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ABSTRACT

The SMIS (Specific Munitions Impact Scenario) experimental series performed at Los Alamos National Laboratory has determined the 3-dimensional shock initiation behavior of the HMX-based heterogeneous high explosive, PBX 9501. A series of finite element impact calculations have been performed in the ALE3D [1] hydrodynamic code and compared to the SMIS results to validate the code predictions. The SMIS tests use a powder gun to shoot scaled NATO standard fragments at a cylinder of PBX 9501, which has a PMMA case and a steel impact cover. The SMIS real-world shot scenario creates a unique test-bed because many of the fragments arrive at the impact plate off-center and at an angle of impact. The goal of this model validation experiments is to demonstrate the predictive capability of the Tarver-Lee Ignition and Growth (I&G) reactive flow model [2] in this fully 3-dimensional regime of Shock to Detonation Transition (SDT).

The 3-dimensional Arbitrary Lagrange Eulerian hydrodynamic model in ALE3D applies the Ignition and Growth (I&G) reactive flow model with PBX 9501 parameters derived from historical 1-dimensional experimental data. The model includes the off-center and angle of impact variations seen in the experiments. Qualitatively, the ALE3D I&G calculations accurately reproduce the "Go/No-Go" threshold of the Shock to Detonation Transition (SDT) reaction in the explosive, as well as the case expansion recorded by a high-speed optical camera. Quantitatively, the calculations show good agreement with the shock time of arrival at internal and external diagnostic pins. This exercise demonstrates the utility of the Ignition and Growth model applied in a predictive fashion for the response of heterogeneous high explosives in the SDT regime.

INTRODUCTION AND BACKGROUD

The computational analysis presented here is part of the Impact Response of Energetic Material Systems program at Lawrence Livermore National Laboratory. The goal of this program is to support the design activities of the Insensitive Munitions (IM) community of the Joint Munitions Program (JMP). This includes developing computational models and performing relevant experiments to predict the response of weapon systems containing energetic materials – both propellants and explosives – to the impact of bullets and metal fragments. The team objective is to develop robust hydrocode models for the weapon system response in a range of regimes from burning to prompt shock detonation in 3D. These models will be calibrated for individual energetic materials and validated by experimental results. These models can then be provided to the DoD community for the design of weapon systems that meet IM requirements.

In pursuit of these objectives, numerous calculations have been completed using ALE3D with the Ignition and Growth reactive flow model. These calculations have been compared with data from the SMIS (Specific Munitions Impact Scenario) 1.2 tests performed at LANL on PBX 9501. Future work will focus on the spiral development of new models that demonstrate the capability to predict weapon system response in XDT (Detonation Transition from recompression of damaged energetic material), DDT (Deflagration to Detonation Transition), and burning reactions.

SMIS 1.2 TEST SERIES

The test diagnostics set-up and target graphic for the SMIS series is shown in Figure 1. The SMIS 1.2 shot series has become an effective metric for providing spherically-divergent loading to a reactive material. In the experiment, non-uniaxial loading is applied by firing a 50 caliber fragment with a powder gun onto a variable-thickness impact face of 1018 steel over a cased sample of PBX 9501. There are 450 keV x-ray images taken 90^{o} apart that are used to capture the angle of impact of the fragment relative to the impact face. The impact velocity is determined from a series of break-screens and make-screens leading up to the impact. The arrival times of the shockwave within the explosive is determined from both PZT pins and manganin gauge records. The occurrence of Go/No-Go for an SDT reaction is determined by inspection.

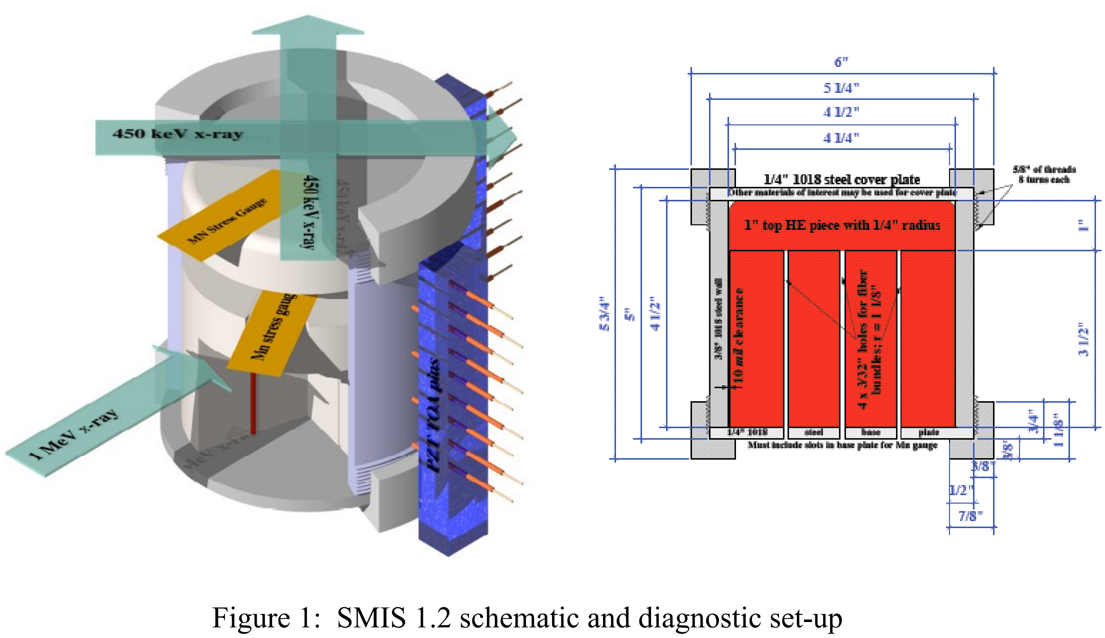
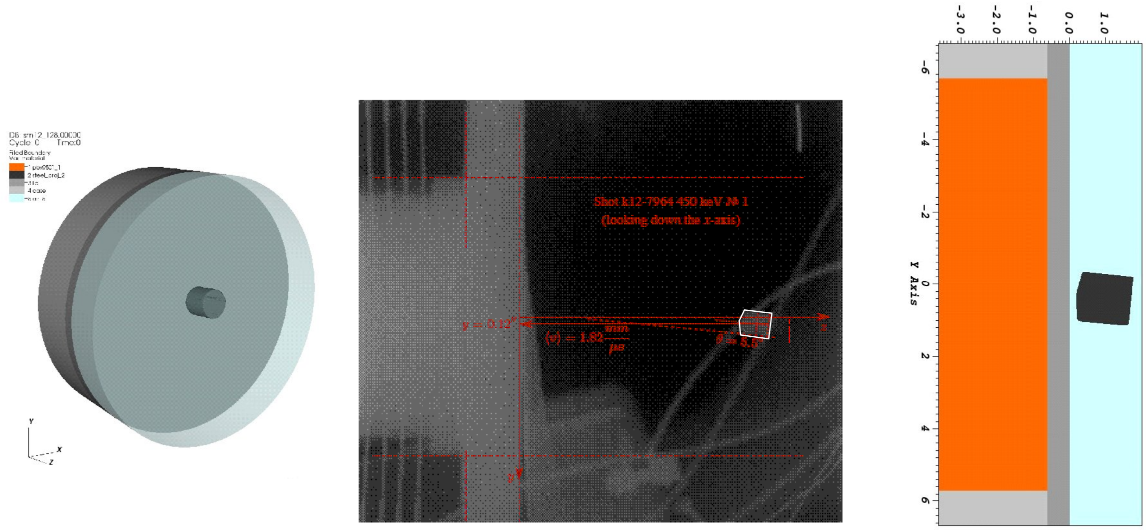


Figure 1: SMIS 1.2 schematic and diagnostic set-up

ALE3D MODEL SETUP AND GO/NO-GO

A computational model has been developed in ALE3D that includes the first 3 cm (1.2") on the 4.5" long, cylindrical, PBX 9501 sample, so the run up to detonation is captured. The model is shown in Figure 2. The model contains 4.7 million elements and runs to completion in 8-16 hours on 128 processors. The reactive flow model of Cochran-Chan, and Lee-Tarver (iform 15 in ALE3D), is applied using parameters documented in Ref [3]. Of the four cases modeled, the Go/No-Go threshold has been accurately predicted by ALE3D when the impact angle and location are properly accounted for in 3-dimensions. These cases are summarized in Table 1.



(a) (b) (c)

Figure 2: ALE3D SMIS 1.2 model: (a) shows the ALE3D model, (b) shows an SMIS 450 keV x-ray capture from the k12-7964 shot, and (c) shows the slice through the ALE3D model that corresponds to that x-ray viewpoint

Table 1: Summary table of SMIS 1.2 shots on which calculations are performed

Shot number	**Average impact velocity [km/s]**	**Impact angle |α| [degrees]**	**SDT response**
1/8" 1018 steel cover plate			
k12-7967	1.57	5.1	Go
k12-7966	1.46	16.9	No-Go
1/4" 1018 steel cover plate			
k12-7964	1.82	5.75	Go
k12-7958	1.70	5.1	No-Go

These results are shown graphically in Figure 3, which plots the mass fraction reacted (variable: fhe, which ranges from 0 to 1) in the reactive flow calculation for each of the different cases. It is shown in the figure that the same threshold reported in the SMIS shot is calculated by ALE3D. In the figure, the duplicative preceding "k12" on the shot numbers has been dropped for simplicity.

These calculations reinforce the conclusion that the Ignition and Growth model, even though it has been developed and calibrated in uniaxial loading, can be applied – without modification – for fully 3-dimensional loading to capture energetic material response in SDT.

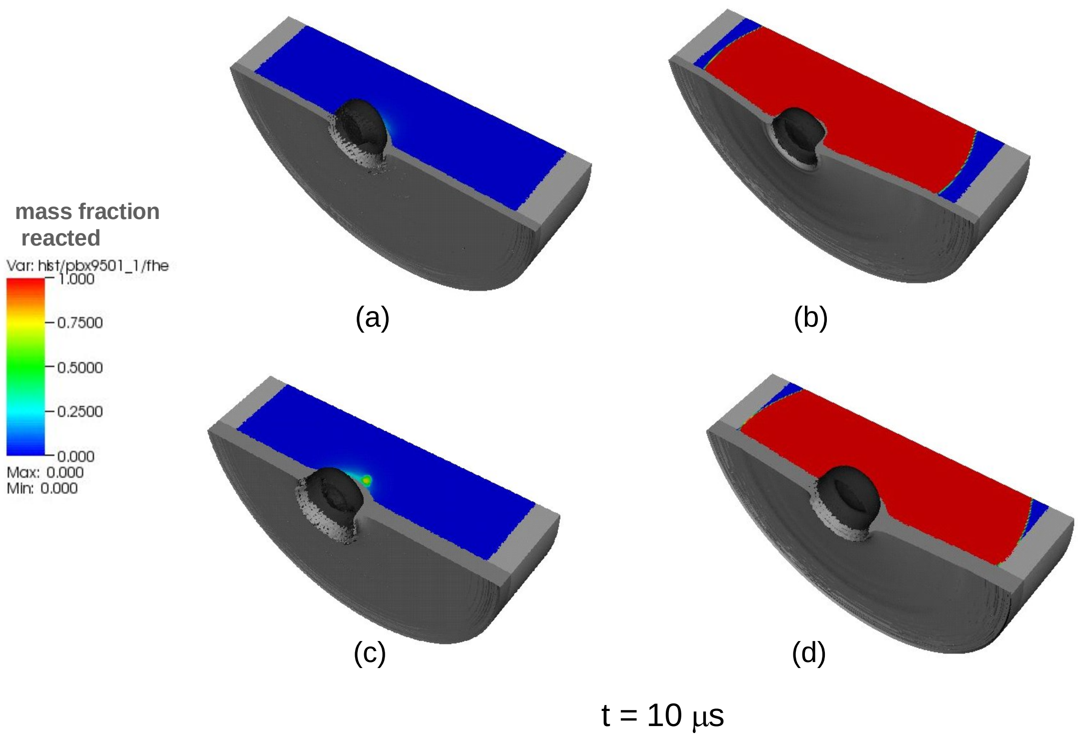


Figure 3: Fringe plots of mass fraction reacted for 4 different cases: (a) 7966, (b) 7967, (c) 7958, and (d) 7964. Cases (a) and (c) are considered SDT "No-Go" while (b) and (d) are considered SDT "Go" reactions.

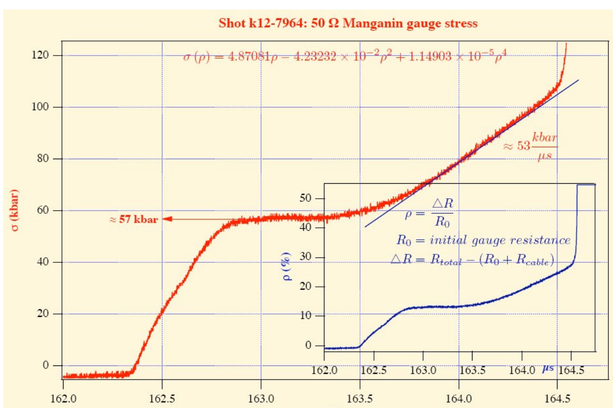
MANGANIN GAUGE RECORDS

There are 2-ea manganin gauge records for each shot in the SMIS 1.2 series (see Figure 1). ALE3D pressure measurement techniques have been inserted in the calculation to compare with the temporal history of these gauges. The manganin gauges measure stress, which is a tensor of the sum of deviatoric (shear) and hydrostatic (pressure) components. For hydrodynamic calculations, the stress is nearly equivalent to the pressure, and they can be compared directly. This will not be the case in the strength-dominated models that are being developed in support of the more comprehensive objectives of the IM program (e.g. XDT, DDT), but it is the case here.

In three dimensions, it is not immediately apparent whether manganin gauge records, ubiquitous in 1D experimentation, are either relevant or meaningful. Certainly, they cause some issues in interpretation of experimental values. Simple point pressure tracers in the computational mesh do not represent the values shown in the experiments.

To understand the physical mechanisms and how they affect the quantification of computational pressure histories, a series of parameter studies have been performed to evaluate the effect of material properties and geometry on the pressure rise time. It is seen in the first (50 Ω) gauge record that there is a rise time, a plateau in pressure, and then another smooth rise until failure (see Figure 4). This could be caused by a potting-filled gap between the case lid and the explosive, or possibly, the material properties of either the fragment or the lid. The second slow pressure rise is expected when there is gauge stretching from a non-uniaxial load. Through an ALE3D computational study, there was no indication that either the Equation of State (EOS) or the strength properties of the steel alter the predicted rise time, and that even a 20-mil Sylgard gap doesn't show enough of a cushioning effect to account for the rise time that was seen in the experiment. It is concluded that this is a result of gauge stretching from the non-uniaxial shock loading.

Some of this discrepancy in modeling an experiment is explained by the nature of the gauge itself. Because of the 3-dimensional loading of the gauges (especially the larger, 50 Ω, gauge), the pressures have been distributed over the surface area of the element (1/4" x 1/4", in this case) when comparing calculation and experiment. In order to get the pressure histories to match experimental data, the pressure tracers in the computational model must be averaged across the area of the resistive element. When this is done, the pressure tracers match the smoothly rising curve that is seen in the data and even reach a similar plateau (Figure 4). It is expected that complete modeling of the gauge package would give even better correspondence with experiment and that it could capture the late-time pressure increases that are attributed to gauge stretching.



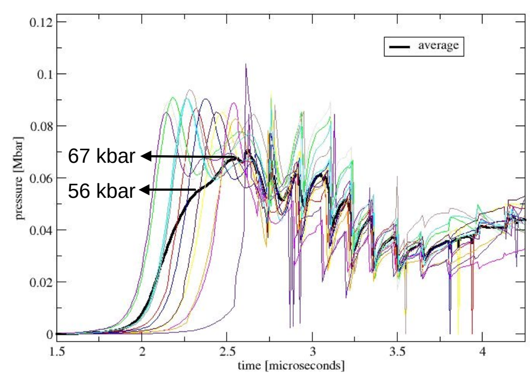


Figure 4: 50 Ω Manganin gauge record from 7964 (left) compared with the ALE3D average pressure tracer calculation (right)

The 50 mΩ gauge that is 1” into the PBX 9501 does not show the same initial rise behavior, but it also has a relatively smaller surface area (1/16” x 3/16”). Figure 5 shows the response of this gauge which shows significantly lower pressures than those calculated in ALE3D. One explanation is that the Ignition and Growth model is running up the detonation wave faster than is shown in the experiment. With only one embedded tracer, it is difficult to come to a complete conclusion that involves the run distance to detonation. Further SMIS shots with embedded pressure tracers could clarify this disagreement.

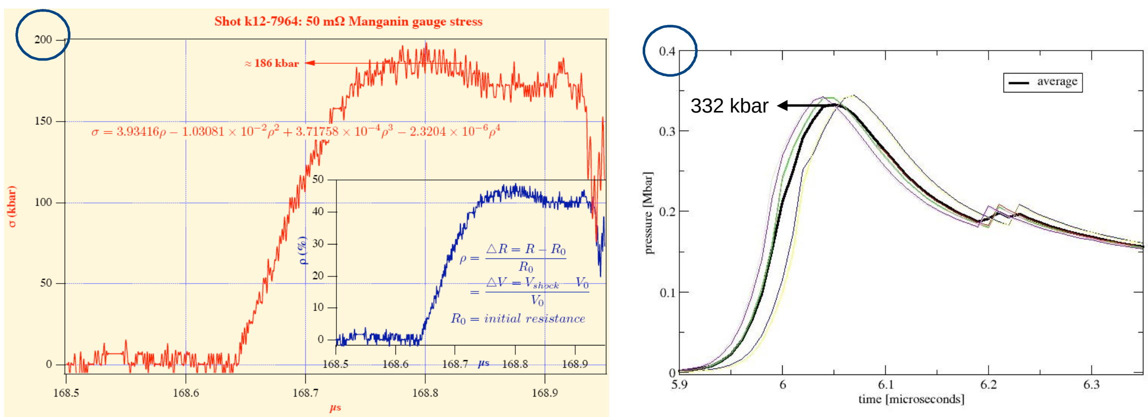


Figure 5: 50 mΩ Manganin gauge record from 7964 (left) compared with the ALE3D average pressure tracer calculation (right), note that the scales are different

GLOBAL TIME OF ARRIVAL COMPARISON

There has been some uncertainty in the velocity of the fragment at impact, as there is no direct measurement of impact time from the experiment. As such, comparison of Time Of Arrival (TOA) data is a bit nebulous. The experimentalists have provided “Absolute Timeline & Associated Position Plots” data for the k12-7964 shot. The timeline starts at the initiation of the first break-screen and continues until the last fast-framing camera fires over 660 μs later. Since the relative times between gauges and PZT pins can be quantified, those values are compared between the SMIS experiments and the ALE3D calculations (see Table 2). In the table, the times are normalized to the TOA on the 50Ω gauge so the “normalized TOA” reported is the difference in travel between the gauge being reported and the 50 Ω gauge. It is notable that there is as much as a 34% variation in the ALE3D and SMIS normalized TOA’s close into the fragment impact zone, but that difference quickly diffuses out at the pin rails. This supports the 50 mΩ manganin gauge data indicating that the Ignition and Growth predicts a slightly faster run-up to detonation.

Table 2: Comparison of normalized Time of Arrival (TOA) for the SMIS experiments and ALE3D calculations

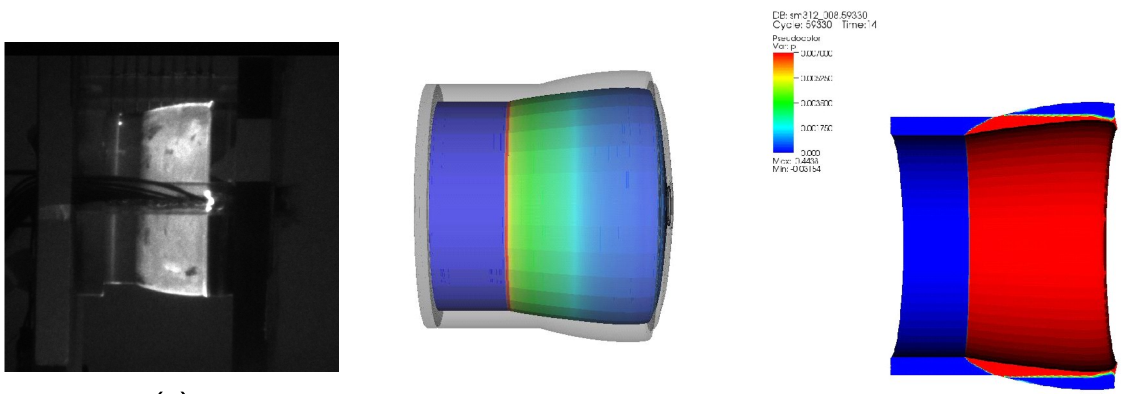
k12-7964 TOA					
	SMIS		Calculation		
	Raw TOA [μs]	Normalized TOA [μs]	Raw TOA [μs]	Normalized TOA [μs]	Δ [%]
Manganin Gauges					
50Ω	640.849		1.80		
50mΩ	647.139	6.3	6.04	4.2	33
Embedded Pins					
pin-19	650.015	2.9	8.12	2.1	28
pin-20	649.875	2.7	7.84	1.8	34
pin-21	649.533	2.4	7.75	1.7	29
pin-22	649.549	2.4	8.04	2.0	17
Pin Rail 1					
pin-1	655.053	7.9	13.18	7.1	10
pin-2	655.409	8.3	13.98	7.9	4
Pin Rail 2					
pin-10	654.783	7.6	13.36	7.3	4
pin-11	655.159	8.0	14.15	8.1	-1

CASE EXPANSION

Early in the post-processing of the SMIS 1.2 Cooke (optical) camera data, a dim line traveling across the PBX 9501 ahead of the optical signature of the reaction front appeared to be a precursor shock of a strong detonation in the explosive (Figure 6 (a)). This behavior is seldom seen in heterogeneous explosives because a non-pristine material has hot-spots that are initiated by the precursor shockwave. The detonation wave will build from a pressure wave to a strong detonation without an observable signature, so it looks like one wave. The observed behavior in the SMIS test resembles a homogeneous reactive material, which is not expected in the detonation of PBX 9501, a well-known heterogeneous explosive. Without an explanation, this could indicate that the physics of the response to a spherically-diverging shockwaves is different than that of a uniaxial load. This could indicate that existing reactive flow models that have been built on 1D experimental data are invalid in 3-dimensions.

The build-up phenomenology of a detonation wave in a heterogeneous reactive material is a fundamental assumption in the Ignition and Growth model, and this assumption has a basis in observed phenomena – which has been demonstrated throughout years of validation work. A series of calculations in 2-dimensions attempt to ascertain the physical mechanisms to explain the perception that there are multiple shockwaves running through the explosive. These calculations demonstrate that a delay exists between the shock front arrival and the perceived reaction front arrival because there is a delay in the outer case expansion. During that delay, the optical signature of the reaction is blocked by the shock-induced opacity of the PMMA case.

There are studies in the literature about the shock-induced opacity of PMMA. Segreti, et. al. [4] discovered that the opacity is created by a crystallization phenomena that can be correlated to the heat evolution of fracture by looking at samples fired in an oven. They saw that shock-resistant PMMA fails like a ductile material and the temperature rises as the plasticity evolves. From Segreti, et. al.: "During plastic deformation, material locally reaches a sufficiently high temperature to trigger crystallization phenomenon". This opacity has also been reported by Barker and Hollenbach [5] in their studies of shock-driven VISAR window materials. In Barker, the onset of plastic response is identified as ~7 kBar under uniaxial loading. Figure 6(b) shows a camera image from the SMIS shot and a corresponding ALE2D plot of the case expansion. The delay between the shock arrival and case expansion response is clearly visible. Figure 6(c) shows a cut-away of the instantaneous pressure magnitude limited to 7 kBar (with a peak pressure of over 400 kBar!). This identifies the region in the wall (shaded in *red*) that has been shocked sufficiently enough to be opaque to an optical camera. It is shown that the region between the shock front and the wall expansion is not expected to have an optical signature. This computational study shows that the heterogeneous assumption of the Ignition and Growth model and the SMIS data are completely consistent and complimentary.



(a) (b) (c)

Figure 6: Comparison of (a) Cooke optical camera data with the ALE2D calculations of (b) case expansion and (c) pressure

CONCLUSIONS

Using the SMIS 1.2 test series, the Ignition and Growth reactive flow model has been validated for the prediction of Shock to Detonation Transition (SDT) consistent with the mission of the Joint Munitions Program. Comparisons have been made between the experimentally observed and computed Go/No-Go occurrence, arrival times, and case expansion. These direct comparisons indicate that the Ignition and Growth model is an effective tool in the prediction of the impact response of energetic materials in the SDT regime.

Fully 3-dimensional experimentation is still rare in the energetic materials community, and shortfalls in the diagnostic capability in 3-dimensions have been identified for future areas of development. In addition, future work will include development and implementation of alternative diagnostics, as well as code development of reactive flow and strength models for the predictive response of XDT (Detonation Transition from recompression of damaged energetic material), DDT (Deflagration to Detonation Transition), and burning reactions to support the Insensitive Munitions community of the Joint Munitions Program.

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