R1-B.2: Characterization of Homemade Explosives (HMEs)

Abstract—The threat of homemade explosives (HMEs) has seen an increase due to the constituent materials used and relatively low costs that allow terrorist to obtain and use them. In contrast to military and DOE explosives, the characterization of these materials is severely lacking. A significant challenge is the little experimental data available due to the large-scale setup that is required for characterization. The main restraint is due to the large, critical diameters needed to sustain a steady detonation in a non-ideal explosive. We are developing and performing small-scale experiments (grams) in tubes with small diameters relative to the expected critical diameter and anticipating unsteady detonations that are likely to fail in many cases. Using microwave interferometry, a highly time resolved profile of the location of the detonation front is measured. The failure dynamics measured with the interferometer allow for the characterization of the non-ideal explosive over a wide parameter space (from overdriven to failure). This approach also allows a relatively quick screening of HMEs using only small amounts of materials.

I. PARTICIPANTS

<table>
<thead>
<tr>
<th>Faculty/Staff</th>
<th>Name</th>
<th>Title</th>
<th>Institution</th>
<th>Email</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Steven F. Son</td>
<td>PI</td>
<td>Purdue University</td>
<td><a href="mailto:sson@purdue.edu">sson@purdue.edu</a></td>
</tr>
<tr>
<td></td>
<td>Lori J. Groven</td>
<td>Assistant Professor</td>
<td>South Dakota School of Mines</td>
<td><a href="mailto:Lori.Groven@sdsmt.edu">Lori.Groven@sdsmt.edu</a></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Students</th>
<th>Name</th>
<th>Degree Pursued</th>
<th>Institution</th>
<th>Month/Year of Graduation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>David Kittell</td>
<td>PhD</td>
<td>Purdue University</td>
<td>5/2016</td>
</tr>
<tr>
<td></td>
<td>Peter Renslow</td>
<td>MS</td>
<td>Purdue University</td>
<td>8/2014</td>
</tr>
</tbody>
</table>

II. PROJECT OVERVIEW AND SIGNIFICANCE

The goal of the work in this period is to link previous experimental and modeling efforts that aim to characterize homemade explosives (HMEs) on a small-scale. Calibrated reactive burn models (RBMs) are needed to simulate the performance of HMEs based on geometry and confinement—these simulations are also valuable for determining the threat posed by HMEs and the design effectiveness of improvised explosive devices (IEDs). However, in contrast to military and DOE explosives, reactive burn models have not been calibrated for most HMEs. Significant challenges include the complexity of traditional large-scale characterization experiments, a wide material parameter space, and non-ideal detonation behavior. In order to achieve a link between the small-scale experiment and modeling effort, a well-characterized high explosive triaminotrinitrobenzene (TATB) was chosen for evaluation under conditions of varying porosity. These experiments utilize a microwave interferometer (MI) and capture highly time-resolved trajectories of the leading shock wave in small (~0.64 cm) dia. cylindrical charges of TATB. The objective of this work is to match data obtained from the small-scale MI experiment with simulations using the shock physics hydrocode CTH. Because TATB is well studied, our goal is to determine whether or not a model calibrated at the large scale can simulate the small-scale experiments. Specifically, three model types—history variable reactive burn (HVRB), ignition and...
growth reactive burn (IGRB), and Arrhenius reactive burn (ARB) – have been found for TATB corresponding
to four different material forms: ultrafine- (U), coarse porous- (CP), coarse high density- (HD), and super-
fine- (SF). Our goal is to show which aspects of the model influence the observed transient response, and
how preexisting model parameters should be adjusted to better fit the data obtained. Reaching this goal will
pave the way for future studies that consider using small scale characterization data to simulate large scale
experiments, and also to return to the characterization of homemade explosives. Preliminary studies were
also conducted during this period to analyze the effect of diameter and confiner material sound speed on the
propagation of detonation waves in ammonium nitrate and fuel oil (ANFO).

III. RESEARCH ACTIVITY

A. State-of-the-art and technical approach

A.1 Experimental

Successful experiments have been performed with the explosive TATB using a microwave interferometer to
measure the detonation front’s position and velocity profile at different porosity levels. By increasing poros-
ity (decreasing theoretical max density TMD) it is possible to give TATB more non-ideal behavior and ob-
serve shock wave velocities near the sound speed of the material. In these experiments, density was varied
between 40-96%TMD. Increased porosity reduces the energy density and tends to increase the reaction zone
thickness. By varying porosity, it is also possible to vary the shock sensitivity of the explosive. This has been
demonstrated with a second set of tests using a PMMA attenuator. It is shown that the critical attenuator
thickness of 1-3mm for 96%TMD can be increased to 5-7mm for 80%TMD. Shock sensitivity should increase
for more porous materials and can be explained by the heterogeneous microstructure and hot spot theory
[1]. The crushing action of the incident shock wave collapses more voids and localizes more hot spots in the
porous explosive yielding a stronger transition to detonation.

Studies with ammonium nitrate and fuel oil (ANFO) were also revisited to investigate the effect of diameter
and lower sound speed confiners. Using a combination of 0.64 and 1.27 dia. steel confiners as well as PVC
materials, new work was able to show detonation failure over a broader spectrum of failure rates. This work
will be continued with prilled ammonium nitrate (AN) and incorporated into simulations utilizing an ignition
and growth reactive burn model. The ultimate goal is to calibrate an IGRB model for different compositions
of ANFO using the new geometries and confiner materials.

A.2 Modeling

One- and two- dimensional mesh resolved simulations were found for the small-scale experiment with TATB.
Due to the relatively ideal nature of TATB, the effect of porosity only resulted in a change to the steady deto-
nation velocity. In all cases, except for the ignition and growth reactive burn (IGRB), the one- and two- di-
mensional velocities were nearly identical, requiring only ~0.5 cm to stabilize. This suggests that the level of
confinement is too high to observe transient failure – a conclusion supported by the 6-7 mm critical diameter
limit (the test dia. was 6.4 mm). Nevertheless, the 40 and 50%TMD cases appeared to fail in the experiment
but did not in the simulation, except with the IGRB model. Other differences between the models are the vary-
ing reaction zone thickness and shock pressures.

Although shock velocity is the only recorded measurement, it became apparent that the input pressure of
the ideal explosive plays a critical role in these simulations. A model was developed for Primasheet 1000,
yielding a shock pressure of ~16 GPa. Using this pressure, the shock initiation experiments were simulated
with and without chemical reaction. It is shown that the burn models that matched the steady detonation
velocities do not match the critical attenuator length, and this has been correlated with the level of realism in
the reaction zone thickness. Models that can predict a reasonable reaction zone (a few mm) can also predict initiation behavior, whereas a temperature-based model which predicts an unreasonable reaction zone (a few μm) could not predict this behavior.

Finally, an IGRB model for ANFO was implemented as a preliminary test of new geometries. This model was used to evaluate low sound speed confiners and predict detonation failure ahead of actual tests. Much work needs to be done to fine tune the model parameters and this will be continued into the next period. Specifically, the larger diameter charges allow for more reaction to occur and a greater chance to observe differences in performance between compositions.

B. Major contributions

Our specific accomplishments this period are summarized below:

1. Finished wavelet analysis code and theory paper; we have also standardized an optimization routine. The Wavelet code is able to recover the detonation velocity profile and was used to produce all of the following results.
2. Measured the detonation velocity of pressed TATB in the small-scale MI experiment as a function of porosity.
   - Calibrated the material wavelength as a function of porosity and fit experimental data with the Landau-Lifshitz/Looyenga equation.
   - Demonstrated that for the current experimental configuration, this velocity is near the ideal Chapman-Jouget limit.
   - Transient detonation failure may have been observed at 50 and 40%TMD.
3. Performed shock initiation studies to determine the critical attenuator thickness for 96 and 80%TMD.
   - Using pressure estimates from CTH, we were able to generate Pop-plot data.
4. Simulated the TATB experiments in CTH with five different models calibrated to large-scale explosive characterization experiments.
   - Temperature-based Arrhenius burn can match velocity, but the reaction zone prediction is not physical and this model cannot match the shock initiation behavior.
   - History variable reactive burn was calibrated to perform like Arrhenius burn; similar results except slightly better prediction of shock initiation.
   - Ignition and growth reactive burn was modified to admit different initial porosities. The resulting steady velocities were off, but the reaction zone thickness and shock initiation behavior were more physical.
5. Performed extensive one- and two-dimensional mesh resolution studies and varied other simulation parameters to achieve a high degree of numerical accuracy.
6. Created an explosive model for the ideal booster charge (Primasheet 1000) used in the experiments to more accurately predict shock pressures.
7. Wrote an accessory tool for CTH to track the position of a moving shock wave, and record shock and reaction zone state variables such as pressure and temperature.
8. Designed a preliminary IGRB model for ANFO to match previous work and successfully predict the effect of low sound speed confiners.
9. Moving forward on ANFO studies varying prill size and utilizing the larger diameters.
   - Low sound speed confiners such as PVC produce interesting failure dynamics but decrease the signal strength of the microwave interference signal.
The following results were collected over the recent funding period and show current project status. Some of these results have been published in a M.S. thesis; the rest will be disseminated in two conference papers at the 2014 International Detonation Symposium and two companion journal articles.

B.1 Detonation velocity with varying porosity for TATB

- Experimental

Calibrated material wavelengths were found for TATB as a function of TMD in order to analyze microwave interferometer data. A microwave mixing equation was used to verify the results (see Figs.1-3).

![Calibrated Material Wavelength](image1)

**Figure 1**: Calibrated material wavelength for pressed TATB used to analyze shock position/velocity.

![Shock Position and Velocity](image2)

**Figure 2**: Shock position (left) and velocity (right) for TATB pressed between 40 and 96%TMD.

![Average Detonation Velocity](image3)

**Figure 3**: Average detonation velocity for the TATB experiment as a function of TMD; also shown are material sound speed, Cheetah calculations, and an empirical fit.
Available models for TATB

Hydrocode simulations of explosives require a reactive burn model (RBM). This includes the equation of state (EOS) parameters for the unreacted and reacted material, a reaction rate law to advance a single progress variable, and a mixing law for intermediate levels of reaction (see Fig. 4).

- Arrhenius Reactive Burn Model (ARB)
  - A temperature-based reaction rate model
  - Used to describe initiation of homogeneous explosives
  - Potential for error as temperature is not a well-measured quantity
- Ignition and Growth Reactive Burn Model (IGRB)
  - A pressure-based reaction model with 12 adjustable constants
  - Most widely-used model for heterogeneous explosives
  - Calibrated with Pop-plot data
- History Variable Reactive Burn Model (HVRB)
  - Reaction rate is a function of time since the passing of a shock wave
  - Also used for heterogeneous explosives like IGRB and calibrated to Pop-plot data
- Equation of State (EOS)
  - Defines pressure-volume-energy (P,V,E) relationship of a chemically non-reacting material
  - EOS is said to be complete if temperature state is known (usually estimated with $C_v$)
  - Types include: Mie-Grüneisen (MGR), Jones-Wilkins-Lee (JWL), and tabulated look-up values (SES AME)
- P-α Porosity Model
  - Adjust an explosive model based on changes to initial density
  - May be applied in conjunction with MGR and SESAME EOSUR only

![Figure 4: Schematic diagram for a reactive burn model description of an explosive in CTH.](image-url)
### Table 1. Available TATB models in CTH calibrated to large scale explosives characterization data.

<table>
<thead>
<tr>
<th>TATB Material</th>
<th>Reactive Burn Model</th>
<th>Unreacted EOS</th>
<th>Reacted EOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ultrafine (U-)</td>
<td>ARB</td>
<td>MGR</td>
<td>SESAME</td>
</tr>
<tr>
<td>Ultrafine (U-)</td>
<td>IGRB</td>
<td>JWL</td>
<td>JWL</td>
</tr>
<tr>
<td>Coarse, Porous (CP)</td>
<td>HVRB</td>
<td>MGR</td>
<td>SESAME</td>
</tr>
<tr>
<td>Coarse, High Dens. (HD)</td>
<td>HVRB</td>
<td>MGR</td>
<td>SESAME</td>
</tr>
<tr>
<td>Superfine (SF)</td>
<td>HVRB</td>
<td>MGR</td>
<td>SESAME</td>
</tr>
</tbody>
</table>

Necessary model changes

1. Density cannot be varied for the IGRB model because of the JWL EOS. To fix the issue, MGR/SESAME EOS were translated for ultrafine TATB while keeping the same JWL parameters. This is not a perfect solution, but gives an idea for the model performance and capabilities.

The HVRB model has a dependence on initial density (roughly as the fourth-power of density). A density correction factor was introduced as suggested by the CTH development team.

- One- and two-dimensional CTH simulations

A mesh resolution study has shown that a minimum of 160 zones per mm is needed to resolve the problem (possibly more for ARB and HVRB). The old approach of simulating the entire experiment was too computationally expensive, especially for material parameter studies. Instead, a 1.6 cm slice of the experiment is simulated at 160 zones/mm requiring 1-4 hours per run. The ideal explosive model is based from the physical properties of Primasheet 1000 and results from Cheetah. The ideal explosive is set to propagate at the Chapman-Jouget detonation velocity with no intermediate state between the reacted and unreacted material. These geometries are shown below in Figure 5.

Figure 5: New and old simulation geometries used to evaluate the different TATB models in CTH.

- The ShockTracker code for CTH

An accessory code was written for CTH to add the capability to track moving shock waves and compare with experimental data. No pre-existing post-processing routine has this capability, so it is an asset to Sandia National Laboratories and the CTH development team. Several adjustable parameters allow the user to tailor the code for the various types of pressure waves observed and track the reaction zone as well. A graphical discussion of the ShockTracker code approach is shown in Figure 6 on the next page.
Simulation results for detonation velocity as a function of porosity

Figure 6: Graphical discussion of the tracer gauge data needed to be analyzed by ShockTracker.

Figure 7: Detonation velocity at varying porosity levels for 1D simulations (dashed lines) and 2D simulations (solid lines) from CTH and the ShockTracker code.
Simulation results for peak shock pressure as a function of porosity

Overall, all models except IGRB compare well to experimental data and the ideal Chapman-Jouget detonation velocity. The TATB explosives are well-supported and far from the failure condition, except for 50 and 40\%TMD. In those cases, the measured velocity is closer to the material sound speed and only the IGRB model predicts failure for low TMD. In that case, the reaction zone is stretched out and decouples from the leading shock wave.

Figure 8: Maximum shock pressure at varying porosity levels for 1D simulations (dashed lines) and 2D simulations (solid lines) from CTH and the ShockTracker code.

Comparison of CTH and experimental data for detonation velocity

Overall, all models except IGRB compare well to experimental data and the ideal Chapman-Jouget detonation velocity. The TATB explosives are well-supported and far from the failure condition, except for 50 and 40\%TMD. In those cases, the measured velocity is closer to the material sound speed and only the IGRB model predicts failure for low TMD. In that case, the reaction zone is stretched out and decouples from the leading shock wave.
B.2 Shock initiation study for TATB

- Experimental results

A PMMA attenuator was used to decrease the input shock pressure to TATB samples and evaluate shock sensitivity as a function of porosity. Experiments were conducted at 96 and 80% TMD and results are shown in Table 2 and Figure 10 on the next page.

<table>
<thead>
<tr>
<th>Test</th>
<th>% TMD</th>
<th>Density (g/cc)</th>
<th>PMMA Length (mm)</th>
<th>Failure?</th>
</tr>
</thead>
<tbody>
<tr>
<td>80% TMD Test 1</td>
<td>79.48</td>
<td>1.5396</td>
<td>5</td>
<td>NO</td>
</tr>
<tr>
<td>80% TMD Test 2</td>
<td>78.60</td>
<td>1.5225</td>
<td>5</td>
<td>NO</td>
</tr>
<tr>
<td>80% TMD Test 3</td>
<td>79.10</td>
<td>1.5321</td>
<td>7</td>
<td>YES</td>
</tr>
<tr>
<td>80% TMD Test 4</td>
<td>79.47</td>
<td>1.5393</td>
<td>7</td>
<td>YES</td>
</tr>
<tr>
<td>96% TMD Test 1</td>
<td>98.80</td>
<td>1.9137</td>
<td>1</td>
<td>NO</td>
</tr>
<tr>
<td>96% TMD Test 2</td>
<td>97.20</td>
<td>1.8828</td>
<td>1</td>
<td>NO</td>
</tr>
<tr>
<td>96% TMD Test 3</td>
<td>96.21</td>
<td>1.8635</td>
<td>3</td>
<td>YES</td>
</tr>
<tr>
<td>96% TMD Test 4</td>
<td>97.47</td>
<td>1.8880</td>
<td>3</td>
<td>YES</td>
</tr>
</tbody>
</table>

Table 2. Shock sensitivity results for TATB.
CTH simulation results and comparison

The critical attenuator thicknesses are summarized in Table 3. No model was able to fully capture the observed shock initiation behavior.

<table>
<thead>
<tr>
<th>Model</th>
<th>96% TMD (mm)</th>
<th>80% TMD (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARB U-TATB</td>
<td>&lt;1</td>
<td>3</td>
</tr>
<tr>
<td>IGRB U-TATB</td>
<td>7</td>
<td>10</td>
</tr>
<tr>
<td>HVRB TATB (CP)</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>HVRB TATB (HD)</td>
<td>N/A</td>
<td>1</td>
</tr>
<tr>
<td>HVRB TATB (SF)</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Actual</td>
<td>1-3</td>
<td>5-7</td>
</tr>
</tbody>
</table>

Table 3. Critical attenuator thickness needed for detonation failure.

Using CTH simulations of inert TATB, we were able to estimate the input shock pressure to the samples in Figure 11 on the next page and back out a crude estimate for data points on a Pop-plot in Figure 12 on the next page.
B.3 Preliminary modeling of ANFO with IGRB

- A composite model with different parameters from different sources:
  - porous AN Mie-Grüneisen EOS from Baer, Gartling, and DesJardin
  - chemical kinetics from JWL++ model used by Kong and Kim for ANFO K-1
  - JWL fit with Cheetah for products (substantiated by other papers)
  - IGRB adjusted to match somewhat with previous experimental data

- Realistic match of experiment

We used the new ANFO model to predict that the detonation would fail in 1.27 cm dia. thick-walled PVC. A new set of experiments were designed and confirmed the result of detonation failure. Some highlights of the new ANFO model are shown in Figure 13 on the next page.
Figure 13: Overview of some features of the new ANFO model in CTH as compared with experimental data and the predictive capability to design a new experimental geometry based on PVC confinement.
B.4 Preliminary experimental work with ANFO in new configurations

A new confiner was designed out of low sound speed (~2 km/s) PVC shown in Figure 14. In addition, the same ANFO material was also tested in the normal configuration and a larger diameter steel confiner. These results are shown in Figure 15.

---

Figure 14: Schematic drawing of a new confiner geometry manufactured out of PVC.

Figure 15: Preliminary results with stoichiometric ANFO under three confinement conditions; two tests were performed at each configuration, and sample density was held constant at 1.0 g/cc.
C. Future plans

The ammonium nitrate currently used for studies is Kinepak and Kinepouch. Microscope images of these materials are shown below in Figure 16. These materials show very little differences and do not permit the variation of prill size as they are already a fine powder. Future work will investigate the effect of prill size on experimental results utilizing the new geometries and confinement.

![Microscope images of two varieties of AN used in previous and current work; Kinepak (left) and Kinepouch (right).](image)

Figure 16: Microscope images of two varieties of AN used in previous and current work; Kinepak (left) and Kinepouch (right).

IV. RELEVANCE AND TRANSITION

A. Anticipated end-user technology transfer

We anticipate transferring these techniques to research labs and companies such as EMPI and RMS.

V. LEVERAGING OF RESOURCES

A M.S. student contributing to this project was funded by Sandia National Laboratories.

VI. PROJECT DOCUMENTATION AND DELIVERABLES

A. Peer reviewed journal articles


   Pending-


B. Other presentations

1. One short course at Picatinny Arsenal
C. Student theses or dissertations produced from this project

1. Peter J. Renslow, A small-scale experiment using microwave interferometry to investigate detonation and shock-to-detonation transition in pressed TATB, May 2014, Master of Science in Aeronautics and Astronautics (M.S.A.A.E.).

VII. REFERENCES
