Model Development for Insensitive Munitions (IM) Simulations

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Abstract

Concerted efforts are underway to make munitions IM compliant and less vulnerable to unplanned hazard scenarios such as shock, shear, and thermal stimuli**.** For munitions to be IM compliant they must fulfill their performance, readiness and operational requirements on demand while at the same time reduce the probability of inadvertent initiation, which can cause collateral damage to weapon platforms and personnel.[1] In the IM-community there are several potential threats to munitions ranging from magazine fires to inadvertant impact into energetic materials. We have narrowed our scope to examine threats capable of creating slow cook-off, fragment impact and sympathetic detonation. We are focusing on the coupled behavior of physical phenomena such as thermal ignition, burning and shock initiation. Currently we are exercising the hydrocodes CTH[2] and ALE3D[3] to determine their ability to simulate these different phenomena and to build new models that enhance our capability to predict constitutive behavior and energetic response.

Introduction

The sensitivity of munitions to unplanned thermal and impact stimuli results in much catastrophic damage to personnel and weapons platform.[4] These catastrophic incidences often occur due to accidents in ammunition storage, normal handling and transport.

Within the Insensitive Munitions (IM) community there are several identifiable threats to munitions due to hazards from fire or from external impacting stimuli. For example, fire hazard could directly impact munitions storage leading to a fast thermal cook-off or the fire next door to an ammunition stowage could lead to much slower thermal reaction (slow cook-off) over time. There are hazards to munitions from external stimuli such as bullet impact, fragment impact, sympathetic detonation and shape charge jet attacks. There are six IM-tests[5] used to study these threats. For each IM-test, there are associated physical phenomena such as thermal ignition, burning, deflagration-to-detonation transition, mechanical ignition, shock initiation, fragmentation and detonation failure, which needs to be better, understood. To be successful in our efforts, we have narrowed our scope to the areas of slow cook-off, fragment impact and sympathetic detonation. More specifically, we are focusing on isolated phenomenon such as thermal ignition, burning and shock initiation.

We realize that addressing IM concerns involves looking at all aspects of the munitions which involves the energetic material, the confinement material and configuration, the venting capability, and the storage and configuration.[1] However, before the latter issues can be addressed one needs to first understand the reactive behavior of the energetic material. Different energetic materials because of their formulations exhibit variations in physical properties, sensitivity, explosive output, and toxicity, etc. Predicting the response behavior of energetic material during fragment impact, sympathetic detonation and slow cook-off is a challenging task. To this end, we have selected a representative cross section of energetic material to study. That is, we are investigating the response behavior of PBXN109, PBXN9, PBX9501, and COMP-B but not necessarily in that order. We are assessing the predictive capability of computational tools and validating their associated thermal, chemical and mechanical models with small scale experiments. Being that this work is in its infancy stage and efforts are ongoing, we are only reporting completed efforts to date at the time this manuscript is written.

Thermal Ignition of Energetic Materials

Under the thermal ignition category, we are concerned with hazards in which the insult to the energetic involves the transfer of thermal energy. Obvious situations are the classical slow and fast cook-off scenarios. More subtle, however, are situations that may arise from other threat scenarios. Impact and penetration of the energetic material by fragments is one example in which thermal ignition may play a role. The penetration process often includes a significant amount of plastic deformation to not only impacting fragment, but to the casing material as well. Given that the energetic does not ignite from any type of shock loading, the work imparted on the penetrating materials may generate sufficient localized heating to initiate the materials.[6]

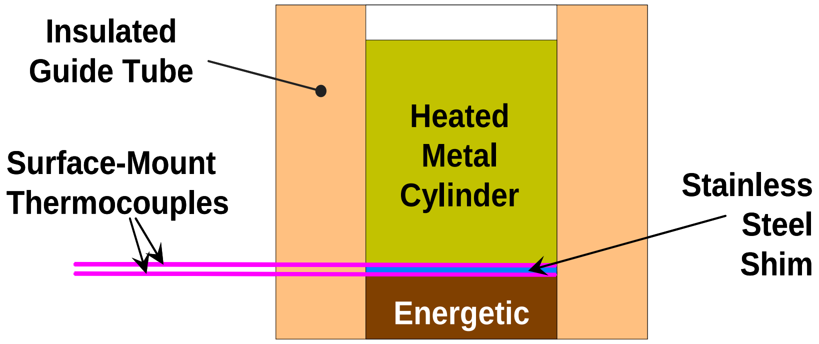

Fig. 1. Hot fragment configuration used to study thermal ignition.

To those familiar with reactive flows, thermally induced reactions are perhaps the easiest to conceptually understand. As thermal energy is imparted on a substance, the molecules comprising the substance are excited. When sufficient energy is realized, the material can decompose. Somewhere along the decomposition path, smaller molecules are formed which, when brought into contact, are exothermically reactive. Some of the energy released by the reaction feeds back up the path, sustaining the reaction.

As a starting point for thermal ignition scenarios, we adopt a configuration, shown in figure 1, similar to classical hot fragment conductive ignition experiments.[7] A 0.500 inch diameter, 1.000 inch long right circular cylinder simulates the fragment. The cylinder is heated to a given temperature, and then dropped from the oven. The cylinder comes to rest atop a thin (0.010 inch) thick shim underneath which is a thermocouple and a 0.375

inch thick energetic sample. While this test, similar to other incarnations, is concerned with establishing conditions describing go / no-go, the thermocouple provides an additional, temporal data trace with which to compare model results.

Even under the simplified configuration, a complex set of resultant behaviors may be realized from the given experiment. While highly complex models for energetic response have been develop,[8] we begin with a greatly simplified model description. Model modifications, introducing more complicated behavior, will be added only as required and as suggested by the temporal data obtained from the experiment. Clearly, a close interaction between bench scale experiments and descriptive models will be required to adequately describe material response.

The model used for the simulations presented below, therefore, is a simple one-dimensional heat transfer approximation. While reactive conversion from one “species” to another is included, mass transport is neglected. Convective losses from the top of the fragment and the bottom of the energetic are modeled using free convection correlations.[9] For the reaction processes of the energetic we adopt global kinetic schemes obtained from experiments such as ODTX.[10] These schemes are attractive due to their simplicity and low computational cost, especially as we proceed toward simulations of more complex weapons systems. Additionally, these mechanism have exhibited reasonable success in determining time to explosion in slow cook-off simulations,[11,12] and are therefore a logical starting point for other thermal ignition work.

To illustrate the type of data that will be obtained from the experiment and compared to the simplified model, we present the results from a series of preliminary simulations. These simulations utilized PBXN-109 as the energetic, composed of approximately 65 % RDX, 20 % aluminum and the balance an HTPB binder. Thermal material properties for the energetic were obtained from the literature.[12] The RDX kinetic model was the reduced mechanism of McGuire and Tarver.[13] The aluminum was considered as an inert. Although minor in overall contribution, the HTPB binder was allowed to decompose according to a first-order Arrhenius style mechanism.[14] The thermal properties of the gaseous products were maintained at those of the parent material. The fragment utilized was considered to be composed of type 316 stainless steel.

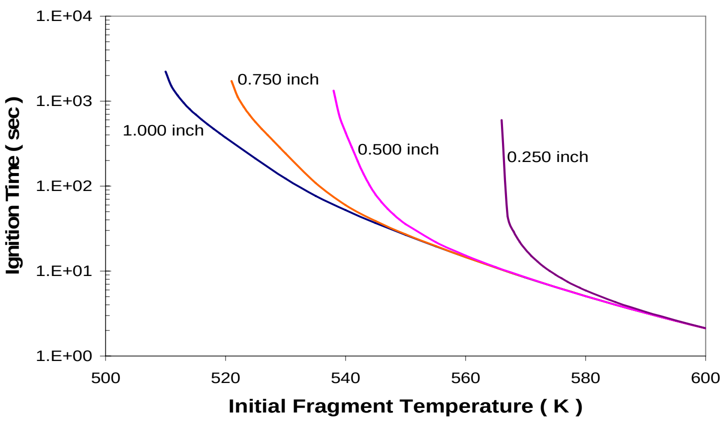

Fig. 2. Simulated ignition time of PBXN-109 as a function of initial fragment temperature at various fragment lengths.

Shown in figure 2 are time to event curves, defined as thermal runaway, plotted against the initial fragment temperature. The individual curves represent various fragment lengths. As is expected, lower initial fragment temperatures can still result in ignition for longer fragments, due to the greater amount of stored thermal energy. The results are observed to collapse to the same curve as the fragment temperature is increased. This type of response is a reflection of the transient conduction across the length of the fragment. While stainless steel is comparatively a good thermal conductor, there will still be a thermal gradient established across the length. As the initial temperature is increased, the depth of fragment material contributing to the ignition of the energetic sample decreases, i.e. ignition is achieved before the thermal wave can proceed across the length of the fragment. This result may be important when considering fragments which have experienced plastic work heating from case penetration. While the initial temperatures may be high, the thickness of heated material is typically very small. Conduction into the energetic material must therefore compete with conduction into the cooler, non-deformed center of the fragment.

Conditions describing go / no-go behavior are extracted from the simulations and shown in figure 3. The critical temperature (lower bound) is presented as a function of fragment length. Similar to the discussion above, longer fragments have lower critical temperatures due to net amount of stored energy in the fragment. Similar response curves can be generated for fragment materials of varying thermal conductivity.

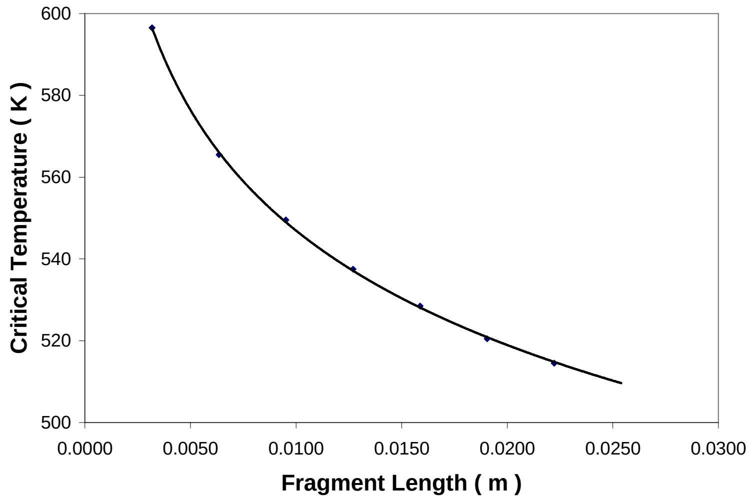

Fig. 3. Simulated go / no-go response curve for PBXN-109 and a 316 stainless steel fragment as a function of fragment length.

Deflagration / Pressurization rates of partially confined energetics

Of ultimate importance to the IM community is an adequate description for the level of violence exhibited by a munition exposed to a given threat scenario. The complexity of the problem is easily observed when one considers the necessity of including such phenomena as case fragmentation, fragment throw and blast. The first step in describing the violence, however, is an accurate portrayal of the rates of pressurization, i.e. mass generation, within at least partially confined volumes. Thus, it is necessary to go beyond establishing ignition conditions and consider sustained reactions within the energetic.

As an example of the processes involved, consider the impact and penetration of a munition, containing energetic materials, by a fragment. If the energetic material initiates in a less than detonative fashion, then there is mass generation from the decomposition of the explosive. Given that the hole produced by the penetrating fragment is not of sufficient size, then the gaseous products produced by the reaction will lead to pressurization of the volume. As the pressure increases, the reaction rates will most assuredly increase, resulting in even more pressure. Thus, there is a feedback mechanism that can lead to a catastrophic failure of confinement and high levels of violence.

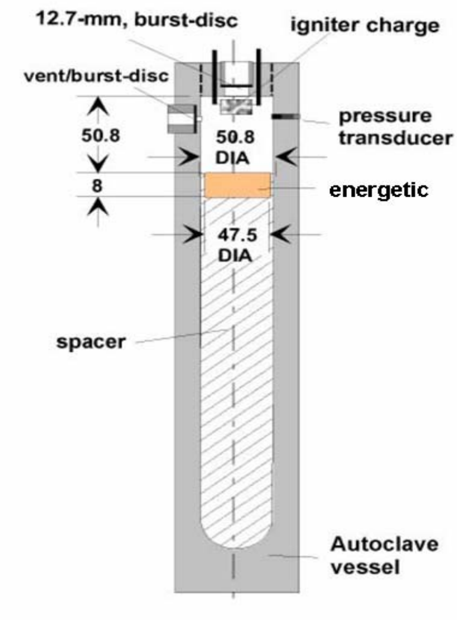

Fig. 4a. Vented chamber used for study of deflagration / pressurization rates of reacting energetic materials.

The prototypical experiment being utilized for this class of problems is a vented chamber in which energetic material is allowed to combust, shown in figure 4a.[15] A small pyrotechnic charge is initiated, rapidly pressurizing the volume with hot gases and igniting the top surface of the sample. Once initiated, the products of combustion lead to additional pressurization of the chamber and enhance the combustion process. At some, predefined pressure, a burst disk of known diameter opens, allowing for venting of the products. The venting may act to slow or perhaps quench the reaction. If not quenched, the reaction will continue, albeit at a slower rate, and eventually lead to a pressure sufficient to open a larger burst disk. The more rapid venting of the chamber ultimately quenches the reaction.

Data obtained during these tests include the pressure within the vessel as a function of time. Additionally, as the reaction is quenched when the large burst disk opens; the remaining energetic can be recovered and used to establish the total amount of reacted material.

The simulations being developed for this experiment treat the reacting energetic as a surface discontinuity between reactant and product. The surface regresses into the unburned reactant at a rate proportional to the pressure within the volume raised to some power. This technique is a typical procedure used for interior ballistic considerations which is similar to the situation being addressed here. Previous simulations have emphasized the need to include heat loss effects, from the hot gaseous products to the initially cold vessel wall, to adequately describe the pressurization rate. Figure 4b, shows the estimated pressure profile in the vent chamber for PBXN109 using the numerical cavity code. From the pressure time curve, two different gas volume, 200 cc and 150 cc were quenched at 60MPa but at different time.

In addition to contributing to ultimate level of violence descriptions, this work can play a significant role in the design of IM mitigation strategies. A known means of mitigating the response of a munition, and a current focus area for IM technology, is the introduction of vents to the munition design. The vents serve to reduce the pressurization rate to such a degree that violent failure of confinement is not reached. Incumbent on a successful strategy is establishing an adequate amount of venting, under the various threat scenarios, to slow the reaction while not hindering the ultimate performance of the munition. Modeling and simulation, when coupled with the bench-scale experiments, can be used to optimize vent design and reduce the number of full-scale experiments.

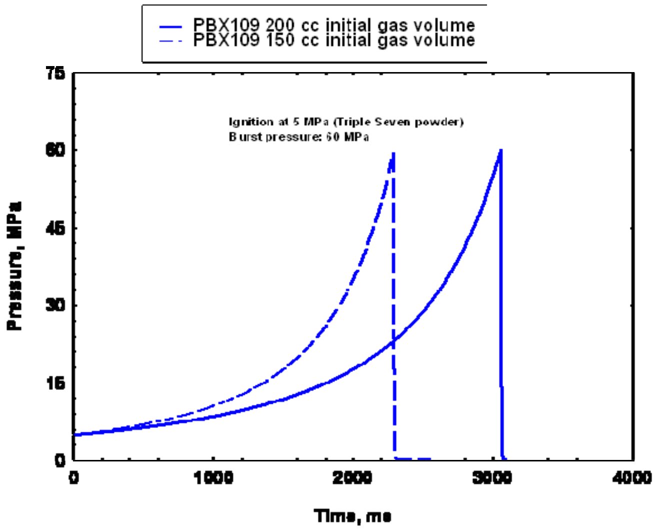

Fig. 4b Estimated pressure profile in vented chamber using the Cavity Code. PBXN109 200cc and 150 cc initial gas volume.

Explosive Shock-Initiation Models under Complex Shock Loading

Simulations of projectile impact, sympathetic detonation, and other hazard scenarios predict shock loading on energetic components which is significantly different from that produced in experiments used to calibrate shock initiation models. Figure 5 displays the simulated pressure time-history from a wedge-test which is designed to create this

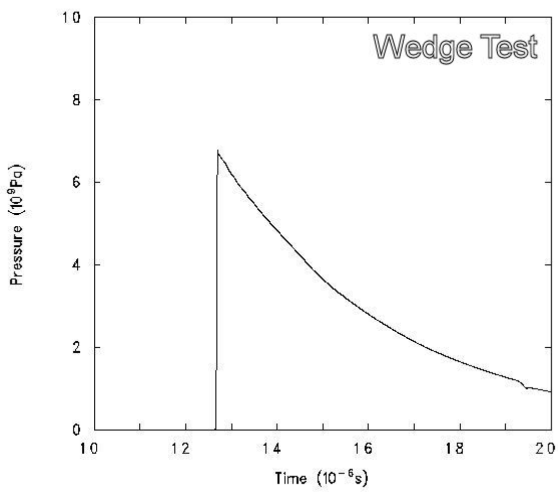

Fig. 5. Pressure time-history produced by typical wedge test.

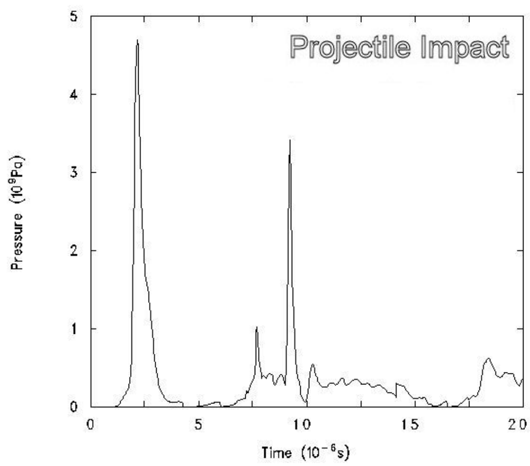

Fig. 6. Pressure time-history produced by cylindrical fragment impact on covered explosive.

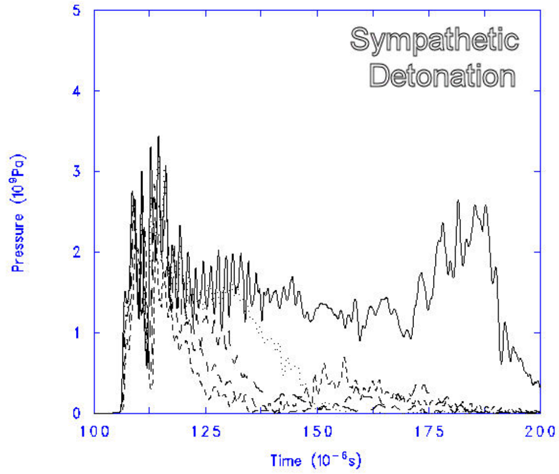

Fig. 7. Pressure time-history produced in acceptor charge by detonation of donor charge across an aluminum buffer.

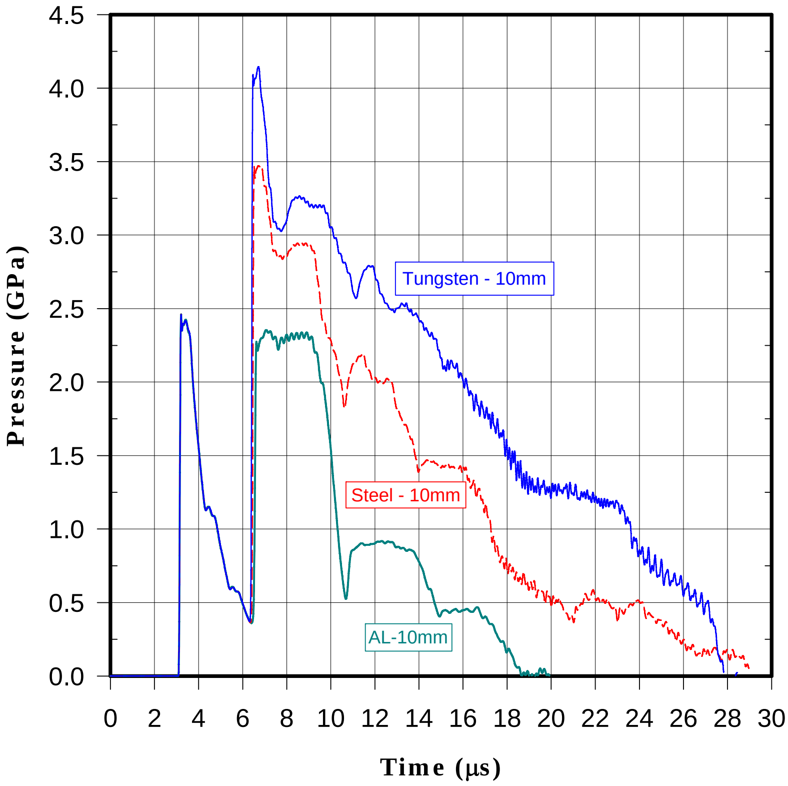

Fig. 8 Pressure–time history in inert explosive from impact of multi-layered flyer plate.

simple form. In contrast, note the more complex pressure-history (multiple strong peaks) in figure 6 from simulated impact of a simple flat-ended cylindrical projectile on a covered charge. Simulation of real - world situations involving sympathetic detonation produce a considerably more complex pressure-time history as shown in figure 7. Reactive models calibrated using Pop-plot data obtained from wedge tests cannot be expected to perform well in these more complex scenarios.

Significant improvement might follow from calibrating shock initiation models with a controlled experiment that produces a wave-form more complex than the wedge-test but less complex than those created by actual hazards. Existing experimental data for response of explosives to controlled complex shocks include that of Campbell and Travis[16] who reported on shock desensitization, and Salisbury, et al.[17] who reported experiments with stepped waves. Although both provided important insight, neither experiment generates the type of wave envisioned here.

We have undertaken an effort to characterize the response of explosive charges to controlled complex shock waves and are employing CTH[2] and ALE3D[3] simulations to develop experimental systems for producing waves with multiple peaks. Possibly an ideal experiment would generate two shock peaks of variable amplitude, duration, and separation. Special consideration is being given to controlling the amplitude of and the interval between the peaks. Both gun-launched flyer-plate arrangements and explosively driven systems have been investigated, including complex (layered) flyers impacting simple targets and simple flyers impacting complex targets. Although wave forms in complex layered targets are difficult to interpret, layered flyers impacting simple targets show promise. Figure 8 illustrates typical results from three gun-launched systems, each with a leading aluminum flyer and following flyers of different materials. The amplitudes of each peak as well as the durations and interval between peaks can be controlled.

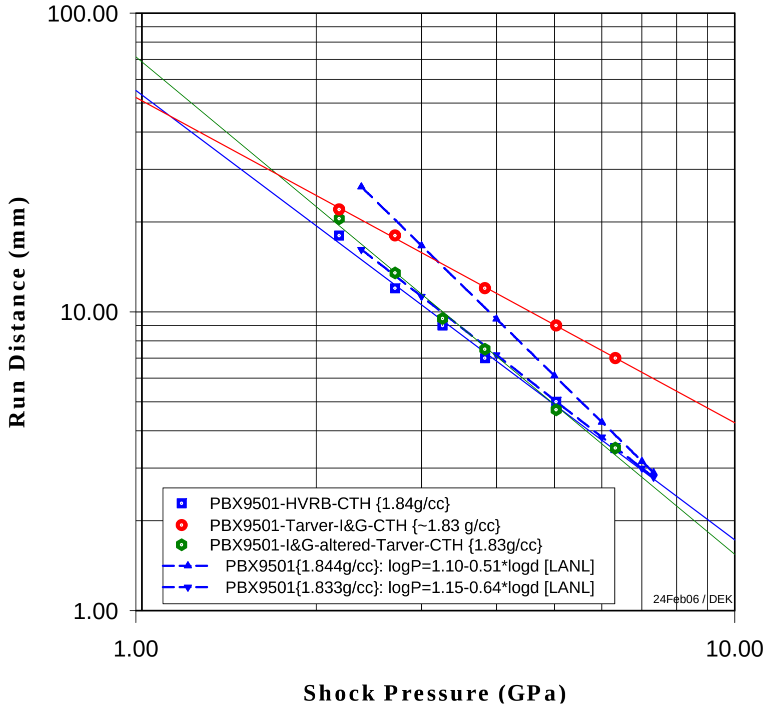

Fig. 9. Run distance to detonation versus impact shock pressure for PBX9501. LANL data => blue dashed lines. CTH with HVRB => blue squares. CTH with Ignition & Growth with original Tarver input => red symbols. Altered Ignition & Growth (pressure index of growth terms changed from 2 to 2.8) => green symbols.

In conjunction with tailoring the impact wave form, we are also exploring the performance of available shock-initiation models including HVRB (History-Variable Reactive Burn) in CTH[2] and Ignition & Growth[18] in ALE3D[3] and CTH[2]. It is not clear that these models will accurately capture the explosive response to a complex wave form. However, at a minimum, they should reproduce the PoP-Plot data (run-distance-to-detonation versus impact pressure). A CTH[2] simulation based on HVRB for the explosive PBX9501 (95% HMX) {using CTH[2] Library parameter values} leads to a fairly close representation {blue symbols in figure 9} of the LANL data {1.833 g/cc}.

Repeating this simulation, with the Ignition & Growth reactive model {based on Tarver's input data set for 9501}, leads to the curve defined by red symbols. The slope of the predicted curve is too shallow, which may suggest that matching embedded gauge data at one or two input conditions does not ensure a match to the PoP-Plot. One remedy is to alter the assumed pressure index of the two growth terms from 2 to 2.8, and then re-adjust the magnitudes of the multiplicative constants. This adjustment leads to the curve defined by the green symbols, which is a good approximation to the LANL data. Finally, the Statistical Hot Spot (SHS) Model found in ALE3D[3] is of particular interest since it has been shown to simulate experiments in which lower-amplitude shock waves desensitize explosives to subsequent higher-amplitude waves. It appears to account for growth and extinction of hot spots which is most likely important in the complex shock environment. Although our effort is continuing, the results to date suggest the SHS model is difficult to employ.

Summary and Conclusion

The preliminary results presented here highlight the focus areas here for this current IM modeling effort. We are interested in developing modeling capabilities to predict munition response to hazard scenarios involving slow cook-off, fragment impact and sympathetic detonation. To achieve these goals, it is first necessary to examine and understand the underlying physical phenomena, which are thermal ignition, burning and shock initiation.

In the area of non-detonative material response, the current state-of-the-art models are able to predict the time to ignition of energetic materials, such as PBXN109 shown earlier. However, the transition of energetic material from ignition response to burning and tracking the level of reaction violence due to slow cook-off hazards are not yet predictable.

The preliminary results also highlight the need for more sophisticated shock initiation models. The current state-of-the-art shock initiation models parameterized from wedge test experiments capture simple planar shock waves. Real world situations, involving munitions subjected to fragment impact and sympathetic detonation hazards, produce complex shocks of multiple waves and varying strengths. Numerical experiments have been developed to demonstrate the type of complex shock behavior that is more typical of real world shock hazards. The Statistical Hot Spot (SHS) Model found in ALE3D[3] is one such model showing promise in this area but the results are yet to be determined.

In order to meet IM designs and criteria it is important to first understand the reactive response of energetic materials. This work is, therefore a step in that direction by developing predictive modeling capabilities.

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