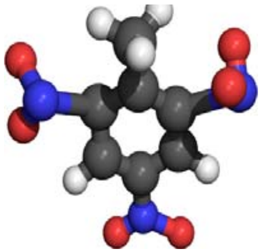

MODELING TNT IGNITION

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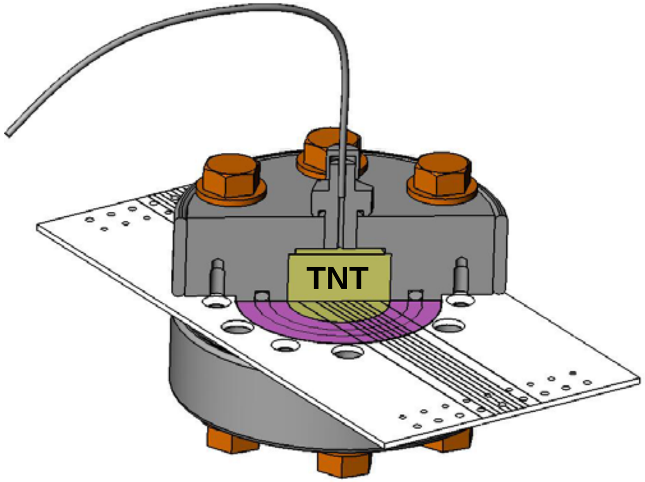
Sandia National Laboratories

Albuquerque, New Mexico

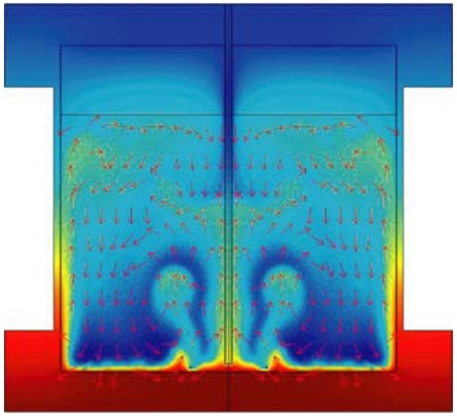
ODTX

0.5” sphere



1” cylinder

Midscale “bucket”



8” cylinder

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
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under contract DE-AC04-94AL85000.

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

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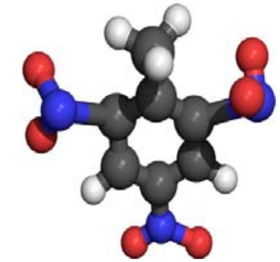
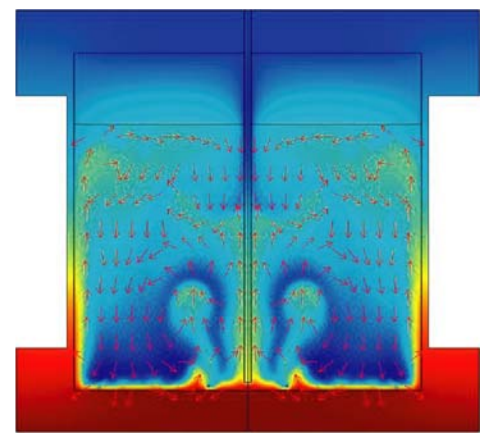
Why Study TNT Ignition?



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

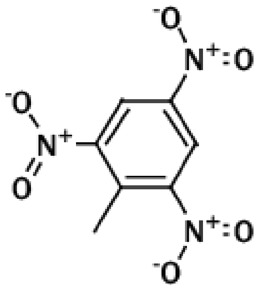
- **Used in numerous explosives**
  - **Composition B or cyclotol (60% RDX and 40% TNT)**
  - **Octol (70% HMX and 30% TNT)**
  - **Pentolite (50% PETN and 50% TNT)**
  - **Tritonal (80%TNT and 20% Al)**
  - **Many more**

- **Standard explosive**
  (e.g. TNT equivalence)



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 conductivity is 8 times larger than solid conductivity
- Thermal expansion, phase change, and reaction included
- Effect of impurity modeled empirically



$$\text{TNT } (C_7H_5N_3O_6) \rightarrow 0.18CH_4 + 2.14H_2O + 1.93\ CO_2 + 1.5\ N_2 + 4.89\ C^* + 5.4 \times 10^6 \text{ J/kg}$$

$$\text{TNT} \rightarrow 0.742\ G + 0.258\ C^*$$

$$\frac{d}{dt}\omega_{tnt} = \xi A \left(\frac{P}{P_o}\right)^n \exp\left(-\frac{E + z\sigma_E}{RT}\right)\omega_{tnt} \qquad \xi = 10^{38\omega_{tnt} - 37.67}, \text{ if } \omega_{tnt} \geq 0.95$$

$$1 - \omega_{tnt} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}z^2\right) dz \qquad \xi = 10^{1.6\omega_{tnt} - 3.04}, \text{ if } \omega_{tnt} < 0.95$$

National Nuclear Security Administration

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Conservation Equations

Energy
(field: material blocks)

$$\rho_b C_p \frac{\partial T}{\partial t} = \nabla \cdot \left(k \nabla T \right) + r h_{rxn} \rho_{b,o}$$

Energy
(integral: bulk elements)

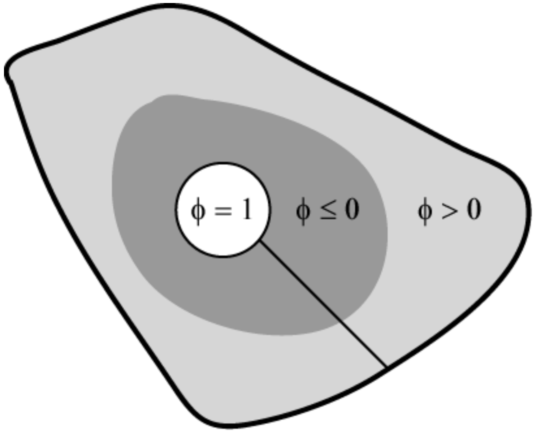
$$\tfrac{d}{dt}\left(V_b \rho_g C_g T_b \right) = -\int_S h(T_b - T) dS + \dot{m}_i h_i - \dot{m}_o h_o$$

Gas Continuity
(integral: permeable regions)

$$\tfrac{d}{dt} M_g = \int_\Lambda r dm_{c,o}$$

Gas Momentum
(integral: permeable regions)

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



Auxiliary

$$\phi = 1 - \omega_{tnt} (1 - \phi_o) \rho_{c,o} / \rho_c$$

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

$$\delta = 0.5 \times \left\{ 1 + \tanh\left[\left(T - T_{pc} \right) / w_{pc} \right] \right\}$$

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

$$\rho_c = \delta \rho_l + (1-\delta) \rho_s$$

$$\rho_s = \rho_{s,o} / \left[1 + \beta (T - T_o) \right]$$

$$\rho_l = 1544.6 - 1.016 \times (T - 273.15)$$

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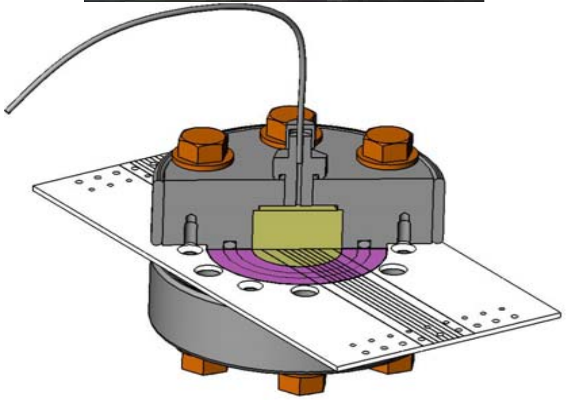
Three experiments

- ODTX (0.5” diameter sphere)
  - Pressed 1350 kg/m^3 (90-100% pure)
  - Volume of bulk TNT is ~1 cm^3
  - Slow and fast cookoff (<1 s to T_{bc})
- SITI (1” diameter cylinder)
  - Flaked (896 kg/m^3) and solid (1633 kg/m^3)
  - Volume of bulk TNT is ~13 cm^3
  - Purity being measured (~98% pure)
  - Slow cookoff (10 m ramp to T_{bc})
- Midscale (8” diameter cylinder)
  - Flaked 800 kg/m^3 (assumed 98% pure)
  - Volume of bulk TNT is ~1600 cm^3



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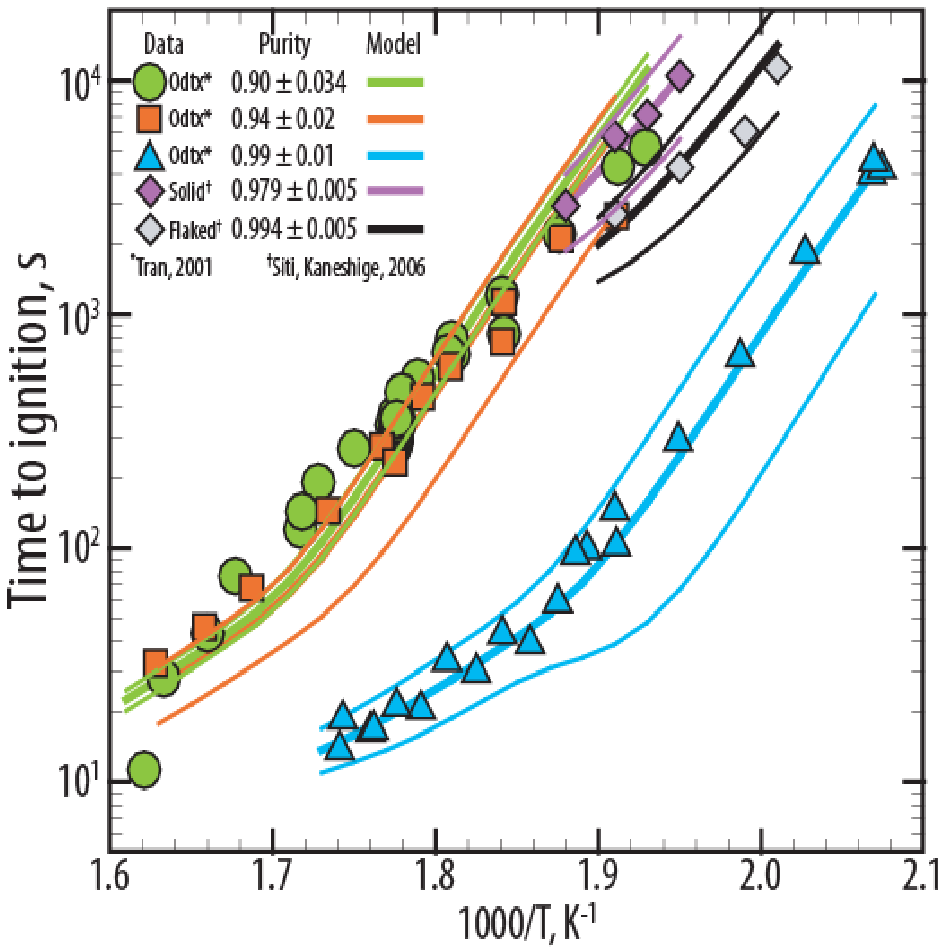
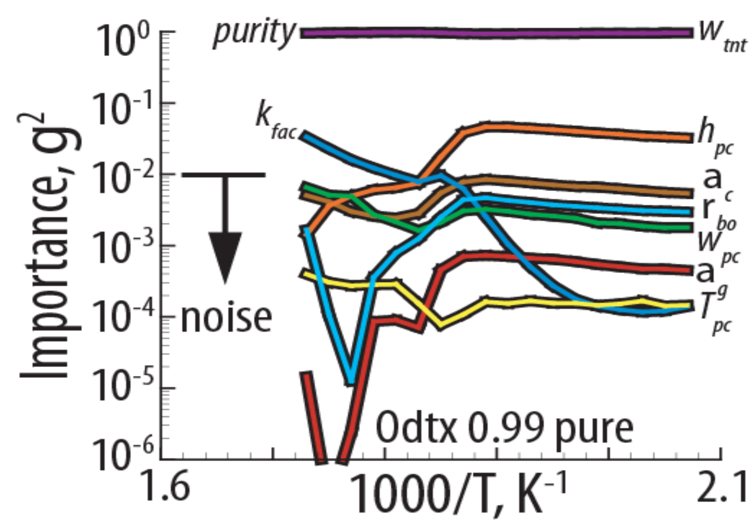
Time-to-Ignition

(ODTX different TNT purities and SITI)

Time to Ignition



Uncertain parameters



Material parameters:

a_c, m^{-1}	50,000 ± 5,000	k_{fac}	1 ± 0.05
a_g, m^{-1}	100 ± 10	T_{pc}, K	354 ± 1
		w_{pc}, K	10 ± 5

Experiment parameters:

	Odtx	Siti-flaked	Siti-solid
ρ_{bo}, kg/m^3	1,350±12	896±25	1,633±1
V_{enc}, cm^3	0	0.605±0.015	1.99±0.02
V_{tube}, cm^3	0	0.2±0.02	0.2±0.02
w_{tnt}	0.9±0.034 0.94±0.02 0.99±0.01	0.994±0.005	0.979±0.005

Impurity causes dramatic change in ignition time

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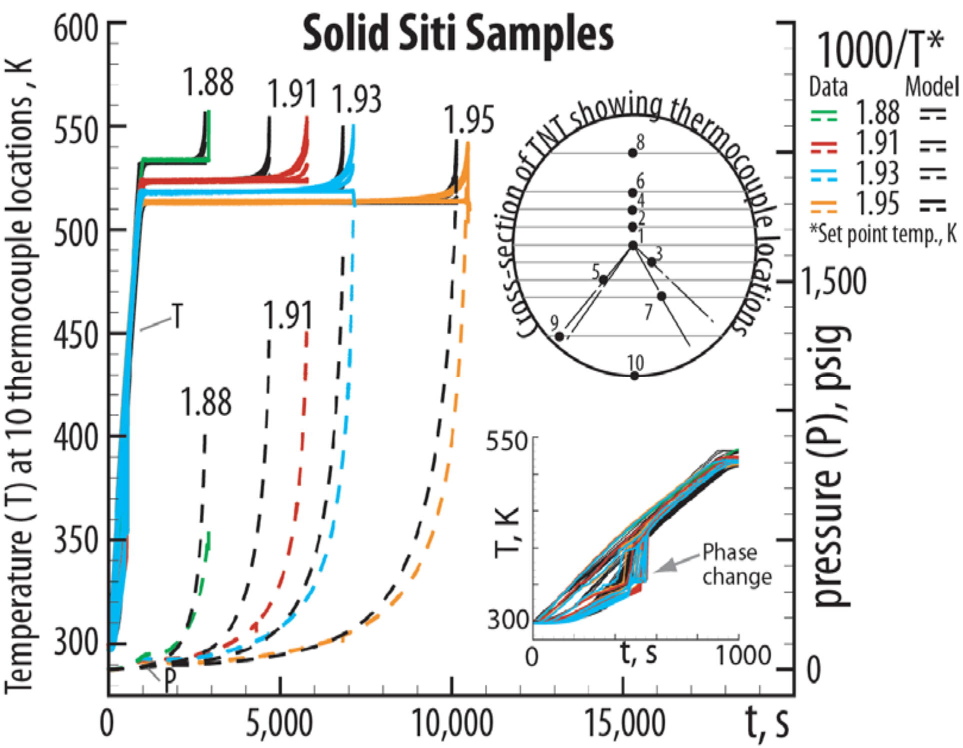
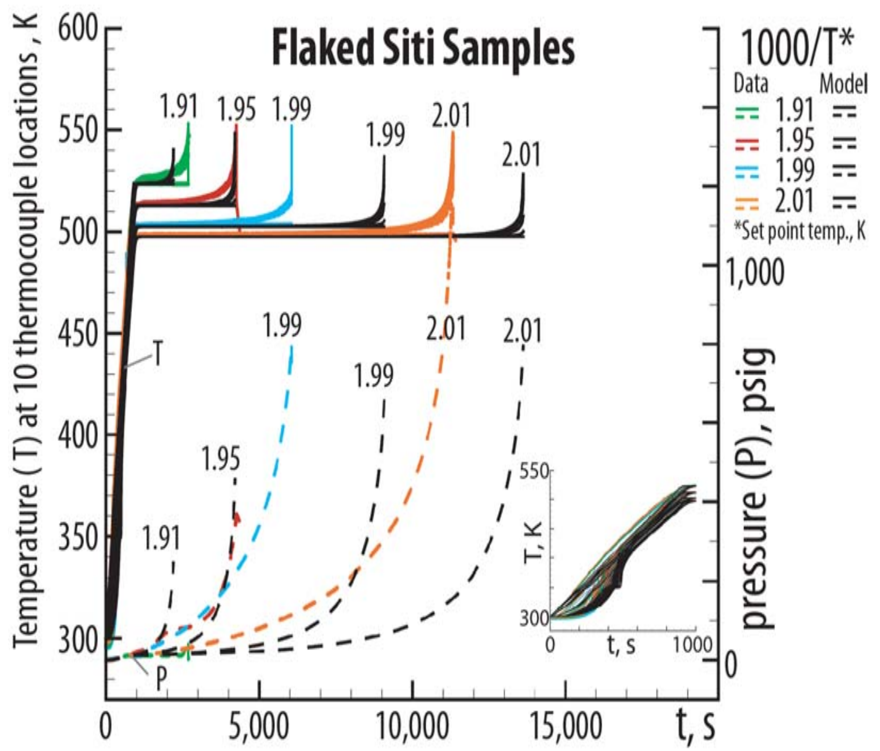
Temperature and Pressure





Kaneshige, 2004

Mean predictions are in fair agreement with data

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Larger scales require convection

Energy

$$\rho_b C_p \frac{\partial T}{\partial t} + \rho_b C_p \vec{v} \cdot \nabla T = \nabla \cdot \left(k \nabla T\right) + r h_{rxn} \rho_{b,o}$$

Continuity

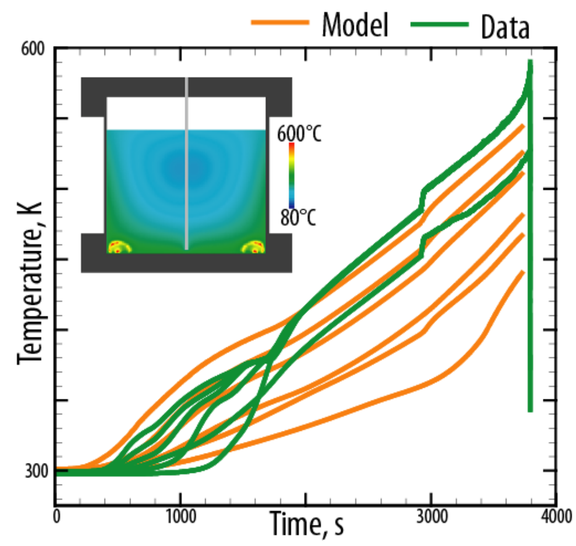
$$\frac{\partial \phi_{tnt} \rho_{tnt}}{\partial t} + \vec{v} \cdot \nabla \left(\phi_{tnt} \rho_{tnt}\right) = -r\left(1-\phi_{g,o}\right)\rho_{c,o}$$

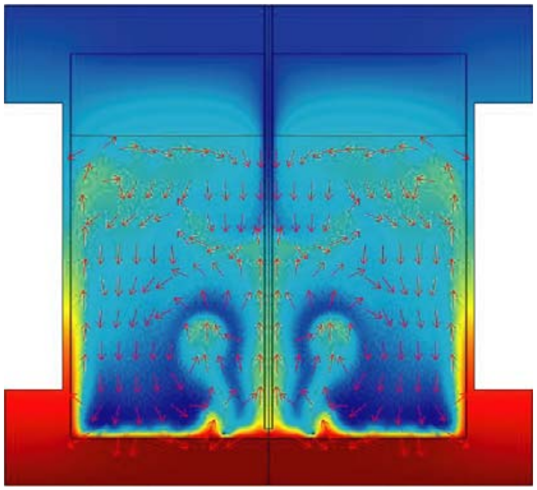
$$\frac{\partial \phi_{g} \rho_{g}}{\partial t} + \vec{v} \cdot \nabla \left(\phi_{g} \rho_{g}\right) = 0.742 \times r\left(1-\phi_{g,o}\right)\rho_{c,o}$$

$$\frac{\partial \phi_{C*} \rho_{C*}}{\partial t} + \vec{v} \cdot \nabla \left(\phi_{C*} \rho_{C*}\right) = 0.258 \times r\left(1-\phi_{g,o}\right)\rho_{c,o}$$

Momentum

$$\rho_b \frac{\partial \vec{v}}{\partial t} + \rho_b \left(\vec{v} \cdot \nabla\right)\nabla = -\nabla P + \mu \nabla^2 \vec{v} + \rho_b \vec{g}$$





Scaling up sometimes requires additional physics

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 many explosives (e.g. HMX, RDX almost complete)
- 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 TNT SITI experiments and fast cookoff SITI experiment