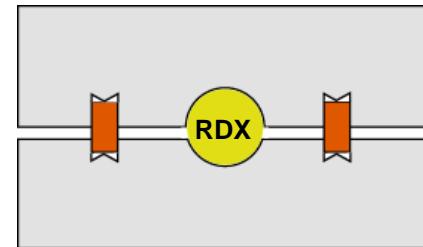
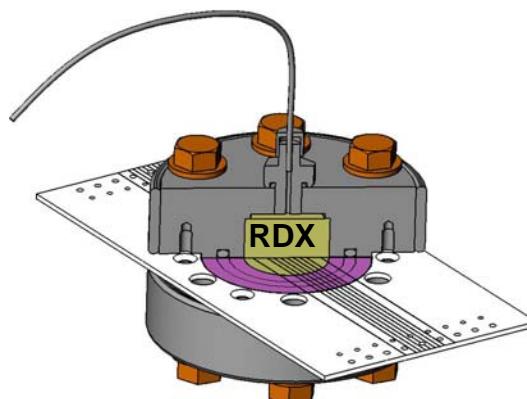
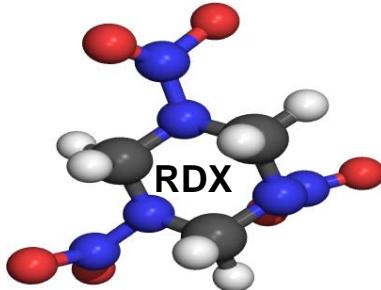


MODELING RDX IGNITION

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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
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Why Study Cookoff?



July 29, 1967 USS Forrestal

Zuni rocket accidentally fired from F4 Phantom
hit 400 gallon fuel tank of A-4D Skyhawk



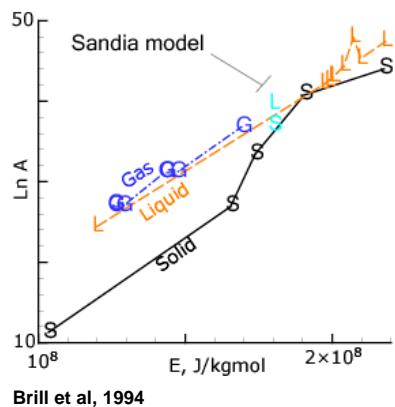
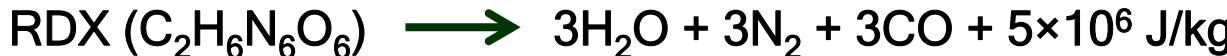
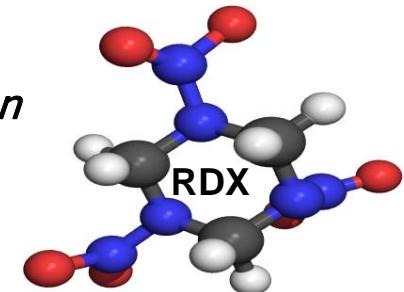
A Zuni rocket accidentally fired from an F-4 Phantom parked on the starboard side of the flight deck aft of the island. The missile streaked across the deck into a 400 gallon belly fuel tank on a parked A-4D Skyhawk. The ruptured tank spew highly flammable JP-5 fuel onto the deck which ignited spreading flames over the flight deck under other fully loaded aircraft ready for launch. The ensuing fire caused ordinance to explode and other rockets to ignite. Spread by the wind, the flames engulfed the aft end of the stricken ship turning the flight deck into a blazing inferno. Berthing spaces immediately below the flight deck became death traps for fifty men, while other crewmen were blown overboard by the explosion.

The four-and-a-half-acre flight deck was littered with pieces of aircraft, as men struggled to clear away bombs and ammunition, throwing the ordnance over the side. One young 130-pound lieutenant found the strength to heave a 250-pound bomb overboard.

134 men lost lives, 64 aircraft destroyed/damaged

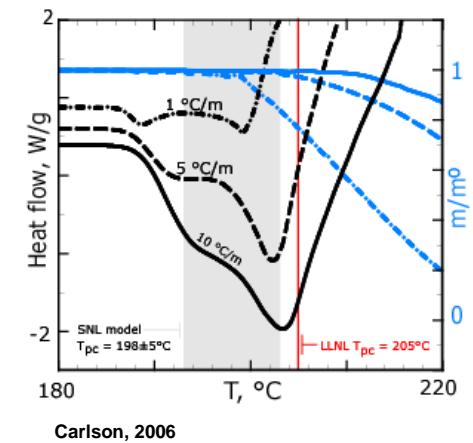
Model Features

- One-step, first-order mechanism
- Distributed Arrhenius rates modified by $(P/P^o)^n$
- Product hierarchy from equilibrium calculation
- Liquefaction modeled thermodynamically
- Liquid rates are 15 times larger than solid rates
- Thermal expansion, phase change, and reaction included



$$\frac{d}{dt} \omega_{rdx} = A \left(\frac{P}{P^o} \right)^n \exp \left(-\frac{E + z\sigma_E}{RT} \right) \omega_{rdx}$$

$$\omega_{rdx} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^z \exp \left(-\frac{1}{2} z^2 \right) dz$$



Conservation Equations

Energy
(field: material blocks)

$$\rho_b C_b \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + rh_{rxn}$$

Energy
(integral: bulk elements)

$$\frac{d}{dt} (V_b \rho_g C_g T_b) = - \int_S h(T_b - T) dS + \dot{m}_i h_i - \dot{m}_o h_o$$

Gas Continuity
(integral: permeable regions)

$$\frac{d}{dt} M_g = \int_{\Lambda} rdm_c^o$$

Gas Momentum
(integral: permeable regions)

$$P(x, y, z, t) = P(t) = M_g / \int_{\Lambda} \frac{M_{wg}}{RT} d\Lambda$$

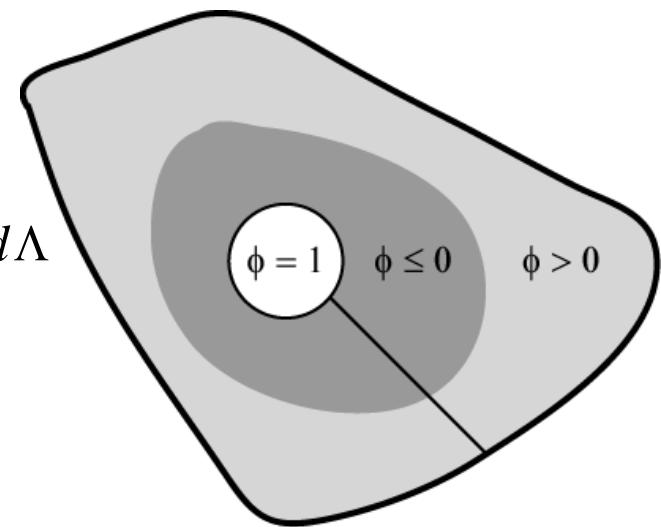
$$\phi = 1 - \omega_{rdx} (1 - \phi^o) \rho_c^o / \rho_c$$

$$\rho_b = \phi \rho_g + (1 - \phi) \rho_c$$

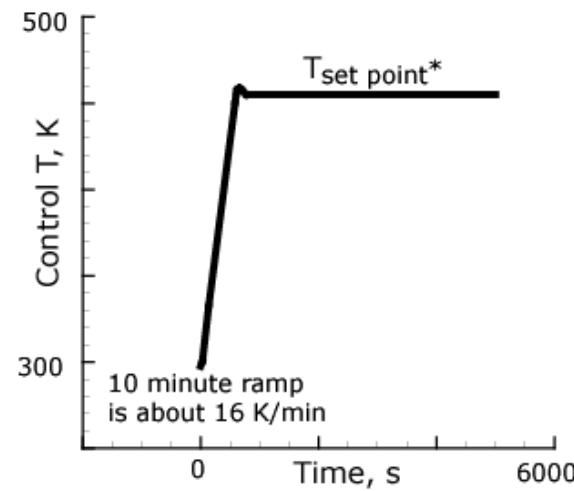
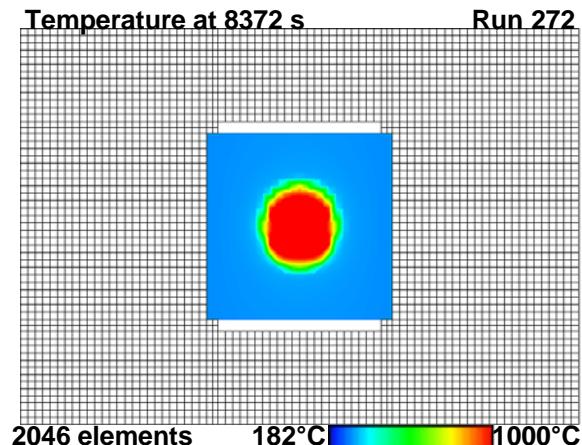
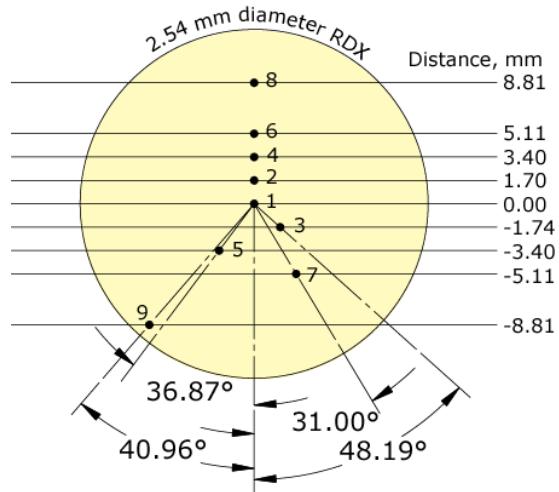
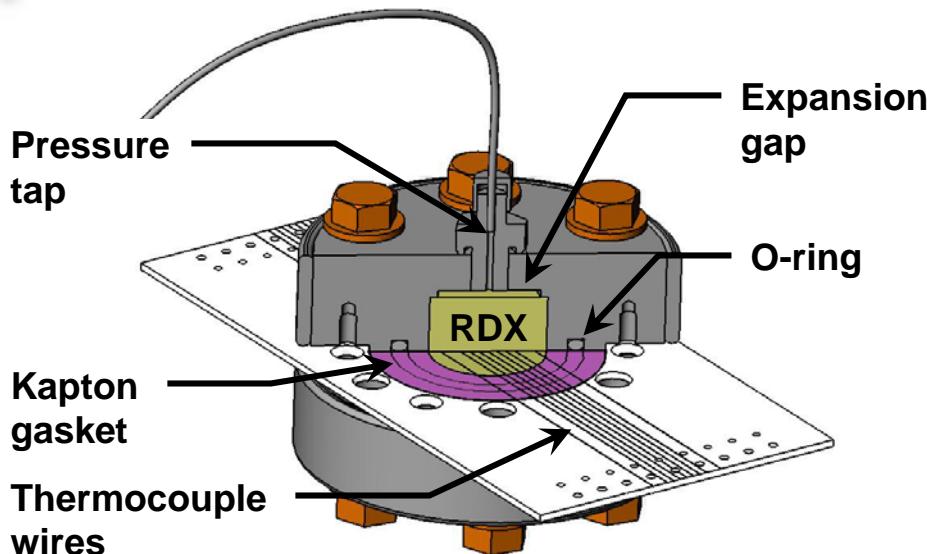
$$\rho_c = \rho_c^o / \left[1 + \beta (T - T^o) + \delta \gamma \right]$$

$$k = \phi k_g + \frac{2}{3} (1 - \phi) k_c + \frac{16 \sigma T^3}{3[\phi \alpha_g + (1 - \phi) \alpha_c]}$$

Auxiliary



Sandia's Instrumented Thermal Ignition Experiment (SITI)

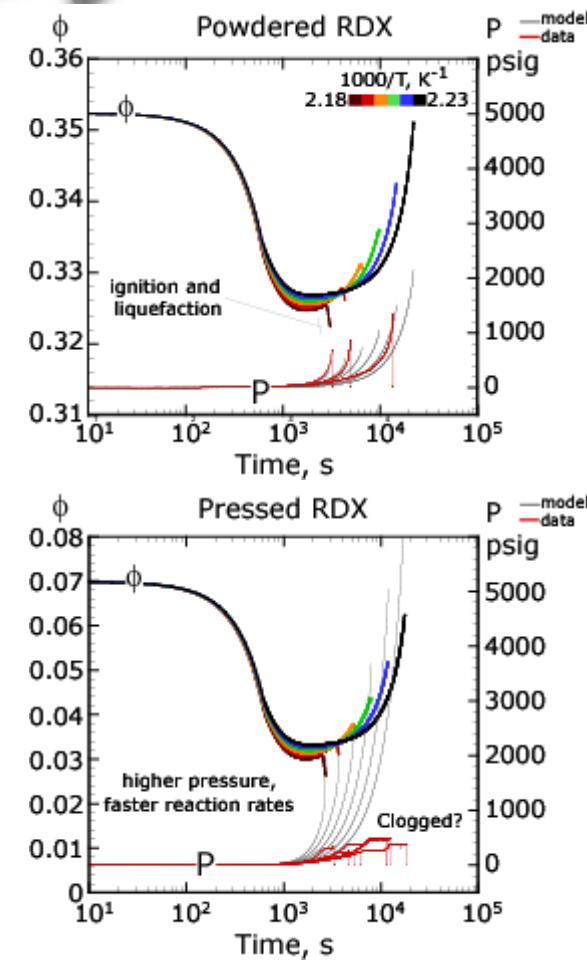


*Example is run 272 with $T_{\text{set point}} = 455$ K

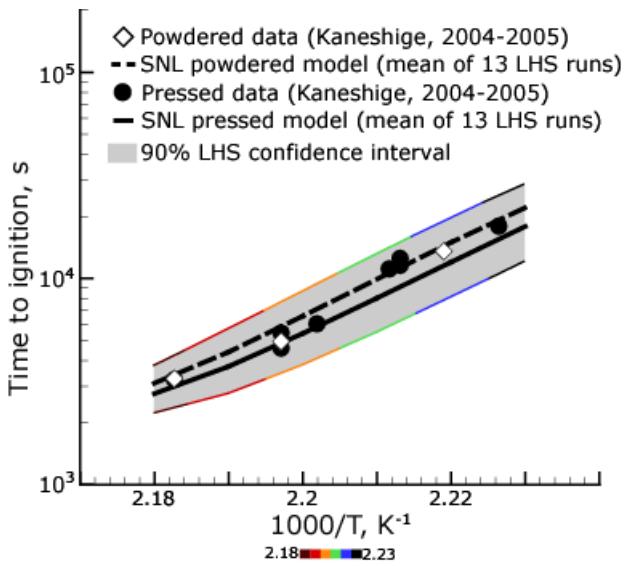
RDX model of SITI

Thermal expansion and phase change effect ϕ and k

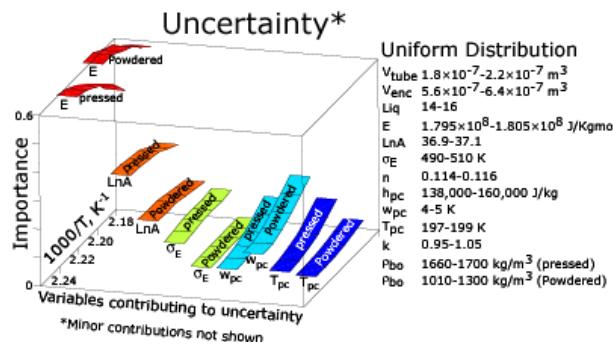
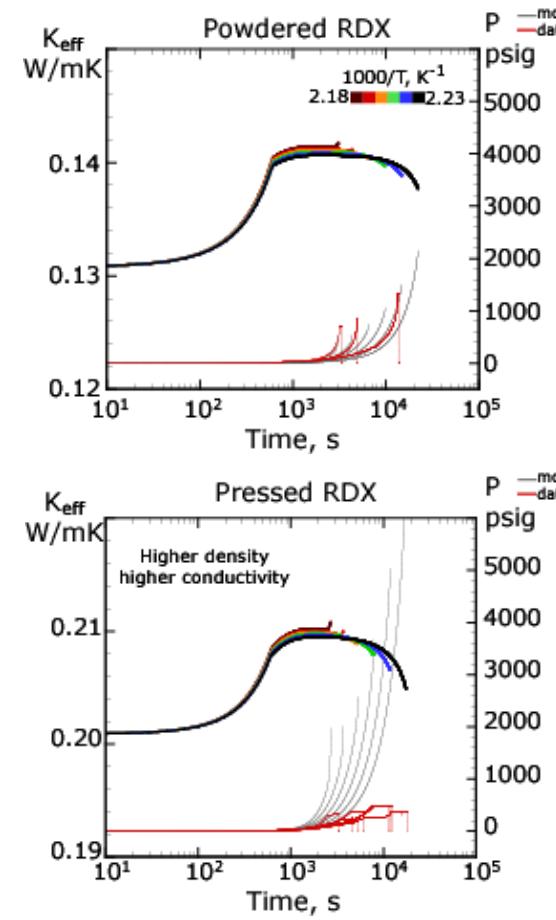
Gas Volume Fraction



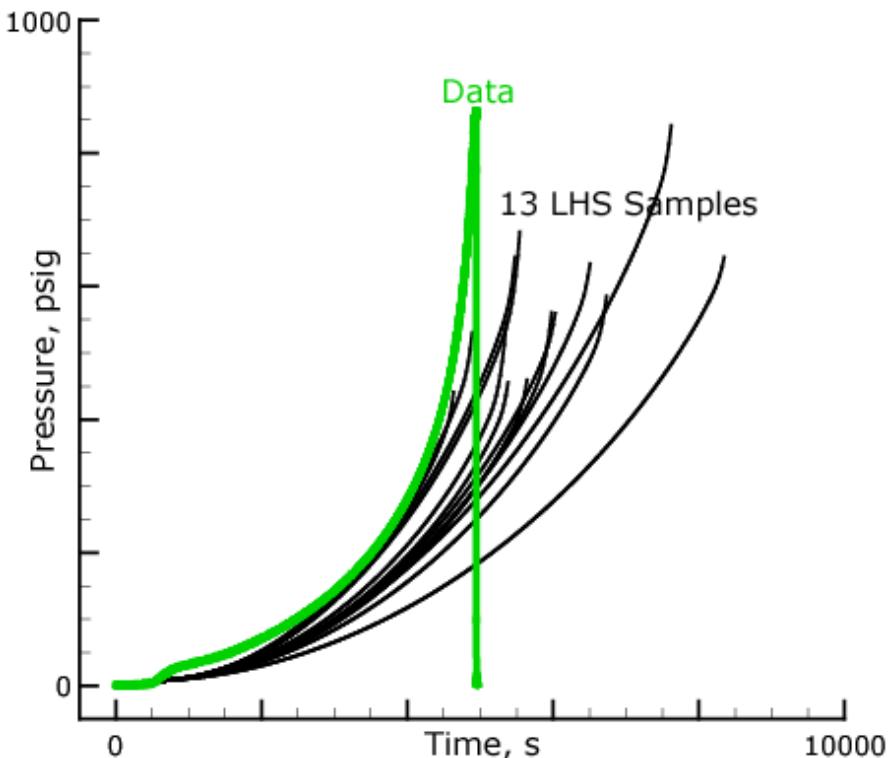
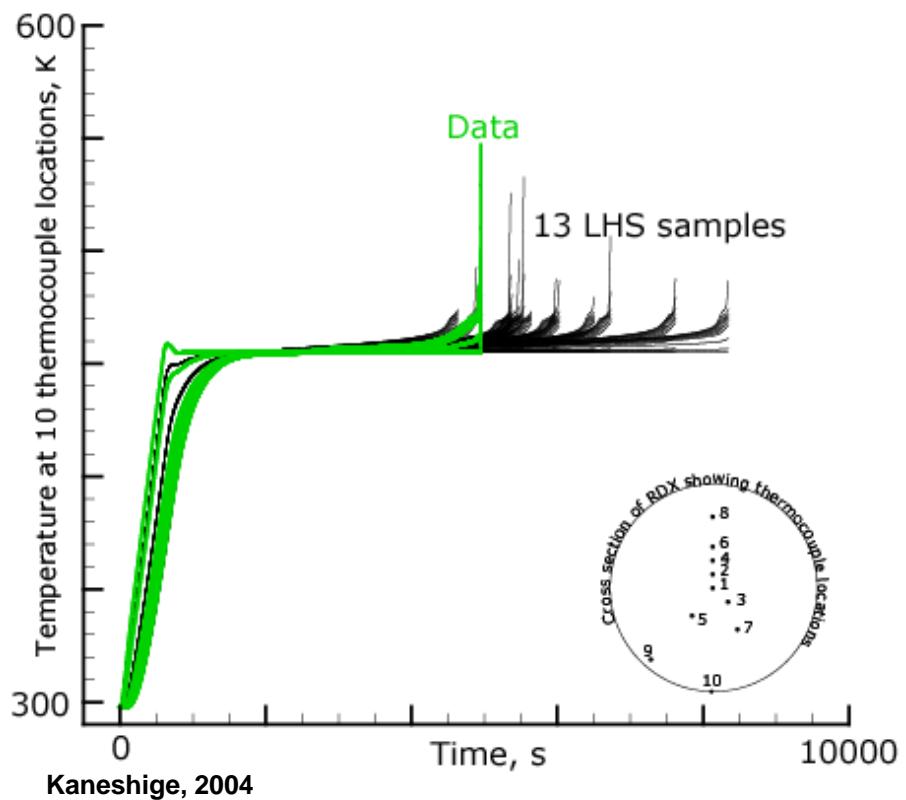
Time to Ignition



Thermal Conductivity



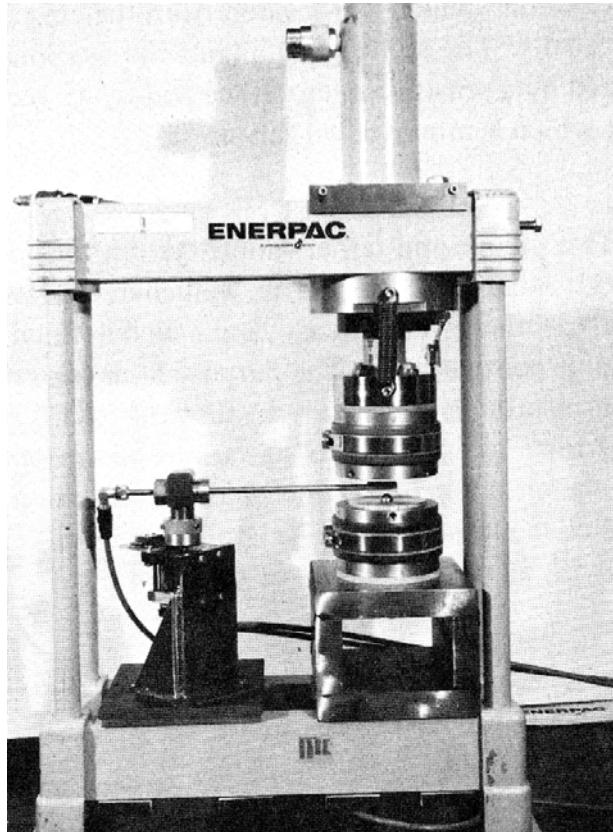
RDX model of SITI run 272





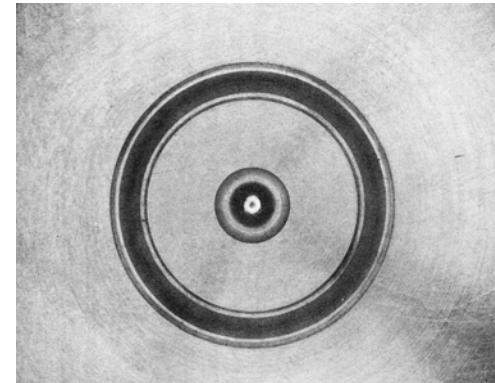
LLNL's One-Dimensional Time to Ignition Experiment (ODTX)

Apparatus



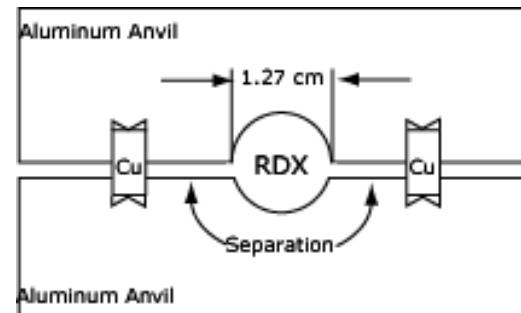
Catalano et al., 1976

Detail of anvil face



Catalano et al., 1976

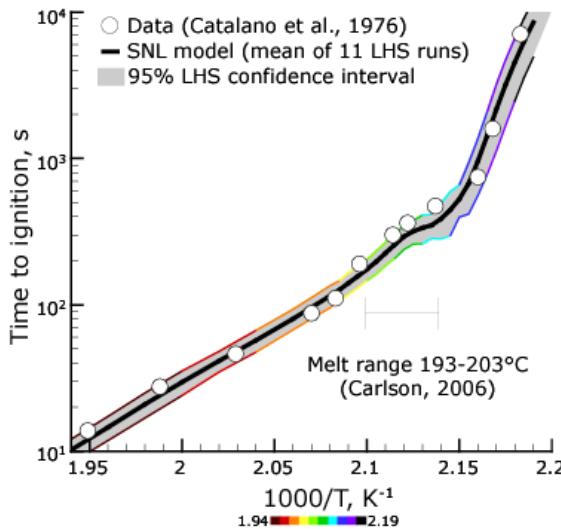
Schematic



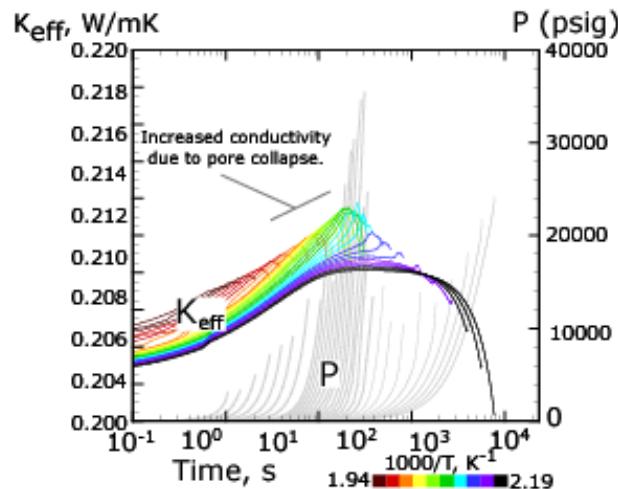
Anvil held at constant T, time to event measured

RDX Model of ODTX Experiment

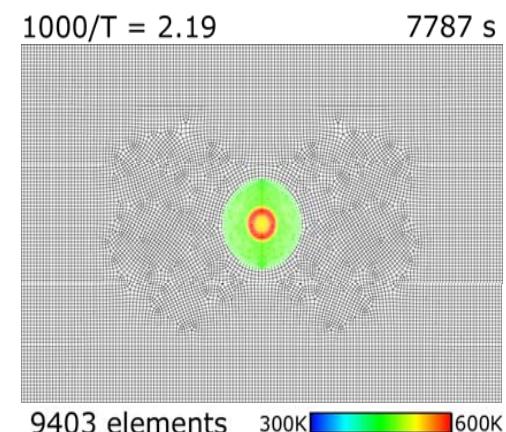
Time to ignition



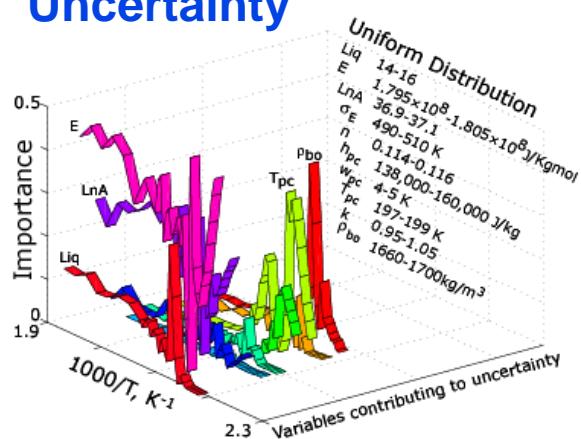
Thermal conductivity



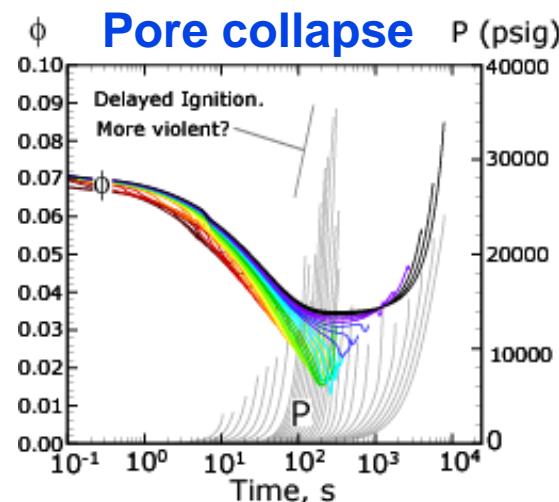
T near ignition



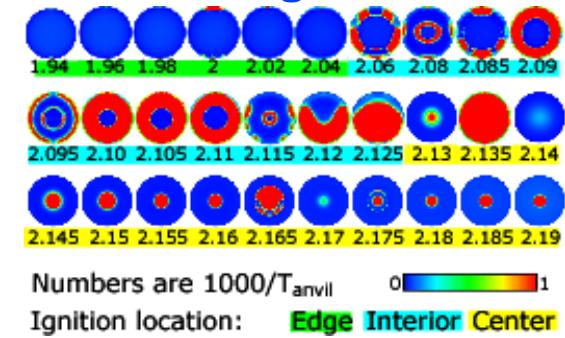
Uncertainty



Pore collapse



Gas volume fraction (ϕ) near ignition



Model fits time to ignition



Summary and Conclusions

- 1-step, 1st-order, distributed activation energy, pressure dependent, thermodynamic phase change, effective thermal conductivity, low Mach pressure model
- Model fits two separate experiments: SNL's SITI experiment and LLNL's ODTX experiment
- Latin Hypercube Sampling (LHS) used for uncertainty
- Model form may be applicable for all explosives
- Need to know 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
- Future desires include pure RDX SITI experiments and fast cookoff SITI experiments (quench whole experiment in hot liquid)