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A Computational Study of Detonation of Propagation in PBX-9404 Using CTH and LASmerf Codes

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Abstract

For many years, the researchers at the Army Research Laboratory (ARL) have been using CTH hydrocode and its History Variable Reactive Burn (HVRB) model to study the reactive behavior of various granular and non-granular explosives. Recently, we acquired another code (LASmerf) to study the response of the munitions. A computational study was undertaken to compare the results from these two codes. A comparison of the computational results will be presented in this paper. Also, a brief description, advantages, and disadvantages of each code will be discussed.

1. Introduction

Several models have been developed to predict reaction/detonation propagation as well as detonation failures in explosives. These models have evolved over the years and have been used in conjunction with numerical simulations to study the reactive behavior of various energetic materials. Recently, the LASmerf code was acquired to study the response of the various munitions when shocked or impacted by the incoming missiles, shells or projectiles.

Two-dimensional simulations, using the CTH and the LASmerf codes, were performed and the results were compared. In the simulations, Composition B explosive was used as a donor round and PBX-9404 was used as an acceptor round. The donor and acceptor rounds were separated by the inert materials (barrier). The barrier consisted of air, Plexiglas, steel, Plexiglas and air.

In the CTH simulations, the Program Burn (PB) model was used to detonate the donor and the HVRB model was used to monitor the initiation and growth of the reaction in the acceptor round. The HVRB model is not available in the LASmerf code and the Forest Fire Burn (FFB) model was used to detonate the donor. The FFB was also used to monitor the reaction and/or detonation in the acceptor round in the LASmerf simulations.

The reaction and propagation of detonation in the acceptor was determined by monitoring reaction variable contours (in CTH code) and mass fraction contours (in LASmerf code). The simulation results from these codes were compared by determining the critical barrier thickness and time of detonation. Both of these codes predicted about the same barrier thickness to prevent sympathetic detonation between the donor and the acceptor rounds.

2. CTH Code and History Variable Reactive Burn Model

The CTH code was developed by Sandia National Laboratories. It provides capabilities for modeling dynamics of multidimensional systems with multiple materials, large deformations, and strong shock waves. Three reactive and two porosity models are also incorporated into the code. Two of the reaction models are: (1) the PB model for detonation and (2) the HRVB model for shock initiation. The PB model forces detonation at the characteristic propagation velocity through a specified portion of the computational mesh. The HVRB model is designed to model the shock-to-detonation of the high explosive.

3. CTH Simulations and Results

Simulations to determine the sympathetic detonation between the acceptor and donor rounds using the CTH code and the HVRB model were performed. Initial simulations were performed using Composition B as a donor and an acceptor. Later, the simulations were done using Composition B as a donor and PBX-9404 as an acceptor. The barrier package was a layered material consisting of air gap, Plexiglas, steel, Plexiglas and air

gap, between the donor and acceptor rounds. A typical computational configuration is shown in Figure 1.

Using the PB model, the explosive in the donor round was detonated at the center of the round. The HVRB Model was used to observe the reaction in the acceptor round. In one simulation, a 16 mm thick steel; a 20 mm Plexiglas thick (total thickness) and 14 mm of total air gap separated the donor and acceptor rounds. Material and reaction variable color band plots and pressure contour plots were made. The plots helped to determine the damage, pressure, and reaction/detonation of the explosive in the acceptor round. Pressure and damage plots will not be given in this paper. Only reaction variable plots are shown here.

Figure 2 shows a sequence of four reaction variable color band plots, spanning the period from 42.0 to 66.0 μs after the donor was detonated. The figure shows bands of the various colors, ranging from blue to red. The upper red color band in the legend, at the right, pertains to detonation and lower blue color band pertains to a minor or no reaction. A minor reaction, in the acceptor, was observed at 42.0 μs. The reaction increased and initiated the detonation in the acceptor, between 64.0 and 66.0 μs.

The response of the acceptor round was also measured by monitoring the pressures, at various locations, inside the acceptor round. A pressure of more than 300 kb was observed in the acceptor, that is equal to or more than the detonating pressure of PBX-9404, confirming that the acceptor did detonate.

Additional simulations were performed by varying the barrier thickness. The thickness of Plexiglas was increased from 20.0 mm to 24.0 mm and the air gap was decreased from 14 mm to 10 mm, but the total thickness of the barrier was kept the same. The simulation was performed and reaction variable color band and pressure contour plots were made. A very low shock pressure was observed in the acceptor round. That shock pressure was not strong enough to detonate the explosive in the acceptor. So, increasing the thickness of Plexiglas and decreasing the air gap, without changing the overall thickness of the barrier, attenuated the shock, and thus prevented the acceptor from detonating.

4. LASmerf Code and Forrest Fire Burn Model

The LASmerf Code is a general purpose two-dimensional/three-dimensional hydrocode. The code uses reactive flow models for explosive response to input shock. The code has the capability to simulate the fragment impact/penetration phenomenon in explosives and other materials. It has the capability to compare the effectiveness of different warhead configurations by comparing the respective threshold values. It, further, can

assist in getting information as well as providing valuable insight for designing the warheads. It has the capability for modeling sympathetic detonation and Shock to Detonation Transition (SDT). The FFB model[3] to predict the response of explosives to loading by sustained shock waves is incorporated in this code.

5. LASmerf Code, Simulations, and Results

Just as in the CTH simulations, only one donor and one acceptor were used in the simulations. The same type of barrier material was used. In the first simulation, 16 mm thick steel; 20 mm of Plexiglas and 14 mm of air gap separated the donor and acceptor rounds (see Figure 1). The total thickness of the barriers was the same as was in CTH simulations. Same computational configuration, as shown in Figure 1, was used to run the simulations. Composition B was used as a donor and PBX-9404 was used as the acceptor. Mass fraction and pressure contours plots were made to monitor the reaction and pressure in the acceptor round. The donor round was detonated by using the FFB model. That produced a very high shock pressure in the donor that was transmitted to the acceptor round. That high shock pressure initiated the reaction in the explosive in the acceptor round.

Figure 3 shows a sequence of four mass fraction contours plots, spanning from 46.0 and 60.0 μs after the donor was detonated. Figure 3 shows bands of the various colors, ranging from green to red. The upper red color band in the legend, at the right, pertains to detonation and the lower green color band pertains to a minor reaction. No reaction in the acceptor was observed at 46.0 μs and only a minor reaction was observed at 50.0 μs. The reaction increased and the explosive in the acceptor detonated at about 56.0 μs.

At 60.0 μs, the rest of the explosive in the acceptor round detonated. Additional simulations were performed by varying the barrier thickness. The thickness of Plexiglas was increased from 20.0-mm to 24.0-mm and the air gap was decreased from 14-mm to 10-mm, but the total thickness of the barrier package was kept the same. The mass fraction and pressure contours plots were made. Only a green colored band was observed in the acceptor round, signifying that the acceptor experienced a minor reaction, but did not detonate.

6. Summary and Conclusions

The simulations were performed to monitor the reaction and determine the sympathetic detonation response of the acceptor round (PBX-9404). The simulations showed that for a barrier package consisting of a 16 mm thick steel, a 20 mm thick Plexiglas and a 14 mm air gap, the acceptor round detonated.

The simulations were repeated by varying the barrier thickness. When the thickness of Plexiglas was increased to 24 mm and the air gap was decreased to 10 mm, the acceptor did not detonate. The shock produced by detonating the donor round was mitigated significantly by this barrier package and a lower shock pressure was transmitted to the acceptor.

That low shock pressure could not detonate the acceptor round. In the LASmerf simulations, the acceptor detonated at 56.0 μs, but in the CTH simulations, the acceptor detonated at about 65.0 μs. This discrepancy could be attributed to the different burn models used in the codes. In the CTH simulations, the PB and the HVRB models were used. But, in the LASmerf simulations, a FFB model was used.

Using sixteen to thirty-two processors, the CTH simulations were performed on High Performance Computing Modernization Program platform (JVN). The LASmerf simulations were performed on a PC. CTH is a parallel code that is widely used in the Army Research Laboratory and in other Department of Energy/Department of Defense laboratories, whereas the LASmerf is not widely used (relative to CTH). The post-processing in the CTH code is more user friendly than in the LASmerf code. The LASmerf is a serial code. Running the LASmerf code on the PC restricts the use of the system for other applications.
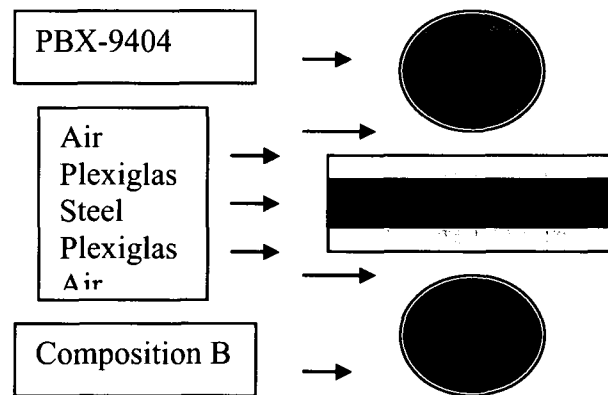
The main objective of conducting the computational study was to compare the results from LASmerf and CTH simulations. The simulation results from these two codes were comparable. Many simulations were performed and the results from some of the simulations are summarized in Table 1.

Table 1. Computational results of CTH and LASmerf hydrocodes

Hydrocode	Air (mm)	Plexiglas (mm)	Steel (mm)	Plexiglas (mm)	Air (mm)	Time of Detonation, μs	Detonation Yes/No
CTH	5.00	12.00	16.00	12.00	5.00		No
CTH	7.00	10.00	16.00	10.00	7.00	64–66	Yes
LASmerf	5.00	12.00	16.00	12.00	5.00		No
LASmerf	7.00	10.00	16.00	10.00	7.00	56–59	Yes

References

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3. Lundstrom, E.A., "Evaluation of Forest Fire Burn Model of Reaction Kinetics of Heterogeneous Explosives." *NWC TP-6898*, Naval Weapons Center, China Lake, CA, 1988.

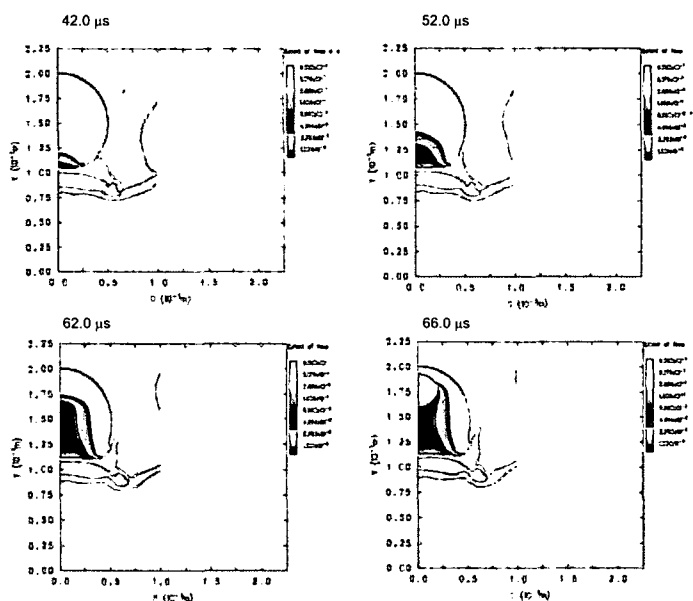Figure 1. A typical configuration showing PBX-9404 (acceptor), inert material and Composition B (donor)

Figure 2. Reaction variable color band plots in the acceptor round, no reaction (blue) to detonation (red)
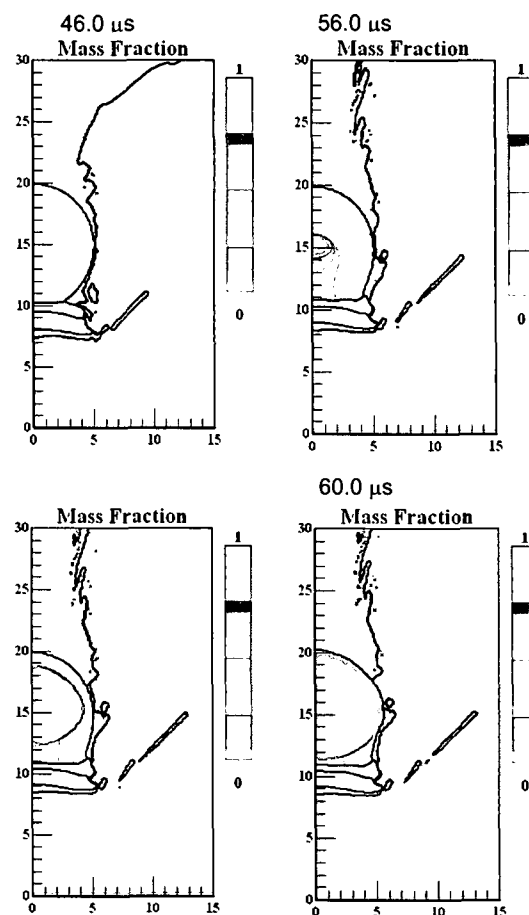
Figure 3. Reaction contours for the acceptor round (detonated). Distance along the axes is in cm. Mass Fraction Legend; minor reaction (green) to detonation (red).