Research paper

A computational study of the effect of grain size distribution on shock initiation of pressed HMX powder

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Abstract

CODEX code is used to study the impact sensitivity of bimodally distributed HMX powders by mixing two monomodally distributed systems having the mean diameters of 70 μm and 220 μm. The sensitivity is examined through the coefficients of the James function for initiation threshold. Predicted thresholds of bimodally distributed systems are bounded mostly by those of the monomodally distributed systems. The coefficient of trigger energy is found to correlate well with equivalent diameter. However, the coefficient of specific energy appears to be independent of mixing ratio and relates to that of the 70 μm monomodal system. This tendency is supported by a close correlation found between the density of dissipated energy and the percentage of grains as a function of equivalent grain diameter, signifying that fine particles predominate the initiation characteristics in mixtures.

Keywords: shock initiation, HMX powder, bimodally distributed powders, CODEX, James initiation threshold

1. Introduction

A holy grail the explosive community has struggled with for many decades is the quantitative understanding and prediction of links between explosive microstructure attributes and engineering level safety and performance characteristics. Historically the study on safety has been focused on the correlation of bulk powder metrics such as particle size and specific surface area to explosive sensitivity ranked by, e.g., drop weight tests, sensitiveness measured in impact and gap tests, and critical detonation diameter tests. A notable recent development is the work of Hugh James[1, 2] who extended the energy criterion for shock initiation by Walker and Wasley[3]. An appealing aspect of this extension is that it has a term that is analogous to an activation energy[1] and through this parameter one may probe the effects played by microstructure attributes quantitatively.

This paper is aimed at exploring one such link between particle size distribution and the James shock initiation threshold through use of a cohesive finite element code called CODEX[4),5]. Special attention is focused on mixing size distributions because this attribute has not been studied as well as particle size, and there are reports of non-monotonous or anomalous behavior[2, 6] which may offer a new window to gain insight into the microstructure -sensitivity link(s).

2. CODEX and ignition threshold

CODEX codes have been in development at Georgia Institute of Technology for almost a decade with an expressed purpose of quantifying the effects of microstructure on impact initiation of energetic materials. It explicitly tracks mechanical and thermal processes that are thought to be key to modeling the links between hot spot creation and shock initiation. Details of the code is referred to the recent publications[7), 8)]. We note, however, that CODEX is not concerned with the growth of chemical reaction to detonation, relying on the historical observation that the ignition process is separate from the buildup to detonation[9)−11)]. Ignition threshold in CODEX is defined by the criticality of hot spots for thermal explosion defined by

$$d(T) \geq d_c(T) \qquad (1)$$

where d is the diameter of a hot spot whose interior maximum temperature is T. d_c is the minimal diameter of a hot spot required for thermal runaway at temperature T. One often-quoted calculation of $d_c(T)$ is that of Tarver et al.[11)]. Other examples are found in Reference[5)]. To the first order these threshold boundaries have been found to be same within a few percent.

The separation of the critical state defined by Equation 1 from the subsequent buildup to detonation or violent reactions dates back to the work[11),12)] in the 1970's. More recently the separation is reviewed by Hugh James who emphasized that his threshold function describes the "trigger" state (or threshold) and does not relate to the subsequent growth to detonation[1)]. Hence the initiation characteristics described by such measurements as Pop-plot needs to be separated from that of "trigger" state defined by an equation such as Equation (1). However, based on the observations above, we assume that there is a one-to-one correlation between the existence of critical hot spots which lead to thermal runaway and the occurrence of eventual detonation.

Probing the effect of particle size distribution described in this paper is based on the above described separation and the response characteristics that are manifested in the James initiation threshold, which is elegantly expressed in the relationship,

$$\frac{E_c}{E} + \frac{\Sigma_c}{\Sigma} = 1 \qquad (2)$$

where $E = pu\tau$, $\Sigma = u^2/2$, p is the shock pressure, u is the shock particle velocity, and τ is the shock duration. Specifically, shock initiation calculated by CODEX emulates thin flyer experiments in which the impact generates one dimensional (global) loading wave such that lateral expansion does not occur. Flyer conditions are effected by prescribing the boundary particle velocity and its duration. The range of the boundary conditions considered is u = 100−1200 m/s and τ = 8−980 ns.

Figure 1 illustrates CODEX predictions for monomodally distributed systems and its comparison with the experimental results for pressed class 3 and class 5 HMX powders.

The trends observed in the computational predictions are in fair agreement with those observed in experimental data. The difference between the two are attributed to non-ideal matching of grain size, lack of porosity in the computational samples, and computational sample size, to name a few. What is important to note is that the overall trends are consistent, with smaller grain yielding lower ignition thresholds.

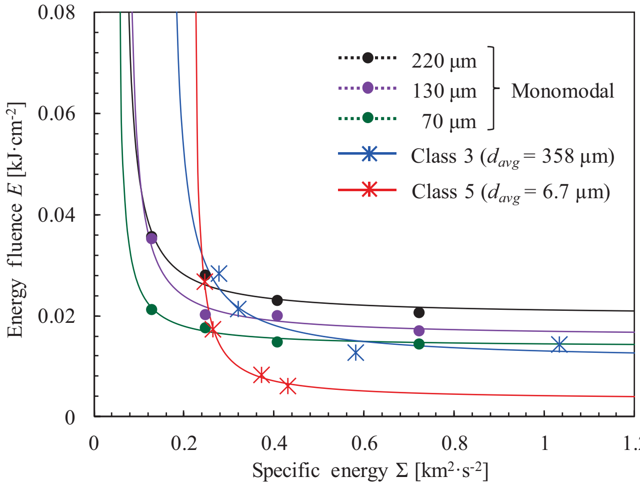

Figure 1 Computationally predicted 50% thresholds for the monomodal systems having the average grain size of 70, 130, and 220 μm and experimentally measured thresholds for pressed class 3 (d_{avg} = 358 μm) and class 5 (d_{avg} = 6.7μm) HMX powders.

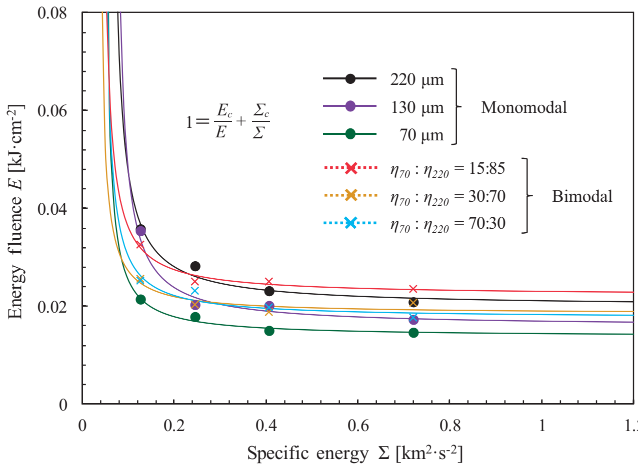

Figure 2 Predicted 50% ignition thresholds for the bimodal systems in comparison with the base monomodal systems[7)]. Solid and broken lines are James functions fitted to discrete computational points.

Encouraged by this agreement, we wanted to further test the capability of CODEX by challenging a harder question of modeling bimodally distributed systems that are created by mixing two monomodally distributed systems. Material and microstructure creation are identical to those used for preparing the monomodals[7)] for which the mean particle sizes are 70, 130, and 220 μm. Standard deviations of the distributions are 19.9, 40.3, 68.5 μm respectively. These average grain sizes are chosen so that they lie between the sizes of Class 3 and Class 5 HMX. Details are referred to the original paper[7)]. In this paper we chose the distributions of 70 and 220 μm as the base systems, and three bimodal systems are created mixing these base systems. The mass ratios are $\eta_{70} : \eta_{220}$ = 70 : 30, 30 : 70, and 15 : 85. η_{70} and η_{220} represent mass fractions of the grain groups with average sizes of 70 and 220 μm respectively. The computational determination of "go" and "no-go" threshold follows the same procedure as used for the monomodal systems[7].

3. CODEX predictions for bimodally distributed systems

Figure 2 shows the calculated threshold points for the bimodal systems and the fitted James functions in the original James space of energy fluence E and specific energy Σ.

In general, the mixture threshold points lie between those of the base systems with the exception of two points for the mixture of $\eta_{70} : \eta_{220}$ = 15:85. At present we do not have any explanation for the deviation. It could be a statistical scatter for the inherently stochastic systems at the grain scale.

Figure 3 is a comparison of the threshold parameters E_c and Σ_c in the James function, Equation (2). Equivalent diameters are calculated as follows.

$$d_{eq} = \sqrt{1/\frac{\eta_s}{d_s^2} + \frac{\eta_L}{d_L^2}} \tag{3}$$

where η_s and η_L are mass fractions of small and large grains in monomodal systems and d_s and d_L are corresponding average diameters of the small and large grains in the same systems.

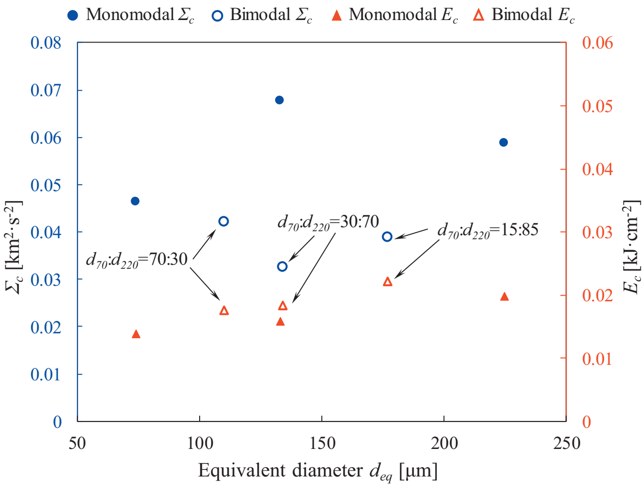

Figure 3 Coefficients of James function fitted to computationally predicted threshold points. The trends of the coefficients partially confirm the James observation about the behavior of E_c and Σ_c. The trigger energy E_c is in line with the monomodal systems, but that the behavior of Σ_c is dominated by fines. Coefficients of the James function fitted to the experimental data on Figure 1 are E_c = 0.01kJ·cm^{-2}, Σ_c = 0.16km^2·s^{-2} for Class 3, and E_c = 0.01kJ·cm^{-2}, Σ_c = 0.22km^2·s^{-2} for Class 5, respectively. The discrepancy between the experimental coefficients and the computational ones may be attributable to the semi-quantitative nature of the computational prediction shown in Figure 1.

To the first order, constant E_c appears to be in line with the base systems and we do not see any anomalous behavior. According to James[1], E_c is considered to be a trigger energy for initiation, so Figure 3 indicates that this energy is not influenced sensitively by mixing grain distributions. This is reasonable in the sense that the systems are well separated, and the critical values are almost independent of the average particle size with the caveat that the calculated range only covers a narrow range of 70−220 μm, compared to say, Class 3 and Class 5 whose average diameters are 358 μm 6.7 μm respectively. Also, the result may not be surprising in that as shown in Reference 7), the cumulative probability of ignition is not too sensitive to the average grain size.

However, the behavior of Σ_c is different, particularly regarding the threshold point for the mixture 30 : 70. When it is compared to that of the comparable monomodal system of d_{avg} = 130 μm, the value is only 1/2 of the base system. This change is reminiscent of the change reported by Hugh James in the value of Σ_c, which is doubled when the average value of coarse particle increased by a factor of 3 while keeping the mass ratio constant. It is also known[2] that binder affects Σ_c significantly. So, there is a possibility that fine grains may be effectively acting as a binder that has its own trigger threshold. Figure 4(a) shows the actual cross section of the bimodal system that supports such an interpretation. In addition, as shown in Figure 4(b), the amount of fines is far greater than that of coarse grains, so it is not surprising, as remarked by Hugh James[2], if the fines predominate the shock ignition characteristics.

To better understand the behavior of Σ_c, we show in Figure 5 a superposition of the particle size distribution and the density of dissipated energy as a function of equivalent particle diameter. It clearly shows a correlation

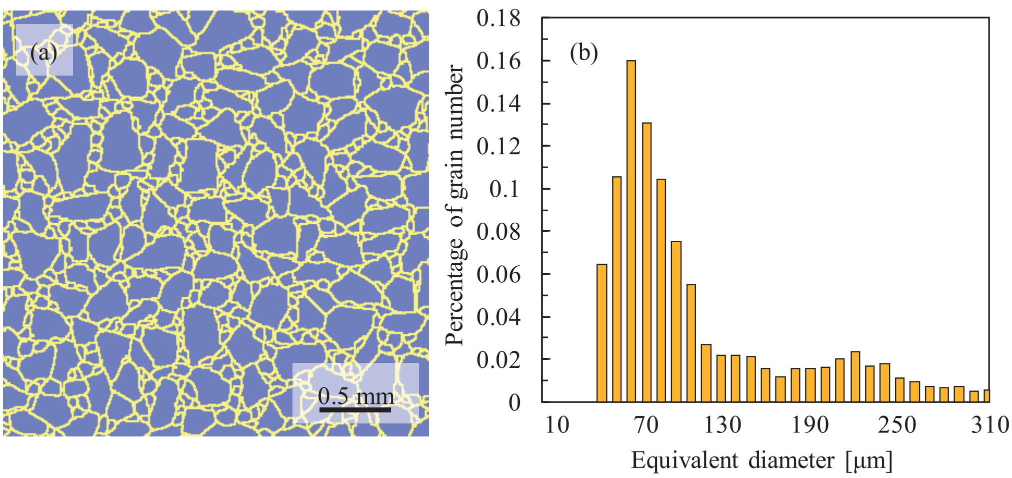

Figure 4 (a) is the cross sectional view of the bimodal system that has the size distribution shown in (b).

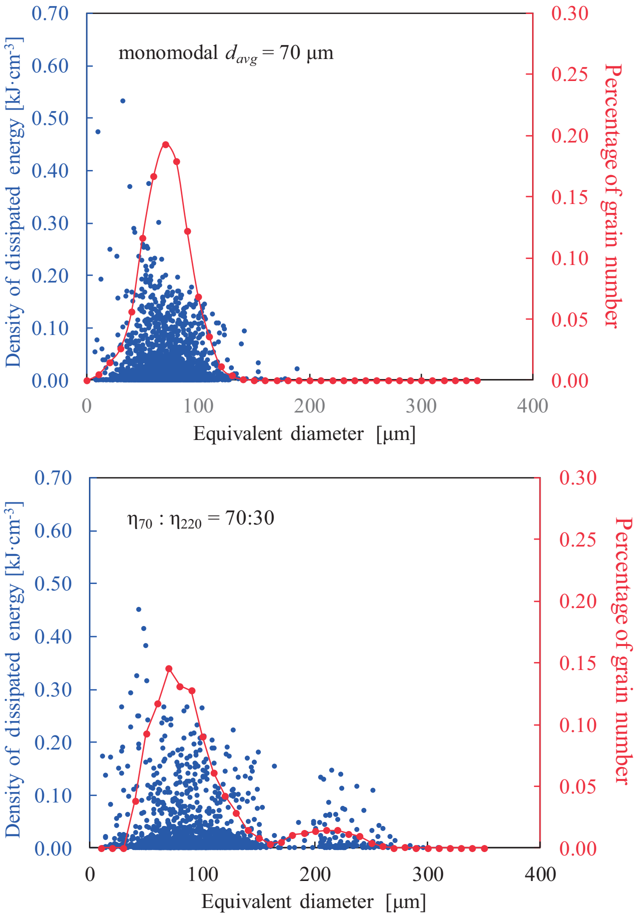

Figure 5 Comparison of the calculated dissipated energy and the particle size distribution as a function of equivalent diameter for the monomodal system having d_{avg} of 70 μm and the bimodal system consisting of $\eta_{70} : \eta_{220}$ = 70:30.

between the two. But it also reveals something that was not anticipated. That is, by yet unidentified mechanisms, small particles on the order of 20–50 μm appear to receive greater amount of dissipated energy. Though not shown here, other systems show a similar behavior. A possible explanation for this observation is that since in CODEX the primary heating mechanism is frictional heating, it may imply that fine particles in the interstitial space between larger particles move more easily and do so over larger distances than the large particles. Also, large particles may act as if they are big balls in a milling machine, and dissipated energy is concentrated in fine particles. This implies that adding coarse grains has little effect on the ignition behavior[2].

4. Conclusions

We tested CODEX code to model the response behavior of bimodally distributed HMX systems in order to predict the effect of mixing particle size distribution on ignition behavior. Predicted results are in qualitative agreement with Hugh James' observations. They are 1) fine grains are principally responsible for the behavior of the mixed system simply because there are more of them than coarse particles and they behave like a binder surrounding the coarse particles, and 2) the trigger energy E_c for the mixed systems appears to follow a lever rule between the two base systems. Definitely more study is needed to understand the links between macroscopic ignition behavior and particle size distributions.

References

1) H. R. James, Propellants, Explos., Pyrotech. 21, 8–13 (1996).
2) H. R. James, Proc., 13th Symp. Detonation, 952–961 (2006).
3) F. E. Walker and R. J. Wasley, Explosivstoffe, 17, 9–13 (1969).
4) B. A. Khasainov, B. S. Ermolaev, H. N. Presles, and P. Vidal, Shock Waves, 7, 89–105 (1997).
5) A. Barua, Y. Horie, and M. Zhou, Proc. R. Soc., A 468, 3725–3744 (2012).
6) A. Barua, S. Kim, Y. Horie, and M. Zhou, J. Appl. Phys., 113, 184907 (2013).
7) S. Kim, C. Miller, Y. Horie, C. Molek, E. Welle, and M. Zhou, J. Appl. Phys., 120, 115902 (2016).
8) S. Kim, Y. Wei, Y. Horie, and M. Zhou, J. Mech. Phys. Solids, 114, 97–116 (2018).
9) B. C. Taylor and L. W. Erwin, Proc. 6th Symp. Detonation, 3–10 (1976).
10) P. Howe, R. Frey, B. Taylor, and V. Boyle, Proc. 6th Symp. Detonation, 11–19 (1976).
11) C. M. Tarver, J. Phys. Chem., 100, 5794–5799 (1996).
12) R. J. Spear and V. Nanut, AD-A187 597 (MRL-R-1077) (1988).