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MODELING THREE-DIMENSIONAL SHOCK INITIATION OF PBX 9501 IN ALE3D

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ABSTRACT

A recent SMIS (Specific Munitions Impact Scenario) experimental series performed at Los Alamos National Laboratory has provided 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 and study code predictions. These SMIS tests used a powder gun to shoot scaled NATO standard fragments into a cylinder of PBX 9501, which has a PMMA case and a steel impact cover. This SMIS real-world shot scenario creates a unique test-bed because (1) SMIS tests facilitate the investigation of 3D Shock to Detonation Transition (SDT) within the context of a considerable suite of diagnostics, and (2) many of the fragments arrive at the impact plate off-center and at an angle of impact. A particular goal of these model validation experiments is to demonstrate the predictive capability of the ALE3D implementation of the Tarver-Lee Ignition and Growth reactive flow model [2] within a fully 3-dimensional regime of SDT.

The 3-dimensional Arbitrary Lagrange Eulerian (ALE) 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 reproduce observed "Go/No-Go" 3D 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 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 fragments. One of the initial team objectives is to extend and develop robust modeling and simulation capabilities that may be applied to weapon system response to a single fragment over a range that extends from burning of the energetic material to prompt 3D SDT. Such modeling and simulation capabilities will be calibrated to individual energetic materials and validated with experimental results. The resulting capabilities are in turn provided to the DoD community to aid in the design of weapon systems that meet IM requirements.

In pursuit of these objectives, 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 divergent 3D loading to a reactive material. In these experiments, non-uniaxial loading is applied by firing a 50 caliber fragment from a powder gun onto a variable-thickness impact face of 1018 steel and into a PMMA-cased sample of PBX 9501. Orthogonal 450 keV x-ray images capture tilt angle and impact position of the fragment relative to the impact face. Impact velocity is determined from a series of break-screens and make-screens leading up to the impact. The arrival time 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.

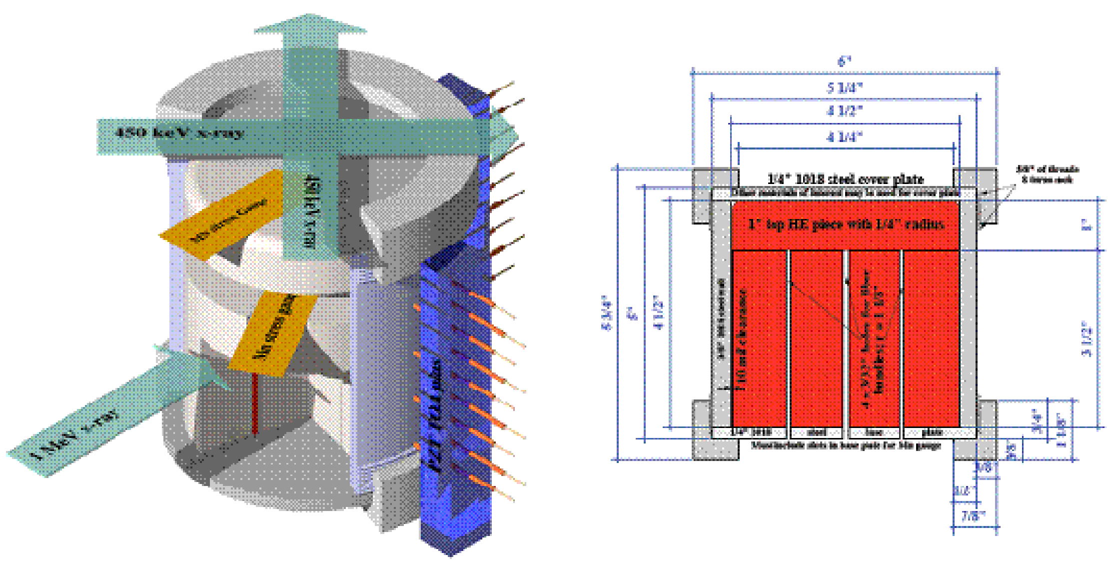

Figure 1: SMIS 1.2 schematic and diagnostic set-up

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, and the run up to detonation is predicted within this distance. 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, is applied using parameters documented in Ref [3]. Of the four cases modeled, the Go/No-Go experimental result 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.

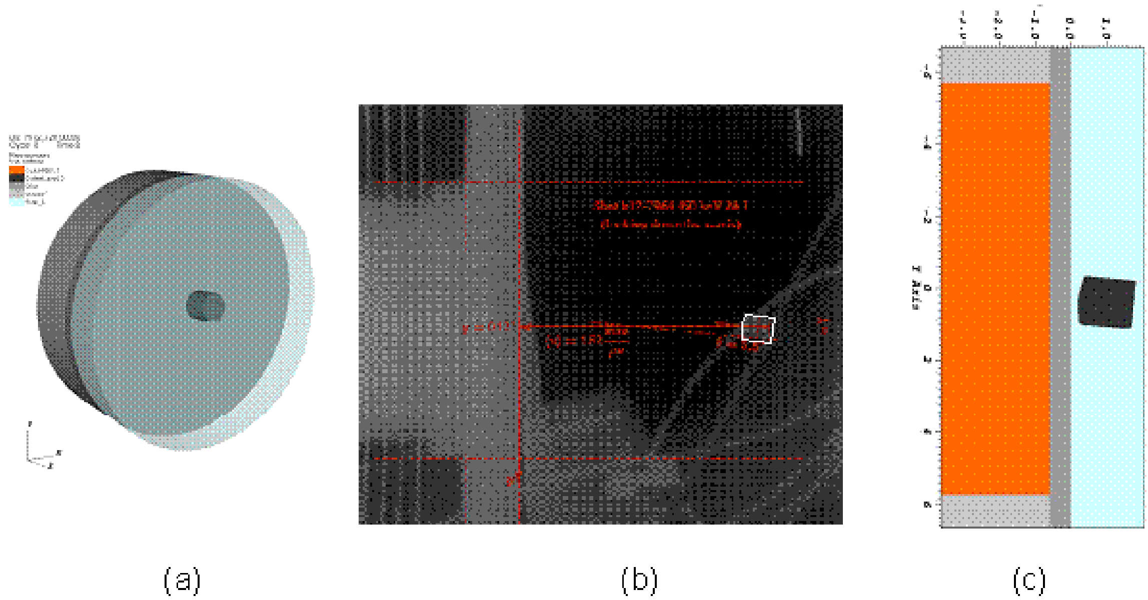

Figure 2: ALE3D SMIS 1.2 model: (a) shows the ALE3D model, (b) shows an SMIS 450 keV x-ray capture from the k12-7964 shot, and (c) shows the slice through the ALE3D model that corresponds to that x-ray viewpoint

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

Shot number	Average impact velocity [km/s]	Impact angle $\|\alpha\|$ [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 illustrated 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 Go/No-Go result 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 usefully applied – without modification – for fully 3-dimensional loading to capture energetic material response in SDT.

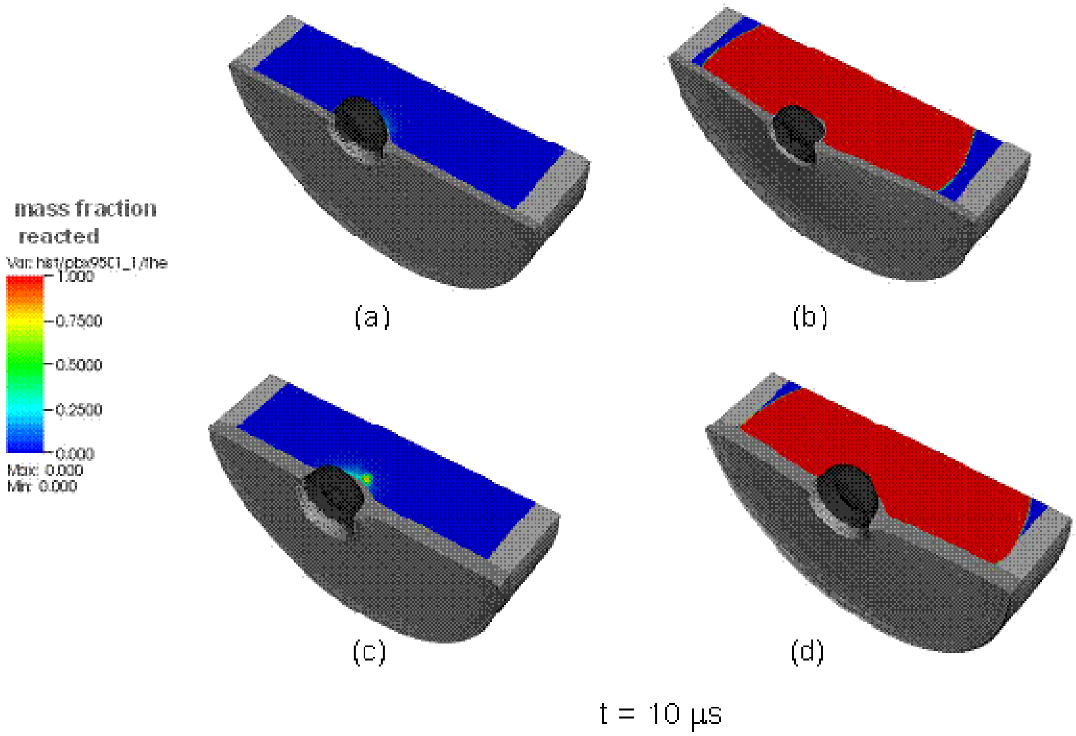

Figure 3: Fringe plots of mass fraction reacted for 4 different cases: (a) 7966, (b) 7967, (c) 7958, and (d) 7964. Cases (a) and (c) are considered SDT "No-Go" while (b) and (d) are considered SDT "Go" reactions.

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 3-dimensions it is not immediately apparent whether the stress measurement obtained with manganin gauge records, ubiquitous in 1D experimentation, are quantitative in nature. Although the recorded time of arrival of waves on these gauges is meaningful (up to the point where the gauge breaks), it is speculated, however, that these stress measurements do represent a lower limit of the actual dynamic stress. Since the manganin gauges are calibrated to measure the component of the stress tensor along the axis of symmetry for normal incident waves, there are some issues in interpretation of the values as determined by these gauges. Simple point pressure tracers in the computational mesh do not represent the values shown in the experiments.

To understand some of these 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 stress, and then another smooth rise until failure (see Figure 4). This initial rise time 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. 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 (in actuality, this gap was most likely ≤ 1-mil). This second slow rise in stress can be explained by gauge stretching. Gauge stretching can result from non-uniaxial shock loading, or the combined effects of reaction and highly divergent flow.

Some of this discrepancy in modeling this 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 stresses are 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 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 first 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 might capture the late-time stress increases.

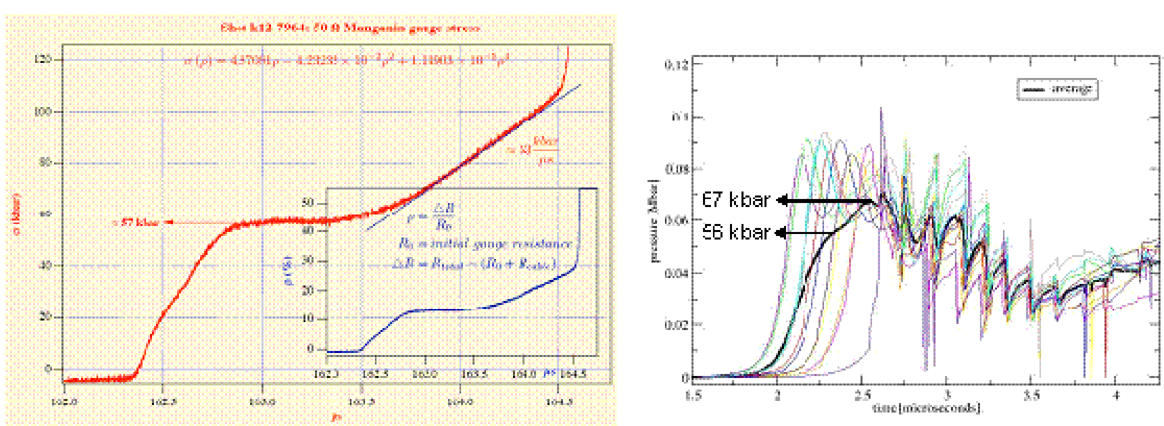

Figure 4: 50 Ω Manganin gauge stress record from 7964 (left) compared with the ALE3D average pressure tracer calculation (right)

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 stresses than the pressures 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 stress tracers could clarify this disagreement.

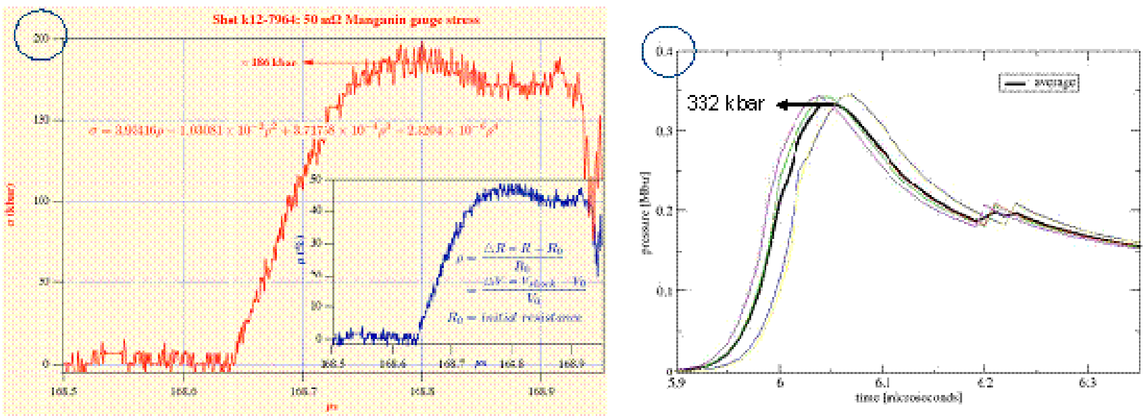

Figure 5: 50 mΩ Manganin gauge stress record from 7964 (left) compared with the ALE3D average pressure tracer calculation (right), note that the scales are different

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 accurately (typically the relative times between these diagnostics is a small fraction of a microsecond), 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 50 Ω 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 this difference quickly diffuses out at the pin rails. This supports the 50 mΩ manganin gauge data indicating that the Ignition and Growth predicts a 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		**ALE3D Calculation**		
	Raw TOA [μs]	**Normalized TOA [μs]**	**Raw TOA [μs]**	**Normalized TOA [μs]**	**Δ [%]**
Manganin Gauges					
50 Ω	640.849		1.80		
50 mΩ	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 (which are typically 1D experiments) because a non-pristine material has hot-spots that are initiated by the precursor shockwave. The detonation wave builds from a stress 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 highly diverging shockwaves is different than that of a uniaxial loading, possibly due to concatenate effects of reaction and highly divergent flow. This could also 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 1D phenomena – which has been demonstrated throughout years of validation work. A series of axisymmetric calculations attempt to ascertain the physical mechanisms to explain the perception that there are multiple shockwaves running through the explosive. These calculations qualitatively 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. This is shown in Figure 6.

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.

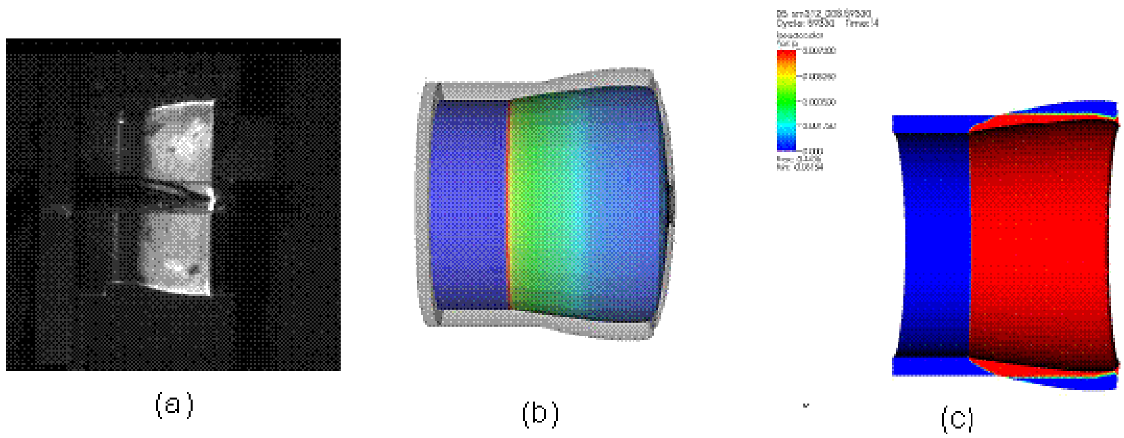

Figure 6: Comparison of (a) Cooke optical camera data with the ALE2D calculations of (b) case expansion and (c) pressure

CONCLUSIONS

Using the SMIS 1.2 test series, the Ignition and Growth reactive flow model, as implemented in ALE3D, has been validated to the extent outlined above for the prediction of Shock to Detonation Transition (SDT) in 3-dimensions. It is anticipated that future SMIS experiments will aid in isolating and answering (some of) the questions that have been discussed here. 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, and conclusions and/or potential discrepancies have been identified. These direct comparisons indicate that the Ignition and Growth model can be 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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