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RESPONSE OF ENERGETIC MATERIALS TO THERMAL HAZARDS

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Eugene S. Hertel, Jr., William W. Erikson,
Michael J. Kaneshige, Anita M. Renlund,
Robert G. Schmitt, and Arthur C. Ratzel, III

Sandia National Laboratories
Albuquerque, New Mexico

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. This work is also supported by the Joint Munitions Program, a collaborative effort between the DOE nuclear weapons laboratories and the DoD.

National Nuclear Security Administration

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Outline

- Problem specification
- Model development process
- Code development platform
- Technical details

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Hazards Analysis of Energetic Materials

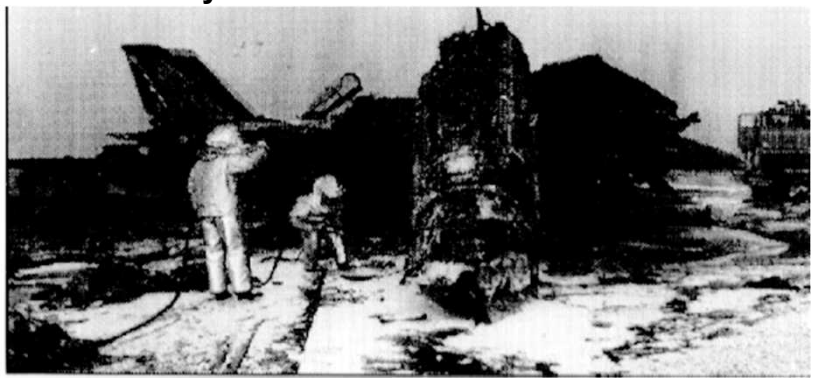
Confined HE in Insulated Box

The DoD & DOE Have Common Needs and Concerns

- Handling
- Storage
- Operations
- Surveillance
- Accidents

Early in the U.S.S. Forrestal Accident

Site after heating for several hours
(Images provided by B. Asay, LANL)



Post-mortem of U.S.S. Forrestal Accident
(Images provided by T. Boggs, NAWC)

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Pool Fire Characteristics

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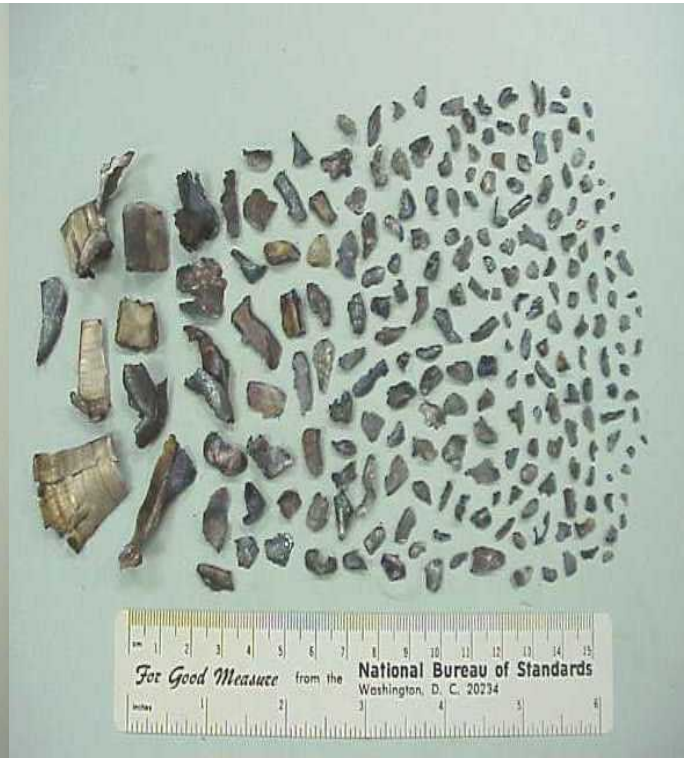
A Spectrum of Thermal Responses

mild pressure burst

moderate violence



high violence,
detonation-like response

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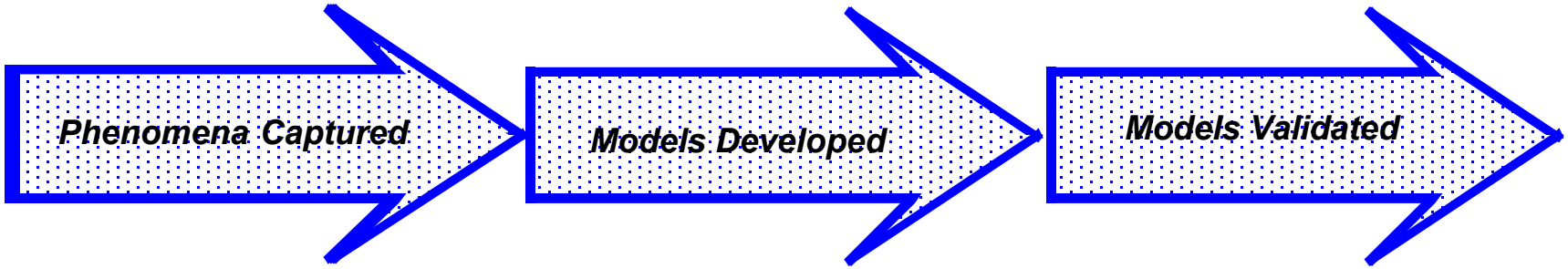
Thermal Explosion Phenomenology

- Stage 1: Thermal insult (hours-minutes-seconds)
  - Mechanical response
  - Heat transfer properties
  - Chemistry descriptions
  - Thermophysical processes (Phase transitions, morphology, etc…)
- Stage 2: Ignition (10-1000's ms)
  - Quasi-static to dynamic mechanical response
  - Ignition state definition
  - Early time flame spread and combustion modes
- Stage 3: Dynamic Mechanics and Combustion (10-100's ms)
  - Confinement dynamics versus energy release rates
  - Continued flame spreading/Combustion mode
  - Detonation transition, explosion, pressure burst
- Stage 4: Post Event Analysis
  - Pick up what is left and answer the question: What happened?
  - Data poor environment

Model Development Process

Sandia's program is a tightly coupled experimental-computational effort focused on developing a suite of validated models that can be used to analyze risk and consequence assessment of ordnance systems



Our focus has been to develop and improve sub-models for energetic material decomposition kinetics, mechanical response, ignition, combustion, rapid energy release (detonation), and system response

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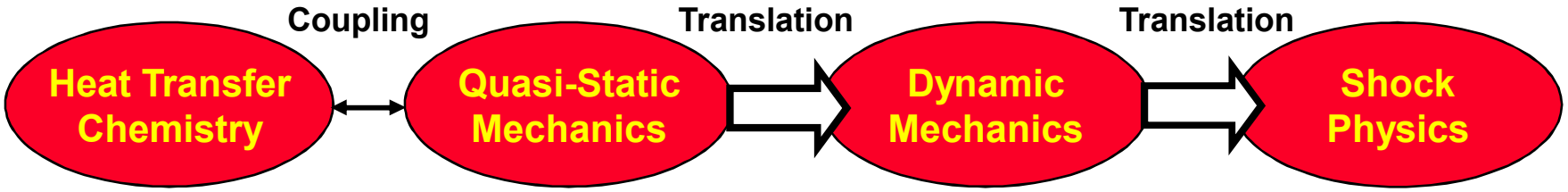
Modeling Thermal Explosions



Heat Transfer Chemistry	Quasi-Static Mechanics	Dynamic Mechanics	Shock Physics
Thermal conductivity	Youngs Modulus	Youngs Modulus	Youngs Modulus
Specific heat	Poissons Ratio	Poissons Ratio	Poissons Ratio
Density	Yield Stress	Yield Stress	Yield Stress
Porosity	Ultimate Stress	Hardening	Hardening
Kinetics	Hardening	EOS models	EOS models
Mixtures	Thermal Expansion	Fracture Strength	Fracture Strength
Permeability	Temperature Dependence	Burn Phenomena	EM constitutive model
Species Transport	EM constitutive model	Burn Models	DDT analysis
Mass Transport	Liquid/molten phase, fluid flow	EM constitutive model	
		Ignition	

Use existing codes to resolve physics at appropriate time and length scales

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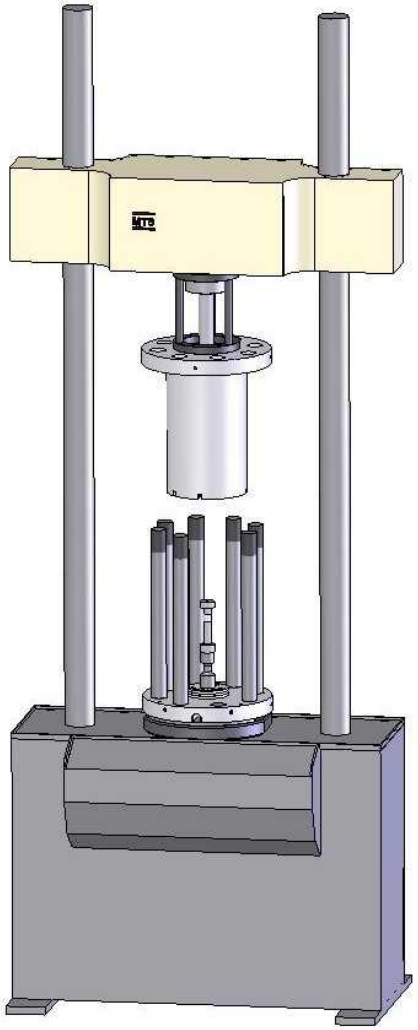
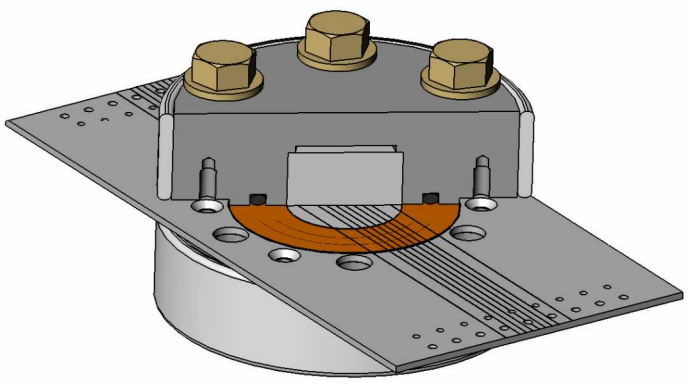
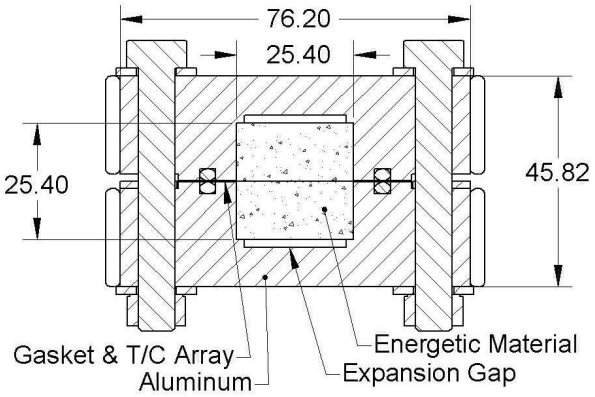
Phenomena/Characterization Experiments



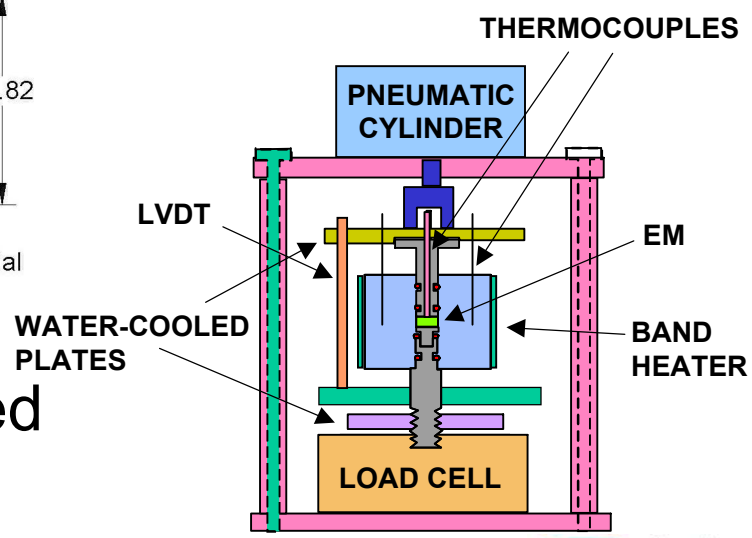
Triaxal MTS





Sandia Instrumented Thermal Ignition (SITI) Apparatus

Hot Cell



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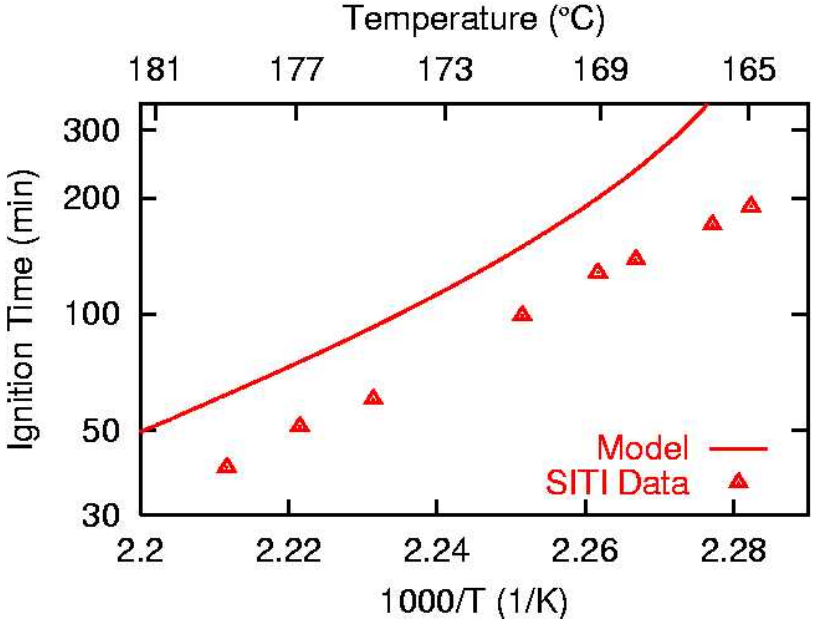
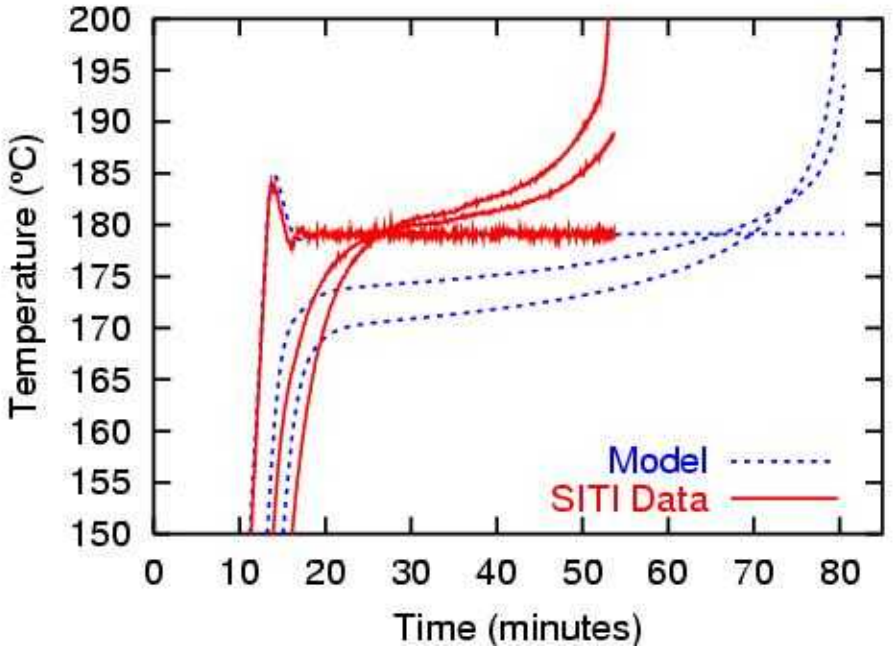
SITI Data Case Study: PBXN-109

"Original" model based on McGuire-Tarver RDX model and PBXN-109 ODTX data

- **ODTX-fit model does not predict SITI ignition time well**
- **In situ temperature measurements suggest why – endothermic first step**





PBXN-109: 64% RDX, 7.4% HTPB, 20% Al, 7.4% DOA

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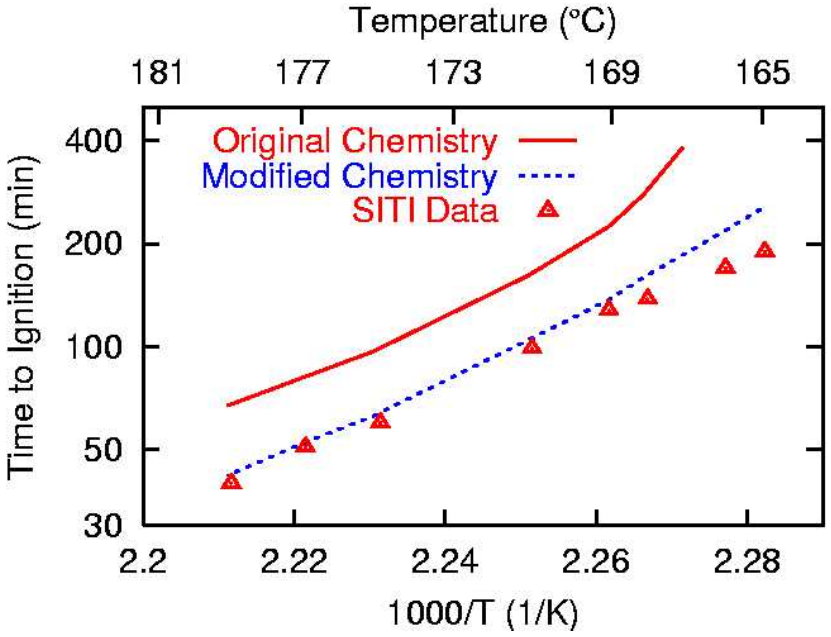
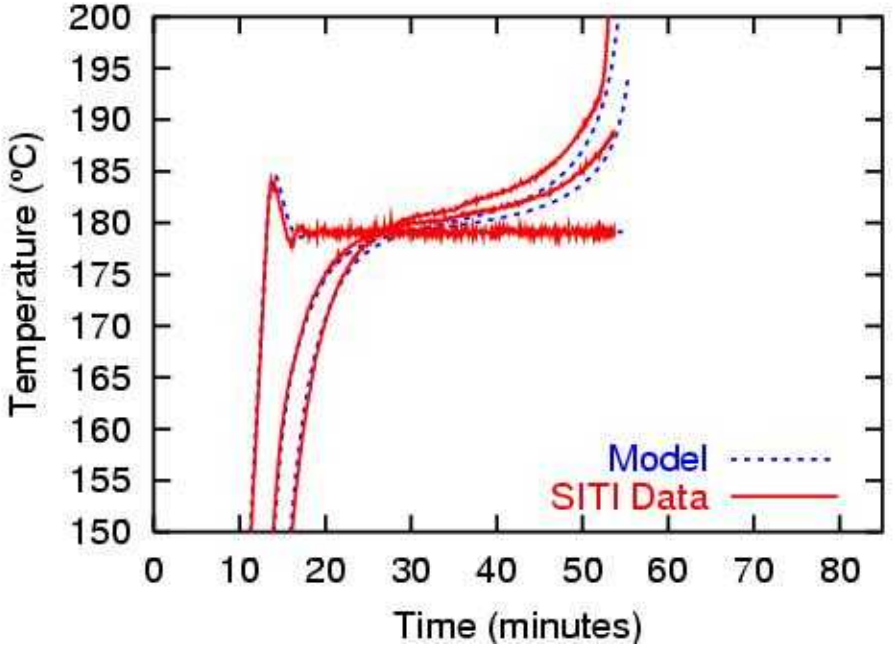
"Modified" PBXN-109 Model

- ***Removed endothermicity of first reaction step***
- ***Readjusted activation energies and prefactors to fit ODTX data***





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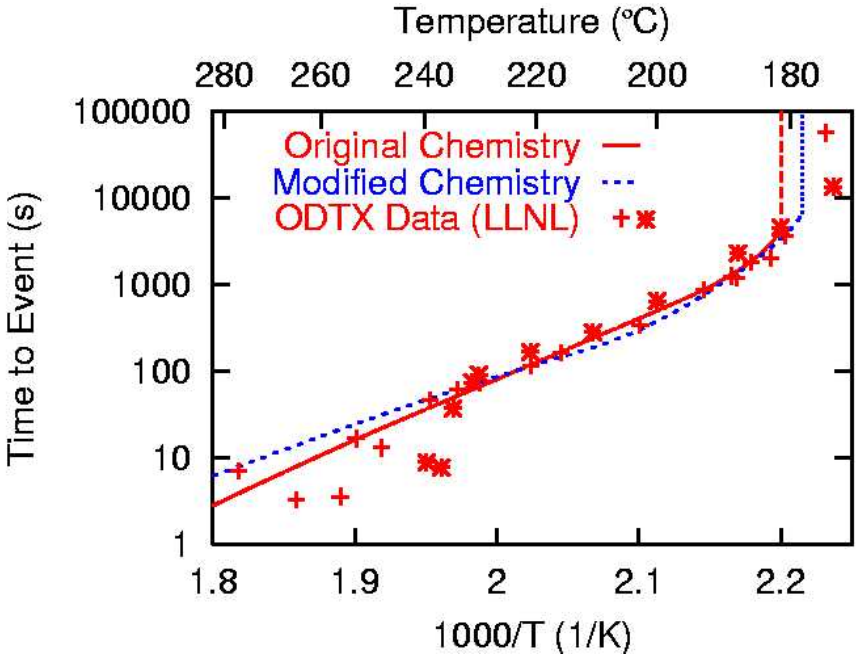
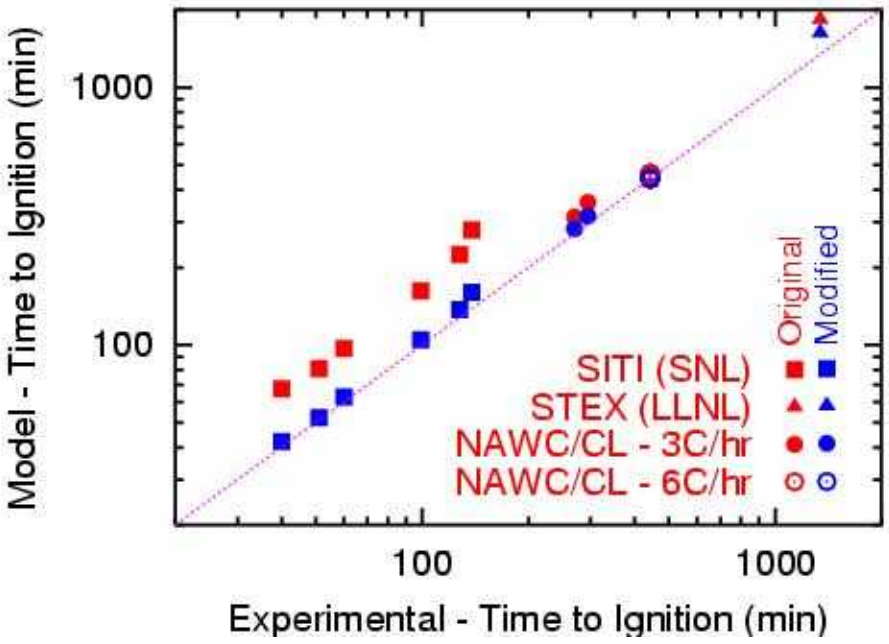
Other Comparisons of "New" Model

Compared to ODTX:

Better at low temperatures

Worse at high temperatures





"Larger" scale tests:

Less over-prediction of time to ignition

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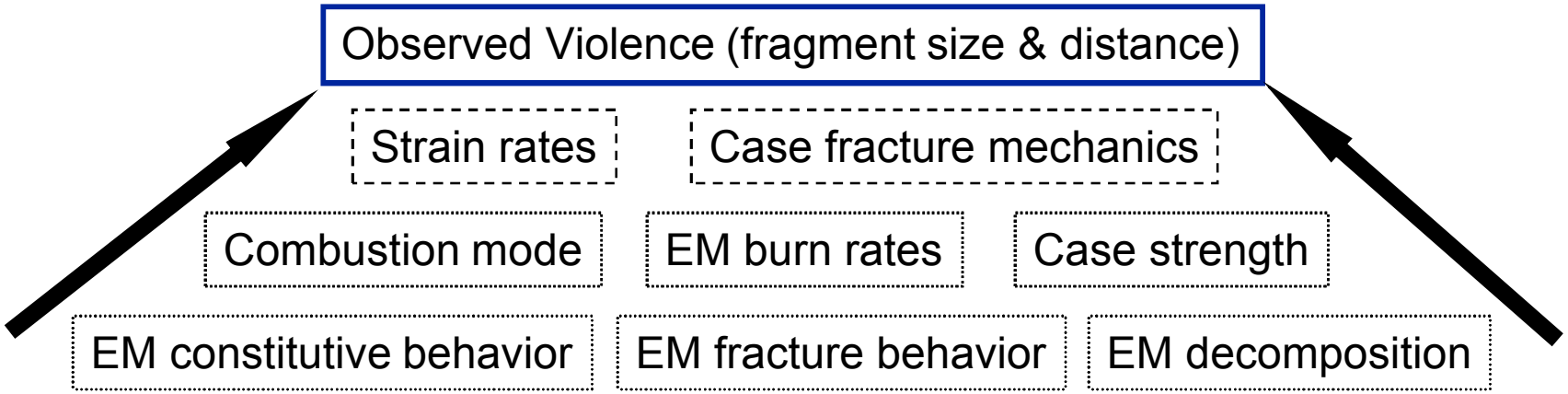
Violence of Reaction

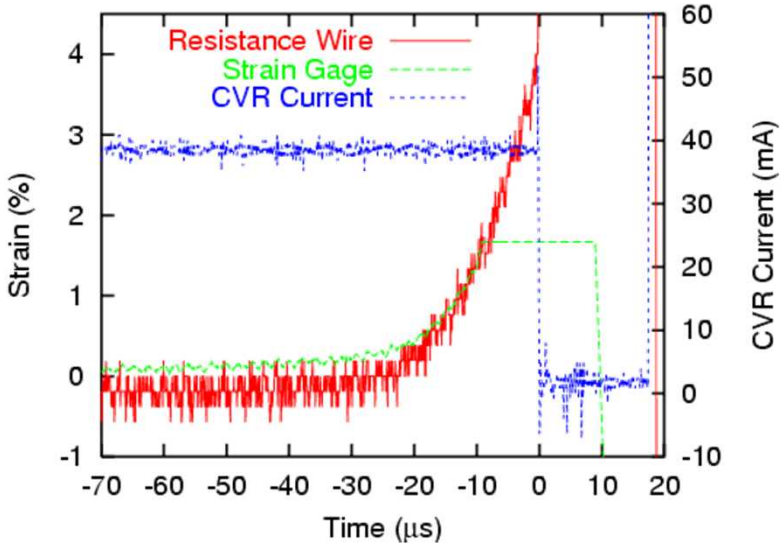
Easiest things to measure are the most difficult to simulate



- **Needed:**
  - **Characterization of fundamental processes and properties that lead to gross measures of reaction violence**
  - **Quantitative measurement of intermediate reaction violence characteristics (velocity, strain rates)**

Reaction Violence Model Development

- Constitutive properties of heated and/or damaged explosives
- Characterization of post-ignition combustion processes – mode and burning rates
- Fiber optic interferometers to measure strain rates
- Resistance wires to measure large strains



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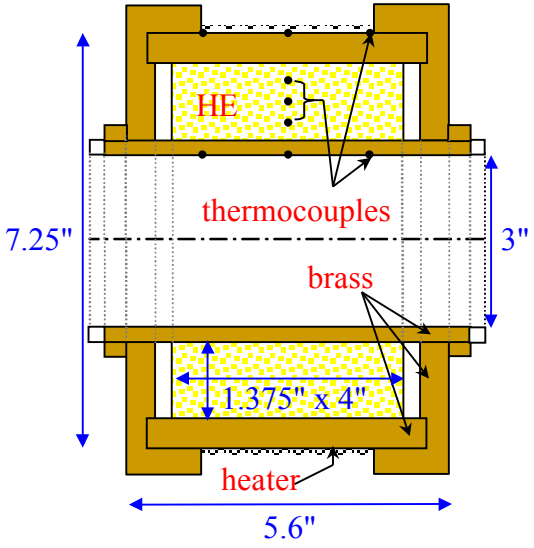
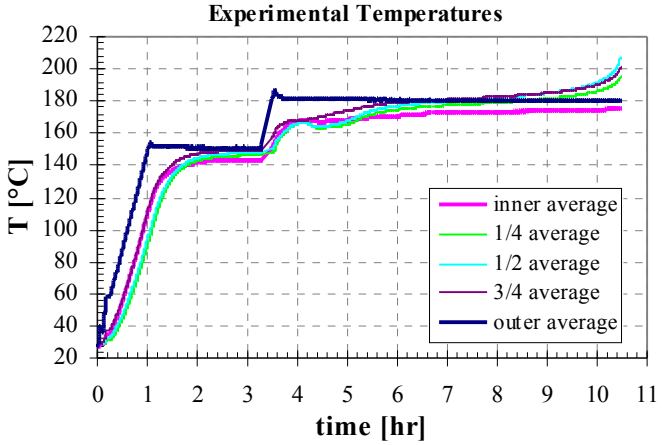
Large Scale Annular Cookoff Experiment

- ~2.5 kg of HE in annular configuration with brass confinement
- Boundary conditions are well defined
- Temperatures measured on inner and outer brass and within HE itself
- heat to 150ºC, hold ~2 hrs., heat to 180ºC, hold
- HE cooked off at ~10.5 hrs (apparent detonation)





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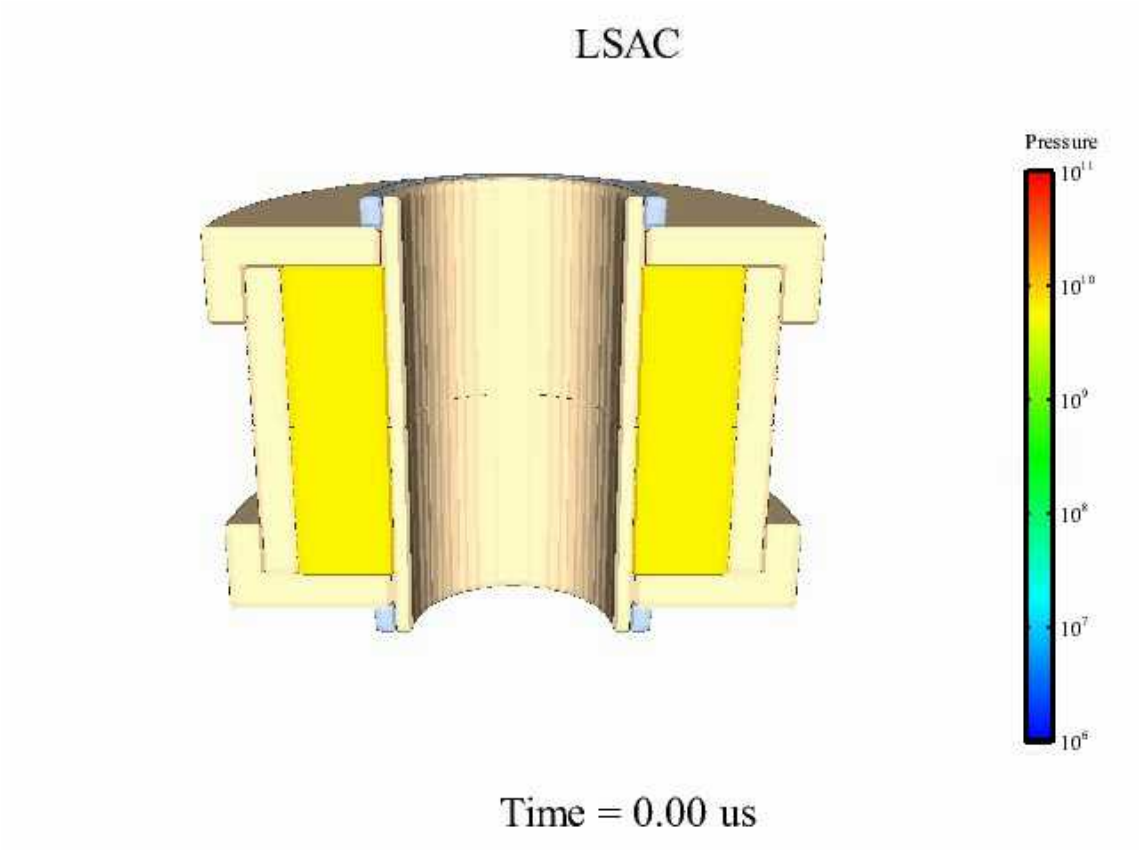
3D Coupled Level Set/Multiphase Calculation



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Summary and Conclusions

- Sandia program is tightly coupled experimental/computational activity
- FEM tools used for pre-ignition
- Shock physics tools for detonation/explosion
- Continuum mixture theory mathematical framework
- Ignition front models have been developed
  - Now capable of responding to dynamically evolving fields
  - Need more experiments to extend post-ignition understanding
- More work needed on improving sub-grid physics models for key phenomena

Supporting OSD Modeling and Simulation Initiative along with developing Insensitive Munitions Initiative

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