Ignition and growth modeling of short pulse shock initiation experiments on fine particle Hexanitrostilbene (HNS)

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Abstract. Hexanitrostilbene (HNS) is a booster explosive that is usually initiated using short pulse duration shock waves produced by high velocity impacts with thin flyer plates. HNS is generally used at a density of 1.60 g/cm³, which implies a porosity of 8%. It has been produced in several forms (I – IV, ultrafine, etc.) with various particle surface areas. The threshold flyer velocities for shock induced detonation versus failure to detonate for these different surface area materials vary slightly, but, in this paper, an average Ignition and Growth reactive flow model parameter set was determined using all of the experimental data from several aluminium and Kapton™ flyer plate studies. This data ranged from shock pressures of 4 GPa to above the Chapman-Jouguet (C-J) detonation pressure (~20 GPa) and from 1 to 120 nanoseconds in time duration. Good agreement was obtained for the available short pulse duration detonation verses failure to threshold flyer velocity data using the Ignition and Growth model.

1. Introduction

Hexanitrostilbene (HNS) is a booster explosive that is usually initiated using short pulse duration shock waves produced by high velocity impact with thin flyer plates. HNS is generally used at a density of 1.60 g/cm³, which implies a porosity of 8%. It has been produced in several forms (I – IV, ultrafine, etc.) with various particle sizes close to the flyer thicknesses. The threshold flyer velocities for shock initiation versus failure to detonate using several flyer thicknesses for these different surface area materials varied slightly. The experimental conditions varied from shock pressures of 4 GPa to those exceeding the Chapman-Jouguet (C-J) detonation pressure of 20 GPa and from 1 to 120 nanoseconds in time duration. The flyer thicknesses varied from 3 µm to 254 µm, and the threshold flyer velocities varied from 1.5 mm/µs to 4.5 mm/µs. All of the flyers had diameters much larger than the HNS failure diameter of approximately 0.25 mm, so the shock initiation was a one-dimensional process. The initiation or failure process depends on the flyer plate thickness, which determines the shock wave pulse duration, and the flyer plate velocity, which determines the shock pressure imparted to the HNS. Aluminum and Kapton™ flyer plates have been used to study HNS. Since aluminum has a higher density and shock velocity than Kapton™, for the same flyer thickness and velocity, aluminum flyers produce higher shock pressures but shorter pulse durations than Kapton™ flyers.

The main objective of this paper was to produce a single HNS Ignition and Growth reactive flow model parameter set using all of the experimental data from several aluminum and Kapton™
flyer plate studies. Similar Ignition and Growth parameter sets have been developed for short pulse duration initiation of several other explosives [1-5].

2. Experimental threshold flyer velocity versus aluminum and Kapton™ flyer thickness data
Several groups have measured threshold velocities at various flyer thicknesses for HNS. Schwarz [6] measured threshold velocities for shock initiation using five Kapton™ flyers ranging from 25 µm to 254 µm thick. Dudley [7] measured 5 threshold velocities for HNS using 5 µm to 50 µm thick Kapton™ flyers. Bowden [8] measured a threshold velocity for a 25 µm thick Kapton™ flyer. Bowden [8,9] measured the threshold velocities of HNS using 5 thicknesses of aluminum ranging from 3 µm to 5 µm. This experimental data is shown graphically in figure 1 for aluminum flyers and in figure 2 for Kapton™ flyers. Input shock pressures range from 5 to 20 GPa with pulse durations of 2 to 120 ns for Kapton™ and from 15 to 24 GPa with pulse durations of 1 to 2 ns for aluminum.

Figure 1. HNS threshold velocity versus flyer thickness for aluminum flyer plates.

Figure 2. HNS threshold velocity versus flyer thickness for Kapton™ flyer plates.

3. Ignition and Growth reactive flow modeling for HNS
The Ignition and Growth reactive flow model uses two Jones-Wilkins-Lee (JWL) equations of state (EOS’s), one for unreacted explosive and one for reaction products:

\[ p = A e^{-R_1 V} + B e^{-R_2 V} + \omega C_v T \]  

(1)

where \( p \) is pressure, \( V \) is relative volume, \( T \) is temperature, \( \omega \) is the Gruneisen coefficient, \( C_v \) is the average heat capacity, and \( A, B, R_1 \) and \( R_2 \) are constants. These EOS’s are fitted to unreacted Hugoniot and reaction product Hugoniot data. The three-term reaction rate equation is used:

\[
\frac{dF}{dt} = I(1 - F)(\rho/\rho_0 - 1 - a) + G_1(1 - F)^2 p^2 + G_2(1 - F) F p^2 + G_{2min} F < 1
\]

(2)

where \( I(1 - F) \) is the initiation rate, \( \rho_0 \) is the initial density, \( a \) is the adiabatic exponent, \( G_1 \) and \( G_2 \) are the rate constants, and \( F \) is the reaction fraction. The reaction rate is limited by the maximum reaction rate and the minimum reaction rate.

\[
0 < F < F_{i\max} \quad 0 < F < F_{G1\max} \quad F_{G2\min} < F < 1
\]
where $F$ is the fraction reacted, $t$ is time in $\mu$s, $\rho$ is the current density in g/cm$^3$, $\rho_0$ is the initial density, and $p$ is pressure in Mbars. $I$, $G_1$, $G_2$, $a$, $b$, $c$, $d$, $e$, $g$, $x$, $y$, $z$, $F_{\text{fgmax}}$, $F_{\text{g1max}}$, and $F_{\text{g2min}}$ are constants.

Pressure and temperature equilibration between the two phases are assumed.

The unreacted HNS JWL equation of state is fitted to the available experimental data. Figure 3 shows the HNS unreacted equations of state defined by the parameters listed in table 1, along with four linear shock velocity ($U_s$) versus particle velocity ($u_p$) fits to different sets of experimental data [10]. Unlike metals, organic energetic materials do not exhibit linear $U_s$ – $u_p$ relationships, so an exponential form like JWL works well. The linear fits lie to the right of the JWL in figure 3, because HNS begins to react when the shock pressure reaches 3.5 GPa [11]. The unreacted JWL Hugoniot yields a reasonable von Neumann spike state for a Chapman-Jouguet (C-J) detonation velocity of 6.8 km/s [12]. The product JWL must predict expansion data below the C-J pressure plus overdriven Hugoniot states above the C-J pressure. The product JWL parameters in table 1 are fitted to a cylinder test [12] using $R_1 = 5.4$ and $R_2 = 1.8$, which should predict HNS overdriven Hugoniot states well.

| Unreacted JWL EOS | Product JWL EOS | Reaction rate parameters |
|-------------------|-----------------|---------------------------|
| $A = 331.8$ Mbar  | $A = 5.3625$ Mbar | $I = 1.4e+6 \mu$s$^{-1}$ |
| $B = -0.025154$ Mbar | $B = 0.2702$ | $x = 4.0$ |
| $R_1 = 11.5$     | $R_1 = 5.4$     | $b = 0.667$ |
| $R_2 = 1.15$     | $R_2 = 1.8$     | $a = 0.26691$ |
| $\omega = 0.5675$ | $\omega = 0.45$ | $G_1 = 14800$ Mbar$^{-1}$ $\mu$s$^{-1}$ |
| $C_v = 2.704e-5$ Mbar/K | $C_v = 1.0e-5$ Mbar/K | $G_2 = 3700$ Mbar$^{-2}$ $\mu$s$^{-1}$ |
| $T_0 = 298K$     | $E_0 = 0.070$ Mbar·cm$^3$/cm$^3$·g | $c = d = e = g = 0.667$ |

Table 1. Ignition and Growth model parameters for HNS initial density = 1.60 g/cm$^3$ (8% porosity)

**Figure 3.** Shock velocity versus particle velocity curves for unreacted HNS.

**Figure 4.** Run distance to detonation versus shock pressure data for sustained pulses in HNS.
4. Comparison of Ignition and Growth model calculations with experimental HNS data

Together with the unreacted JWL EOS and the product JWL EOS, the HNS reaction rate parameters are compared to sustained shock pulse data from Kipp et al. [13] and the short shock pulse data shown in figures 1 and 2. Setchell [11] measured very little chemical energy release below 3.5 GPa, which corresponds to a critical compression of 0.266 91 using the unreacted JWL in table 1. Above that compression, the ignition term in the Ignition and Growth rapidly reacts a maximum of 8% of the HNS defined by the parameter Figmax. Then the growth and completion terms are normalized to the sustained pulse data. Figure 4 shows the agreement between the experimental and calculated run distances to detonation for the 8 different shock pressure experiments by Kipp et al. [13]. Good agreement was obtained, especially for the high pressure (> 6 GPa) regime of the short pulse data.

For the Kapton™ flyers that are 25 to 254 µm thick and produce shock pressures of 5 to 11 GPa and pulse durations of 10 to 120 ns, the HNS Ignition and Growth parameters in table 1 with Figmax = 0.08, together with a Kapton™ Gruneisen equation of state with density = 1.414 g/cm³, c = 2.737 km/s, s = 1.41, and gamma = 0.76 [4], accurately calculate the threshold velocities for shock initiation of detonation. The comparisons are shown in figure 5.

![Figure 5](image-url)

**Figure 5.** Experimental and calculated HNS threshold velocities for Kapton™ flyer plates with thicknesses of 25 µm to 254 µm.

For aluminum, which has a Gruneisen equation of state with density = 2.703 g/cm³, c = 5.24 km/s, s =1.4, and gamma = 1.97 [4], and for Kapton™ flyer plates thinner than 20 µm, igniting only 8% of the HNS does not allow the rest of reaction to build to detonation fast enough. The higher velocity impacts produce shock pressures exceeding the C-J pressure (20 GPa) with time durations of only 1 to 5 ns. More HNS has to be ignited during shock compression to model the threshold velocities. Setting Figmax = 0.18 yielded the calculated results shown in figures 6 and 7 for aluminum and Kapton™ flyers, respectively. The calculated results for both aluminum and Kapton™ flyer plates agree with the experimental results. The shock pressure and pulse duration differences caused by aluminum’s higher density and shock velocity compared to those of Kapton™ were simulated well.
Similar increases in $F_{\text{ign}}$ have been needed for successful modeling of 1D short pulse initiation and 2D small diameter, very short pulse initiation of other explosives [4,5]. Some of the possible reasons for the higher amount of ignition in the very short duration, high pressure shock fronts are: the formation of more “hot spots”; the more rapid growth of ignited volumes to the highly heated surrounding explosive molecules; more rapid amplification of the shock front by faster energy release; and the immediate formation of Mach stem interactions in a three dimensional shock front like those in self-sustaining detonation waves. Further experimental and modeling efforts are required to explain the shock initiation of detonation by very thin, very high velocity and small diameter flyer plates.

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