Short pulse duration shock initiation experiments plus ignition and growth modeling on Composition B

Chadd M May and Craig M Tarver
Lawrence Livermore National Laboratory
Livermore, CA 94551 U.S.A.
Email: tarver1@llnl.gov

Abstract. Composition B (63% RDX, 36% TNT, 1% wax) is still a widely used energetic material whose shock initiation characteristics are necessary to understand. It is now possible to shock initiate Composition B and other secondary explosives at diameters well below their characteristic failure diameters for unconfined self-sustaining detonation. This is done using very high velocity, very thin, small diameter flyer plates accelerated by electric or laser power sources. Recently experimental detonation versus failure to detonate threshold flyer velocity curves for Composition B using several Kapton™ flyer thicknesses and diameters were measured. Flyer plates with diameters of 2 mm successfully detonated Composition B, which has a nominal failure diameter of 4.3 mm. The shock pressures required for these initiations are greater than the Chapman-Jouguet (C-J) pressure in self-sustaining Composition B detonation waves. The initiation process is two-dimensional, because both rear and side rarefactions can affect the shocked Composition B reaction rates. The Ignition and Growth reactive flow model for Composition B is extended to yield accurate simulations of this new threshold velocity data for various flyer thicknesses.

1. Introduction
Composition B (63% RDX, 36% TNT, and 1% wax) and Composition B-3 (60% RDX, 40% TNT) are still widely used energetic materials, because they can be melt cast into complex geometries. Their shock initiation and detonation properties have been studied experimentally and calculated using reactive flow models [1]. Recently it has been reported that solid explosives can be shock initiated using very high velocity, very thin flyer plates at diameters significantly smaller than their unconfined failure diameters. For example, LX-10 (95% HMX, 5% Viton™ binder) was initiated by 1 mm diameter flyer plates at a velocity of 4.3 km/s, even though LX-10’s failure diameter is about 1.5 mm [2]. LX-17 (92.5% TATB, 7.5% KelF™ binder) has shown the same property [3]. This paper describes an experimental study of the short pulse duration initiation of melt cast Composition B (density 1.70 to 1.71 g/cm³) using Kapton™ flyer plates with diameters less than its failure diameter of 4.3 mm [4]. The Ignition and Growth reactive flow model parameters for shock initiation and detonation developed by Urtiew et al. [1] are extended to include this new experimental data.
2. Experimental results

In this experimental setup, a chip slapper [5] is used to accelerate a Kapton™ flyer into a 6.3 mm diameter by 6.3 mm long cylinder of Composition B. An aluminum witness plate is placed on the Composition B to determine detonation, defined by a dent in the aluminum, versus failure to initiate, defined by no dent. Various thicknesses and diameters of Kapton™ flyers are used. The flyer velocity is determined by the dimensions of the flyer and the quantity of electrical energy deposited into the chip slapper. The energy deposited into the slapper is varied to change the flyer velocity in a systematic manner. The threshold velocity for detonation is determined in a reasonable number of shots. Determining the threshold velocity for several flyer thicknesses with the same diameter and for several diameters with the same thickness are two ways to characterize the explosive shock initiation. For Composition B, which has an unconfined failure diameter of 4.3 mm, three flyer diameters (0.381 mm, 0.635 mm, and 2.000 mm) were fired. All of the 0.381 mm and 0.635 mm diameter Kapton™ flyers failed to initiate detonation. The 2 mm diameter flyers of three thicknesses (0.0508 mm, 0.0762 mm, and 0.127 mm) all caused detonation at threshold velocities of 4.72 km/s, 4.24 km/s, and 4.08 km/s, respectively. These experimental results, along with the number of shots fired for each thickness of the 2 mm diameter flyers, are listed in table 1.

Table 1. Experimental threshold velocities versus flyer diameter data for Composition B.

| Flyer diameter (µm) | Flyer thickness (µm) | Threshold velocity (km/s) | Result          |
|---------------------|----------------------|---------------------------|-----------------|
| 381                 | 4.8                  | 8.86                      | Failure         |
| 381                 | 19.6                 | 6.02                      | Failure         |
| 381                 | 50.0                 | 4.47                      | Failure         |
| 635                 | 50.0                 | 4.83                      | Failure         |
| 2000                | 50.8                 | 4.72                      | Detonation (12 shots) |
| 2000                | 76.2                 | 4.24                      | Detonation (12 shots) |
| 2000                | 127.0                | 4.06                      | Detonation (18 shots) |

3. Ignition and Growth reactive flow model

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:

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

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:
\[
dF/dt = I(1 - F)^{(\rho/\rho_0 - 1 - a)} + G_1(1 - F)^{p_1} + G_2(1 - F)^{p_2}
\]

\[
0 < F < F_{\text{igmax}} \quad 0 < F < F_{\text{Gi1max}} \quad F_{\text{G2min}} < F < 1
\]

where \( F \) is the fraction reacted, \( t \) is time in \( \mu \text{s} \), \( \rho \) is the current density in g/cm\(^3\), \( \rho_0 \) is the initial density, \( p \) is pressure in Mbars. \( I, G_1, G_2, a, b, c, d, e, g, x, y, a, z, F_{\text{igmax}}, F_{\text{Gi1max}}, \) and \( F_{\text{G2min}} \) are constants. Pressure must be equilibrated between the two phases, temperature equilibrium is assumed, and converged zoning must be used. The unreacted JWL equation of state is fitted to the available experimental data. Figure 1 shows the Composition B unreacted equation of state defined by the parameters listed in table 2, along with seven linear shock velocity \( (U_s) – \text{particle velocity (u_p)} \) fits to various sets of experimental data listed in Dobratz and Crawford [6]. Unlike metals, organic energetic materials do not exhibit linear \( U_s – u_p \) relationships, so the exponential JWL form works better. The linear fits lie to the right of the JWL in figure 1, because the explosive reacts to some extent when the shock pressure is high enough. The unreacted JWL Hugoniot also yields a reasonable estimated von Neumann spike state at detonation velocity of 7.98 km/s [7]. The JWL product JWL must agree with cylinder test and other expansion data below the Chapman-Jouguet (C-J) [1,6]. In this study, the product JWL must also be accurate at pressures exceeding the C-J state, which have been measured for Composition B in overdriven detonation experiments by Skidmore and Hart [8] as well as Kinneke and West [9]. Figure 2 shows these two sets of experimental data with their large error bars and two product JWL equations of state, one fit only to C-J and below data with \( R_1 = 4.2 \) and \( R_2 = 1.1 \), plus another fit to overdriven data and other data that includes pressures greater than C-J with \( R_1 = 6.2 \) and \( R_2 = 2.2 \). The \( R_1 = 6.2 \) and \( R_2 = 2.2 \) JWL parameters fit the overdriven data better and are used here.

The reaction rate law has to calculate the available high pressure experimental data. Only Cowperthwaite and Rosenberg [7] have measured the reaction zone profile, the C-J particle velocity, and the product expansion using embedded aluminum particle velocity gauges. Figure 3 contains these particle velocity history records, along with the corresponding Ignition and Growth calculations. Campbell and Engelke [4] measured the detonation velocity versus inverse radius curve for detonating Composition B. That data and the Ignition and Growth calculated curve are shown in figure 4. The agreement using the Ignition and Growth parameters in table 2 with the experimental data on Composition B in figures 3 and 4 is excellent. These model parameters listed in table 1, together with a Kapton™ Gruneisen equation of state with density \( = 1.414 \) g/cm\(^3\), \( c = 2.737 \) km/s, \( s = 1.41 \), and \( \gamma = 0.76 \) [2], were then applied to the short pulse duration threshold velocity experiments.

**Table 2. Ignition and Growth model parameters for Composition B (Initial density = 1.712 g/cm\(^3\))**

| Unreacted JWL EOS | Product JWL EOS | Reaction rate parameters |
|-------------------|-----------------|-------------------------|
| A=778.1 Mbar      | A=13.4815 Mbar  | I=4.0e+6 \mu\text{s}^{-1} \text{d}=0.667 |
| B=0.05031 Mbar    | B=0.5896 Mbar   | b=0.667 \text{y}=2.0    |
| R_1=11.3          | R_1=6.2         | a=0.0367 \text{F}_{\text{G1max}}=0.9 |
| R_2=1.13          | R_2=2.2         | x=4.0 \text{G}_2=75 \text{Mbar}^{-1} \mu\text{s}^{-1} |
| \omega=0.8938     | \omega=0.5      | \text{F}_{\text{igmax}}=0.175 \text{e}=0.286 \text{F}_{\text{G2min}}=0.667 |
| Cv=2.487e-5 Mbar/K| Cv=1.0e-5 Mbar/K| \text{G}_1=546 \text{Mbar}^{-2} \mu\text{s}^{-1} \text{z}=1.0 |
| To=298K           | Es=0.085 Mbar-cm\(^3\)/cm\(^3\)-g | \text{c}=0.333 \text{F}_{\text{G2min}}=0.9 |
4. Results and conclusions
The small diameter short pulse shock initiation experiments listed in Table 1 were modeled using the Composition B parameters listed in Table 2. All of the 0.381 mm and 0.635 mm diameter calculations failed to detonate at the experimental flyer velocities. The rarefaction waves from the edges of the Kapton™ flyers reached the centers of the Composition B charges before significant reaction was initiated, reduced the shock pressures, and caused the reaction rates to rapidly decrease. For the 2.000 mm diameter flyers, more time is available for the initiating reaction to grow. When the regions of complete reaction grow outward to the failure diameter of Composition B (4.3 mm) before the rarahctions arrive, then full detonation occurs. Table 3 compares the calculated threshold velocities.
for the three flyer thicknesses with 2 mm diameters to the experimental threshold velocities.

Table 3. Experimental versus calculated Composition B threshold velocities for 2 mm diameter flyers.

| Flyer thickness (µm) | Experimental velocity (km/s) | Calculated velocity (km/s) |
|----------------------|-----------------------------|---------------------------|
| 50.8                 | 4.72                        | 4.85 +/- 0.05             |
| 76.2                 | 4.24                        | 4.25 +/- 0.05             |
| 127                  | 4.06                        | 3.95 +/- 0.05             |

To initiate sufficient reaction in the very short times before the rarefaction wave from the back of the Kapton™ flyer overtakes the shock front, approximately 17.5% of the chemical energy must be released. This is done by setting the maximum fraction ignited to 0.175. Similar values have been necessary to match the threshold velocities for 2D initiation for LX-10 [2] and LX-17 [3]. This maximum fraction reacted that must be ignited is much larger than igniting an amount equal to the void volume of the pressed or cast charge, as is done for much lower shock pressure, longer pulse duration shock pressures. For Composition B, the void volume at 1.712 g/cm³ is 2.2% [1]. Some of the possible reasons for the higher amount of ignition are: formation of more “hot spots” as the shock pressure increases; more rapid growth of ignited volumes into the highly heated surrounding explosive; more rapid amplification of the shock front by closer energy release; and the formation of Mach stem interactions and a three dimensional shock front, as in self-sustaining detonation waves.

Further planned research on two-dimensional Composition B shock initiation includes: using Kapton™ flyer diameters between 0.635 mm and 2 mm to determine the minimum flyer diameter that can initiate detonation; using other flyer materials to investigate the effects of impedance of the minimum diameter; and determining the effects of Composition B porosity and initial temperature.

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