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

I. PARTICIPANTS

<table>
<thead>
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</thead>
<tbody>
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<tr>
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<th>Degree Pursued</th>
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<th>Month/Year of Graduation</th>
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<tr>
<td>David Kittell</td>
<td>PhD</td>
<td>Purdue University</td>
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II. PROJECT DESCRIPTION

A. Overview and Significance

Terrorists increasingly use homemade explosives (HMEs) because of low-costs and availability. The specific compositions of HMEs are nearly limitless, so making accurate assessments of the threat from these materials is challenging. Consequently, there is significant interest in quickly characterizing HMEs so that these threats can be more accurately modeled. A significant challenge is the time and cost associated with traditional large-scale tests required to sustain a steady detonation in non-ideal explosives. In this work, we are developing experiments that require only a few grams of material involving transient detonation failure. One approach, employed by us and others, uses microwave interferometry (MI) to continuously track the position of shock and detonation waves inside the test sample; other approaches use the detonation wave to close and continually change the resistance of a simple circuit, and this will be explored for use in this work. Overall, a highly time-resolved profile of the location of the detonation front can be measured. These measured failure dynamics allow for the characterization of non-ideal explosives over a wide parameter space (from overdriven to failure). These small-scale experiments provide detailed data relatively quickly and at a lower cost than alternatives.

B. State-of-the-Art and Technical Approach

Microwave interferometry (MI) is a technique to measure shock and detonation velocities in explosives. However, it has not been applied to homemade explosives in this configuration (failing detonation). This MI technique is used to measure the phase and amplitude of microwave signals that are transmitted through an unreacted explosive and reflected back at locations of interest. These reflection points are located at dielectric discontinuities such as a shock wave or a reaction front [12, 13], which occur in the media during a detonation event. The phase measurements can then be used to infer the relative position and velocity of the phenomena. MI is a unique nonintrusive diagnostic for explosives research with high temporal resolution; however, challenges exist due to transmission losses and partial reflection of the signal. Achievable MI signals in explosives are often of a low quality and velocity measurements in non-ideal systems remain challenging.
Total reflection of the MI signal is never realized due to partial transmission through the wave front of interest [13], as well as attenuation of the signal due to absorption and dispersion effects in the explosive media [14]. Furthermore, the shock or detonation wave may be a nonplanar reflector due to sample diameter effects as well as material heterogeneities resulting in poor signal quality. Other factors which may affect the signal quality include the possibility of a decoupled shock-reaction zone (e.g., shock initiation and detonation failure) giving rise to multiple harmonic frequencies, as well as the confinement of the test explosive acting as a waveguide for the MI signal [14]. When several of these non-idealities are present simultaneously, it may still be possible to extract useful velocity information with an advanced time-frequency analysis.

B.1. Objectives

The goal of the work for the current period is to study various compositions of ammonium nitrate (AN) and fuel (e.g. diesel or aluminum) and show how the explosive performance is influenced by physical material characteristics (e.g. porosity, density, particle size and shape). Similar tests using AN and fuel oil (ANFO) or AN and aluminum (ammonal) have been performed by Rocky Mountain Scientific Laboratory (RMSL) and Los Alamos National Laboratory (LANL); however, these tests are performed at a large-scale. We are collaborating with both facilities to compare the results of large- and small-scale tests and, overall, provide a greater wealth of experimental data to calibrate models for these non-ideal explosives. MI is used to obtain highly time-resolved detonation velocity data for the small-scale experiments; however, development is ongoing to augment or replace the MI system for explosive compositions which are not compatible with MI due to the absorption of the microwave signals. The primary objective of the work is to determine whether or not different trends in material characteristics can be compared between the large-scale (steady detonation) and small-scale (transient failure) results. Another objective for the work is to simulate the small-scale experiments using the shock physics hydrocode CTH. To capture all relevant physics, the simulation will be fully 3D, and should provide a roadmap for how the small-scale data might possibly be used to calibrate or validate different reactive burn models (RBMs) for ANFO or ammonal. With the increasingly complex models for ANFO, sensitivity studies and multi-variable optimization algorithms will be used to determine which parameters are most influential in matching the observed transient detonation response.

B.2. Experimental

B.2.a. Material characterization

B.2.a.i. Ammonium nitrate (AN)

Different forms of AN were studied while preparing compositions of ANFO and ammonal. The four different AN products obtained were Kinepak, Cold-Pack, Tripwire and Brenntag. These materials are used for a wide range of applications, including rock blasting, mining, fertilizer and first-aid cooling packets (refer to Table 1 on the next page). Microscopic images were obtained in order to identify the particle morphology; corresponding images for each of the different AN products are shown in Figure 1 on the next page. To match the sample preparation performed by RMSL, the Brenntag prills were further ground by hand using a standard food processor and are considered as a different material altogether from the original Brenntag prills. The number of ways that a terrorist could prepare these different types of AN blends is nearly limitless.
<table>
<thead>
<tr>
<th>Product Name</th>
<th>Particle Morphology</th>
<th>Mean Particle Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kinepak</td>
<td>ground fines and small prills</td>
<td>51 μm</td>
</tr>
<tr>
<td>Cold-Pack</td>
<td>ground / crystalline</td>
<td></td>
</tr>
<tr>
<td>Tripwire</td>
<td>prills (explosive grade)</td>
<td>2.02 mm</td>
</tr>
<tr>
<td>Brenntag</td>
<td>prills (fertilizer grade)</td>
<td>2.06 mm</td>
</tr>
<tr>
<td>Brenntag (blend)</td>
<td>ground / crystalline</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Different types of AN obtained for study.

Figure 1: Microscope images for different types of AN: (a) Kinepak, (b) Cold-Pack, (c) Tripwire prills, (d) single Tripwire prill, (e) Brenntag prills, (f) single Brenntag prill, (g) and (h) are different Brenntag hand blends.

**B.2.a.ii. Aluminum powders**

Compositions of AN and aluminum powders (ammonal explosives) may have increased explosive performance due to the afterburning of the aluminum. Different powders were selected to match those recently evaluated by RMSL. These tests were conducted to quantify the effects of particle size and morphology...
(spherical or flake) on ammonal performance. Aluminum powders were received directly from RMSL in order for direct small- vs. large-scale comparisons to be made. The aluminum used at RMSL was characterized using a laser diffraction technique, and further microscope images were taken at Purdue University to qualitatively describe the morphology and verify the aluminum size distributions. Further details, including material ID and median diameter, are given in Table 2 as well as Figures 2 and 3 on the next page. Of note, the flake aluminum powder F2 appeared to be mistakenly classified as flake, as it consisted of an assortment of different shapes (mostly needle-like).

<table>
<thead>
<tr>
<th>ID</th>
<th>Particle Morphology</th>
<th>Product Name</th>
<th>Median Dia. (μm)</th>
<th>Microscopy Notes</th>
</tr>
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<tbody>
<tr>
<td>S1</td>
<td>sphere</td>
<td>H-30</td>
<td>37</td>
<td></td>
</tr>
<tr>
<td>S2</td>
<td>sphere</td>
<td>H-95</td>
<td>128</td>
<td></td>
</tr>
<tr>
<td>S3</td>
<td>sphere</td>
<td>RSA-600</td>
<td>733</td>
<td>teardrop-like</td>
</tr>
<tr>
<td>S4</td>
<td>sphere</td>
<td>RSA-900</td>
<td>1030</td>
<td>teardrop-like</td>
</tr>
<tr>
<td>F1</td>
<td>flake</td>
<td>Chromal</td>
<td>40</td>
<td>amorphous appearance</td>
</tr>
<tr>
<td>F2</td>
<td>flake</td>
<td>K-105</td>
<td>140</td>
<td>assorted shapes (not flakes)</td>
</tr>
<tr>
<td>F3</td>
<td>flake</td>
<td>K-109</td>
<td>701</td>
<td></td>
</tr>
<tr>
<td>F4</td>
<td>flake</td>
<td>K-102</td>
<td>1250</td>
<td></td>
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Table 2: Different types of aluminum powders obtained for study.

Figure 2: Microscope images for different types of spherical aluminum powders: in order (a) S1, (b) S2, (c) S3 and (d) S4 (refer to Table 2 for details).
B.2.b. Transmission signal verification

For application of the MI technique, it is important to have the ability to quickly determine if the dielectric properties of an explosive will result in the MI signal being transmitted, absorbed and/or attenuated. For example, the inclusion of aluminum in ammonal samples can result in signal loss or attenuation. Not only is the relative weight percent of aluminum important in the overall composition, but also the size and morphology of the particles. In addition to aluminum, the particle morphology of AN (prills vs. ground) was also investigated with respect to MI signal transmission. Without resorting to explosive testing, a simple piston-cavity reflector was used to determine the amplitude of the MI reflection through the material of interest, and compared against a transmission standard (air). Transmission results are reported in Table 3 on the next page, and shown graphically in Figures 4 and 5 on the next page.

In summary of the transmission verification tests, a flexible polytetrafluoroethylene (PTFE) waveguide was attached to a 1/4-inch dia. piston-cylinder assembly having a thin aluminum foil on the piston face. The piston is actuated by hand and the MI signal is recorded. When air fills the cavity, a high-amplitude interference pattern is obtained. If the cylinder is partially filled with a mixture other than air; the microwave signal must first travel through the mixture before reflecting off of the moving piston face. Loose Kinepak, prills and ANFO were tested in this manner, with the corresponding signals shown in Figure 4 on the next page. Samples of ammonal with 20 wt.% aluminum are shown in Figure 5 on the next page. In particular, larger aluminum particle sizes and flake shapes will inhibit the transmission of the MI signal. All types of dry AN allow transmission of the MI signal, but small amounts of moisture will almost completely absorb the full signal also. These results also motivate future work to develop an alternative intrusive probe technique.

Figure 3: Microscope images for different types of flake aluminum powders: in order (a) F1, (b) F2, (c) and (d) F3, (e) and (f) S4 (refer to Table 2 for details).
AN Type* | MI | Al (spherical) | MI | Al (flake) | MI
---|---|---|---|---|---
Kinepak | Yes | S1 | Yes | F1 | No
Cold-Pack | Yes | S2 | Yes | F2 | Yes
Tripwire | Yes | S3 | No | F3 | No
Brenntag | Yes | S4 | No | F4 | No
Brenntag (blend) | Yes

*Note: for dry AN and planar reflectors only. Real shocks in samples with prills are non-planar and MI signal quality is lower during explosive testing.

Table 3: MI signal verification results showing material compatibility for signal transmission.

Figure 4: MI transmission verification study for loose Kinepak AN, Tripwire prills and stoichiometric Kinepak ANFO; all materials pass the transmission test.

Figure 5: MI transmission verification study for loose ammonal samples with 20 wt.% Al. Spherical powder S3 and larger sizes as well as flake powders F1, F3 and larger size fail the MI transmission test. Note that F2 is not truly a flake geometry and would likely diminish the signal if a flake geometry were present at that size.
B.2.b.i. MI signal quality for explosive testing

The transmission verification study is used as a material screening tool before explosive testing. However, non-ideal MI signals may still be obtained due to signal scattering and attenuation. For prilled AN, the transmission properties are favorable, yet the actual shock waves in these materials are non-planar and scatter the MI signal. Examples of the MI signal obtained from dynamic testing are shown in Figure 6 and compare a typical result for Kinepak AN vs. Tripwire AN prills. Advanced analysis techniques based on wavelet analysis [1] could possibly analyze segments of the Tripwire prill MI signal; the shock front could also be made to appear more planar by testing at larger diameters, or by grinding the prills into a finer powder.

![Figure 6: Typical MI signal for the transient detonation failure of ANFO samples using Kinepak AN (left) and Tripwire AN prills (right).](image)

B.2.c. Experimental results

B.2.c.i. Effects of packing density on ANFO failure behavior

Stoichiometric ANFO using Kinepak AN was tested at a wide range of initial densities to determine the effect of initial density on failure behavior. Initial density is reported as the percent of theoretical maximum density (%TMD) in order to emphasize correlations in performance with the amount of void space in the sample; MI position and velocity data is shown in Figure 7 on the next page. ANFO is unique in that it can become insensitive at higher packing densities (less void space). This physical phenomenon is known as the “dead-pressing” effect [2], and actual densities of ANFO used for rock blasting can be as low as ~50% TMD. What is unique with this study is that the lowest density tested at 38% TMD (hand poured) results in completely reacted samples and appears to be the most sensitive density tested for ignition. This result is likely dependent on the type of confinement used for testing – weaker confinement than 304 stainless steel would likely result in non-ignition for the same low-density samples.

For most of the small diameter (6.52 mm) tests with Kinepak and Cold-Pack ANFO, the failing detonation wave did not consume the entire sample, leaving a dense compact in the remainder of the confiner tube. The remaining confiner length was measured and the unreacted ANFO weighed to determine the final density and %TMD; these results are shown in Figures 8 and 9 on the next page. A clear trend is observed for this type of small-scale test: that increased reaction is achieved by decreasing %TMD and increasing void space in the sample. This is somewhat counterintuitive when considering conventional explosives, where performance is increased by increasing the initial density. However, explosive yield and sensitivity are different characteristics and the lower densities increase the ignition sensitivity as described by an energy localization hot-spot theory [3]. RMSL has reported qualitative observations of the sensitivity of density in their experiments also.
Figure 7: Position and velocity data for variable initial density of Kinepak ANFO.

Figure 8: Remaining confiner length and change in %TMD (due to passing shock/compression wave) of the unreacted ANFO as a function of the initial sample %TMD.

Figure 9: Remaining explosive confiners after dynamic testing. No confiner remains were recovered for compositions initially below 66% TMD pressed density.
B.2.c.ii. Effects of AN type on ANFO performance

The effect of different AN types on ANFO performance was investigated with larger diameter (11.3 mm ID) steel conifers. The larger diameters allowed the shock wave in prilled ANFO to appear more planar (evidenced by less erratic signal), and be compared with the Kinepak and Cold-Pack ANFO with less difficulty analyzing the MI signals. Velocity profiles are shown in Figure 10 and images of the confiner remains are shown in Figure 11. One major conclusion of this study is that the Kinepak and Cold-Pack ANFO behave nearly identically; this implies that the AN readily available in Cold-Pack sold at many retail stores may exhibit the same performance as explosive grade Kinepak used for rock blasting. Compared to ANFO samples prepared with Tripwire prills, the velocities are slightly lower; in addition, the prilled samples do not leave any confiner remains. It is unclear whether or not the prilled velocity is slightly higher due to the lower initial %TMD or particle morphology. Future tests with the prilled material could be conducted at larger diameters to improve the MI signal reflection.

Figure 10: Velocity profiles for stoichiometric Kinepak, Cold-Pack and Tripwire prill ANFO using 11.3 mm dia. steel thin-walled confiners.

Figure 11: Typical confiner remains for stoichiometric Kinepak and Cold-Pack ANFO tests using 11.3 mm dia. confiners. No remains are recovered for the prilled ANFO.

B.2.c.iii. Effects of aluminum particle size and morphology on ammonal explosives

Different aluminum particle sizes having spherical or flake morphology were mixed with the ground Brenntag blend AN to make samples of ammonal similar to those prepared by RMSL. Velocity and position data,
recovered confiner images and the measured remaining confiner length for the samples are shown in Figures 12-14 and Table 4 on the next page. The most distinguishable trend in the analyzed MI data is that flake powder F2 exhibits a slightly increased detonation velocity than the other powders tested. There is also a possible correlation between the confiner length remaining and particle size; this trend is observed primarily with the spherical particles (refer to Fig. 14 and Table 4). Future work is needed to test more samples and gain a greater confidence in the statistical significance of results. Collaboration with LANL and RMSL will pursue this further.

![Figure 12: Position and velocity profiles for ammonal detonation tests having different aluminum particle size and morphology.](image)

![Figure 13: Recovered confiners from ammonal tests. From left to right: Brenntag blend AN with F2, S1, S2 and F1 respectively.](image)

![Figure 14: Remaining confiner length from ammonal detonation tests according to aluminum particle size categories (refer to Table 4).](image)
B.3. Modeling

B.3.a. Overview

An accurate simulation of the small-scale MI characterization experiment depends on several model and geometry considerations. Some of these include explosive parameters for ANFO, as well as strength and mechanical failure models for the 304 stainless steel conϐiner. A 2D or 3D simulation is necessary to capture the effects of radial losses on detonation wave propagation. However, only a fully 3D simulation will reproduce the intricate “petals” or “strips” formed out of the conϐiner wall by abrupt detonation failure, which controls how the pressure in the test article is released. Significant progress was made in two areas: (1) a computationally feasible and relevant 3D simulation; and (2) the development of optimization algorithms which might be used to calibrate the unknown material parameters for ANFO. The immediate objective of this work seeks to calibrate a tabular variable-density model for ANFO, which may then be used to simulate larger-scale experiments. This type of model development is unprecedented within the explosives community and has the potential to launch a paradigm shift in explosive model calibration. The largest technical challenge is constraining the model so that convergence is possible over several (~10-20) unknown parameters. This challenge could be readily met with additional measurements in addition to the highly time-resolved detonation wave velocity profiles. Work is ongoing to design additional novel diagnostics to supplement the MI system and will be incorporated into the associated parameter optimization routines.

B.3.b. Model parameters

B.3.b.i. Mie-Grüneisen EOS for polycrystalline ammonium nitrate

The unreacted equation-of-state (EOS) for ANFO is approximated using a full density shock-particle relationship for polycrystalline AN. It is assumed that the contribution of fuel oil is negligible in the overall shock loading of this material. Parameter values were obtained from M. Baer [4] and correspond to the linear shock-particle relationship (see Table 5),

\[ U_s = c_0 + s_1 u_x \]  

### Table 4: Particle size categories for different Al powders.

<table>
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<th>Particle Size Category</th>
<th>Aluminum Types</th>
<th>Median Diameter</th>
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<tbody>
<tr>
<td>1</td>
<td>S1, F1</td>
<td>&lt; 50 μm</td>
</tr>
<tr>
<td>2</td>
<td>S2, F2</td>
<td>&lt; 150 μm</td>
</tr>
<tr>
<td>3</td>
<td>S3</td>
<td>&lt; 1 μm</td>
</tr>
</tbody>
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### Table 5: Mie-Grüneisen EOS parameters for polycrystalline AN.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>( \rho_0 ) (g/cc)</td>
<td>1.725</td>
</tr>
<tr>
<td>( c_0 ) (cm/s)</td>
<td>2.2e5</td>
</tr>
<tr>
<td>( s_1 )</td>
<td>1.96</td>
</tr>
<tr>
<td>( \Gamma_0 )</td>
<td>1.0</td>
</tr>
<tr>
<td>( \rho_0 ) (g/cc)</td>
<td>1.725</td>
</tr>
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</table>
Using a constant Grüneisen parameter value of 1.0, the complete EOS was evaluated for stability with respect to the slope of the Hugoniot and isentrope [5], as well as the sign of the fundamental derivative [6]; no instabilities were found. Variable initial density is treated as an extrapolation of the fully dense Hugoniot via the P-α porosity model discussed next.

**B.3.b.ii. P-α porosity model**

The initial density of ANFO is critical in determining performance, including explosive yield and ignition sensitivity. For initial densities less than 100% TMD, the passage of a shock wave through the non-reacting material will collapse void space resulting in a modified Hugoniot relationship and possibly a compaction wave (instead of a shock). The P-α porosity model is used to modify the non-reacted material behavior, whereas the effects of initial density on chemical reaction are taken into consideration via the calibrated burn model. The P-α porosity model contains three unknown parameters, which must be fitted using the experimental data and are described in Table 6.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Physical Interpretation</th>
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<tbody>
<tr>
<td>$P_s$</td>
<td>Pressure where all voids are crushed out</td>
</tr>
<tr>
<td>$P_e$</td>
<td>Upper pressure limit for elastic crushing behavior</td>
</tr>
<tr>
<td>$C_e$</td>
<td>Material sound speed within the elastic region</td>
</tr>
</tbody>
</table>

**Table 6: Experimentally determined parameters for the P-α porosity model.**

**B.3.b.iii. Jones-Wilkins-Lee EOS for detonation products**

The detonation product EOS is estimated through thermochemical equilibrium calculations of the Chapman-Jouguet (CJ) detonation state. These calculations were performed with the thermochemical equilibrium code CHEETAH (LANL), where a Jones-Wilkins-Lee (JWL) EOS was fitted using the equation for a pressure adiabat given by,

$$p(\Delta) = A e^{-R_2 V} + B e^{-R_2 V} + CV^{-\omega -1}$$  \hspace{1cm} (2)

passing through the CJ state [7]. These calculations were performed for multiple initial densities so that a look-up routine was implemented to determine the EOS for each initial density under investigation. The variation of these parameters with initial density is shown graphically in Figure 15 on the next page.

**B.3.b.iv. Ignition and growth reactive burn model**

Similar to the P-α porosity model, the ignition and growth reactive burn model (IGRB) [8] contains parameters which must be calibrated using experimental data. The IGRB model has been used to capture the initiation and failure behavior of high explosives (HEs), and is typically calibrated with larger-scale tests using either Pop-plot, in-material particle gauge and/or corner turning data. The IGRB model expresses the reaction rate as the sum of three terms,

$$\dot{\lambda} = \dot{\lambda}_1 + \dot{\lambda}_2 + \dot{\lambda}_3$$  \hspace{1cm} (3)

where these terms stand for the ignition of the reaction ($\dot{\lambda}_1$), growth of the reaction ($\dot{\lambda}_2$) and reaction completion ($\dot{\lambda}_3$). Model parameters and the equations associated with each term are shown in Table 7 on the next page. Overall, the reaction rate is a function of the reaction progress variable, density and pressure.
B.3.b.v. Mixture EOS

For an incomplete reaction, the reaction progress variable, \( \lambda \) is used to average the unreacted and detonation product EOS. For non-ideal explosives such as ANFO, the mixture model is an active area of research within the field. For this work, a simple mixture model is used which assumes both mechanical and thermal equilibrium [9]. Other mixture models relax the condition of thermal equilibrium [10], however these models are not readily available in hydrocode CTH used for analysis; and moreover, none of the IGRB equations have thermally based terms.
B.3.c. 3D simulation results

The 3D fixed mesh rectangular geometry (3DR) used for the MI experiment is shown in Figure 16. This geometry includes the MI waveguide, 304 stainless steel conﬁner, booster explosive, ANFO and ambient surrounding air. The simulation is a 1/4-model of the experiment; having 160 x 160 x 640 zones for a resolution of 6.4 zones/mm. (Similar work by the U. S. Army Engineer Research and Development Center (ERDC) simulating close-in air blasts of ANFO has a comparable resolution of 4 zones/mm [11].) Symmetry boundary conditions are enforced on the bottom of the x, y and z-axes, whereas material is allowed to freely leave the mesh at the top of the x, y and z-axes. The symmetry condition on the bottom z-axis acts so that the explosive charge is set against an inﬁnitely thick wall. Finally, four thin slits (x=y mirrored in each quadrant) were cut into the bottom of the conﬁner to pre-crack the wall and encourage the formation of four petals (refer to Table 8 for a petal count observed from conﬁners recovered in the MI experiments). The ideal petal count of four was determined after inspection of several of the recovered conﬁners.

<table>
<thead>
<tr>
<th>No. of Petals</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.52 mm dia.</td>
<td>2</td>
<td>7</td>
<td>17</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>11.28 mm dia.</td>
<td>0</td>
<td>0</td>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 8: Number of petals observed in MI experiments.

Figure 16: 3DR geometry of the 1/4-model for small diameter ANFO experiments, showing the conﬁner material only (left) and a cut of the materials on the xy-plane (right).

B.3.c.i. Performance of baseline model parameters

An initial 3DR simulation was stabilized using baseline model parameters for ANFO; simulation output is shown in Figure 17 on the next page. The original simulation was sensitive to material fragmentation and could crash due to the time step being ratcheted down to an infinitesimal size.
Figure 17: Image sequence of the 3DR simulation for the confiner material (top), all materials except air (middle) and pressure history (bottom). A baseline set of ANFO model parameters was used to produce this image sequence.
This problem has been mostly solved using the SMYRA interface option in CTH; one additional source for
time step crashes is the algorithm used to advance the distension parameter of the P-α porosity model and
work is ongoing to address the issue. Baseline 3DR simulation results were post-processed and, compared to
a clean MI signal, corresponding to detonation failure in stoichiometric Kinepak ANFO having initial density
1.02 g/cc. Overall, the fit is decent but not optimal (refer to Fig. 18). New methodologies were considered to
match the experimental MI data including genetic optimization algorithms.

![Figure 18: Comparison of baseline 3DR position and velocity with MI data for Kinepak ANFO.](image)

**B.3.d. Optimization**

**B.3.d.i. Genetic Algorithms (GA)**

A genetic algorithm (GA) attempts to find the global optimum of an engineering problem using discretized
variables. These variables could originally be continuous but discretized into different bin sizes or discrete
settings such as the choice of a certain material or different treatment options. The collection of all parame-
ter values expressed in binary is combined into a single binary string called the chromosome, which is then
evaluated for overall fitness. The steps of the algorithm evaluate, pair, crossover and mutate the chromo-
somes comprising a single generation. As the algorithm continues, each successive generation approaches a
relatively uniform population near the (hopefully) global optimum. For the current work, the combination
of IGRB and P-α introduces a total of 18 unknown model parameters. To improve the speed and feasibility of
the algorithm, it was hypothesized that the “completion” term of IGRB is unnecessary, as the detonation wave
fails in ANFO and never reaches complete reaction. By disabling this term, 5 parameters were removed from
the study; details of the 56-bit chromosome and parameter discretization used for the genetic algorithm are
shown in Table 9 on the next page.
<table>
<thead>
<tr>
<th>Param.</th>
<th>Bits</th>
<th>Min</th>
<th>Max</th>
<th>Bin Size</th>
<th>Convert to 4-bit or 5-bit integer</th>
<th>2DC Opt. Val.</th>
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<td>Ignition</td>
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<tr>
<td>G₀</td>
<td>5</td>
<td>10⁰</td>
<td>10³¹</td>
<td>Log₁₀[G₀] ± 1</td>
<td>Log₁₀[G₀]/₃₁</td>
<td>10⁰</td>
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<tr>
<td>S₀</td>
<td>4</td>
<td>0</td>
<td>1.5</td>
<td>0.1</td>
<td>(2/3) · S₀</td>
<td>0.3</td>
</tr>
<tr>
<td>A₀</td>
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<td>0.3</td>
<td>0.02</td>
<td>(10/3) · A₀</td>
<td>0.26</td>
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<tr>
<td>Y₀</td>
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<td>0</td>
<td>31</td>
<td>1</td>
<td>(1/31) · Y₀</td>
<td>18</td>
</tr>
<tr>
<td>W₀</td>
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<td>0</td>
<td>0.75</td>
<td>0.05</td>
<td>(4/3) · W₀</td>
<td>0.1</td>
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<tr>
<td>Growth</td>
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<td></td>
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<tr>
<td>G₁</td>
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<td>10⁻³¹</td>
<td>10⁰</td>
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<td>-Log₁₀[G₁]/₃₁</td>
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<tr>
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<td>0.9</td>
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<tr>
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<td>7.5</td>
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<td>(2/15) · Y₁</td>
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<tr>
<td>W₁</td>
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<td>1.0</td>
<td>0.05</td>
<td>(4/3) · [W₁ - 1]</td>
<td>0.25</td>
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<tr>
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<td></td>
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<td></td>
</tr>
<tr>
<td>Pₛ</td>
<td>4</td>
<td>10⁰</td>
<td>10⁻¹⁵</td>
<td>Log₁₀[Pₛ] ± 1</td>
<td>Log₁₀[Pₛ]/₁⁵</td>
<td>10⁻¹⁴</td>
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<td>0.75</td>
<td>0.05</td>
<td>0.2e4</td>
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<td>0.25</td>
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<td>0.2e⁴</td>
<td>(50/31) · [Cₛ/1e⁵ - 0.3]</td>
<td>3.2e⁴</td>
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</tbody>
</table>

Table 9: Discretization of IGRB and P-α parameters used for the genetic algorithm optimization study. Optimum values determined by the algorithm for a 2DC simulation are shown as well.

B.3.d.ii. 2DC simulations

Overall, the CPU cost was too expensive to perform the GA on a fully 3DR simulation. It is estimated that 3,000 to 6,000 simulation runs are required for the GA to converge for the 56-bit chromosome. A compromise is a 2D cylindrical geometry (2DC) which approximates the effect of the confiner but does not petal in the same way (refer to Fig. 19). It is hoped that the 2DC simulations may be used to optimize the parameters before detailed simulations are run in the fully 3DR geometry.

Figure 19: Comparison of 3DR and 2DC simulation geometries for the baseline ANFO parameters. Qualitatively, the shape of the confiner during failure is similar.
B.3.d.iii. Convergence and results

Over 3,000 simulations with 2DC geometry were run for the first test of the GA implementation. Fitness was measured with a correlation coefficient (calculated from the sum-of-squared errors, SSE, to the MI data, and the sum of total squares, SST). Of these runs, 253 of the cases had $R^2$ values greater than 0.95. The best case parameters are shown in Table 9 on the previous page, and the resulting curve fit to the MI data is shown in Figure 20.

![Figure 20: Comparison of GA optimized 2DC simulation with MI data for Kinepak ANFO.](image)

Statistical analysis of the top 253 cases (see Figs. 22 and 23 on the following pages for example output cases) was performed in order to assess the most influential model parameters. A good metric for sensitivity was determined to be the parameter bin size divided by the standard deviation of the top cases (refer to Fig. 21 on the next page). Parameters with the most influence are similar or identical among the top cases so the standard deviation is low (much less than the discretized bin size). From Figure 21, it is clear that the pressure exponent, $Y_1$, of the reaction growth term has the most influence; however, the optimum value is zero. This means that the reaction rate model for detonation failure should be pressure independent and only a function of the initial density of ANFO. These results are invaluable and will be used to eliminate non-relevant model parameters from the optimization study of the small-scale characterization experiments.

![Figure 21: Influence of model parameters determined by statistical analysis of the best cases with R2 values greater than 0.95.](image)
Figure 22: Image sequence of pressure for select cases of the GA optimization study.

Figure 23: Image sequence of reaction progress for select cases of the GA optimization study.
C. Major Contributions

The major contributions of this work this past year, the second year of the project, are:

- Graduated a student (Peter Renslow) who will contribute to security research.
- Ammonium nitrate + aluminum (AMMONAL) tested at small diameter, and comparisons being made to large scale experiments.
- ANFO: Kinepak, cold pack, and prilled AN characterized.
- TATB/Teflon mixtures with tailorable detonation failure characteristics demonstrated and initial modeling compared to these results (results published).
- Wavelet analysis developed and paper accepted to Review of Scientific Instruments.
- Initial development and calibration of ignition and growth modeling to ANFO results.
- Sample density shown to have large effects on detonation dynamics.

The major contributions of this work from the previous year, the first year of the project, are:

- Microwave interferometry developed as a non-intrusive diagnostic.
- Analysis techniques developed Fourier transform, quadrature and peak-to-peak calculations of MI data.
- Varied mixture ratio, sample geometry and confinement (results published).
- Initial modeling of TATB results (results published).

D. Future Milestones

Major future milestones of this work include:

- Obtain data on the effect of diameter on ANFO and AMMONAL materials with MI technique. Much of this work will be done in collaboration with LANL this summer.
- Develop alternative continuous diagnostic (see Section E below).
- Fully develop calibrated ignition and growth model and apply it to large-scale experiments to show capability.
- Characterize more HME materials, including materials that cannot be characterized with MI system.
- Graduate two more students that will contribute to security research.

E. Future Plans

The need for an additional diagnostic has been discussed in the previous sections. Figure 24 on the next page shows a schematic of a new technique to be implemented along with the microwave interferometer system. This diagnostic may allow the decoupling of the shock wave (tracked by the microwave interferometer) from the ionization front (tracked by a closed circuit, the resistance of which continuously changes as the ionization front travels through the confiner) to be observed. This diagnostic may also be used to measure detonation failure of energetic materials that are not compatible with the microwave technique due to microwave absorption or attenuation, such as nitromethane.
Collaboration with facilities outside Purdue University will continue, particularly with RMSL and LANL, in order to further relate small-scale experimental data with that of large-scale detonation experiments. We will determine the effect of diameter on ANFO and AMMONAL materials with MI technique. Much of this work will be done in collaboration with LANL this summer.

We will fully develop a calibrated ignition and growth model and apply it to large-scale experiments to show capability. This is proceeding well and the genetic algorithm applied appears to be robust and useful. We also want to demonstrate the capability of this model to predict results.

As noted, there is an almost limitless range of HMEs that can be formulated. We plan to continue to characterize more HME materials, including materials that cannot be characterized with MI system.

III. EDUCATION AND WORKFORCE DEVELOPMENT ACTIVITY

We are involved in workforce development and education in many ways, including:

A. Course, Seminar or Workshop Development

Teaching a course on the combustion of energetic materials every other year (fall 2014 was the latest offering). The course number is ME 697C and there are typically 10-15 students that take the class. A section of the course covers detonation processes, including diagnostics and non-ideal (homemade) explosives. About one week includes content/relevance to this project.

B. Student Internships, Jobs or Research Opportunities

- David Kittell is interning at Sandia National Laboratories (SNL). He is doing modeling related to this project.
- Nick Cummock is interning at LANL. He is using our MI methods on HME materials of interest to both DHS and DOE.
- Graduated M.S. student, Peter Renslow is working at SNL.

C. Interactions and Outreach to K-12, Community College, Minority Serving Institution Students or Faculty

- Mentoring a local Chemistry high school teacher with a CSS/CI outreach program titled, “Rocket Design, Construction and Engine Synthesis”.

Figure 24: New diagnostic to be implemented in order to track the ionization front in a detonation test.
IV. RELEVANCE AND TRANSITION

A. Relevance of Research to the DHS Enterprise

If we can characterize homemade explosives quickly using small samples, we can provide the relative detonability of different compositions, as well as provide data for modeling efforts so that threats can be more accurately predicted. Transferring detonation and composition information and modeling data to users, small companies such as “Rock Mountain Scientific Laboratory (RMSL), and National Laboratories (SNL, LLNL) will be significant to the DHS enterprise and educating highly trained personnel for those labs will also be significant to the DHS enterprise.

B. Potential for Transition

We are transitioning our testing approach and test data to both companies (e.g., RMSL) and national labs (SNL and LANL) to assist them in their research and technology development.

C. Data and/or IP Acquisition Strategy

Our technical approach is described above.

D. Transition Pathway

The data collected and models developed will help end-users assess threats of various HMEs. We are engaging with small businesses and national labs directly. Students are doing internships now at the labs and will likely take permanent positions when they graduate.

E. Customer Connections

- Cole Yarrington (SNL), mentoring David Kittell
- Scott Jackson (LANL), mentoring Nick Cummock
- Brian Bockmon (RMSL), founder of RMSL

V. PROJECT DOCUMENTATION

A. Peer Reviewed Journal Articles


B. Peer Reviewed Conference Proceedings


C. New and Existing Courses Developed and Student Enrollment

1. Prof. Son teaches a course on the combustion of energetic materials every other year (fall 2014 was the latest offering).

D. Software Developed

1. Models
   a. We are developing a model for ANFO that is built on ignition and growth. This is discussed above in detail. Once developed, others can implement it in CTH or similar codes using our calibrated model.

VI. REFERENCES

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