LA-UR -85-3375

CONF-860616--2

OCT 09 1985

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

LA-UR--85-3375

DE86 000807

TITLE: EFFECTS OF PHYSICAL PROPERTIES ON THE INITIATION BEHAVIORS OF HETEROGENEOUS HIGH EXPLOSIVES

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SUBMITTED TO: International Symposium on Intense Dynamic Loading and Its Effects, 3-7 June, 1986, Beijing, China

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FORM NO 836 R4
ST NO 2629 5/81

EFFECTS OF PHYSICAL PROPERTIES ON THE INITIATION BEHAVIORS OF HETEROGENEOUS HIGH EXPLOSIVES

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We present the results of an investigation into the shock initiation of high explosives with respect to the effects of density and grain sizes. We used a model of treating high-explosive reaction with a multistep process which includes the hot-spot excitation, decomposition, and the propagation of reaction into the region outside the hot spots. The roles of various parameters are discussed; in particular, the hot-spot mass fraction, the reference hot-spot temperature, and the temperature sensitivity parameter are cited as the key factors in the observed behaviors.

INTRODUCTION

The initiation process of heterogeneous high explosives is very complex; the initial loading density and temperature are strong influences, but so is the grain size. Thus we believe that the physical aspects of the high explosive are just as important as the chemical ones in controlling initiation behavior. The run distance to detonation as a function of initial shock pressure, generally known as Pop plot,[1] has been widely used as a measure of the sensitivity of the explosive under shock condition. The experimentally observed result usually follows a linear relation in a log-log scale. Increasing density reduces the sensitivity, as does increasing grain size;[2] however, with regard to the latter, recent works have indicated different trends when the shock pressure is sufficiently low.[3,4] Using a burn model for simulation, we tried to quantify the aforementioned effects, an evaluation never done before, even indirectly. Details of the model have been presented elsewhere, along with review of other models[5] and computational examples.[6]

THE MODEL

The heterogeneous nature of explosives is widely recognized--especially the role of hot spots. However, the mechanisms leading to the condition of early reaction are still speculative. Even without knowledge of details, it is reasonable to expect that hot spots behave quite differently from the rest of the material in responding to the shock. A model is summarized in this section. In the hot-spot region, the reaction progress variable, λ_h, is expressed as follows:

$$\frac{d\lambda_h}{dt} = \frac{1}{\tau_d}\ (1 - \lambda_h) \quad , \tag{1}$$

where t represents time and τ_d the characteristic time of the decomposition process. The overall reaction progress variable, λ, is determined by

$$\frac{d\lambda}{dt} = \frac{\mu}{\tau_d}\ (1 - \lambda_h)$$
$$+ \frac{\mu}{\tau_e}\ [(1 - \lambda) - \mu\ (1 - \lambda_h)] \left[\frac{\lambda_h - f_o/\mu}{1 - f_o/\mu}\right] \quad , \tag{2}$$

where μ is the hot-spot mass fraction, f_o the threshold of hot-spot burn and τ_e the energy transfer characteristic time. Here the dependence on f_o differs slightly from the previous formulation so that the absolute amount of the hot-spot burn is accounted for.[6] Equations (1) and (2) must be solved simultaneously.

The passage of an initial shock wave of amplitude p_s produces an average hot-spot temperature θ_s given by

$$\theta_s = \theta_0 \left[1 - m\,\frac{\theta_0}{\alpha}\,\ln\left(\frac{p_s}{p_0}\right)\right]^{-1} \quad , \tag{3}$$

where m, θ_0, and p_0 are constant and α is the Arrhenius activation temperature. For a given hot-spot temperature θ_s there is an induction time of thermal explosion which we identify with the characteristic time τ_d:

$$\tau_d = \frac{\theta_s^2}{\alpha\beta Z}\ \exp\left(\frac{\alpha}{\theta_s}\right) \quad . \tag{4}$$

In Eq. (4), β is the temperature coefficient resulting from chemical reaction and Z is the frequency factor for Arrhenius reaction. After the shock process, any further change of θ_s will be caused by the compression process:[6]

$$\frac{d\theta_s}{dt} = \theta_s \Gamma \kappa \frac{dp}{dt} \quad , \tag{5}$$

with Γ being the Grüneisen coefficient and κ the isentropic compressibility. Both are assumed constant. Here $\frac{dp}{dt}$ is the time rate of pressure change.

We now discuss the correlation of τ_e with the thermodynamic state. τ_e represents the process of energy transfer. Since the detail knowledge is not available and we intend no formalism here, we therefore propose the following correlation:

$$\tau_e = [G_0 p + G(p)]^{-1} \quad . \tag{6}$$

The linear term in p represents the weaker energy transfer phase, but at higher pressure range, G is the dominant one. In fact, we can identify that term with the pressure dependence in Forest Fire rate.[7]

$$G(p) = \exp\left(\sum_{i=0}^{n} a_i p^i\right) \quad . \tag{7}$$

where a_i's are constant. The roles of the hot-spot mass fraction, μ, the reference temperature, θ_0, and the temperature sensitivity parameter, n, are discussed in the next section.

EFFECTS OF PHYSICAL PROPERTIES AND RESULTS

The different degree of compaction or loading in the high explosive produces differing porosity that in turn is reflected in the density. Lower-density material contains more voids and therefore more surface area to increase the hot-spot mass fraction. A formal relation between the porosity and the hot-spot mass fraction is not feasible at this stage. Also, there is a characteristic length associated with the cavity size, D, which must be bigger for the more porous case. The resulting hot-spot reference temperature has to be greater because of more severe dissipation. Mathematically, θ_0 is likely a monotonically increasing function of D, but again we cannot establish that formulation here. This argument is supported by the results of some micromechanic studies on the hot spots with respect to the cavity size.[8,9] Using PBX-9404 (94% HMX/3% NC/3% CEF), we examined the density effect on the initiation behavior with the Pop plot data for the densities of 1.84 g/cm^3 and 1.72 g/cm^3.[10] For calibration, we used the experimental Pop plot and gauge data from the higher density case.[5] To simulate the initiation behavior at lower density, we must select the equation of state for that particular density but use most of the burn parameters from the higher density case except two. Those are the higher values of the hot-spot mass fraction, μ, and the reference temperature θ_0. With DYNA2D as the computation tool,[11] the calculated run-to-detonation distances versus initial shock pressures, along with the experimental data for densities of 1.84 g/cm^3 and 1.72 g/cm^3 are shown in Fig. 1. The feature in the model to simulate the density effect is evident.

To determine the role of grain size, the hot-spot mass fraction, μ, must be related to the grain size through the surface area and intergranular inhomogeneity. The smaller the grain size, the larger the hot-spot mass fraction. Therefore it is natural to conclude that finer grain should lead to shorter run distance, as some experiments indicate.[2] However, the grain size has the opposite effect on the initial reference hot-spot temperature θ_0 through the irreversible process. As the grain becomes smaller, the material becomes more homogeneous. D becomes smaller, so the dissipation coming from the irreversible stress components is reduced. The effect is the lowering of reference hot-spot temperature thus increasing the explosion time, decreasing the hot-spot burn rate, and eventually resulting in longer run distance. We can argue that larger grain size favors the initia-

tion phase, but smaller grain is advantageous to the propagation. Experimental evidence also supports this trend when the grain is very fine unless the shock intensity is high enough.[3,4] Finally, the temperature sensitivity parameter m reflects the effectiveness of the shock in producing the locally hot condition and is certainly related to the dissipation. An analysis has determined that as the voids become smaller viscoplastic work depends much more on the characteristic dimension of the voids than does inviscid plastic work. In fact, the hot-spot temperature must be higher when viscoplastic work is dominant.[9] The preeminence of one form of dissipation over others as the cavity drastically changes size leads us to speculate the increasing value of m when the grain gets really small.

Using the porous TATB data of porosity about 6.7%, both superfine and micronized (ultrafine) with the latter being much finer than the former,[4] we simulate the effect of grain size following the reasoning we have just discussed. First we obtain the burn parameters from the experimental Pop plot and gauge data[12] for superfine TATB then we calculate the run distances at given shock pressures to confirm the adequacy of those parameters in reproducing the Pop plot. By increasing both the sensitivity parameter m and the hot-spot mass fraction μ but decreasing the hot-spot reference temperature θ_0, we can replicate the Pop plot for the micronized TATB with the information based on the superfine one. Results are shown in Fig. 2. The initiation behavior of porous micronized TATB differs from the superfine not only in larger grain surface area and smaller void size, but also in the dissipative mechanism of producing local hot condition. The ability of the model to simulate the experimental initiation behaviors with physical insight rather than curve fitting is again illustrated. We shall report the data used in the future.

CONCLUSION

We have demonstrated the ability of the model to simulate the density as well as the grain size effects with the data available. More cases, including gauge records, must be studied to validate this relatively simple concept in interpreting their effects on the initiation. Future effort will include the effect of initial temperature. Now, the data needed for the model are limited and in some cases, preliminary. More investigation work is required to support the model refinement and actual application.

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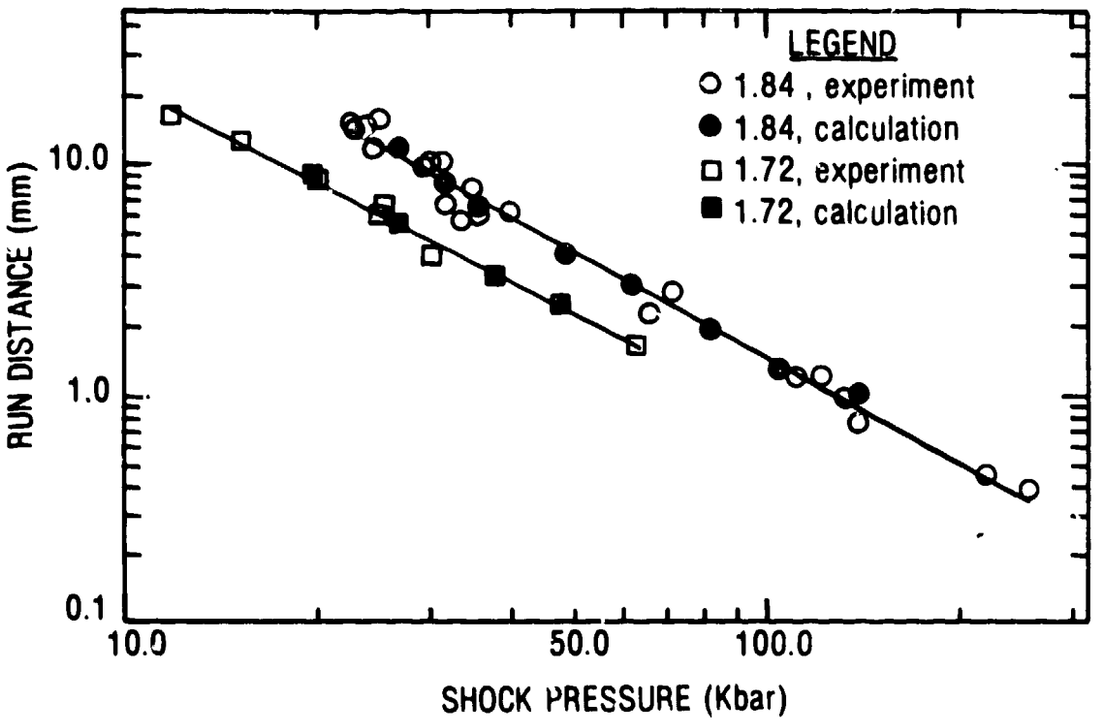

Figure 1. PBX-9404, de sity effects

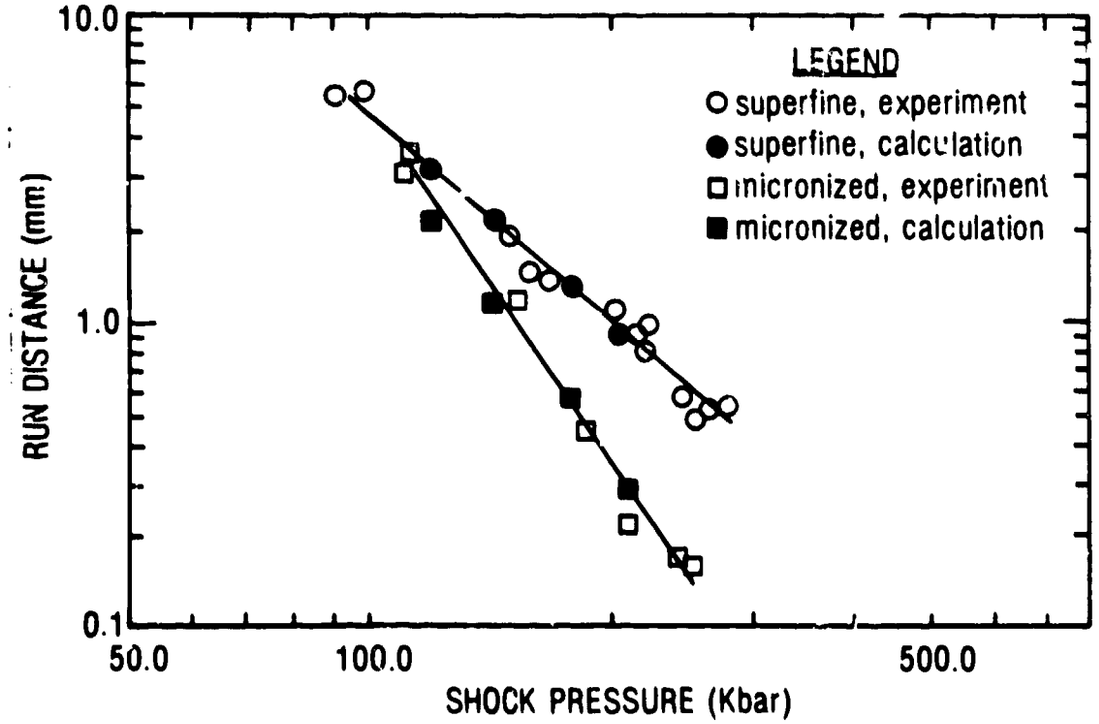

Figure 2. Porous TATB grain size effects