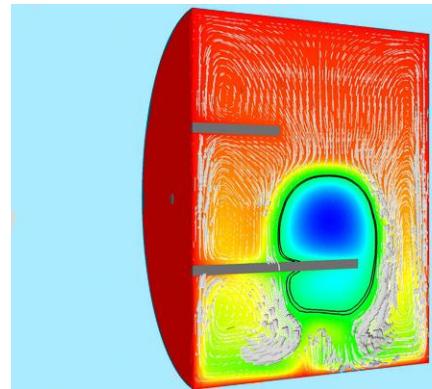
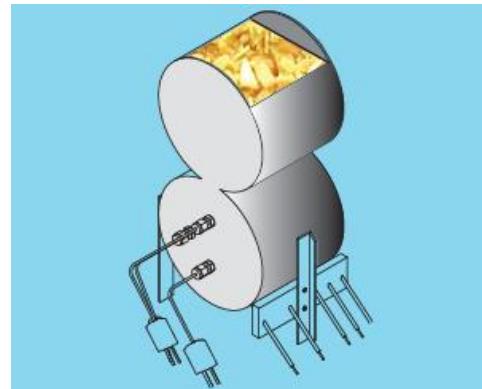
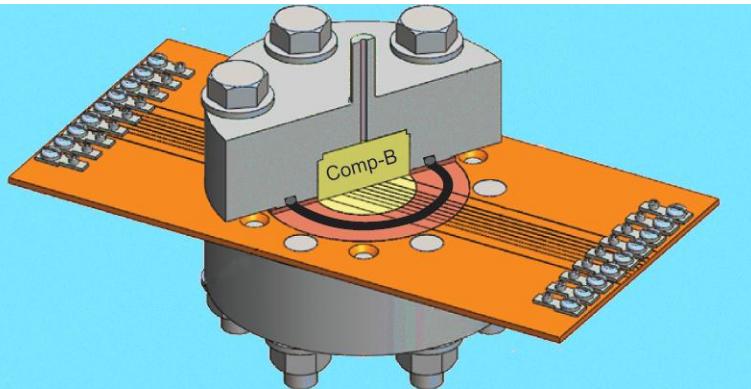
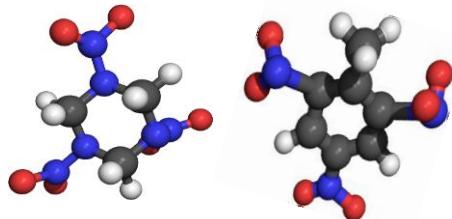


Exceptional service in the national interest



Cookoff of a Melt-castable Explosive

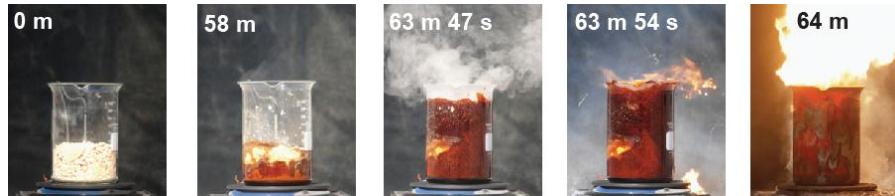


M. L. Hobbs, M. J. Kaneshige, M. U. Anderson



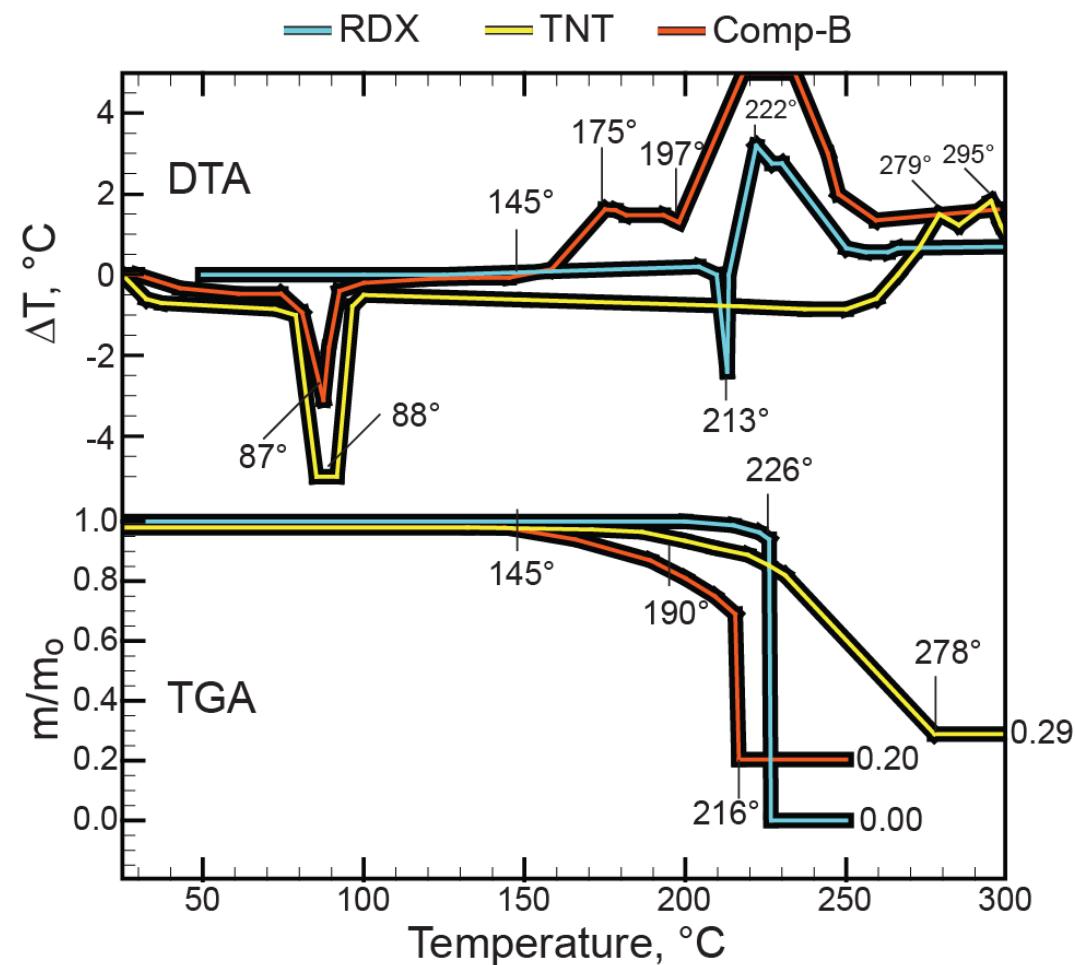
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXX

Introduction



- Composition B (Comp-B) explosives consist of mixtures of RDX and TNT, and a desensitizing wax. In the current work, Comp-B is assumed to be composed of 60/40 RDX/TNT by weight.
- Developed prior to WWI and used in mortar shells, torpedoes, demolition charges, warheads, shaped charges, and bombs.
- Prepared by melting TNT in a steam-jacketed kettle, adding wet RDX slowly, heating and stirring until the water is evaporated. Comp-B is cast into desired shape and cooled.
- Comp-B is easy to process, has a high detonation pressure, but fails many insensitive munitions (IM) requirements.
- Comp-B does not pass slow and fast cookoff IM tests. Consequently, the response of Comp-B during an accident, such as a fire, is important for safety analysis.

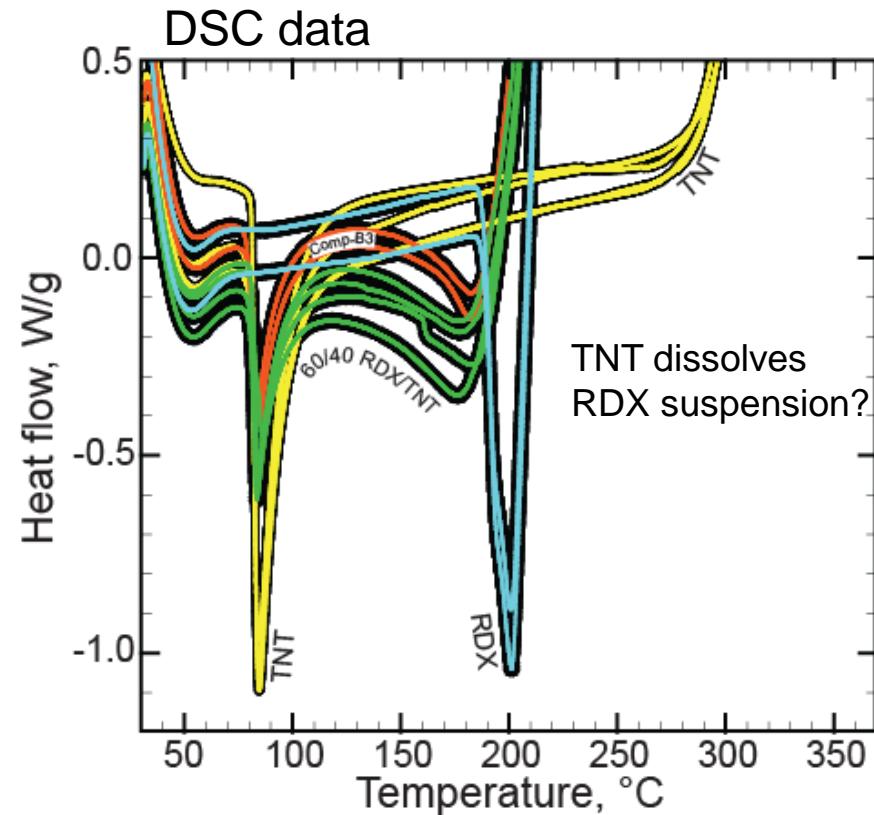
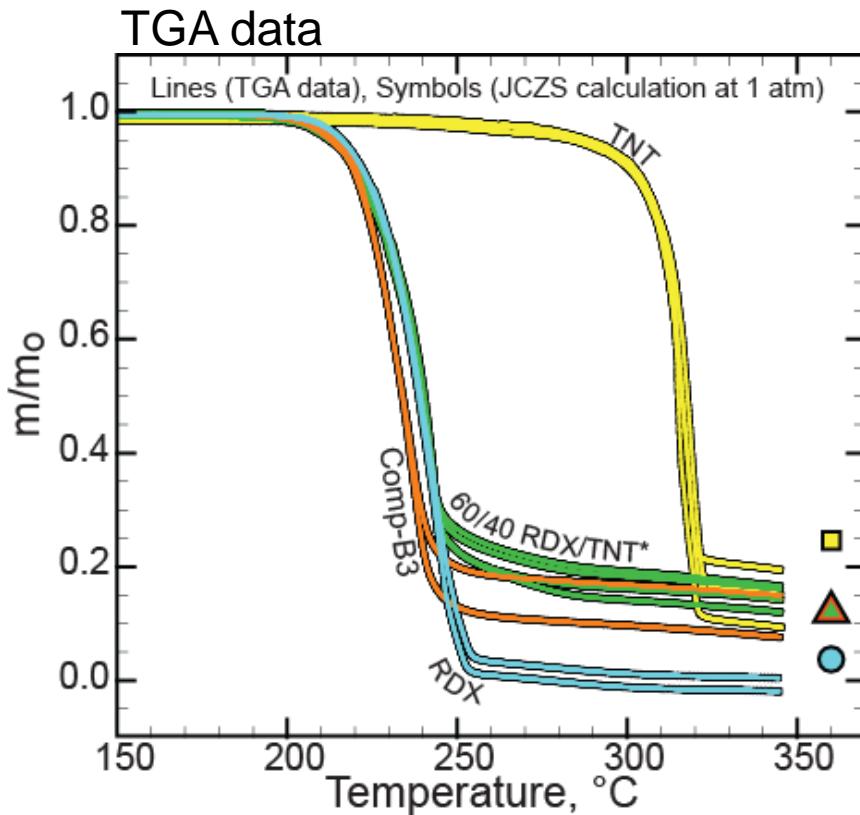
Thermal Analysis by Others*



- TNT in Comp-B melts at same temperature as in pure TNT.
- RDX melt is absent in the Comp-B DTA data.
- Early onset of Comp-B may be caused by hot Comp-B liquid dissolving the RDX suspension.
- Some discrepancy in data (e.g. DTA shows exotherm after TGA indicates no reaction)

*LLNL Explosives Handbook, LLNL report DE85-015961 (1981).

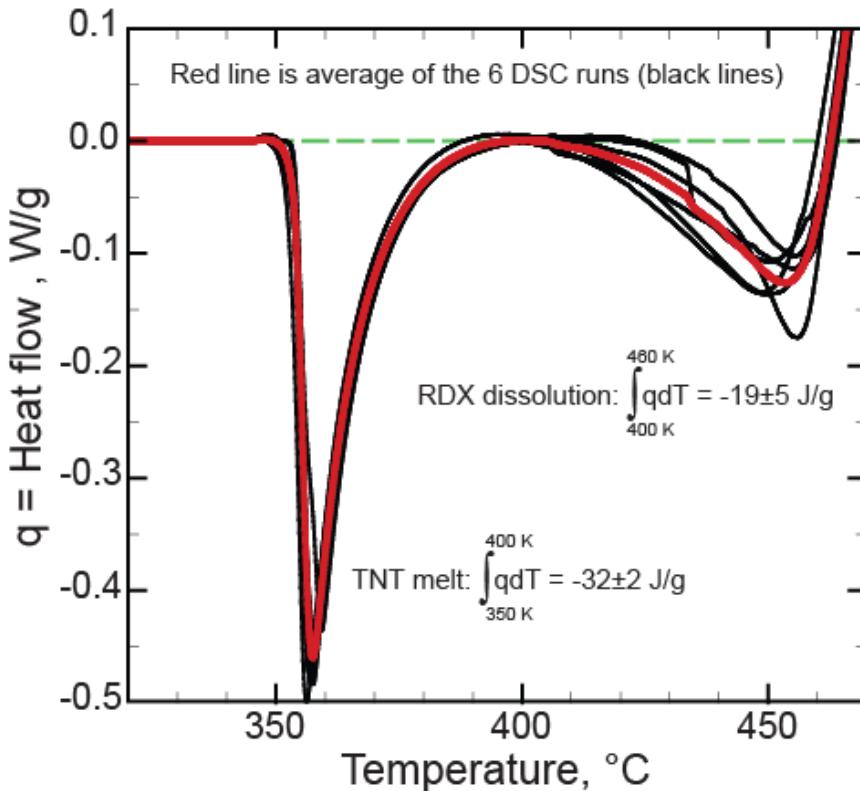
Simultaneous TGA/DSC Data



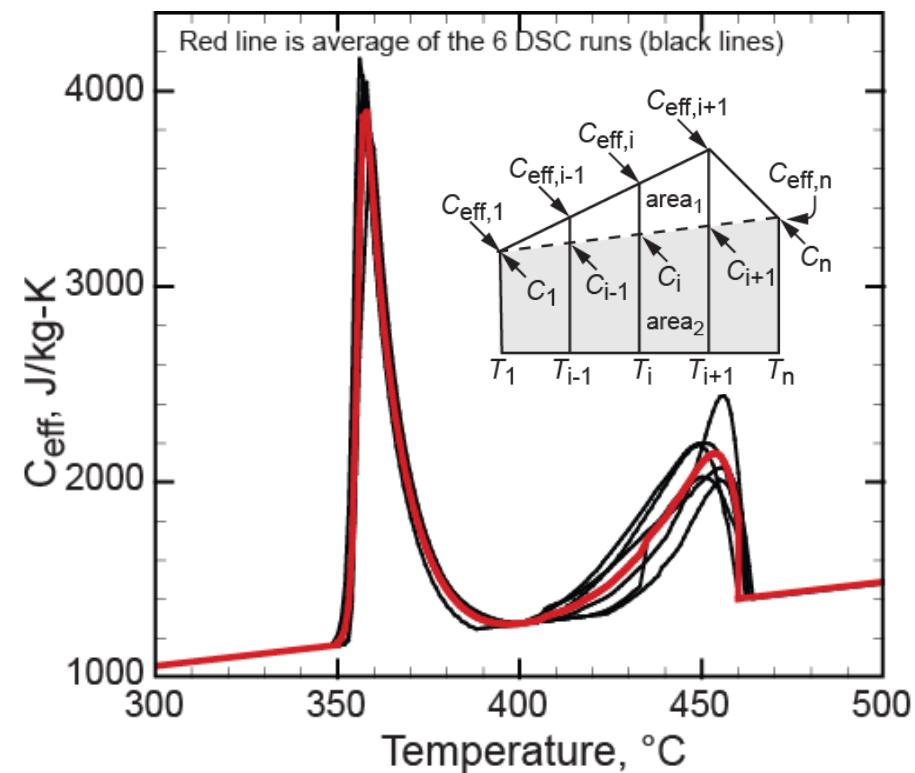
**RDX and TNT are from the same lot used to make the 60/40 mixtures.*

TNT Melt & RDX Dissolution

Baseline corrected DSC

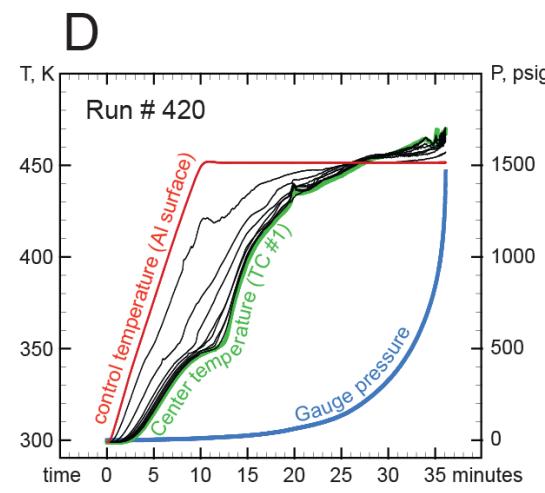
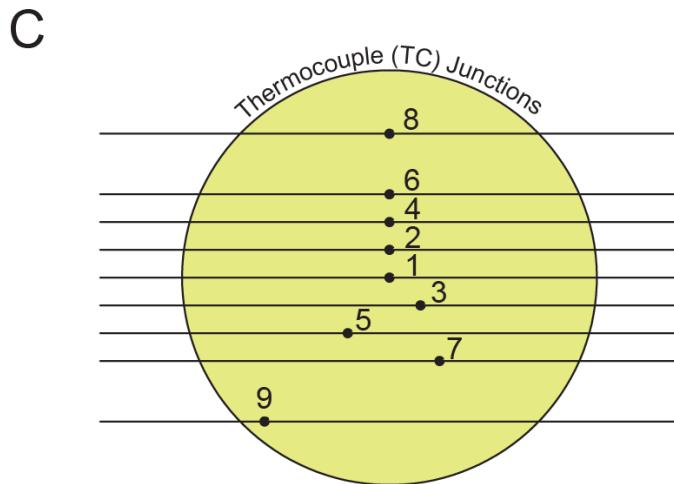
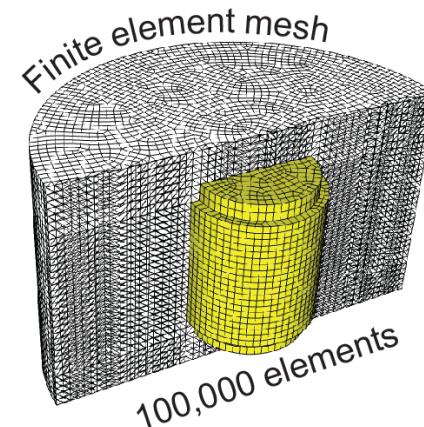
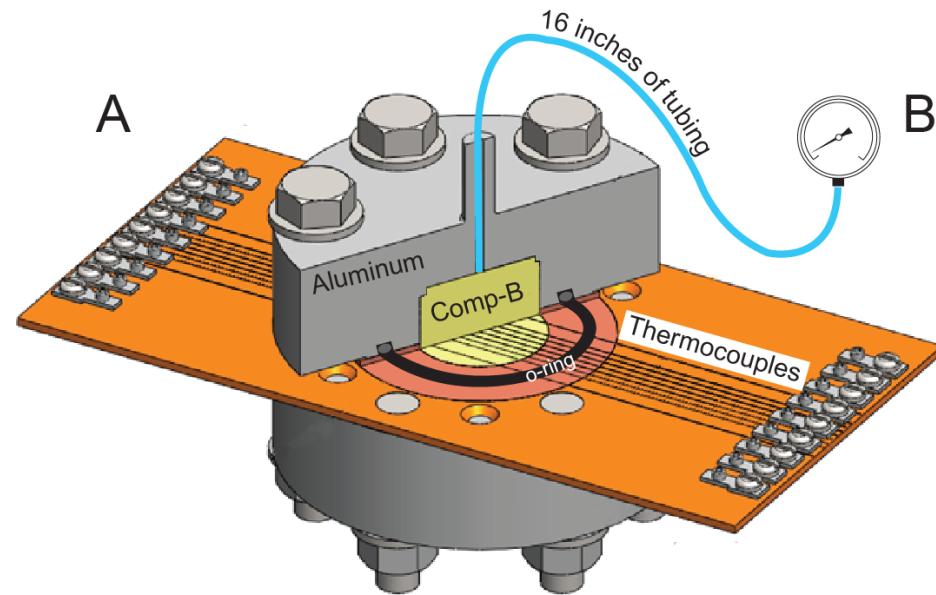


Effective capacitance model



Latent enthalpy taken directly from DSC data. TNT latent enthalpy matches literature. Energy of RDX dissolution is less than RDX melt.

Sandia's Instrumented Thermal Ignition (SITI)



Open half shell



4 m



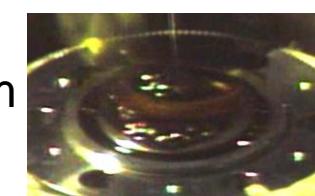
8 m



12 m



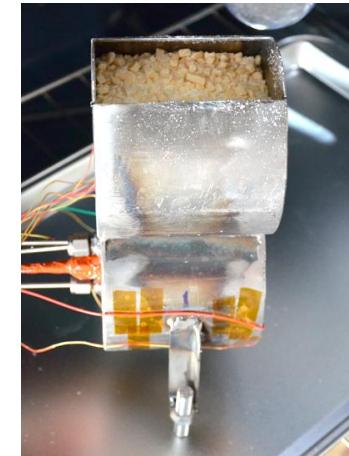
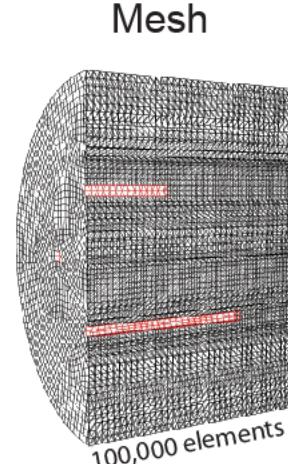
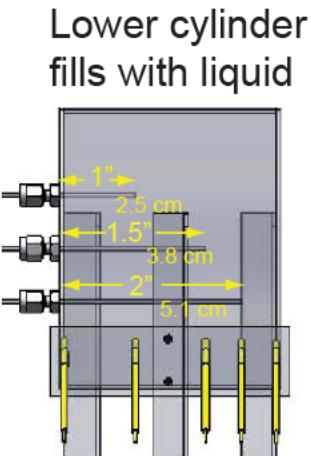
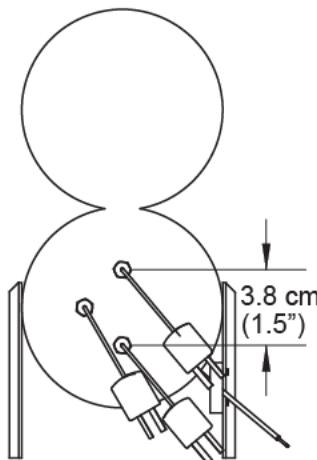
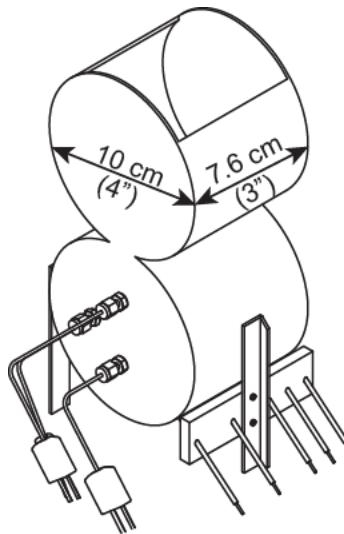
16 m



36 m

6

Oven Test (a.k.a. snowman)



45 minutes



135 minutes



270 minutes



Post test oven



Model Features

- One-step, first-order mechanism
- Distributed Arrhenius rates modified by $(P/P^o)^n$
- Product hierarchy from equilibrium calculations
- Liquefaction modeled thermodynamically
- Liquid rates are 15 times larger than solid rates
- Thermal expansion, TNT phase change, RDX dissolution
- One energy equation, one momentum equation, three continuity equations (Comp-B, Gas, Carbon), various auxiliary equations for gas volume fraction, pressure, etc.



$$r = A \left(\frac{P}{P^o} \right)^{n_p} \lambda \exp \left[- (E + \xi \sigma_E) / RT \right] [\text{compb}] \quad r_{\text{gas}} = \frac{d}{dt} [\text{gas}] = +6.845r \quad r_{\text{carbon}} = \frac{d}{dt} [\text{carbon}] = +2.450r$$

Model Features (continued)

- Single energy equation with convection and reaction source.

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \vec{v} \cdot \nabla T = \nabla \cdot (k \nabla T) + qr$$

- Single momentum equation with Bousinesq volume force.

$$\rho \frac{d\vec{v}}{dt} + \rho \vec{v} \cdot \nabla \vec{v} = -\nabla P + \mu \nabla^2 \vec{v} + (\rho - \rho_o) gh$$

- All wetted surfaces assumed to have a no-slip boundary.

$$\vec{v}_{\text{wetted surfaces}} = 0$$

- Local gas/solid velocities/temperatures equal.

$$T_C = T_g = T(x, y, z, t) \text{ and } \vec{v}_C = \vec{v}_g = \vec{v}(x, y, z, t)$$

- Low Mach flow (velocities much less than sound speeds).

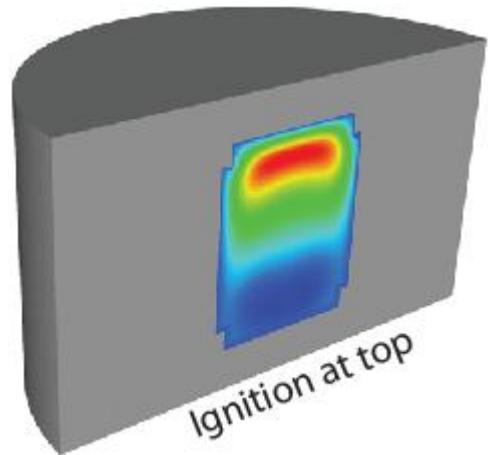
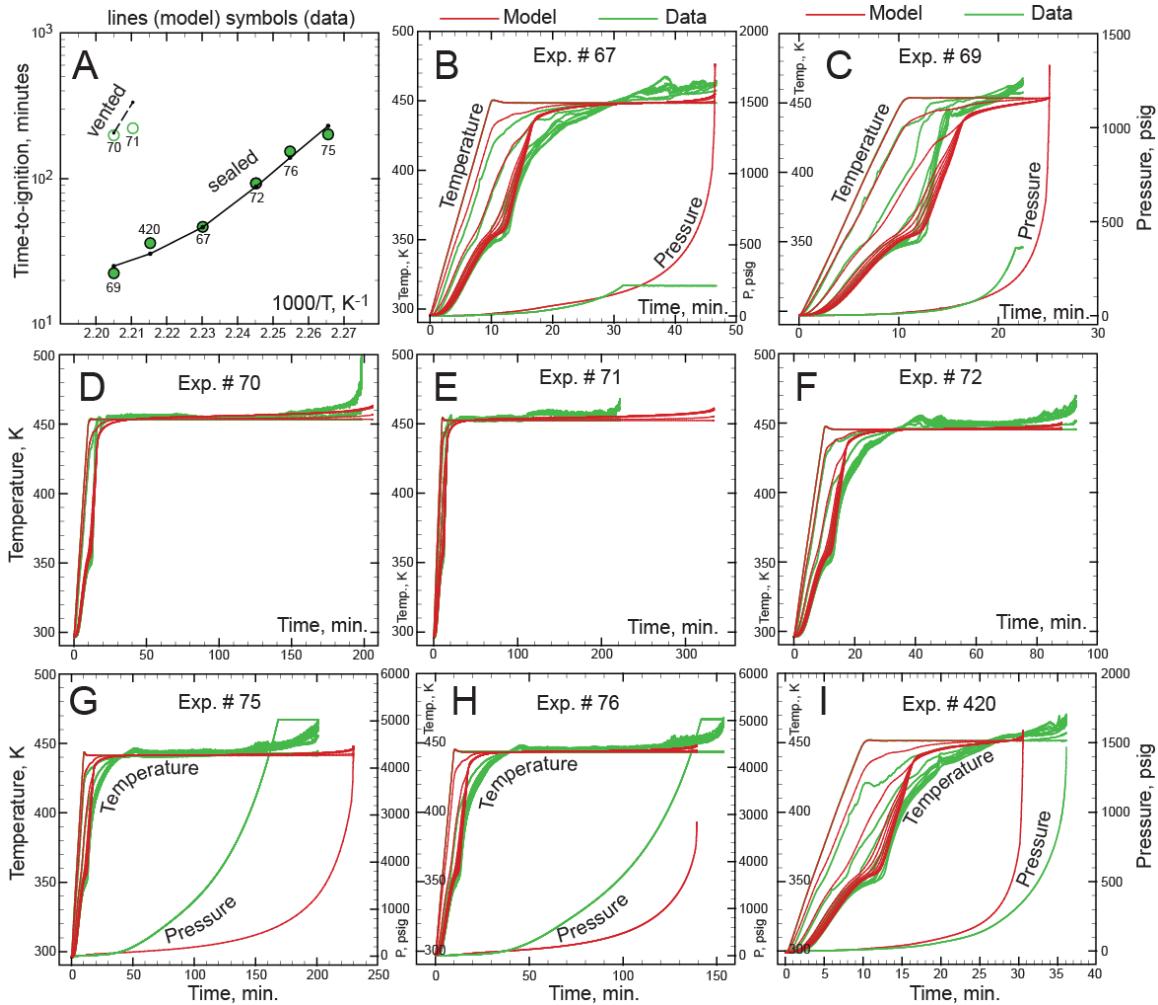
$$P(x, y, z, t) = P(t)$$

- BKWS-EOS used for pressure $P_g(x, y, z, t) = P_g(t) = \frac{\bar{z} n R \bar{T}}{V_g}$

$$\bar{z} = 1 + X \exp(0.298X)$$

$$X = \left(\frac{n}{V_g} \right) \left(\frac{0.0105 \times \text{Covol}}{\sqrt{\bar{T} + 6620}} \right)$$

SITI Test Results

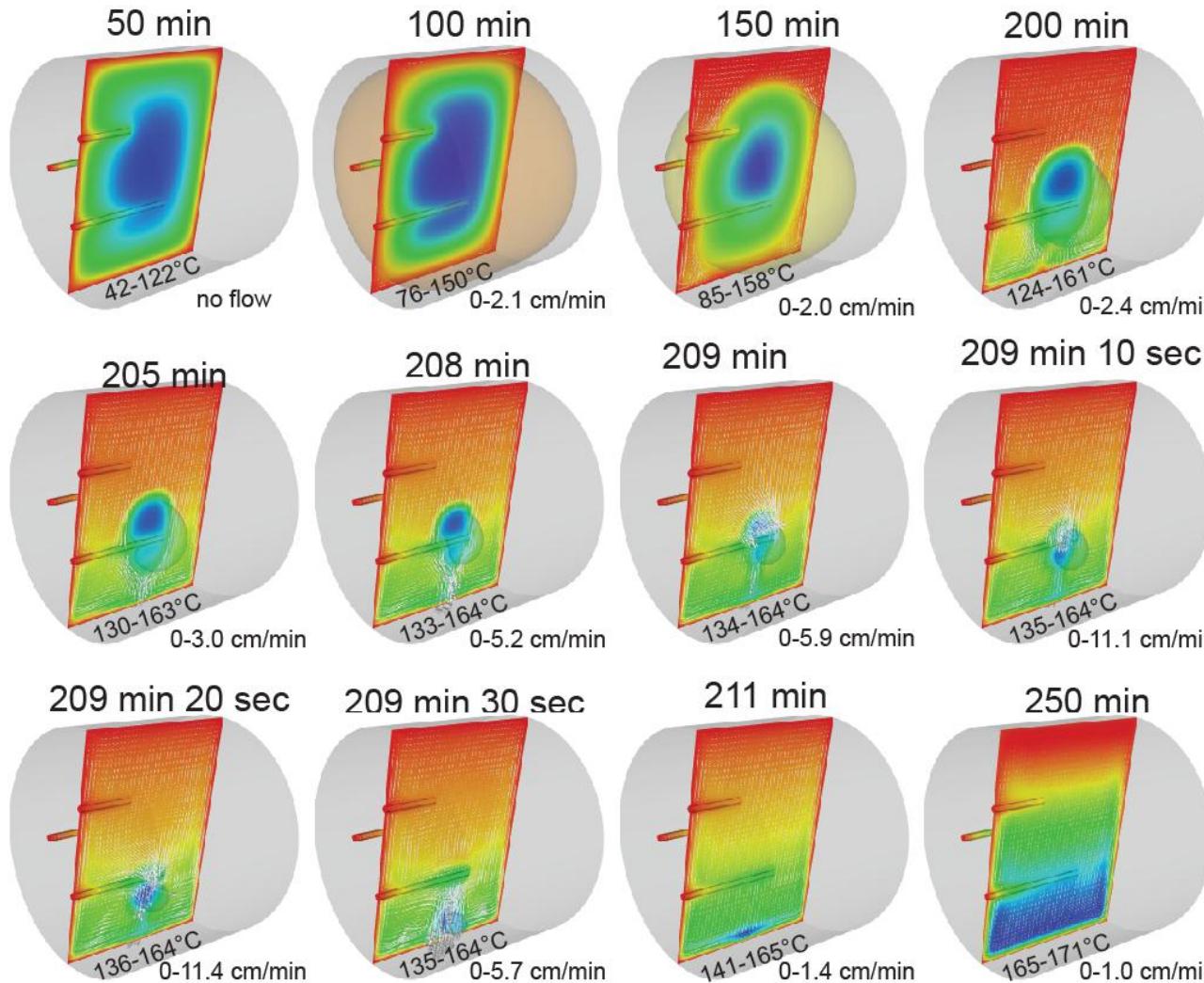


- #71 ignited faster than predicted. Possible plug?
- Good temperature match to 430 K, then model transition from solid to liquid is too fast.

$$T < 412.5K \quad \mu = 0.25 \times 10^6 \text{ Pa} \cdot \text{s}$$

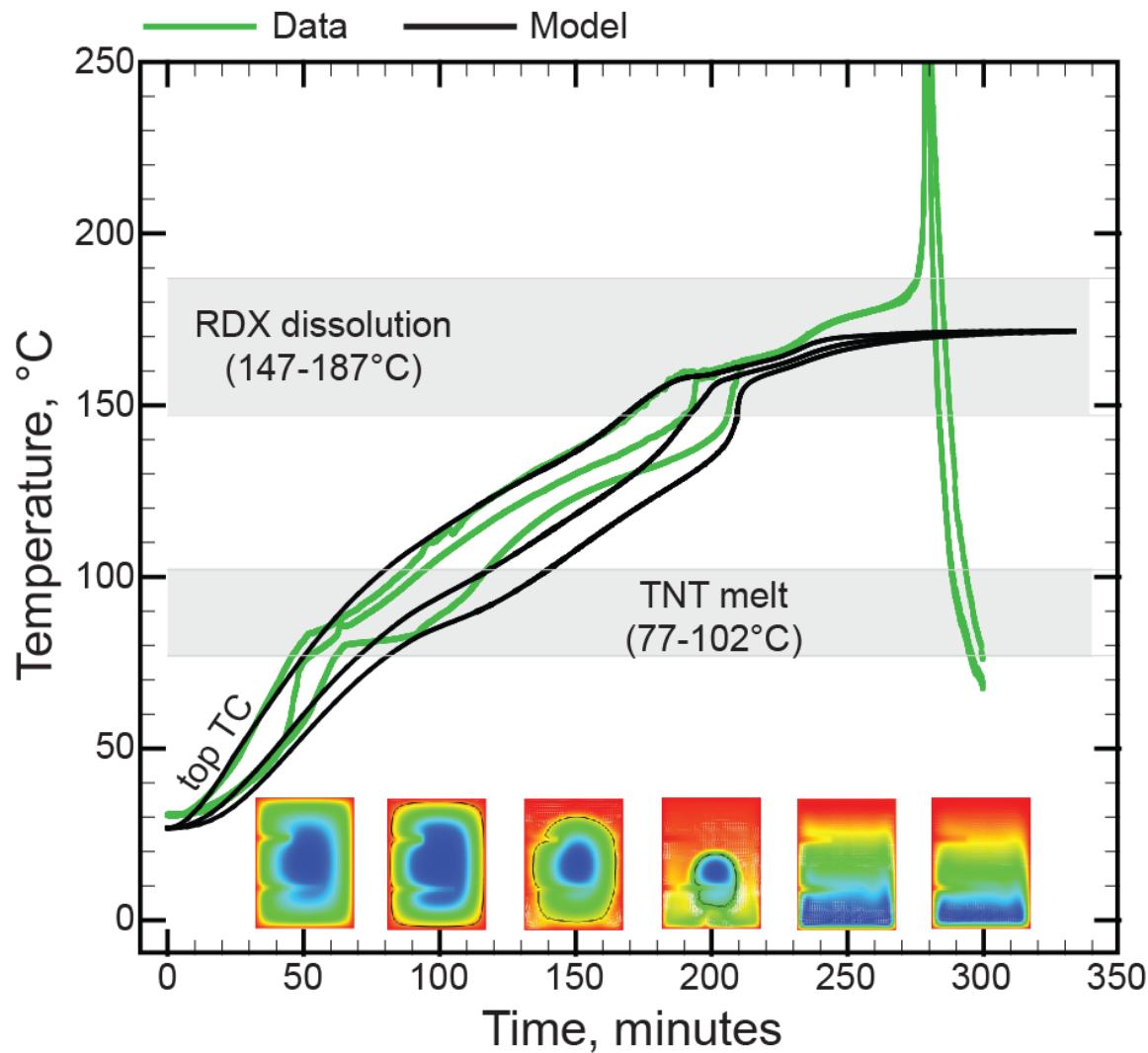
$$T > 413.5K \quad \mu = 0.2 \text{ Pa} \cdot \text{s}$$

Oven Test Results



- Melts from outside to the inside.
- Solid plug gets smaller and starts to fall toward the bottom of the can.
- Liquid heats up and eventually self-heats and ignites at the top of the can.

Oven Test Results



- Temperature pinch occurs in middle of RDX dissolution range.
- Model predicts slightly longer ignition times.
- Discrepancy in ignition time could be related to the method of melting the Comp-B flakes.
- In the experiment, the flakes were melted in the combined system.

Summary and Conclusions

- Decomposition of Comp-B decomposes differently as a mixture than the individual components RDX and HMX.
- TNT melts between 77-102°C in Comp-B.
- The RDX suspension in hot TNT dissolves between 147-187°C
- The dissolution of RDX is not as sharp as a phase change and favors a distributed activation energy model.
- The model captures the time-to-ignition for the SITI experiments.
- The modeled SITI internal temperatures are good until about 157°C and then the temperatures pinch together faster than the measured temperatures.
- Temperature dependent volumetric expansion data is needed at elevated temperatures.
- Viscosity data above 157°C is needed.
- More data is needed for both open and closed systems using melt-cast Comp-B as well as flaked Comp-B.