Predicting Large-scale Effects During Cookoff of PBXs and Melt-castable Explosives

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1 Abstract

We have made reasonable predictions of the cookoff response of large-scale systems containing plastic bonded explosives (PBXs) and a melt-castable explosive using kinetics determined from small-scale experiments. The key to scaling is to include relevant physics for the systems of interest. In the current work, we discuss cookoff of PBX 9502, PBX 9501, LX-14, and Comp-B. PBX 9502 is composed of 95 wt% triaminotrinitrobenzene (TATB) and 5 wt% chlorotrifluoroethylene/vinylidine fluoride (Kel-F). PBX 9501 is composed of 95 wt% octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) and 2.5 wt% Estane® 5703 (a polyurethane thermoplastic), and 2.5 wt% of a nitroplasticizer (NP): BDNPAF, a 50/50 wt% eutectic mixture of bis(2,2-diniropropyl)-acetal (BDNPA) and bis(2,2-dinitropropyl)-formal (BDNPF). LX-14 is composed of 95.5 wt% HMX and 4.5 wt% Estane® 5702-F1. Comp-B is nominally composed of 63 wt% hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), 36 wt% 2-methyl-1,3,5-trinitrobenzene (TNT), and 1 wt% wax. Figure 1 shows various stages of damage for each of these explosives in Sandia's Instrumented Thermal Ignition (SITI) half-shell configuration [1].



Figure 1. Images of PBX 9502, PBX 9501, LX-14, and Comp-B showing various stages of damage.

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2 Observations Guide Simplified Physics

Our decomposition model for each of these explosives has been simplified by using pressure dependent reaction rates, which are a simple way to account for significant gas phase reactions, without knowing the specific details of the reaction mechanism. The pressure dependency was determined by performing small scale experiments that were either vented or sealed. Some of these experiments were performed using molding powders, such as shown in Fig. 1.C for LX-14, to prevent the decomposition gases from being trapped within the explosive. Other experiments were performed with fully pressed explosives. We also performed several experiments with different free gas volume sometimes referred to as ullage. Furthermore, we used a borescope in some experiments to visually observe the explosive as it decomposed *in situ*.

Understanding the role of the binder in our PBX formulations, such as propensity for damage and reactivity, was necessary to predict cookoff response in large-scale systems. Factors to consider include retention of gas within the explosive, damage of the explosive, gas release into the ullage, and gas leakage from the confining vessel. Knowing the working pressure of the large-scale systems was needed to accurately predict ignition times for these pressure sensitive explosives. The pressure was assumed to be ambient when the confining vessel ruptured or leaked. In the current work, our thermal-chemical models did not consider mechanical failure of the explosive or confining vessel. In general, our predictions bound the experimental response by assuming the explosive was either intact (e.g. fully pressed) or fully damaged (e.g. powders).

Damage in the melt-castable explosive, Comp-B, was different than in the plastic-bonded explosives. In Comp-B, the TNT component melts, leaving a suspension of RDX particles that partially dissolves in the hot liquid TNT. At low pressures, decomposition gases accumulate in bubbles and enhance mixing and heat transfer. At higher pressures, bubble formation is suppressed as observed in our borescope images. We found that our predications of sealed small scale experiments matched the data better when we assumed that flow was inhibited by the suspension and lack of significant bubbles. However, in vented systems, flow was observed, primarily induced by bubble formation.

The remainder of this abstract describes predictions and data comparisons for PBX 9502 [2], PBX 9501 [3], and Comp-B [4]. Details regarding the various models and parameters can be found in the references.

3 PBX 9502

We found that the decomposition gases in PBX 9502 were initially retained within the explosive. As the internal pressure increased, material would crack and spall on the surface and release some of the trapped decomposition gases as shown in Fig. 1.A. This release was accompanied by an audible popping sound. Prior to the gas release, internally measured temperatures would increase, and then decrease as the material spalled and the internal pressure was released. Eventually, these explosives thermally ignited.

Our simple PBX 9502 model [2] only solves the conductive energy equation with a source term for the reaction energy using the simple four step mechanism shown in Fig. 2.A. The model does not solve for mechanical damage, which is needed to predict the initial temperature excursion measured in our SITI experiment which confines a 2.54-cm diameter by 2.54-cm tall cylinder of PBX 9502 as shown in Fig. 2.B. for one our large ullage configurations. However, the uncertainty in our model predictions using Latin Hypercube Sampling (LHS) was sufficient to bound the temperature response in the experiment as shown in Fig. 2.C. The predicted internal pressures of the gases trapped within the interior of the explosive are higher in Fig. 2.C. than the measured pressure on the exterior of the explosive. This model was applied by Aviles-Ramos et al. [2, 5] to successfully simulate the thermal response of systems containing 2 to 1312 g of PBX 9502, which is a two order of magnitude increase in sample size.

Predicting Large-scale Effects during Cookoff



Figure 2. PBX 9502 A) simplified mechanism, B) SITI configuration, and C) run #277 results [2].

4 PBX 9501

Initially, we thought that the same framework used for cookoff of PBX 9502 could be used for PBX 9501 since our sealed and vented SITI experiments showed similar trends. However, we observed a reactant limited exothermic reaction, which we attributed to decomposition of the nitroplasticizer in our vented low density SITI experiments. We assumed that the 2.5 wt% nitroplasticizer (NP) in PBX 9501 reacted exothermically causing a temperature excursion in our thermocouple measurements. In our vented experiments, this temperature excursion did not continue into ignition since the amount of NP was small. However, in our sealed low density experiments, the rate of energy release associated with the NP reaction was faster and resulted in cookoff. The faster rates were assumed to be caused by a significant gas phase reaction, which was modeled as a pressure dependent reaction.

In some of our high density SITI runs such as shown in Fig. 1.B, we observed migration of the NP to the outer edge of our experiments, wherein the energy release associated with the NP was quickly dissipated via the conductive aluminum confinement. For these cases, the thermal excursion was not clear. We suspect that the low porosity associated with significantly different expansion properties for our binder and explosive caused migration of the binder in our high-density experiments.

Figure 3.A and 3.B shows our simple mechanism for PBX 9501 as well as measured and predicted temperatures for our low density SITI run #414. Using this mechanism, we successfully simulated various systems from five other laboratories covering three orders of magnitude in PBX 9501 mass (e.g. 2 g to 2.5 Kg). Figure 3.C shows a comparison of three of these experiments performed at other laboratories. Success is partially attributed to ensuring the pressure dependent reactions are modified when the working pressure of the vessel is exceeded. This is done by changing the pressure exponent to zero when the vessel working pressure is exceeded and the gases vent. Also, for systems wherein the explosive mass is small and the density high such as the One-Dimensional Time-to-explosive (ODTX) experiments [6], the NP reaction is suppressed to account for the migration of the nitroplasticizer to the explosive edge with the NP reaction enthalpy dissipated through the aluminum confinement. The ODTX simulations were also limited to the working pressure of the experiment (152 MPa).



Figure 3. PBX 9501 A) mechanism and B) composition. Experiment and model comparison of C) SITI temperatures [3], D) ODTX ignition times [6], E) NAWC pipe temperatures [7], and F) LANL LASC temperatures [8].

5 LX-14

The composition of LX-14 (95.5 wt% HMX and 4.5 wt% Estane[®]) is similar to PBX 9501 (95 wt% HMX, 2.5 wt% Estane, and 2.5 wt% NP). The binder in LX-14 does not contain an energetic plasticizer. We thought that the LX-14 would be less sensitive than PBX 9501 since LX-14 essentially replaces the NP with Estane[®]. Our preliminary experiments indicate that LX-14 is in fact, more sensitive than PBX 9501 as shown in Fig. 4, which depicts SITI center plane temperature data for both LX-14 and PBX 9501. These experiments were performed with low density LX-14 molding prills as depicted in Fig. 1.C and low density PBX 9501 molding prills. We believe the Estane in LX-14 retains the gases within the prills and the pressure dependent reactions are accelerated. In contrast, the gases are not contained as well in PBX 9501 and are relatively slower. More research is needed to determine the pressure effects in LX-14.



Figure 4. Measured center plane temperatures in A) sealed and B) vented SITI configuration with LX-14 and PBX 9501.



Figure 5. Box experiment A) schematic, predicted temperature contours near ignition with B) flow and C) without flow, and D) comparison between predicted and measured temperatures. In B and C, red and blue represent hot and cold, respectively. The thermocouple locations in D are in the center of the heater and 2.5 cm above the heater.

5 Comp-B

Clearly the explosive binder interaction in LX-14 and PBX 9501 are more complex than our initial thoughts. Melt-castable explosives such as Comp-B are even more complex. Previously, we have simulated Cookoff of Comp-B by solving the energy equation with a source term for reactions coupled to the momentum equation with a Boussinesq approximation. This model with flow captured ignition time adequately for our SITI experiments, but did not scale to larger experiments such as shown in Fig. 5. For the simulations with flow, we incorporated the viscosity model of Zerkle et al. [9]. This model did not capture the details of the experiment as well as the same model without flow. We believe that the RDX suspension hinders the natural convective flow, which might be modeled more effectively with a viscosity that has a yield stress. More work is needed to properly scale cookoff predictions of melt-castable explosives.

We have shown in the current work that it is possible to take small-scale experiments, create models, and apply the models to larger systems of practical interest. The key to scaling is recognizing and accounting for relevant physics that may not be significant in the small-scale experiments. For example, we found that pressurization increases our reaction rates and needs to be considered. Also, accounting for reactive binder components such as the NP in PBX 9501 was necessary to predict some systems. Also, accounting for flow when needed for melt castable explosives. We believe more work is required to properly scale cookoff predictions of melt castable explosives.

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