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TITLE HIGH EXPLOSIVES REACTION MODEL AND ITS APPLICATION TO BOOSTER PERFORMANCE

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HIGH EXPLOSIVES REACTION MODEL AND ITS APPLICATION TO BOOSTER PERFORMANCE

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SUMMARY

Initiation of insensitive high explosives requires a boosting system using more sensitive and usually more energetic explosives. However, problems arise if the booster material is too energetic. The initiability of some insensitive but less energetic high explosives can be enhanced by lowering the density and decreasing the grain size or by adding a sensitive component; thus these explosives can be used as booster materials. This paper presents a unified initiation and detonation reaction model and then the simulation of the development of the detonation wave in a PBX-9502 main charge using three booster explosives: low-density superfine TATB, low-density ultrafine TATB, and X-0407. The last two are found to be acceptable for booster application.

I. INTRODUCTION

In many high explosive (HE) systems, a small detonator is needed to initiate the main charge if conventional explosive is used. With TATB based HEs such as PBX 9502 (95% TATB, 5% Kel-F 800) that are generally, but not necessarily, less sensitive; that same small detonator cannot support a strong shock with sufficient duration to initiate the main charge because of the longer run distance required for the shock to detonation transition. The diverging wave configuration weakens the shock strength further and makes the situation even worse; the detonation wave may eventually vanish. With a staging approach, for example, using a booster, we can initiate insensitive high explosive (IHE) main charge without difficulty. Of course, the explosive in the booster should be more sensitive and usually more energetic than the IHE main charge. The booster is typically hemispherical and should be large enough to support a detonation with sufficient intensity and long enough duration to be the wave propagating into the main charge. For safety, on the other hand, we do not want to use too large a booster; that would defeat the purpose of using IHE as the main charge. Therefore, determination of booster performance is crucial.

In some applications, the energetic aspect of conventional booster HE (HMX based, for example) is undesirable since it tends to overdrive the systems. Booster explosives with softer push are preferable. We find that low density (1.8 g/cm^3) TATB has higher shock sensitivity than regular density TATB (1.9 g/cm^3), and ultrafine grain (arithmetic mean diam, 10 μm) is much more sensitive than superfine (arithmetic mean diam, 30 μm). Because low density TATB is less energetic than PBX 9502, it does not overdrive

the system. The use of low-density TATB for booster HE seems quite attractive if the sensitivity is adequate. Another way of enhancing initiability is to add some sensitive HE to the basically insensitive main component. X-0407 (70% TATB, 25% PETN, 5% Kel-F 800) belongs to this class of HE. The energetic aspect of X-0407 is quite compatible with PBX-9502 with no significant overdriven evidence.

The selection of booster explosive and size relies usually on experiment. A class of experiments, commonly known as onionskin, has been conducted to examine the divergence of the detonation pattern as the wave emerginfrom a hemispherical surface recorded by a streak camera. With better modeling of HE behavior, it is now possible to perform numerical simulations and to predict performance.

Hydrodynamic calculation is becoming routine in guiding designs of HE systems. We are concerned not only with detonation, but also with initiation. A unified model that can handle both phases without user intervention is not only of academic interest, but also of practical importance. A model containing both initiation and detonation features considers the special characteristics of physics and chemistry in determining reaction rates for initiation as well as detonation. Such a model is definitely useful because of its smooth transition from one phase to another.

Initiation and detonation of HE involve many complex mechanical, thermal, and chemical processes, some of which defy description. However, in hydrodynamic simulation, characteristic time can be used to estimate the significance of the process, regardless of the origin. In the simplest theoretical treatment, characteristic times are considered extremely short in comparison with the wave transit time and are therefore ignored completely in calculation. The consequence is a reaction model called programmed burn (Chapman Jouguet burn), in which a constant detonation velocity is prescribed.

Initiation of HE, a nonsteady process, requires time and traveling distance for the initially weak shock that is usually below Chapman Jouguet (CJ) pressure to develop into a detonation. Obviously, the time required for such a transition is caused by some finite characteristic times in the initiation process. Even after the explosive is initiated, the question remains of what should be used to describe the detonation behavior, generally believed to be exceedingly fast. Recent studies indicate the need to include a relatively slow process near the end of the reaction, probably caused by slow, exothermic carbon clustering. As a result of these studies, even the detonation cannot be regarded as very fast. The objective of this paper is to summarize a unified model that characterizes the reaction processes in initiation and detonation of heterogeneous high explosives. Then, we apply the model to the evaluation of booster performance. The first modeling effort reported is given in Ref. 1.

II. REACTION MODEL

We only present a summary of an HE reaction model here. The detail has been documented extensively,[2-6] and the model has been used in some applications.[7-8] More on the model will be presented in the forthcoming detonation symposium.[9] Most heterogeneous HEs consist of a main constituent, usually in granular form, plus some binding material, and perhaps secondary explosive. Although adiabatic compression can increase the internal energy and therefore raise the temperature in general, dissipation associated with the irreversible processes is even more effective under the dynamic effect of a passing shock in some highly local regions near the surface of the grains. The internal energy, and subsequently the temperature, becomes higher than that of the surroundings. The locally hot condition initiates decomposition much sooner and thus is called a "hot spot." A quantity known as the hot-spot mass fraction, representing the fraction of the HE susceptible to the shock action, is related to the exposed specific grain surface area and depends on the degree of compaction and therefore density. It is treated as an empirical constant parameter that is typically small. The region exclusive of the hot spots is called the balance of explosive. After the reaction in the hot-spot region has reached a certain intensity, it will propagate into the balance of explosive through some form of energy transfer. The major part of the reaction is controlled by this mechanism. We recognize that although the chemical process in the balance of explosive is mainly decompositional, some recombinations occur, particularly near the end of the reaction. A most prominent one is solid carbon congulation; the process is exothermic and slow. The process time can be quite long and therefore cannot be ignored. Rather than accepting the decomposition products as final, we assume them to be transitional (or partially reacted) and of two different kinds: one goes to the final product form rather quickly, but the second takes considerably longer to reach the final state. Eventually, we obtain three rate equations that govern the hot spot, propagation, and slow reaction for the initiation and detonation of heterogeneous HE; each of the equations is characterized by a process time for that particular stage.

The total reaction (or product) fraction Λ consists of three parts:

$$\Lambda = \eta\Lambda_h + \psi\Lambda_s + (1 - \eta - \psi)\Lambda_f; \tag{1}$$

Λ_h is the reaction fraction in the hot spot region; Λ_f and Λ_s represent the fast and slow reaction fractions in the balance of explosive region. η is the hot spot mass fraction and ψ the mass fraction contributing to the slow reaction. Both η and ψ are constants; η depends on the grain size and density whereas ψ is related to the amount of carbon in the HE. The hot spot reaction fraction is determined by the hot spot process

$$\frac{d\lambda_h}{dt} = \frac{1}{\tau_h}(1 - \lambda_h), \tag{2}$$

with τ_h being the hot-spot process time. The fast reaction λ_f is controlled by the energy transfer between the hot-spot product and the reactant, and the rate is

$$\frac{d\lambda_f}{dt} = \frac{\eta}{\tau_e}(1 - \lambda_f)\frac{(\lambda_h - f_o/\eta)}{(1 - f_o/\eta)}, \tag{3}$$

where τ_e is the energy transfer characteristic time. f_o represents the threshold value which the hot-spot product fraction λ_h must exceed in order to support the reaction propagation. Finally the rate of the slow reaction fraction λ_s is given by

$$\frac{d\lambda_s}{dt} = \frac{\eta}{\tau_s}(\lambda_f - \lambda_s). \tag{4}$$

where τ_s is the slow process time. The hot-spot process time τ_h is related to the shock state and the chemical kinetics properties of the region, whereas the energy transfer time τ_e in the propagation phase depends on the local hydrodynamic condition through the current pressure. Because the slow process time τ_s is believed to be insensitive to the actual thermodynamic state, it is taken as a constant. The correlations of τ_h and τ_e and additional detail can be found in Ref. 2.

To illustrate the ability of the model to reproduce the initiation behavior, we choose to Pop plot as an example. The experimental Pop plot behaviors of low-density superfine TATB, low-density ultrafine TATB and X 0407 are given in Fig. 1 (curves), along with the calculated results using modeling (markers). At high shock pressure level, because of the larger hot spot mass fraction caused by the greater grain surface area, ultrafine TATB is more sensitive than superfine; however, the cooler hot-spot temperature associated with the smaller grain of ultrafine TATB leads to lower sensitivity when the shock is weak. The sensitivity of X 0407 is boosted by the presence of PETN. In general it falls between those low density TATBs except in the low shock pressure range, but X 0407 is more energetic because of its higher density (1.87 g/cm^3) and PETN content as compared with low density TATB. The nominal CJ pressure of X 0407 is 290 kbar versus 270 kbar for low density TATB.

III. BOOSTER PERFORMANCE

Figure 2 shows the configuration for numerical simulation of a boosting system, common in onionskin experiments and in many applications. The booster diameter is 50 mm.

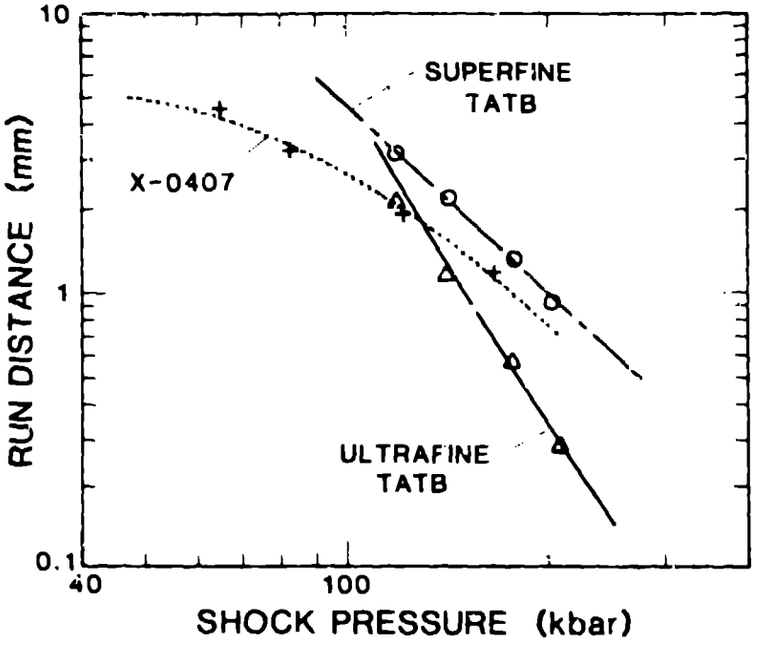

Fig. 1. Pop plots of superfine TATB, ultrafine TATB, and X-0407. Curves are experimental fittings; markers are from modeling.

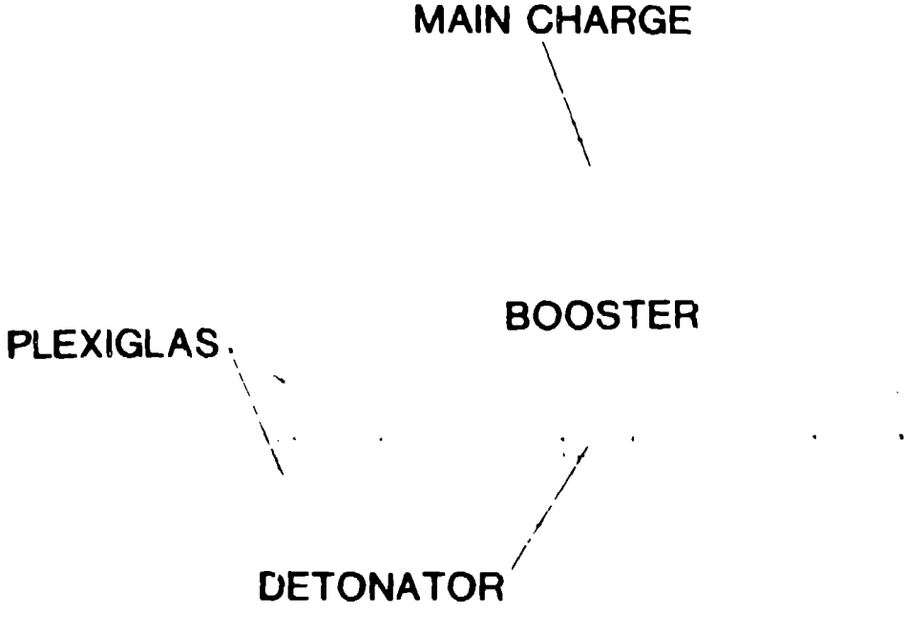

Fig. 2. Booster system configuration.

A 10-mm-thick layer of PBX-9502 envelopes the booster. The unified reaction model and HOM equation of state[10] are used. The booster is initiated by a small detonator that is represented by a region of explosive with 8-mm diameter and 4-mm thickness. The counter bore is 2 mm. The reaction model used for this detonator is the programmed burn with a fraction of surface on the bottom of the detonator used for initiation. The detonator explosive is LX-10 (95% HMX, 5% Viton A) with JWL equation of state used.[11] For computational convenience, the system is bound by layers of Plexiglas (PMMA) to provide some pressure boundary and to prevent excessive mesh distortion. Computation is done on DYNA2D code.[12]

Figures 3-a through 3-e show a sequence of reaction fraction contours at different times using three different booster materials: low-density superfine TATB, low-density ultrafine TATB, and X-0407. A detonation front is represented by closely packed contour lines; the extended reaction zone is depicted by wide line separation. At 1 μs (Fig. 3-a), the detonation front is well defined except for the slight rarefaction on the side in the ultrafine TATB and X-0407 boosters. On the other hand, in the superfine TATB booster, the detonation propagates mainly along the axis of symmetry in a planar fashion, reflecting the effect of the detonator without significant divergence. There is shock-induced reaction, but no significant sideways detonation. The detonation wave, in fact, reduces its frontal area somewhat with the shock-induced reaction zone extending further at 2 μs, as seen in Fig. 3-b; the other two boosters perform quite well at this time. With the inclusion of a nonsteady detonation feature in the model, the effective CJ pressure gradually becomes higher as the detonation propagates further. This condition helps the superfine TATB booster tremendously, re-establishing the detonation wave as shown in Fig. 3-c at 3 μs, an improvement over the earlier study[7] without the benefit of force field enhancement through nonsteady behavior of detonation. Even so, the performance of the superfine TATB is far from desirable. The other two booster explosives continue to develop in a nearly hemispherical wave pattern; the X 0407 booster shows a larger partially reacted region around the detonator, whereas the ultrafine TATB has a smaller, but more definite dead zone. At 4 μs (Fig. 3-d), the detonation front is well inside the main charge region. The shape is quite close to hemispherical when X 0407 or ultrafine TATB is used in the booster, whereas the front just barely passes the interface between the booster and the main charge if the booster material is superfine TATB. Finally, the detonation front has passed the computation region at 5 μs with X 0407 or ultrafine TATB booster explosive (Fig. 3-e), but the detonation front with superfine TATB booster has just reached the pole, and the shape of the front is far from hemispherical.

By examining the pressure at the interface between the PBX 9502 main charge and the Plexiglas layer, we can construct the breakout pattern of the detonation wave as observed in onionskin experiments. The result is presented in Fig. 4. The zero time is lined with the time of the first breakout; consequently, we can compare the uniformity and the divergence of the waves using those three booster explosives. Immediately we can see

Fig. 3-a. Reaction fraction contours at 1 μs.

Fig. 3-b. Reaction fraction contours at 2 μs.

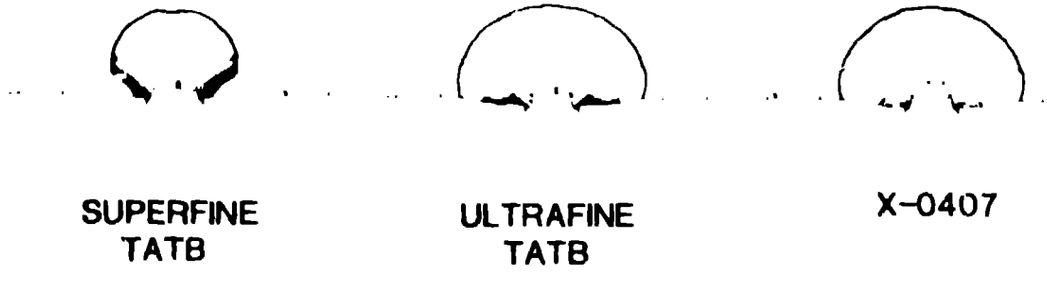

Fig. 3-c. Reaction fraction contours at 3 μs.

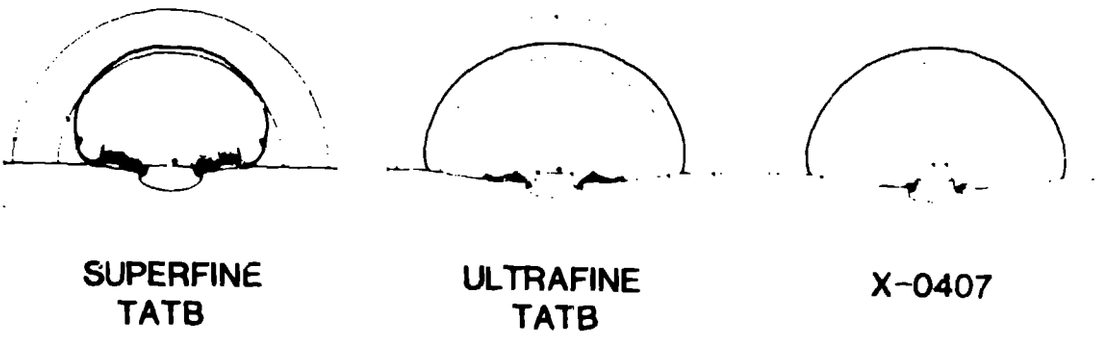

Fig. 3-d. Reaction fraction contours at 4 μs.

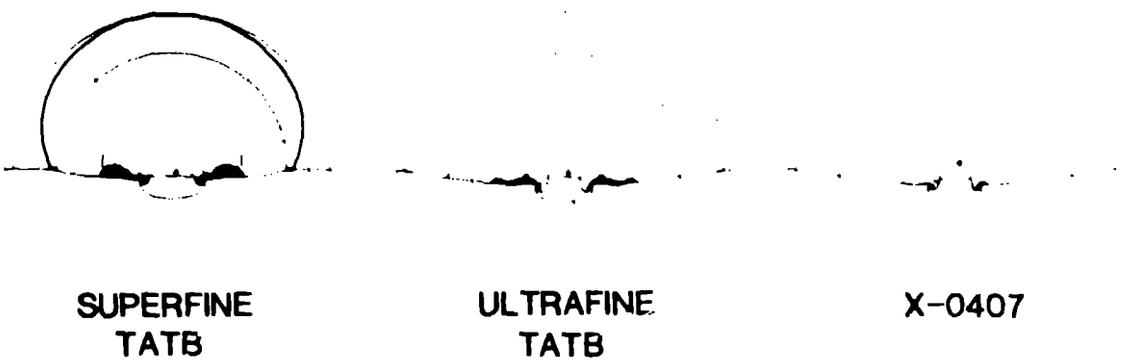

Fig. 3-e. Reaction fraction contours at 5 μs.

that ultrafine TATB and X-0407 are quite similar in developing a good divergent wave. The slight lack of uniformity using ultrafine TATB is caused by a slower detonation velocity, but the deficiency can be overcome by moving the detonator farther inside the booster. On the other hand, the performance of the superfine TATB booster is quite poor, as evident by the slow spread of the detonation wave. The divergence pattern is unacceptable for practical purposes. Some onionskin experiments using X-0407 booster explosive have been conducted; Fig. 5 shows one particular calculation (curve) that agrees quite well with the experiment (markers), considering that the lot-to-lot variation in material properties is not uncommon.

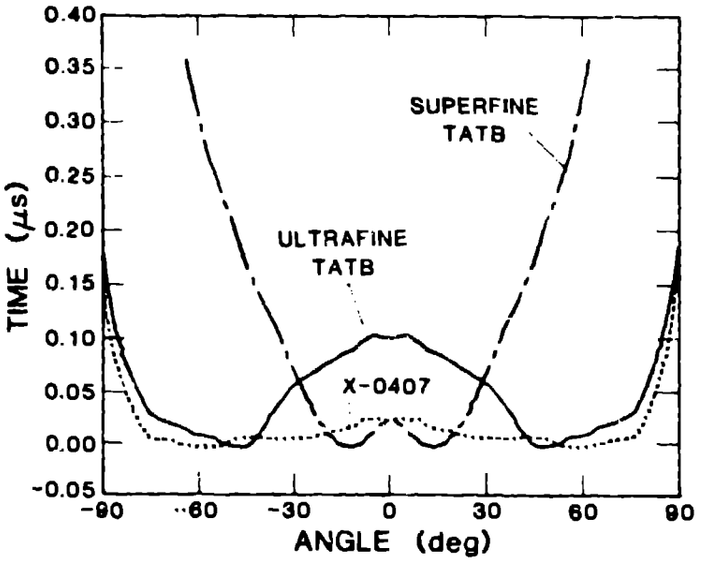

Fig. 4. Breakout patterns of superfine TATB, ultrafine TATB, and X-0407 boosters.

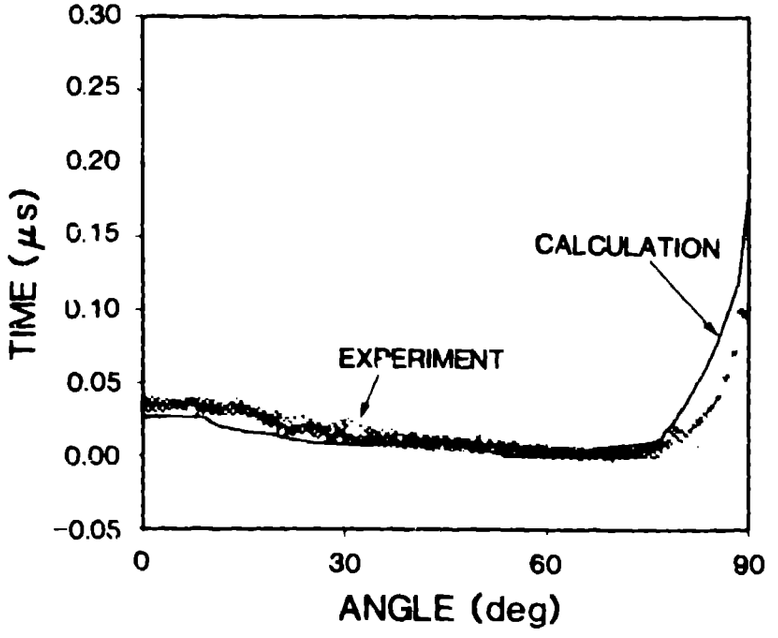

Fig. 5. Breakout pattern of X-0407 booster, calculation vs. experiment.

IV. CONCLUSIONS

We have demonstrated the great potential of using a modeling approach to evaluate the boosting system performance; the agreement between calculation and experiment is quite good. We have also used numerical simulation to investigate booster size, detonator explosives, size, and location effects. Costly experimental programs can, therefore, be substantially cut back in scale.

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