COOKOFF ANALYSIS USING AN IMPLICIT AMR APPROACH

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Introduction

- Objectives
- Problem Definition
- Modeling Framework
- Parameter Definition
- Benchmark example
- Full-scale system simulation examples

Objectives

- Advance the use of digital engineering in the IM assessment & design process
- Need to move to point of true prediction of IM concepts to include materials and configurations
- Here highlight analysis of the slow cookoff scenario; fast cookoff, frag/bullet impact, shape charge and sympathetic reaction also being worked
  - Fast cookoff requires thermal loading process discussed here + “flow” analysis
- Help drive better IM system level testing; currently performed as qual tests
- Multi-component energetics represent unique challenges; ingredients may have well known response but when combined “global” response differs

Governing Equations

- IM scenarios have challenges of heat transfer, chemical reactions and fluid dynamics
- For slow cookoff primary response is a thermal decomposition so can be represented using heat transfer equations
- For fast cookoff, response includes quick gasification and flow of material so must additionally solve
- Definition of reaction rate parameters will be discussed

Heat Transfer Equations

$$\rho C\frac{\partial T}{\partial t} = k(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}) - \frac{\partial \lambda}{\partial t}Q,$$

$$\frac{d\lambda}{dt} = A_\lambda f(\lambda)\exp(\frac{-E_\lambda}{RT}).$$

Flow Equations (2D Axisymmetric)

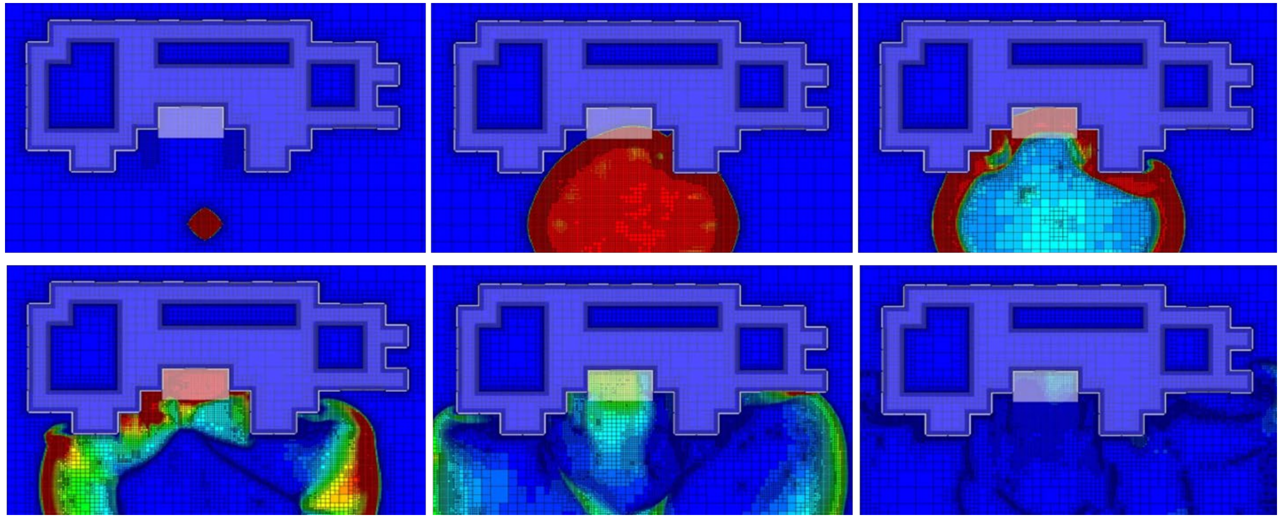
$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{E}}{\partial r} + \frac{\partial \vec{F}}{\partial z} = \vec{S}(\vec{U}),$$

$$\vec{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho\lambda_{explosive} \end{bmatrix} \vec{E} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ u(\rho E + p) \\ \rho\lambda_{explosive} u \end{bmatrix} \vec{F} = \begin{bmatrix} \rho v \\ \rho v u \\ \rho v^2 + p \\ v(\rho E + p) \\ \rho\lambda_{explosive} v \end{bmatrix} \vec{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ k\nabla^2 T + \rho Q\dot{\lambda}_{exp\ losive} \\ \rho\dot{\lambda}_{explosive} \end{bmatrix}.$$

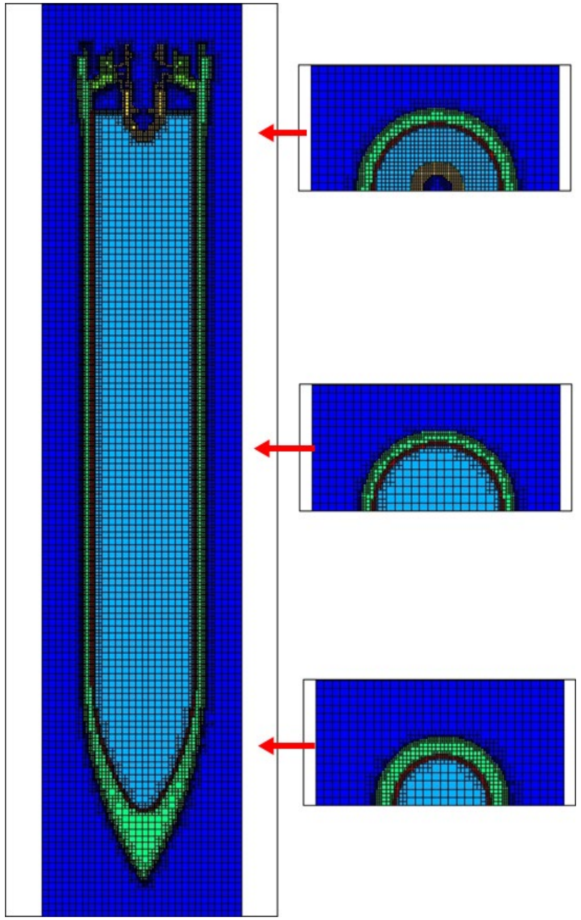
Adaptive Mesh Refinement (AMR) Framework

- Simulations shown here made with a Cartesian Adaptive Mesh code for Blast Explosions & Releases (CAMBER)
  - Finite-volume, multi-material framework
  - Variety of reaction models available
- Greatly increases efficiency, maintaining accuracy
- Adaptation to the solution – refinement in areas with gradients
- Refining to moving waves unique challenge – a method is used that defines location and expected movement of fronts

AMR Used for Blast Modeling



AMR Definition of Object

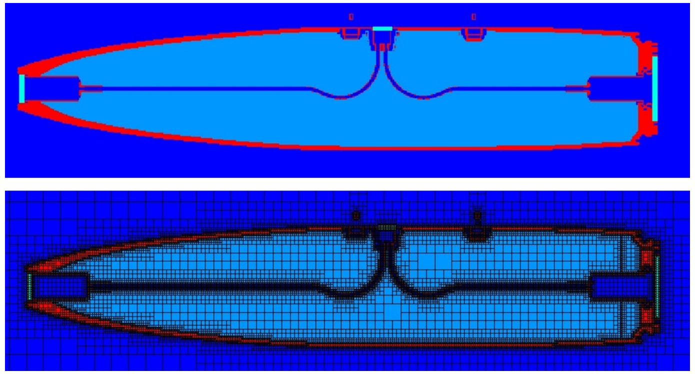


Implicit Approach

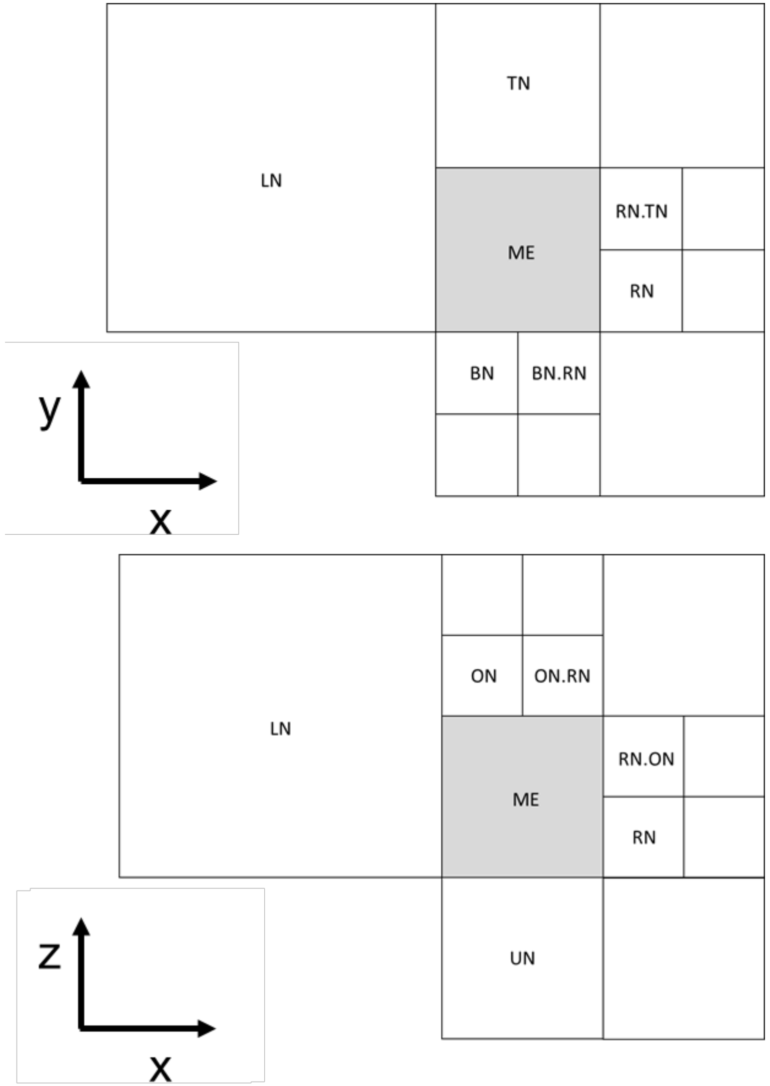
- Timescale of process is such that explicit time integration not practical due to stability requirement is fraction of a second
- Scenarios to be simulated can cover events on the order of several hours or days – implicit methods necessary
- Here an iterative solution method is used
- Leverages fact that AMR structure allows only 1 of 3 potential “neighboring” situations; (1) same, (2) 1/4th, (3) 4x
- Governing equation cast into general form

$$C_{ME}T_{ME} = \sum C_{NB}T_{NB} + S_{ME}$$

- Zero out C_{NB}s based on nature of adaptation

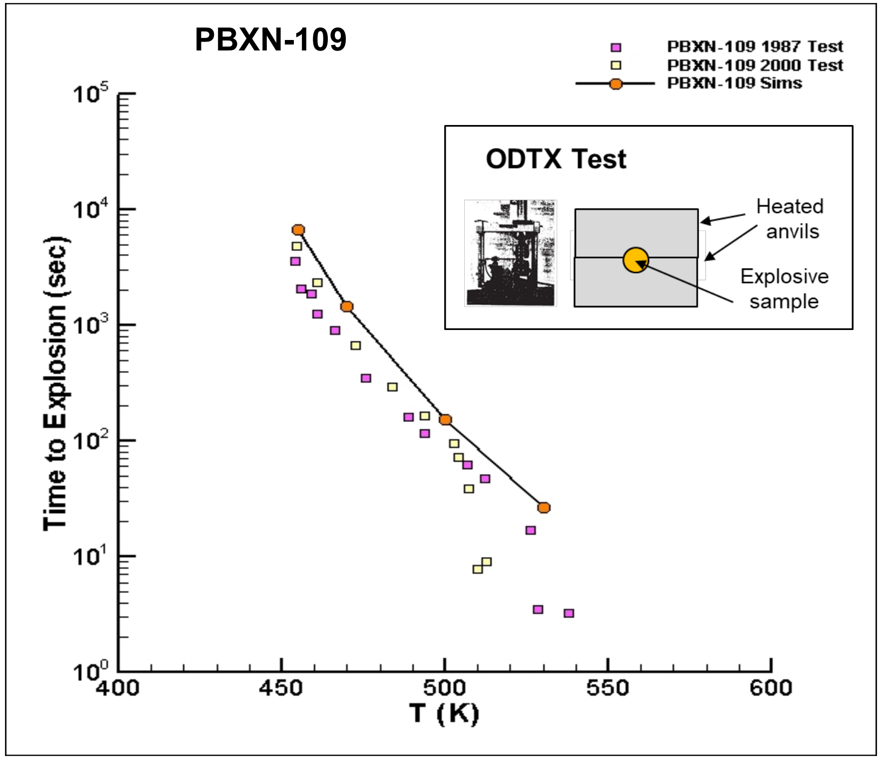


Example Adaptation



Parameter Definition - Multi-step Finite Rate Model

- Key phenomena is transformation & reactions in the energetic during heating
- Two approaches typically taken to address this process
- Studies[1] have shown response to heating can be modeled using a multi-material, multi-step Arrhenius type model
- Parameters derived & validated using ODTX data
- More complex the energetic, the more difficult to define modeling parameters
  - Must work to make “global” characteristics consistent with known behavior of each component
  - Evaluating when a “composite” vs “component” representation is needed



PBXN-109 Kinetic Scheme

$$\begin{aligned} A \rightarrow B \qquad & r_1 = Z_1 exp(-Ea_1/RT)\rho_A \\ B \rightarrow C + Al \qquad & r_2 = Z_2 exp(-Ea_2/RT)\rho_B \\ C \rightarrow D \qquad & r_3 = Z_3 exp(-Ea_3/RT)\rho_C^2 \end{aligned}$$

PBXN-109 Kinetic Parameters

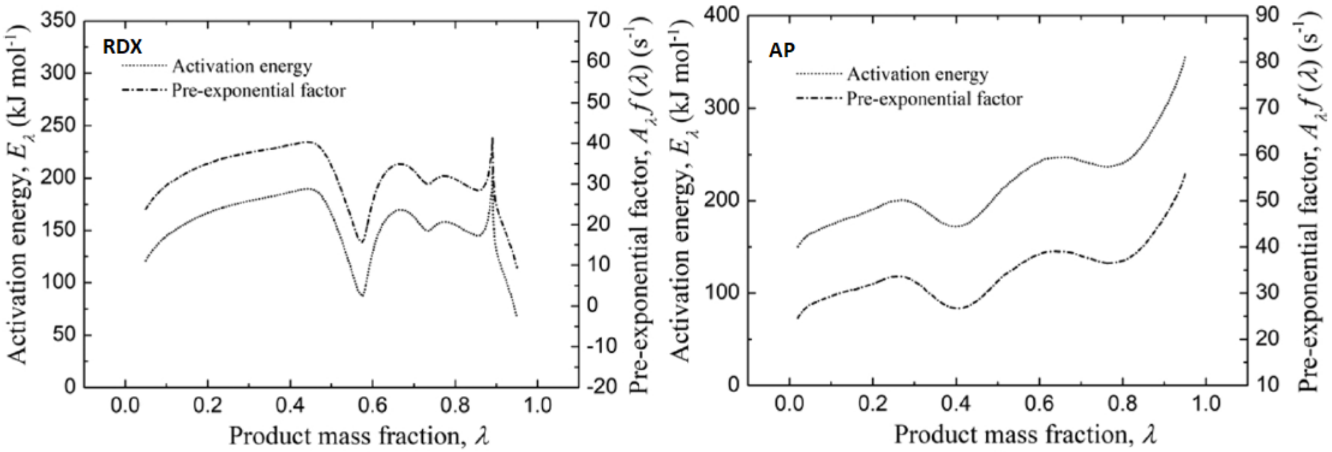
Reaction step	$\ln Z_k$	E_k (kJ/g mole K)	q_k (J/g)
$A \rightarrow B$	43.84 s^{-1}	194.7	268.0 (endothermic)
$B \rightarrow \overline{C}$	39.04 s^{-1}	182.5	−803.9 (exothermic)
$C \rightarrow D$	32.84 $cm^3/s\ g$	141.1	−4241.2 (exothermic)

[1] Yoh, et al,, UCRL-CONF-201173, Nov 25, 2003

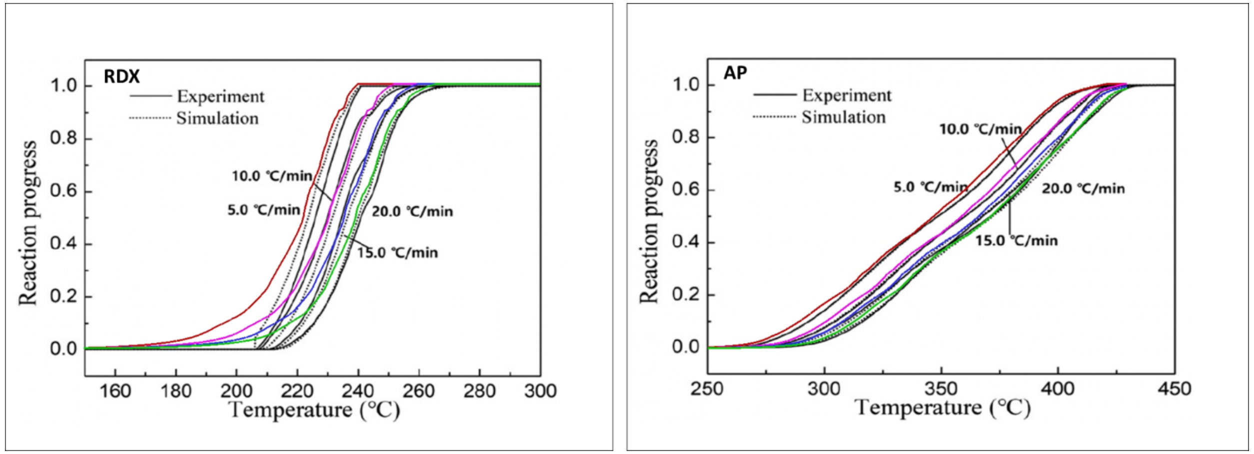
Parameter Definition - Single-step Finite Rate Model

- Another common definition of energetic response uses Self-Accelerating Decomposition Temperature tests [2]
  - Use DSC, TGA
- Single step used to represent the process but not a simple rate law
  - Varying rate parameters replicates the endothermic / exothermic phases
- Max heating temperature was 500 °C, too low for an Al reaction

Rate Parameters for RDX & AP[3]

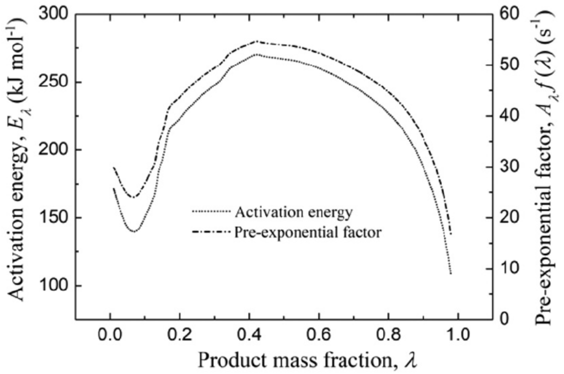


Simulation of RDX & AP Response (Colored curve are current modeling.)



Note: Figures mislabeled in Ref [3]

Rate Parameters for PBX#2 (66% HMX, 25% Al)[3]



[2] Roduit, et al, J. Therm. Anal. Calorim. 93 (2008)

[3] Kim, et al, *Thermochimica Acta,* 678 (2019).

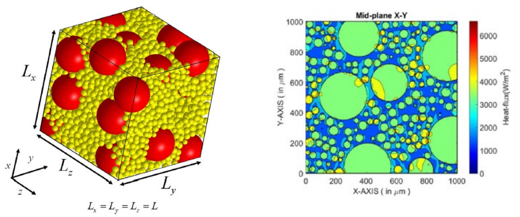
Thermal Properties Definition

- Thermal properties key to process; issue arises if no experimental information is available
- Multi-component energetics; unique challenge
- Density & heat capacity are volume dependent
- Conductivity is a surface property so depends on particle size of each component
  - Originally addressed by Maxwell in 1904

$$k_{eff} = \frac{k_f + 2k_m + 2\phi\left(k_f - k_m\right)}{k_f + 2k_m - \phi\left(k_f - k_m\right)} \cdot k_m$$

  - Currently working better representation
  - Some approaches uses micro sims of define macro parameters[3]

Example from Ref [3]



AP/Al Energetic
K_{eff} (W/mK)

Calc. = 0.51
Exp. = 0.62

RDX25 in Ref [1], PBX #3 in Ref [2]

Component	% weight	ρ (kg/m^3)	C (J/kg-K)	k (W/m-K)
RDX	25	1,858	1,256	0.167
Al	35	2,700	904	205
AP	25	1,950	1,602	0.430
HTPB	15	930	2,900	0.167
Calculated		1,806	1,466	0.74*
Experimental		1,820	1,080	0.20

PBX #2 in Ref [2]

Component	% weight	ρ (kg/m^3)	C (J/kg-K)	k (W/m-K)
HMX	66	1,716	1,427	0.350
Al	25	2,700	904	205
AP	0	1,950	1,602	0.430
HTPB	9	930	2,900	0.167
Calculated		1,742	1,429	2.42*
Experimental		1,900	1,096	0.997

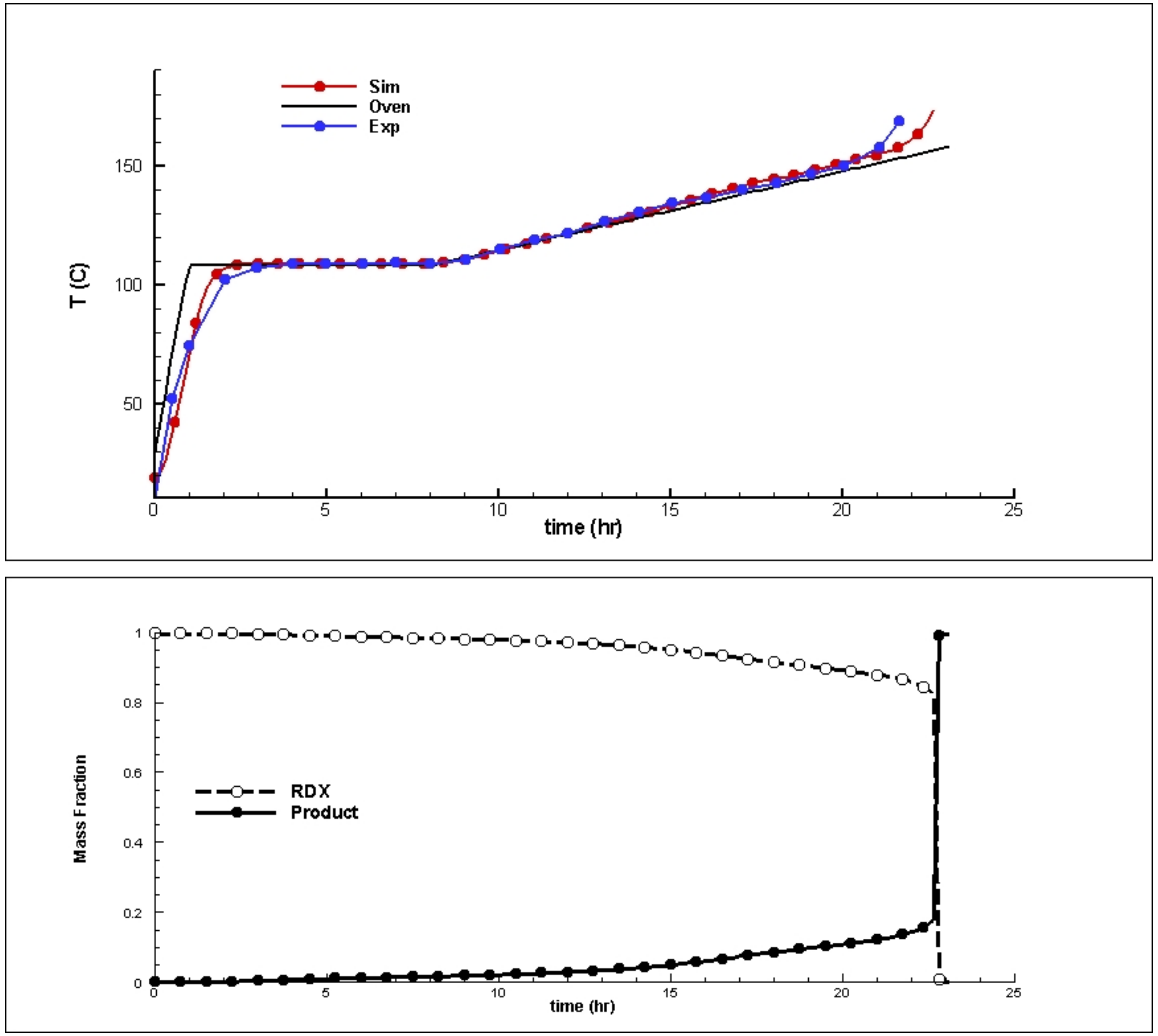
**Using Maxwell eqn.*

[3] Rajoriya, et al, *International Journal of Thermal Sciences,* 127 (2018).

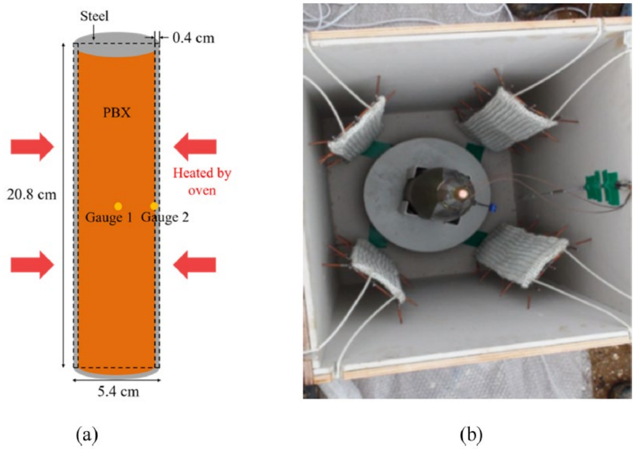
Small-Scale Slow Cookoff Benchmark

- Test item was the RDX25 fill with steel case [3]
- Heating load was 3.3 °C / hr after 7 hr at 108 °C
- Both RDX & AP reactions considered
  - Heat rate causes RDX to respond before AP
  - Temperature well below what is needed for Al to contribute
- Evaluating “composite” vs “component” representation

RDX25 (20%RDX, 35% Al, 25% AP)



Test Configuration

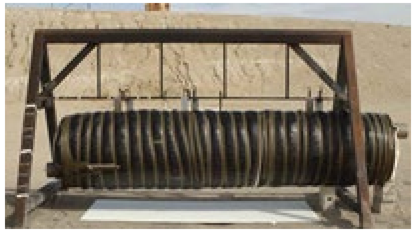


(a)

(b)

Full-Scale Analysis Example (PBXN-109 Fill)

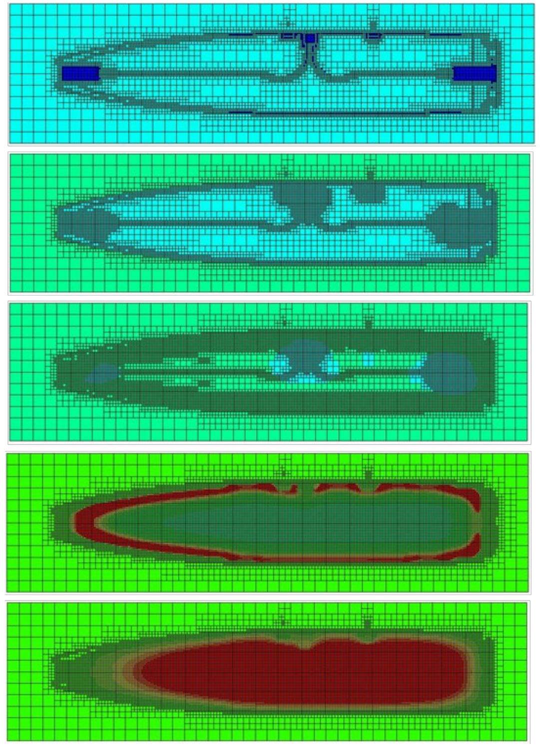
- Test involves engulfing item with heat and elevating load over time
- There is an “induction” process related to the endothermic process
- Implicit/AMR framework allows for efficient analysis



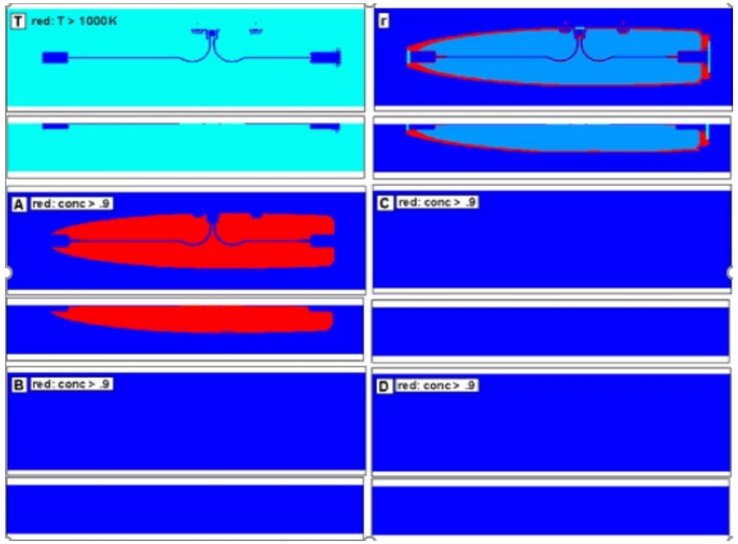
Change in Temperature & Composition

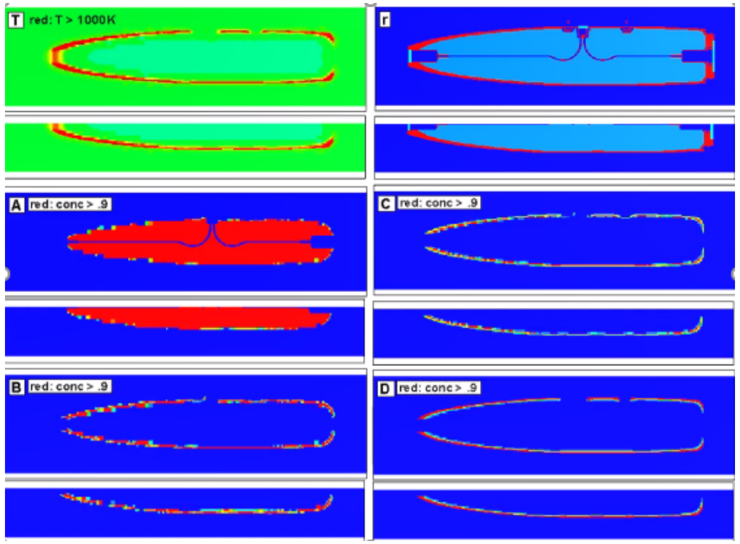
Video

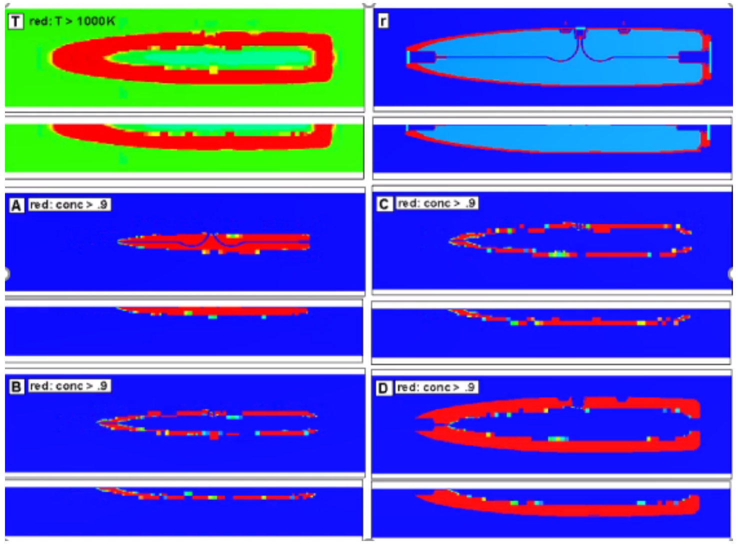
Evolution of Mesh

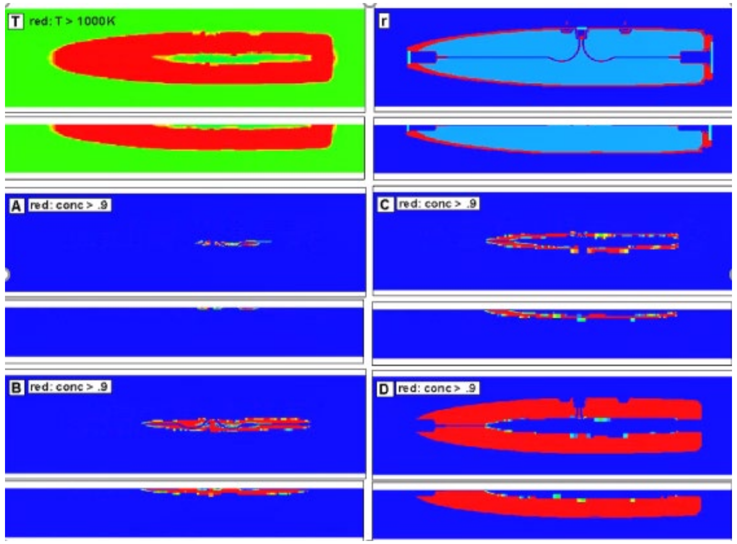


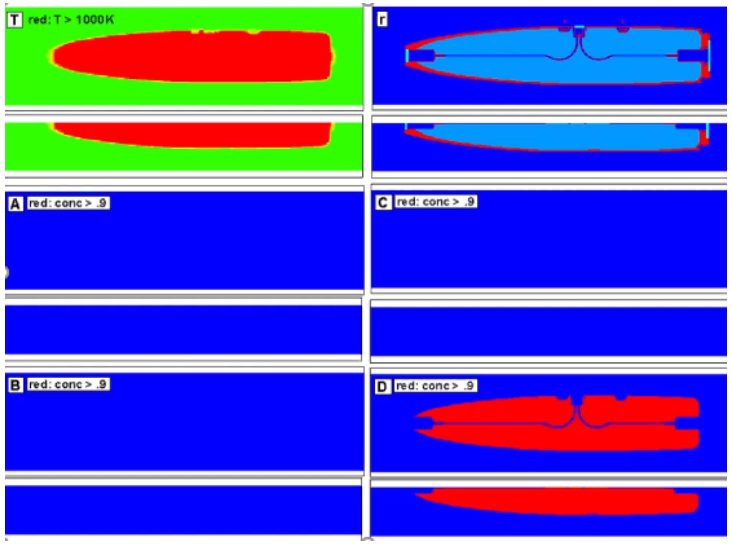
Full-Scale Analysis Example (PBXN-109 Fill) – Still Images

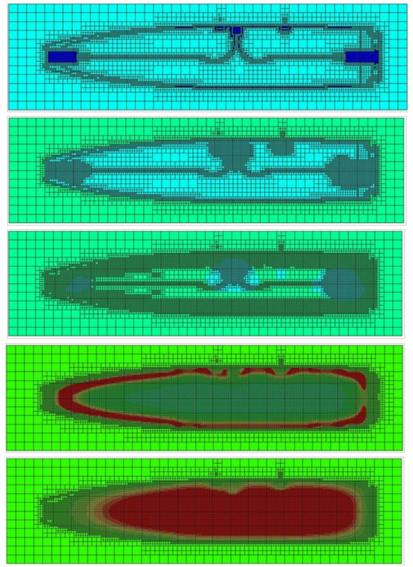






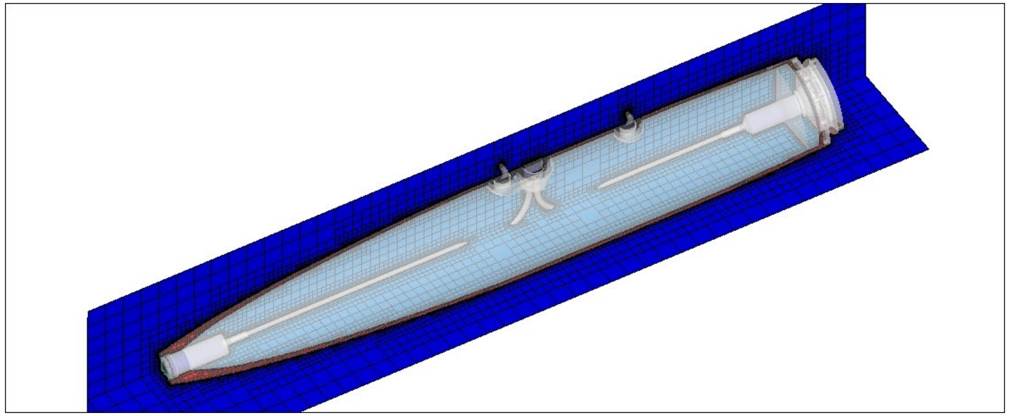


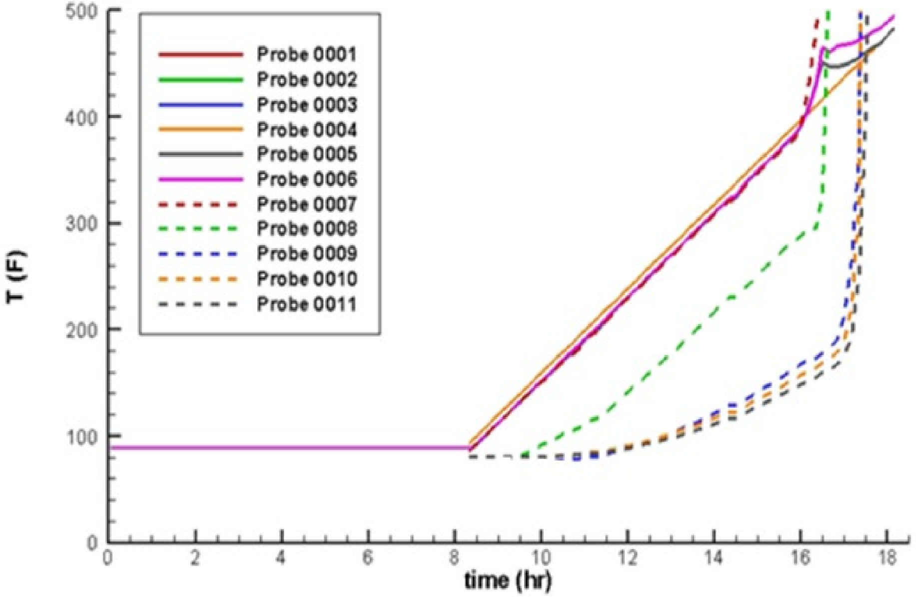




Full-Scale Analysis Example (PBXN-109 Fill)

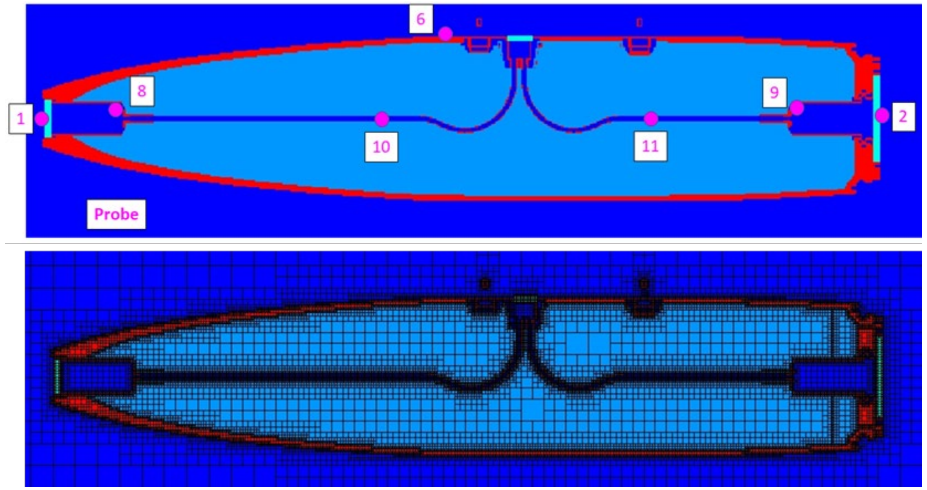
- Predicted “time to explosion” consistent with test data
- Response of the energetic, such as the induction phase, key to overall system response
- 3D modeling framework captures non-uniform response such as difference in front & rear fuze well
  - Early reactions at one end can cause differential forces resulting in billet movement





Results consistent with test data

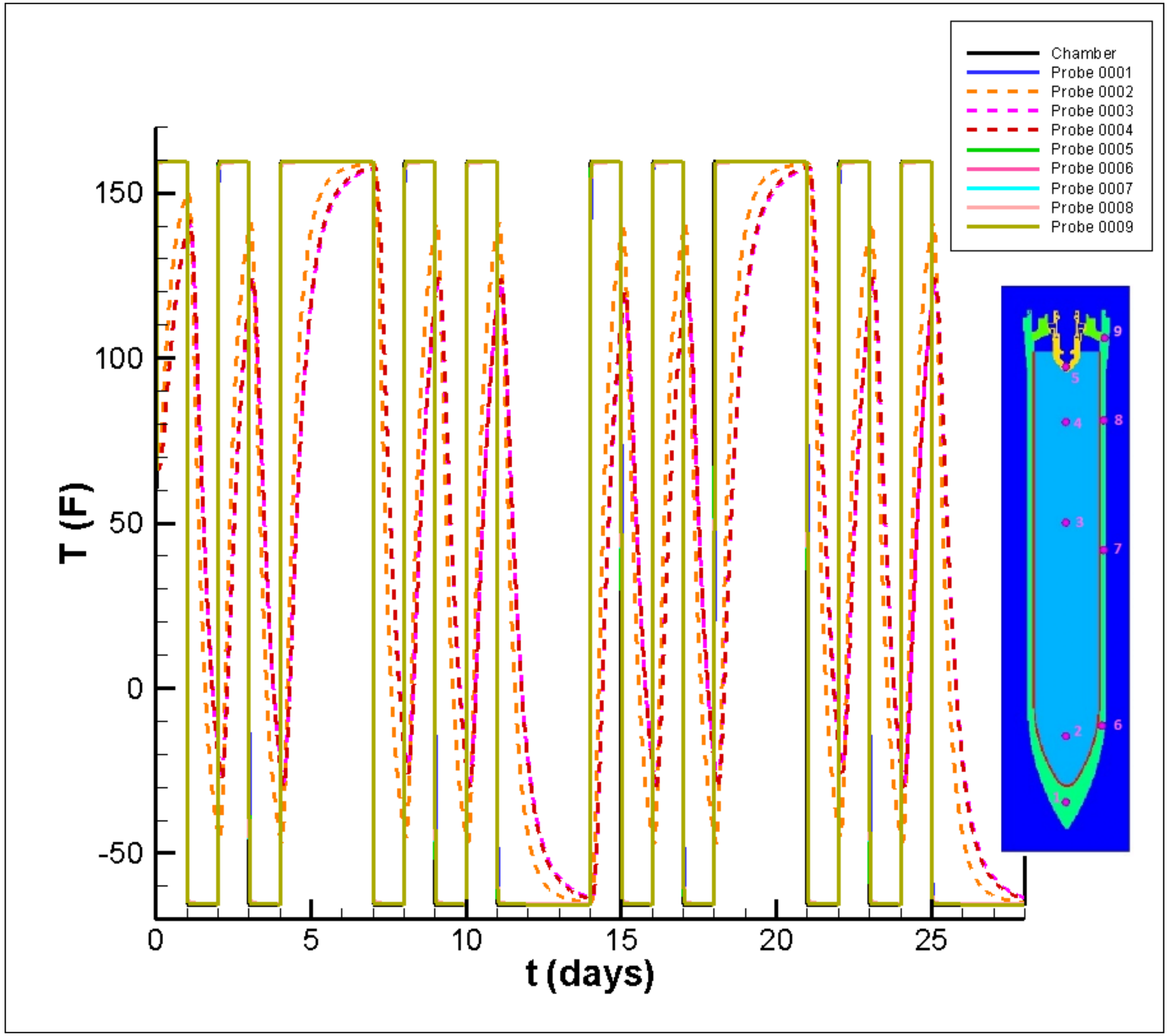
Location of Recording Probes



Long Term Environmental Qual Test (RDX Fill)

UNCLASSIFIED

- Another slow process that involves heating and cooling
- Performed to meet MIL-STD-2105D & 810G, DoD Test Method Standard, Hazard Assessment Tests for Non-Nuclear Munitions
- Munition exposed to 28-day temperature cycle of hot & cold
- Example of full-scale munition test
- Note - response of internal fill slower than what is probably thought to happen

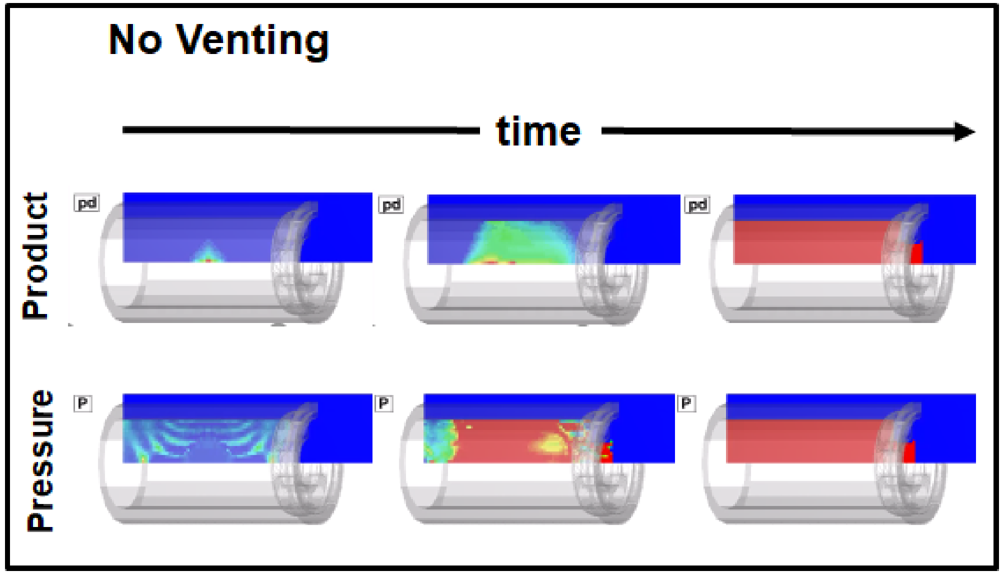


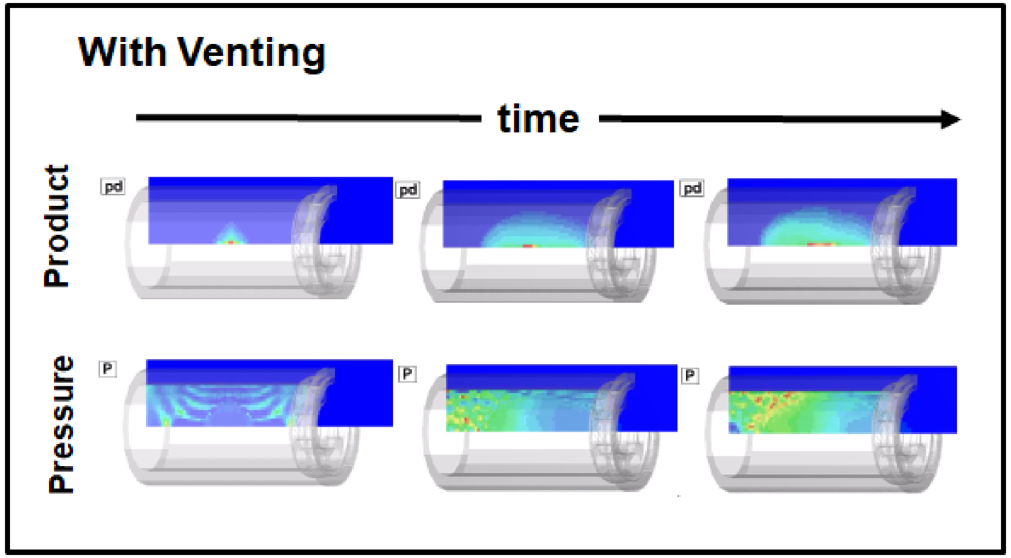
Fast Cookoff Example

- Heating process is modeled as in the slow cookoff scenario
- Response after ignition is modeled – requires solution of full set of governing equations
- Reaction model transitions to a pressure-dependent burn rate model[4]

$$V = aP^n$$

- Solution captures the feedback process from confinement to the reaction rate





[4] Yoh, et al, UCRL-JRNL-207203, Oct 2044 *Journal of Applied Physics*

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Conclusions

- Tremendous potential for leveraging digital engineering in the IM design process
  - Requires tools that capture key phenomena in weapon-scale scenarios
  - Robust and efficient numerical approaches key to have tools that integrate into the design and evaluation process
- Scenarios range from slow cookoff to detonations - robust modeling tools needed
  - Multi-material code with variety of reaction models addresses the phenomena
  - AMR / Implicit approach has proven efficient & promotes integration with design process
- Challenges exist when addressing composite energetics
  - Working theoretical and experimental processes to address this issue
  - Potential for additional useful information collection during qual tests