_4 + 0.66 C*



*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 increases with fast, confined decomposition

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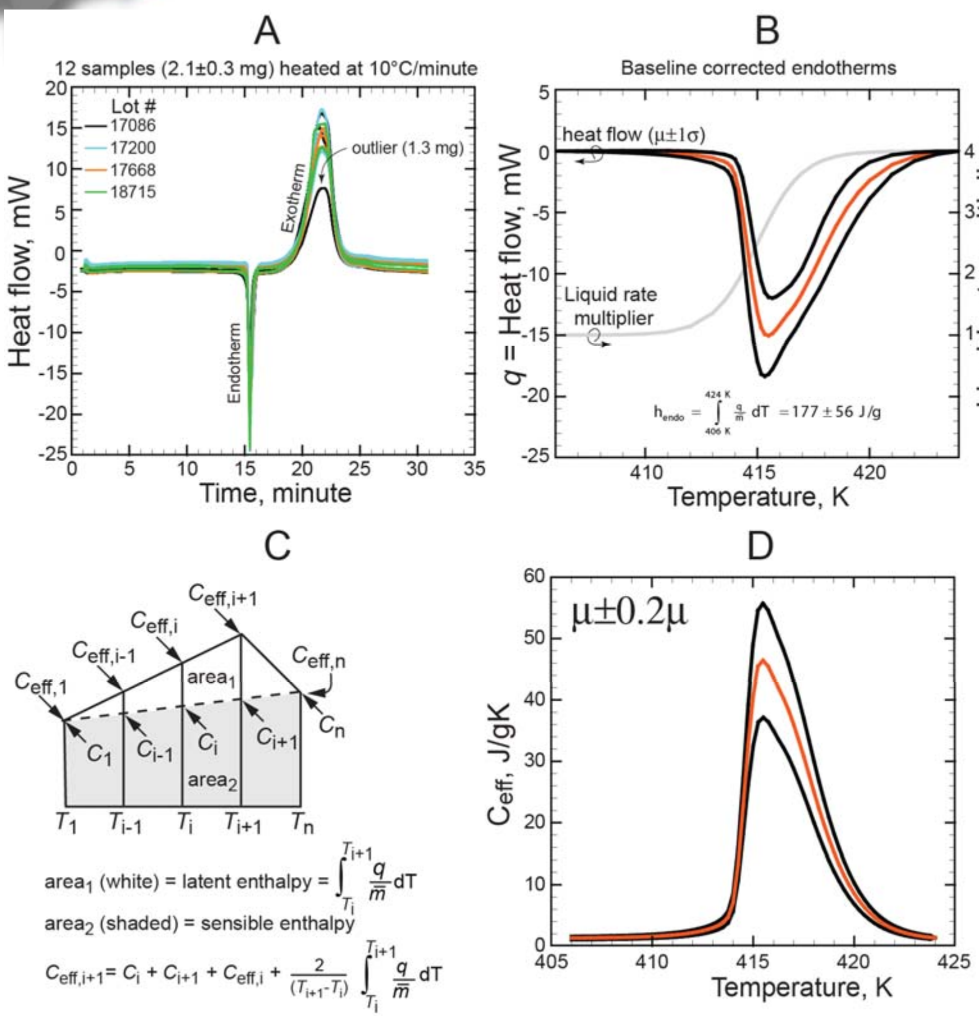
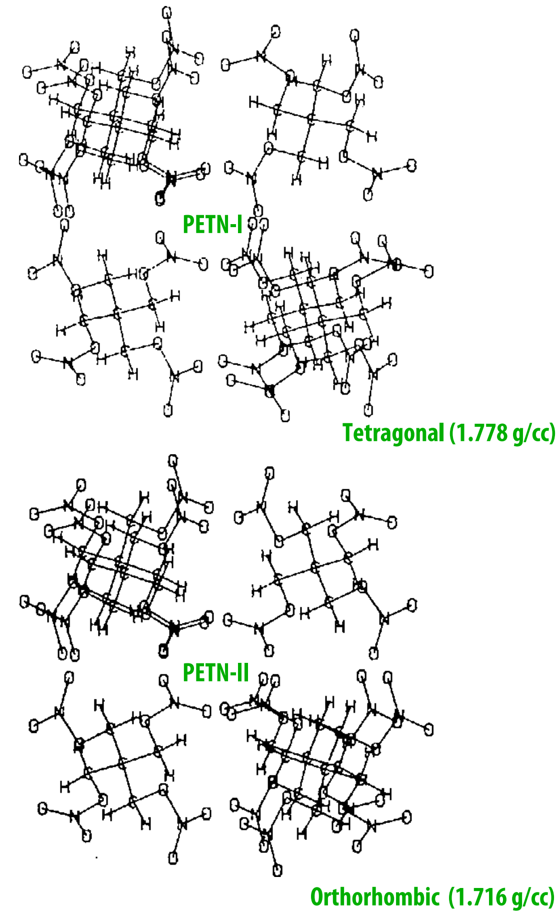
Endotherms modeled using effective capacitance



2 polymorphs



*Cady, HH; Larson, AC, *Acta Crystallographica B(31), 1864 (1975)*

Overlapping endotherms associated with solid-to-solid (PETN-I to PETN-II) polymorphic phase change, sublimation of PETN, and the solid-to-liquid phase transition (i.e. melting).

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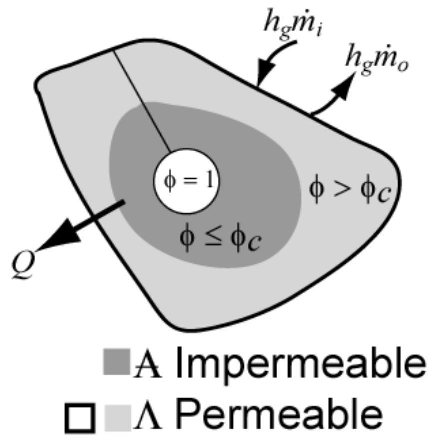
PETN ignition model

Gas continuity (integral)	$\frac{dM_g}{dt} = \int_\Lambda r \rho_c^o \left(1-\phi^o\right) d\Lambda + \dot{m}_i - \dot{m}_o$	(1)
Gas momentum (low Mach)	$P(x,y,z,t) = P(t) = M_g \Big/ \int_\Lambda \frac{M_{wg}}{RT} d\Lambda$	(2)
Energy (integral: bulk elements)	$\frac{dV_b \rho_g C_g T_b}{dt} = -\int_S h\left(T_b - T\right) dS + \dot{m}_i h_i - \dot{m}_o h_o$	(3)
Energy (field: material blocks)	$\rho_b C_b \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \rho_b h_r r$	(4)



Mechanism	mole basis:	$C_5H_8N_4O_{12} \rightarrow 4.17\ CO_2 + 2\ N_2 + 3.66\ H_2O + 0.17\ CH_4 + 0.66\ C$ or	
	mass basis:	$petn \rightarrow 0.975\ gas + 0.025\ carbon$	(1)
Reaction Rate		$r = \frac{d}{dt}(petn) = \xi A \exp\left[-\left(E + z\sigma_E\right)/RT\right] petn$, where $petn_o = 1$	(2)
Distribution parameter		$1 - petn = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-z^2}{2}\right) dz$ or $z = \mathbf{norminv}(1 - petn)$	(3)
Gas volume fraction		$\phi = 1 - \left[S_f \left(1-\phi^o\right) \rho_c^o / \rho_c\right]$ where $S_f = petn + carbon$	(4)
Bulk density		$\rho_b = \phi \rho_g + (1-\phi)\rho_c$	(5)
Thermal conductivity		$k = \phi k_g + \frac{2}{3}(1-\phi)k_c + \frac{16\sigma T^3}{3\left[\phi \alpha_g + (1-\phi)\alpha_c\right]}$	(6)

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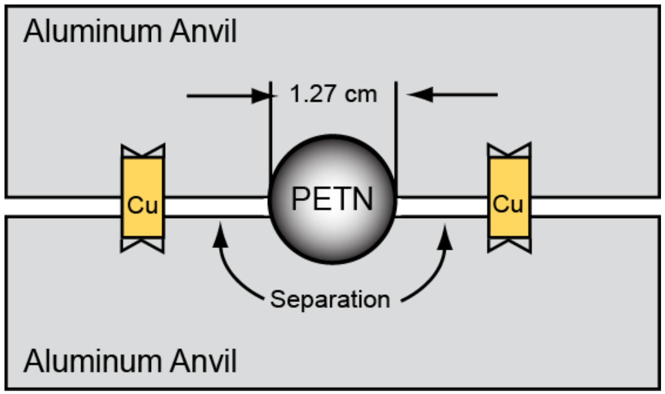
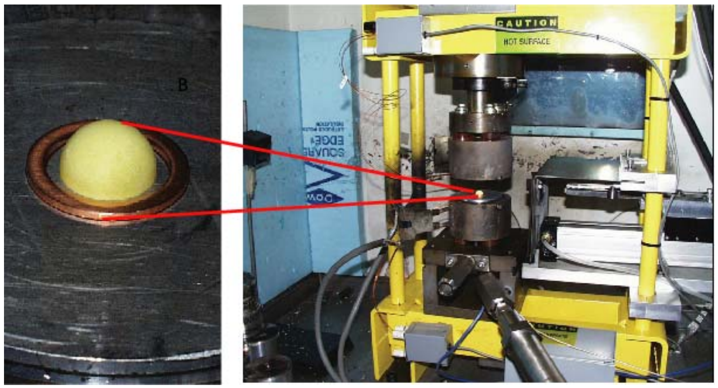
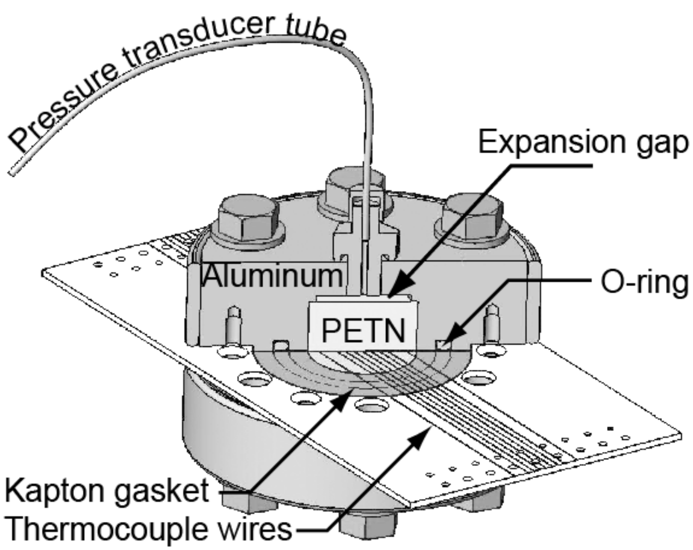
Validation experiments

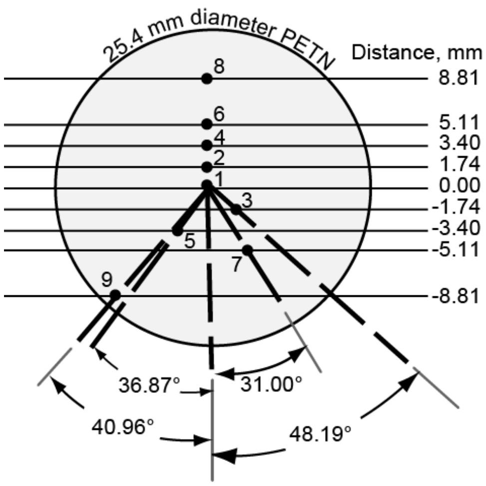
ODTX

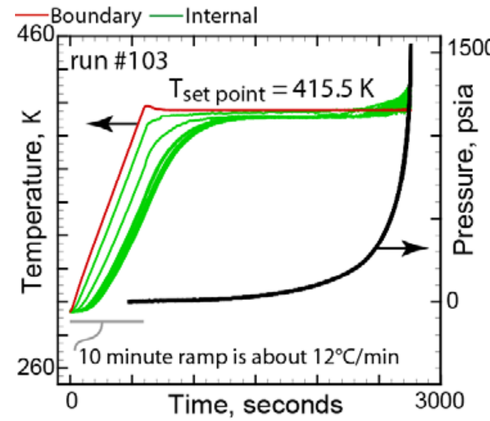




SITI







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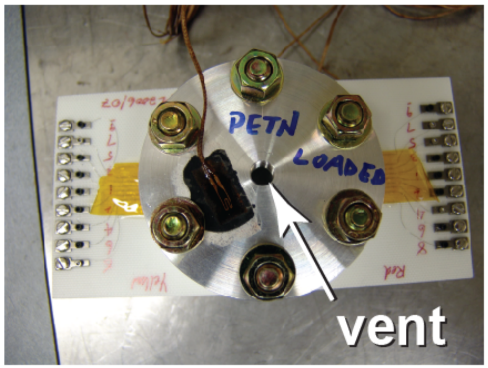
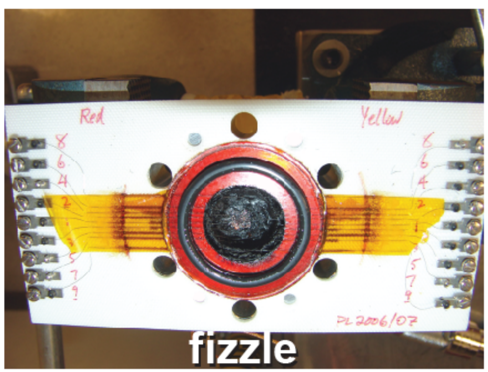
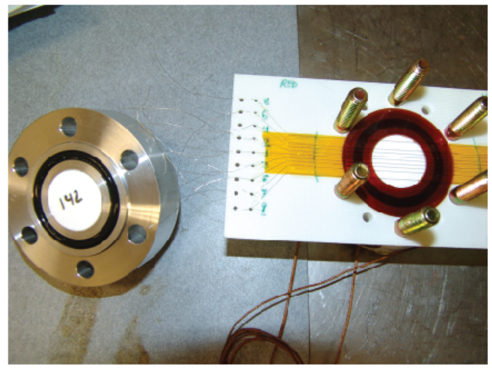
Violence prediction is of interest

Run #102
(unconfined powder)

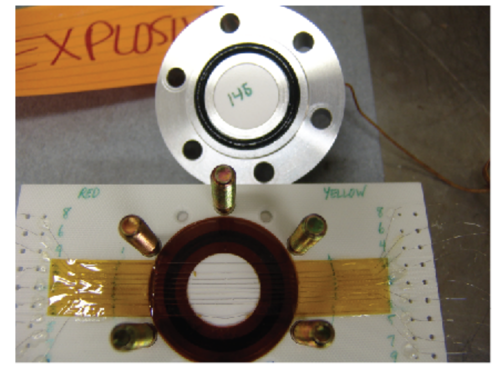




Run #103
(confined pressed solid)



Run #105
(confined pressed solid)



Does it go pop, bang, or kablooey?

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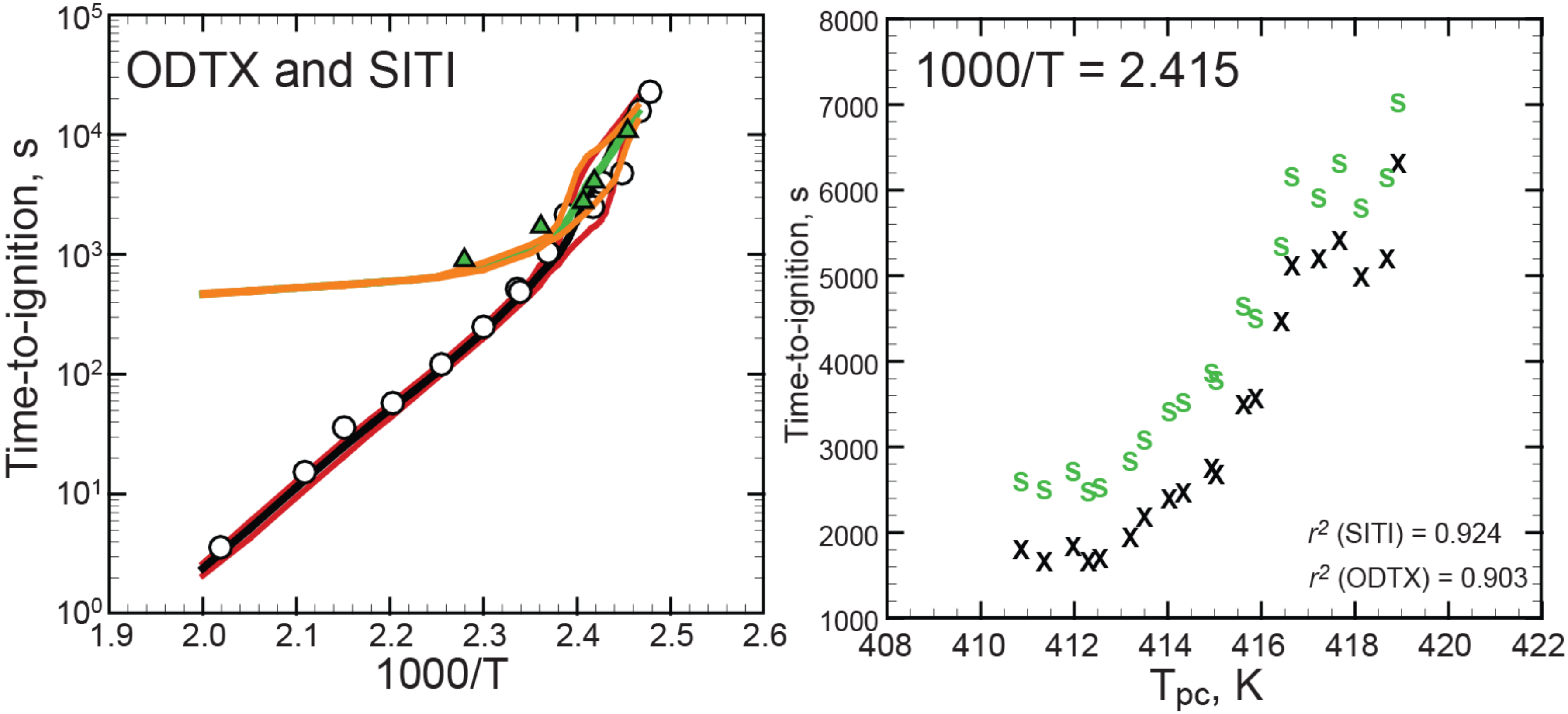
Model predicts ignition time



Uncertainty calculated with 20 LHS samples

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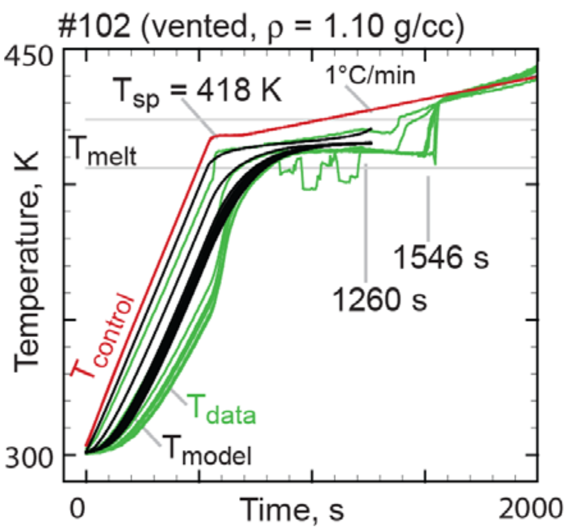
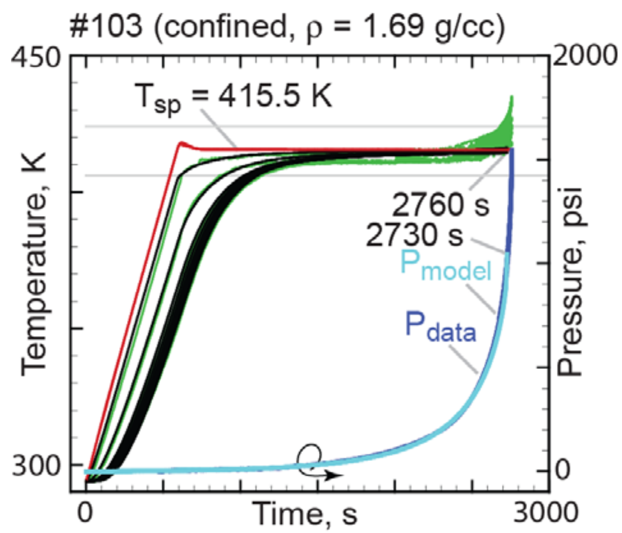
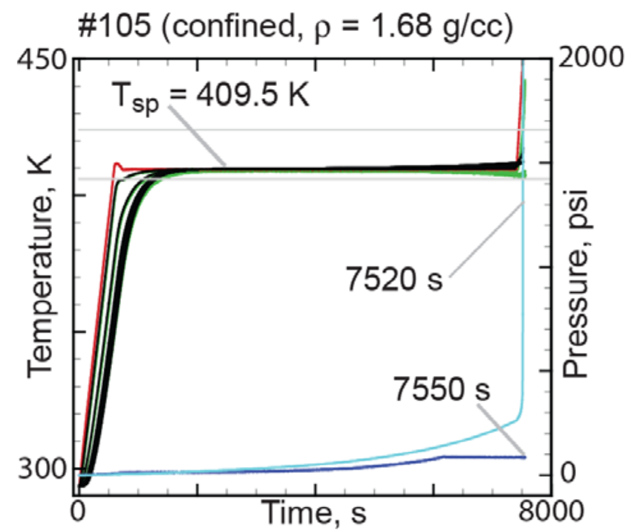
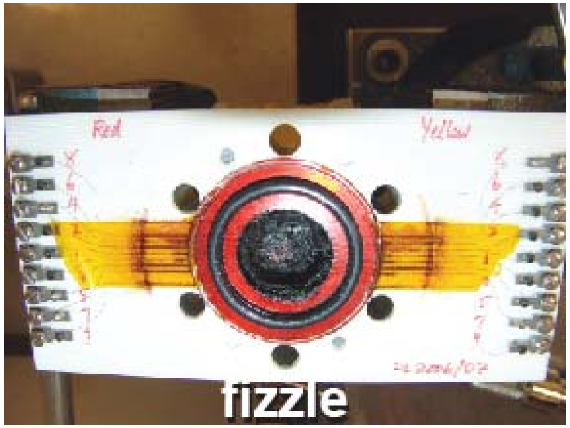
Model predicts temperatures/pressures





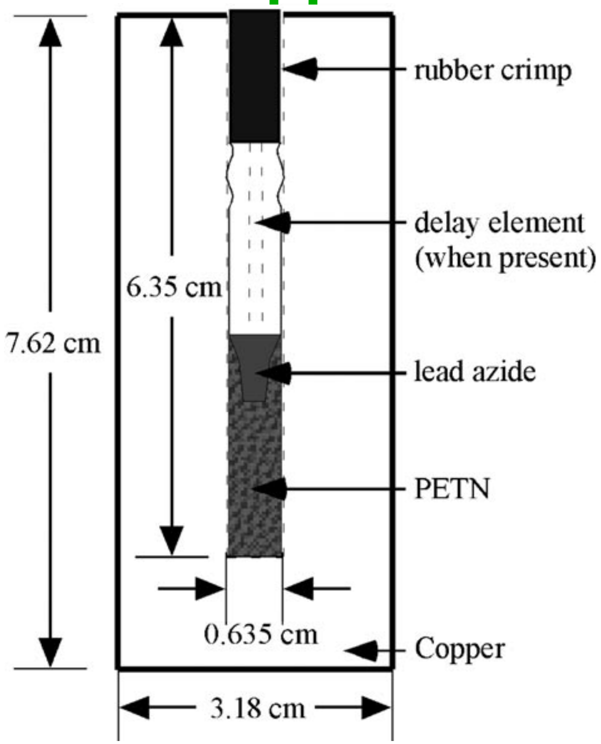




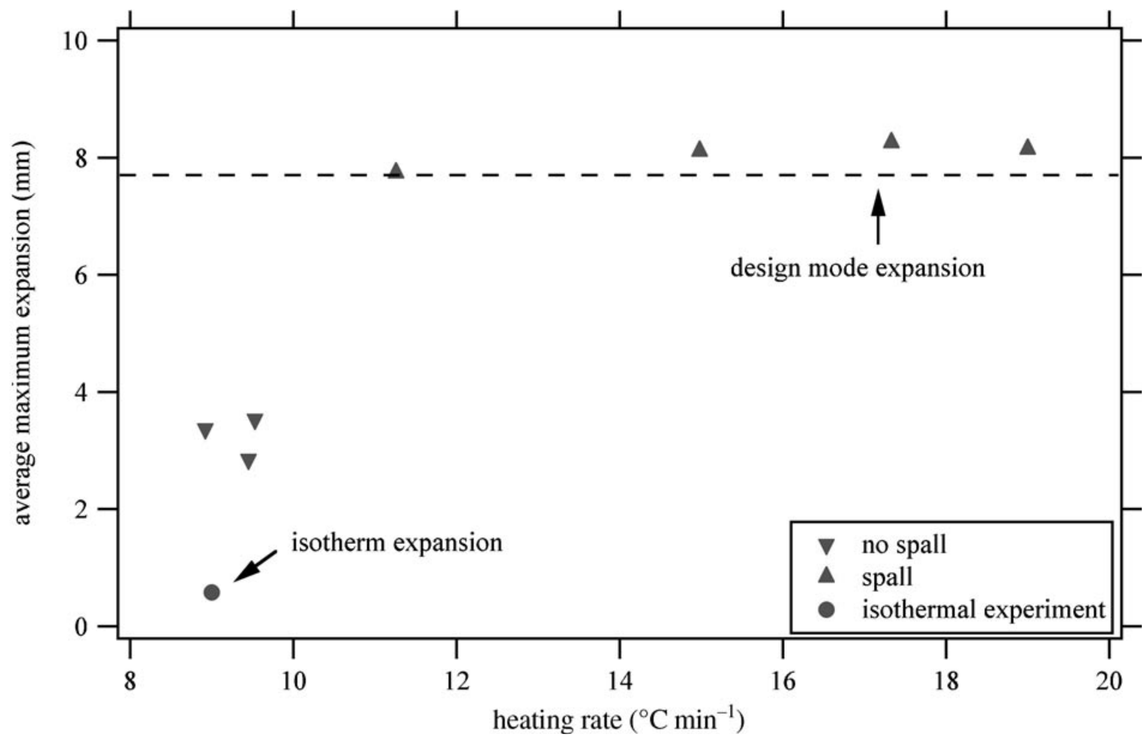
Model does not calculate violence

Does ignition guarantee failure?

Detonator in copper



Expansion of copper



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

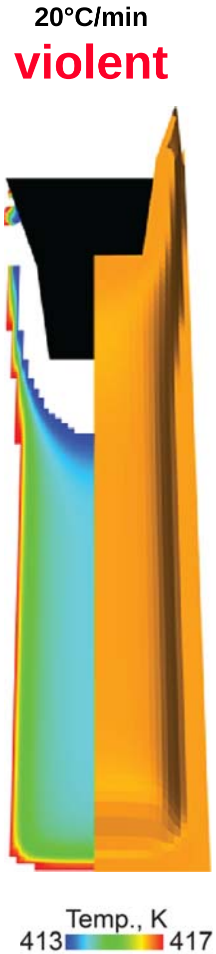
Can violence be correlated to conditions at the onset of ignition with Damköhler (group IV) number, DaIV, or something similar?

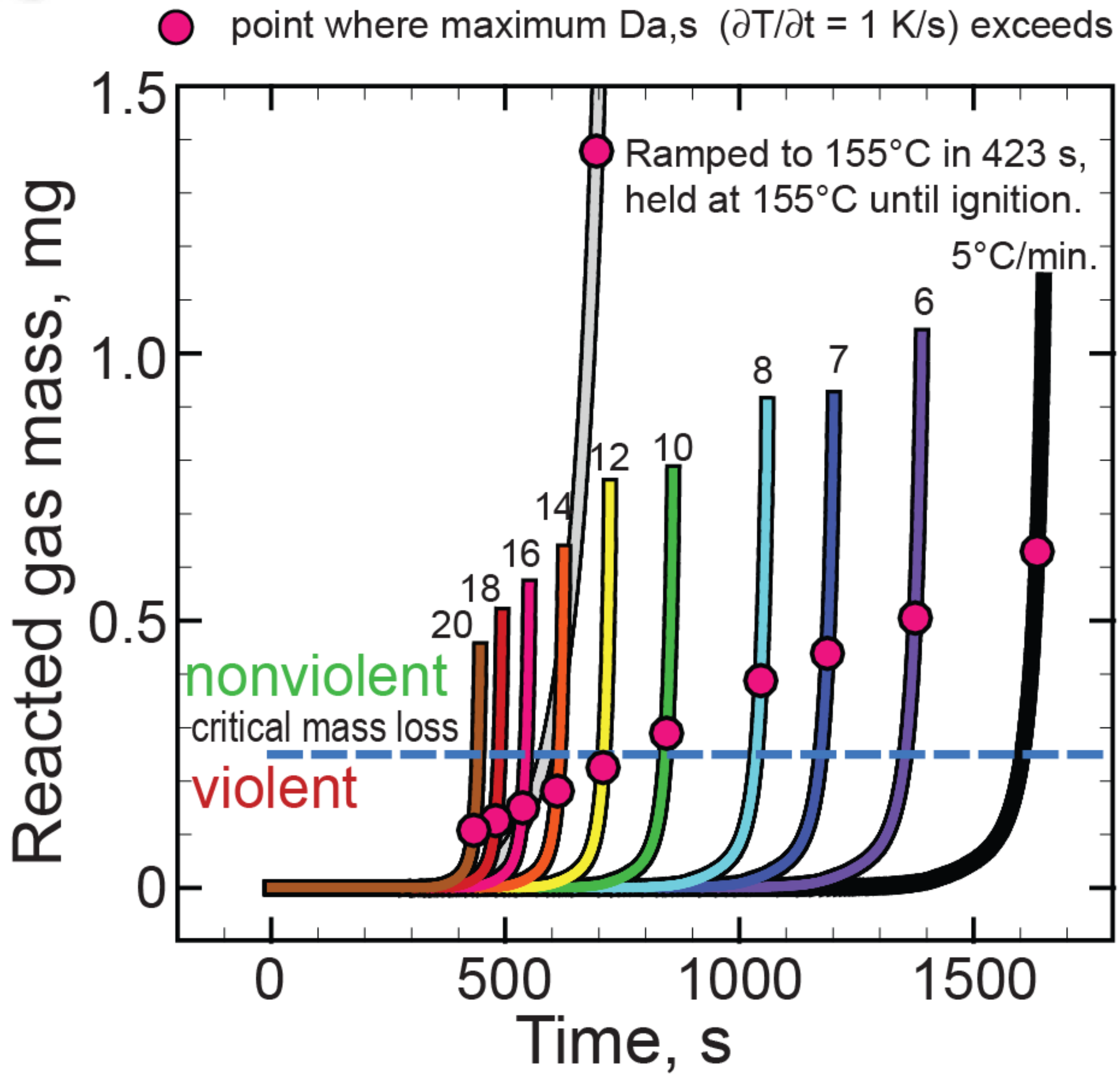
$$D_{a,c} = D_a\mathrm{IV}^* = \frac{\text{reaction time scale}}{\text{conduction time scale}} = \frac{\rho_b h_r r}{\nabla\cdot(k\nabla T)} = \frac{h_r r}{C_b\frac{\partial T}{\partial t} - h_r r}$$

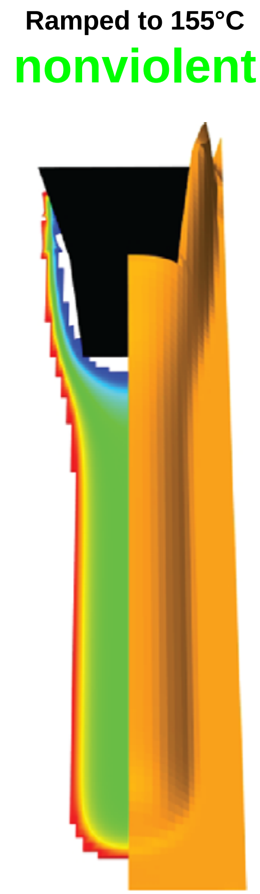
$$D_{a,s} = \frac{\text{reaction time scale}}{\text{storage time scale}} = \frac{h_r r}{C_b\frac{\partial T}{\partial t}}$$

*derived from $\rho_b C_b \dfrac{\partial T}{\partial t} = \nabla\cdot(k\nabla T) + \rho_b h_r r$

Cookoff violence correlated with extent of reaction







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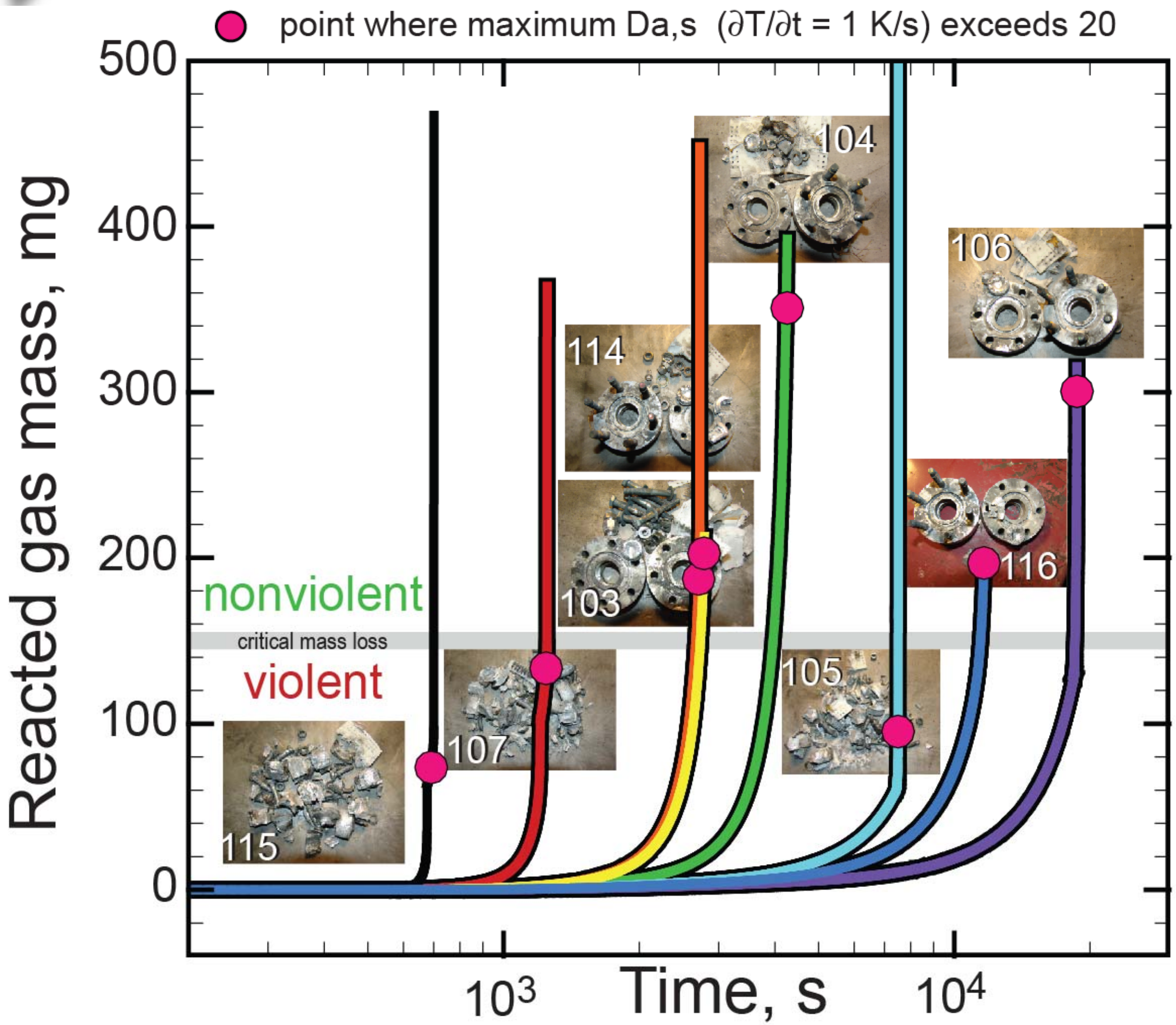
SITI cookoff violence correlated with extent of reaction at onset of ignition



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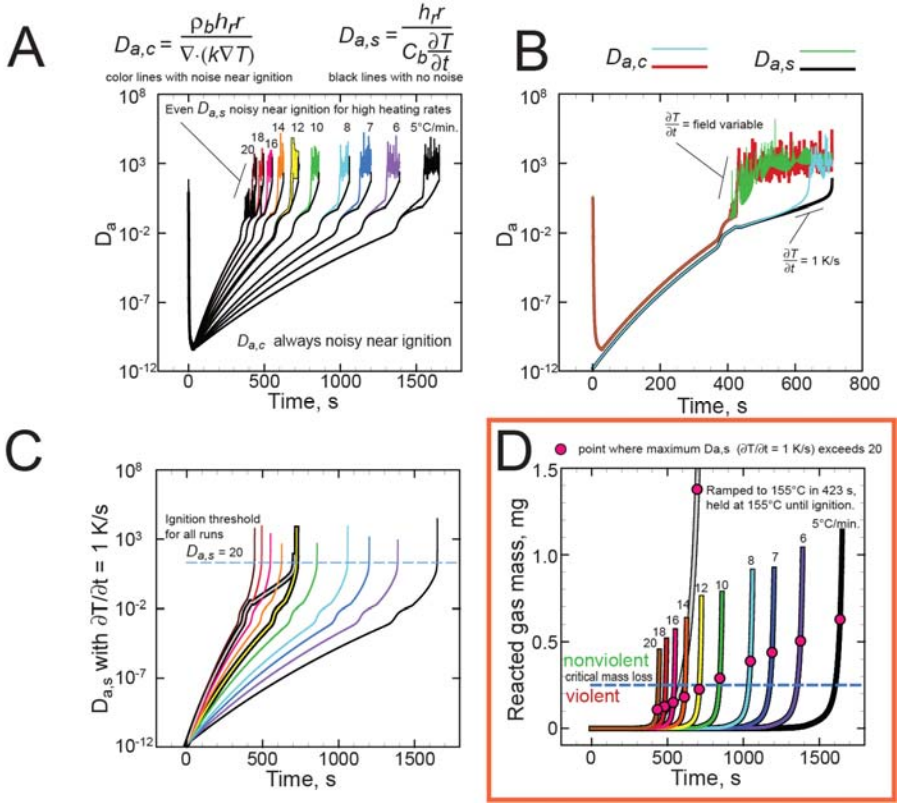
Summary and Conclusions

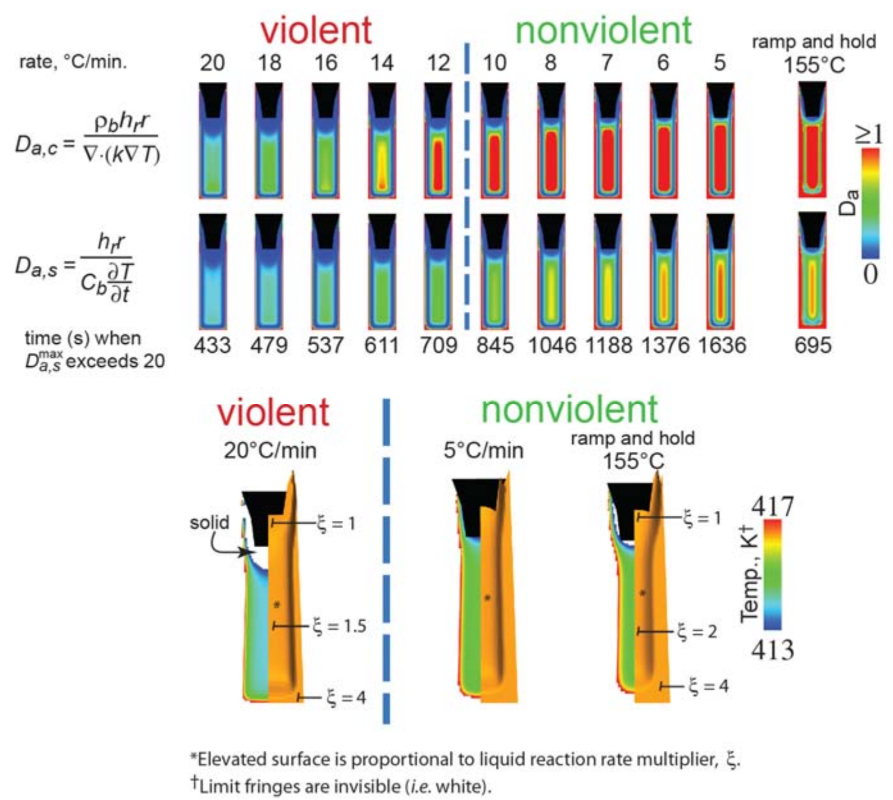
- 1-step, 1st-order, distributed activation energy, pressure dependent, thermodynamic phase change, effective thermal conductivity, low Mach pressure model with decomposition products in equilibrium.
- Model fits ignition times from three experiments: SNL's SITI experiment, LLNL's ODTX experiment, LANL's detonator experiments. Predicts time, location, pressure, but not violence. Cookoff violence correlated with state of material at onset of ignition determined using storage Damköhler number.
- Need to know the thermophysical properties such as thermal conductivity, phase change temperature, phase change enthalpy, reaction enthalpy, reaction products, specific heat, bulk density, volumetric expansion coefficient, and phase density.
- Model form applicable to many explosives (e.g. HMX, RDX, TNT, PETN, TATB, etc.).
- Need to confirm cookoff violence correlations with experiments.

Simulations correlate violence with…

Extent of reaction



Damköhler numbers

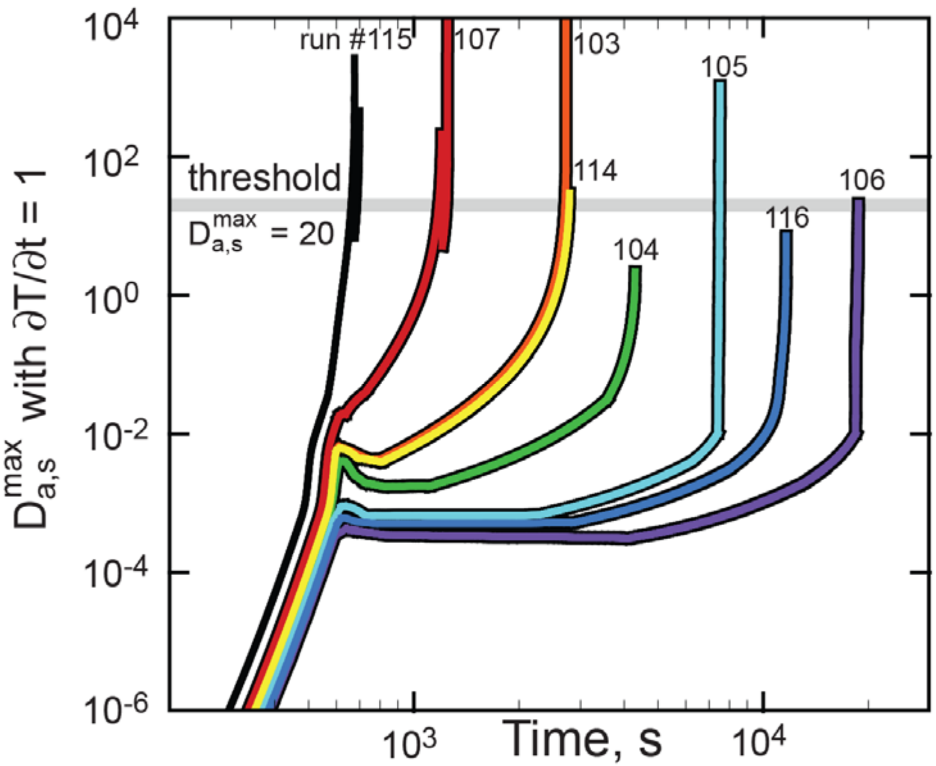


Think liquid formation and hot spots!

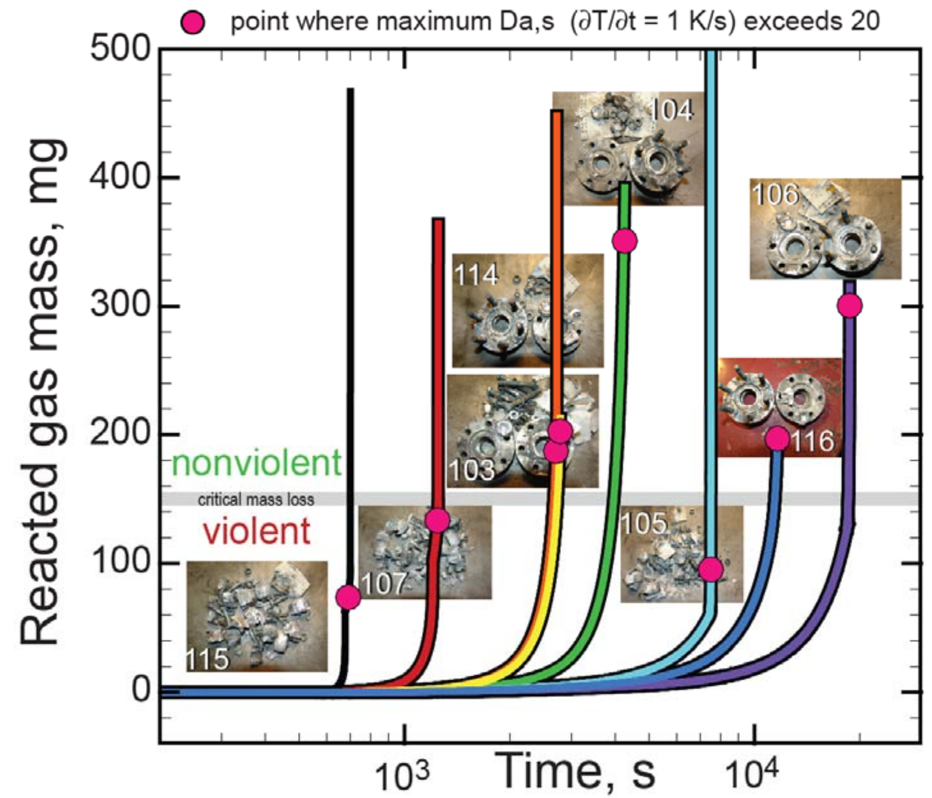
Detonators attained *full output* when the extent of reaction was small and were *duds* when the extent of reaction was large at the onset of ignition.

SITI violence correlated with extent of reaction at onset of ignition

Onset of ignition when $D_{a,s}^{max}$ exceeds 20



Violence correlated with extent of reaction at ignition



Run #105 intentionally ignited after 2 hours.

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