Modeling Challenges on Reactive Structural Materials: Congressional Plus-Up HECE Phase II

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Requirement: Agent Defeat

Complete neutralization of chemical or biological agents, within and without the enemy target structure
Requirement: Hard Target Defeat

- Outer Diameter: 31.5 in.
- Inner Diameter: 24.5 in.
- Total weight: 27,684 lbs
- Explosive Wt: 5386 lbs

Enter and/or penetrate into hard targets to cause severe inside blast damage
Issues – Technical Challenges

- Agent Defeat (AD)
  - Demonstrated improved, but insufficient answer to collateral effects problem
  - Still hasn’t addressed tougher problems: Large targets, complex targets, mobile or above ground targets
    - More powerful energetic material is needed for thermal effects, plus biocidal effects
- Hard Target Defeat (HTD)
  - Not enough blast energy is projected in current weapon concepts
    - More powerful energetic material is needed for blast effects
- Reduce kinetic energy of warhead fragments
Proposed Solutions - A Congressional Plus-up

- Develop more powerful energetics, Guided by M&S
  - Develop thermobarics, reactive structural materials, thermobaric high temperature incendiaries, new weapon concepts
- 1\textsuperscript{st} year: \textbf{Payloads} with TNT detonation energy times 5 or 6
  - Funded in FY08
- 2\textsuperscript{nd} year: \textbf{Reactive structural materials} and bring the energy level to 10 times TNT detonation energy
  - Proposed for FY09
- 3\textsuperscript{rd} year: Agent defeat payloads and Warhead concepts
  - To be proposed for FY10
HECE Phase I: Thermobarics

If we use nano-energetics, ---
Say, $T_{ign} = 1300K$

We are working on it now. Any help is welcome.
HECE Phase II: Reactive Structural Materials (RSM)

- Inert case is parasitic at target:
  - 50 – 85% of munition weight is metal case
  - Further, 50% or more of remaining explosive output energy is lost to case fragments and not available for blast
Energy Goal of RSM on Warhead

- An additional 4,000~5,000 cal for 1 g casing (out of potential 5,000-14,000 cal) to be added
  - Balance between energy, strength and density
  - Quick breakup and ignition/combustion of casing
  - Less loss to fragment kinetic energy to be translated into blast or thermal energy

<table>
<thead>
<tr>
<th>Metal oxidation, Explosive detonation</th>
<th>oxides</th>
<th>ρ, g/cm³ (metal)</th>
<th>Q, cal/g of metal</th>
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<tbody>
<tr>
<td>B</td>
<td>B₂O₃</td>
<td>2.47</td>
<td>13970</td>
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<tr>
<td>Al</td>
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<td>2.7</td>
<td>7422</td>
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<tr>
<td>Ti</td>
<td>TiO₂</td>
<td>4.5</td>
<td>4714</td>
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<tr>
<td>HMX</td>
<td>H₂O, CO₂</td>
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<td>1524</td>
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<tr>
<td>PBXN-109</td>
<td>H₂O, CO₂, Al₂O₃</td>
<td>1.68</td>
<td>1698</td>
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<tr>
<td>TNT</td>
<td>H₂O, CO₂</td>
<td>1.65</td>
<td>1000</td>
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</tbody>
</table>
Systematic Approach

- How do we optimize it?
  - Do we have good ingredients?
  - How do we formulate new RSM with these ingredients?
  - How do we predict performance so that we can convince warfighters that we can do targeteering?
- Need for a roadmap for M&S capability
What are Good Potential Candidates?

- Fuel rich with high energy content
- Prompt shock initiation of *anaerobic* chemical reaction
  - Mechanical deformation $\rightarrow$ create hot spots
  - Hot spots $\rightarrow$ immediate local reaction
  - Propagation of chemical reaction $\rightarrow$ other regions
    - Controlling mechanisms (mass diffusion, etc?)
- Frangibility of reacted materials (as a new fuel) for further *aerobic* reaction
  - Easy ignitability of fuel (droplets/particles/gasses)
  - Fast enough burn rate of fuel
  - Optimum droplet/particle size for better mixing with air
Investigated extensively for reactive fragments

Unsuitable for RSM
- Reaction doesn’t start when explosively launched
- Fluorine in Teflon is an oxidizer, reducing fuel potential of RSM – a minor shortcoming

Impact-to-reaction performance observed, but details never investigated/understood
- Very broad-brush phenomenology modeling only
- No detailed understanding from mechanical behavior to chemical reaction
- Not much of a help as a lead to other formulations
A Better Example

- Start with MnO₂ – Al powders in epoxy as a casing
  - Has shown blast improvement
  - Is it optimal? .. No.
Mechano-Thermo-Chemical Process

- Shock wave from left
- Grinding of one particle against another
- Plastic shear deformation
- Localized heating
- Localized thermitic reaction?
- Further local heating
- Heat transfer to other parts of particles
- Melting?
- Material diffusion

➢ To be continued
Further Processes

- Diffusion controlled reaction
- Heating of epoxy
- Fragmentation or dissociation of epoxy
- Recombination reaction of dissociation products of epoxy
- Al or Mn (produced during thermitic reaction) particle reaction with dissociation products such as H2O or CO2
- Further heating of epoxy fragments/dissociation products
- Acceleration and separation of thermite powders (aggregates?) and epoxy fragments/dissociation products
- Turbulent mixing with ambient air
- Heating and ignition of Al or Mn particles (or aggregates) and gasified epoxy, epoxy dissociation product gas or solid epoxy fragments
- Combustion of these fuels
Naresh Thadani Mesoscale Simulation
(showing mechanical deformation at high porosity)

Al flattening

Al vortex motion

spherical Ni+Al

flake Ni + spherical Al

P (GPa)

P (GPa)

t = 0

t = 10 ns

t = 20 ns

16

14

12

10

8

6

4

2

2

5 µm

10 µm

260 µm

Im of Possibility
Two Main Observations on the Epoxy Formulation and in General

- Inefficient reaction
  - Condensed phase material diffusion controls the overall reaction process
  - Doubtful if the reaction can be effected in the short time scale of blast applications

- Difficulty in modeling
  - So many possible pathways of uncertain strengths
  - Even a vague understanding would be expensive
Desired Efficient Formulations

- Ignition and burn characteristics can be enhanced?
- Would porosity enhance the first step?
- What types of manufacturing processes are available?
- Fragment (flying out) size can be controlled?
- Nano-energetics?
Nano-Energetics?

- Possibilities from nano-energetics
  - Improvement of ignition kinetics (connected with condensed phase reaction kinetics) - both issues are to be affected by nano-scale mixing
  - Strength and porosity of consolidated reactive materials (effect of nano-sized or nano-structured components)
  - Mechanical initiations of energetic formulations: mechanisms need to be understood, nano-sized particles/domains can behave very differently (better?) compared to micron-sized ones
Nano-energetics?

- Can some of the above processes be manipulated?
  - Material diffusion time eliminated (premixed at nano-scale)?
  - Ignition assured and delay time shortened (enhanced reactivity)?
  - Burn rates accelerated, (or delayed – Phase III)?
  - Fragmentation pattern dictated (gas generators as binder?)?
  - Control of porosity?

- More efficient M&S capability?
  - Can a clear (easier) road map be constructed?
    - Can some of the processes can be approximated or eliminated (e.g. infinite rate of kinetics or diffusion)?

- Need help
Phase III – Agent Defeat Payloads and Warhead Concepts

- Payload and reactive casing burning in a localized volume (a couple of hundred feet radius) surrounding a target structure for a sustained period (a few seconds)
  - Maximum energy from Phase I and Phase II
  - Fuel particle size control for balance between buoyancy and gravity, and for adequate limited range
  - Enhanced agent neutralization capability by introduction of Cl or F compounds
- Will need help