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Ignition and Growth Modeling of the Shock Initiation of PBX 9502 at -55°C and -196°C

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Abstract. Gustavsen et al. reported the results of 26 shock initiation experiments using embedded particle velocity gauges on various lots of PBX 9502 (95% TATB/ 5% Kel-F binder) cooled to -55°C . A previously developed Ignition and Growth reactive flow model for -55°C PBX 9502 was compared to this newer data to ensure that it still applies. More recently, Hollowell et al. published similar data on PBX 9502 cooled to -196°C ($+77\text{K}$) with liquid nitrogen. An Ignition and Growth (I&G) model parameter set for -196°C PBX 9502 was developed and yielded good agreement with the measured shock initiation process and transition to detonation. Hollowell et al. also measured the interface particle velocity histories between the detonating PBX 9502 charges and various windows (PMMA, Kel-F, and LiF) placed at the rear PBX 9502 surfaces. This detonation data was accurately calculated using the -196°C PBX 9502 I&G parameters.

Keywords: PBX 9502, shock initiation, detonation, Ignition and Growth modeling

PACS: 82.33.Vx, 82.40.Fp

INTRODUCTION

Gustavsen et al. [1,2] reported the results of 26 shock initiation experiments using embedded particle velocity gauges on various lots of PBX 9502 (95% TATB/ 5% Kel-F binder) cooled to -55°C . Ignition and Growth (I&G) reactive flow model parameters for the shock initiation of LX-17 (92.5% TATB/ 7.5% Kel-F binder) at -55°C were developed using both embedded manganin pressure gauges and embedded particle velocity gauges by Urtiew et al. [3]. Several detonation experiments on PBX 9502 and LX-17 at -55°C have been successfully modeled using the I&G model [4] based on improved experimental data on both the unreacted [5] and the reaction product equations of state [6] of PBX 9502, but the Gustavsen et al. shock initiation data had not been calculated. They found that the PBX 9502 shock initiation at -55°C depended somewhat on the lot of PBX 9502 used. One of these lots (HOL86A891-004) yielded similar initiation results to several other lots and was also the lot used by Hollowell et al. [7] at -196°C . The embedded particle velocity gauge experiments on this lot (six at -55°C and five at -196°C) were studied using the PBX 9502 I&G shock initiation model. Very small changes in the reaction rate parameters from those of Urtiew et al. [3] were needed to match the newer -55°C experimental data. Due to page limitations, only the I&G modeling results at -196°C are reported here. At the rear of the 23 mm long PBX 9502 charge in each -196°C experiment, a transparent window was used along with the PDV technique to measure the interface particle history between the detonating PBX 9502 and the window. PMMA, Kel-F, and LiF windows were employed. The I&G modeling results compare well to the PDV records and are included in this paper.

EXPERIMENTS

Hollowell et al. [7] shock initiated five 50 mm diameter by 23 mm long cylinders of PBX 9502 at -196°C using 6 mm thick Kel-F 81 flyers accelerated to various velocities. The flyer velocities ranged from 2.654 to 3.506 km/s, creating shock pressure in the PBX 9502 targets ranging from approximately 12.7 to 19.6 GPa. The initial density

of the -196°C PBX 9502 was estimated to be 1.950 g/cm³. A “stirrup” gauge on the front surface of the PBX 9502 measured the initial particle velocity. Ten thin particle velocity gauges at various depths in the PBX 9502 measured shock front and subsequent increasing particle velocities due to reaction. PMMA, Kel-F, or LiF windows were used to measure the interface particle velocities of detonating PBX 9502 and windows using the PDV technique.

THE 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:

$$p = A e^{-R_1 V} + B e^{-R_2 V} + \omega \square C_v T \quad (1)$$

where p is pressure, V is relative volume, T is temperature, ω 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:

$$\frac{dF}{dt} = I(1 - F)^b(\rho/\rho_0 - 1 - a)^x + G_1(1 - F)^c F^d p^y + G_2(1 - F)^e F^g p^z \quad (2)$$

$0 < F < F_{igmax} \quad 0 < F < F_{G1max} \quad F_{G2min} < F < 1$

where F is the fraction reacted, t is time in μ s, ρ is the current density in g/cm³, ρ_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_{igmax} , F_{G1max} , and F_{G2min} are constants. Pressure and temperature equilibration between the two phases are assumed.

The unreacted PBX 9502 JWL EOS is fit to experimental data. The reaction product PBX 9502 JWL EOS is fit to expansion data below the C-J pressure and overdriven Hugoniot states above the C-J pressure. Since there is no EOS data for PBX 9502 at -196°C, the unreacted and reaction products EOS's for -55°C PBX 9502 [4] are used. The five experiments were simulated using the PBX 9502 parameters in Table 1 and the inert Gruneisen EOS's in Table 2. The best results were obtained by decreasing all the reaction rate parameters (I, G_1 , and G_2) from the -55°C PBX 9502 values. Comparisons of the experimental and calculated results are shown in the next section.

Table 1. Ignition and Growth model parameters for PBX 9502 at -195°C and $\rho_0 = 1.95$ g/cm³

Unreacted JWL EOS	Product JWL EOS	Reaction rate parameters
A = 632.07 Mbar	A = 13.6177 Mbar	I = 1.5e+5 μ s ⁻¹ a = 0.214 x = 4.0 b = 0.667
B = -0.029509 Mbar	B = 0.7199 Mbar	$F_{igmax} = 0.5$ $F_{G1max} = 0.5$ $F_{G2min} = 0.0$
$R_1 = 11.3$	$R_1 = 6.2$	$G_1 = 0.3$ Mbar ⁻¹ μ s ⁻¹ c = 0.333 d = 0.111
$R_2 = 1.13$	$R_2 = 2.2$	y = 1.0
$\omega = 0.8938$	$\omega = 0.5$	$G_2 = 180$ Mbar ⁻³ μ s ⁻¹
$C_v = 2.704e-5$ Mbar/K	$C_v = 1.0e-5$ Mbar/K	z = 3.0
$T_0 = 77$ K	$E_0 = 0.069$ Mbar-cm ³ /cm ³ -g	e = 0.333 g = 1.0

Table 2. Gruneisen EOS parameters for inert materials

$$p = \rho_0 c^2 \mu [1 + (1 - \gamma_0/2)\mu - a/2\mu^2] / [1 - (S_1 - 1)\mu - S_2\mu^2 / (\mu + 1) - S_3\mu^3 / (\mu + 1)^2]^2 + (\gamma_0 + a\mu)E \quad (3)$$

where p = pressure, $\mu = (\rho/\rho_0 - 1)$, and E is thermal energy

INERT	ρ_0 (g/cm ³)	c(mm/ μ s)	S_1	S_2	S_3	γ_0	a
Kel-F 81	2.14	2.65	1.65	0.0	0.0	0.66	0.0
PMMA	1.186	2.59	1.52	0.0	0.0	0.85	0.0
Kel-F 800	1.99	1.838	1.824	0.0	0.0	0.66	0.0
Brass	2.638	5.15	1.35	0.0	0.0	0.34	0.0

COMPARISON OF EXPERIMENTAL AND MODELING RESULTS

The measured and calculated particle velocity histories for the five -196°C PBX 9502 experiments are shown in Figs. 1 – 5 in order of increasing shock pressure. The gauge records and detonation locations agree well.

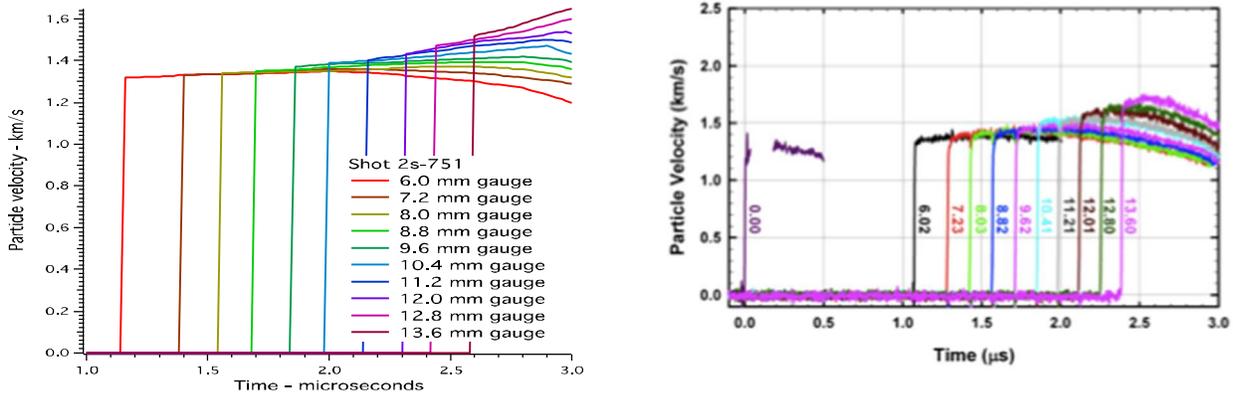


FIGURE 1. Experiment 2s-751; initial pressure = 12.7 GPa; detonation distance = 18.2 mm; model (left) and experiment (right)

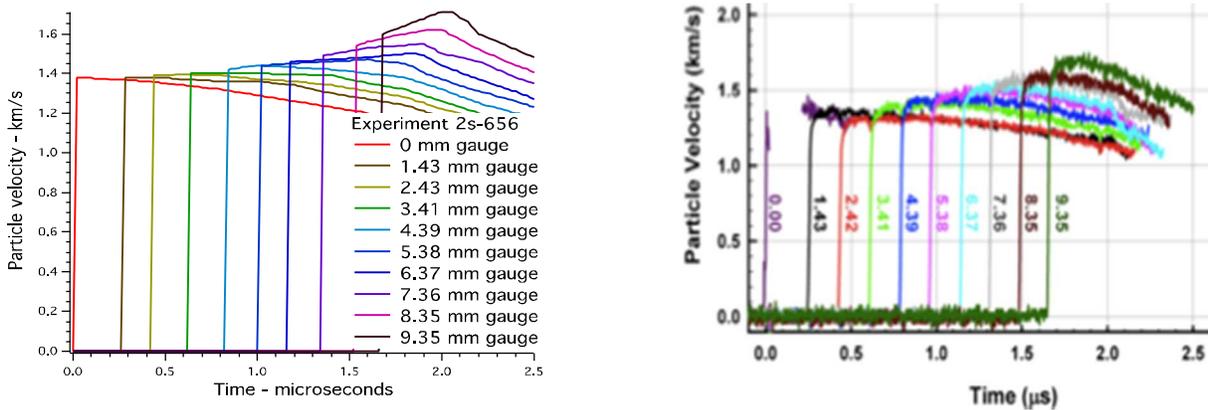


FIGURE 2. Experiment 2s-656; initial pressure = 14.1 GPa; detonation distance = 13.9 mm; model (left) and experiment (right)

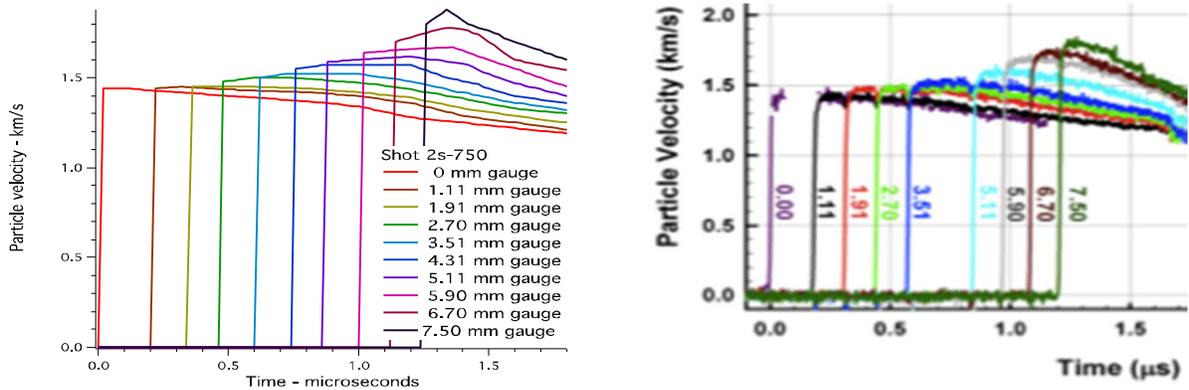


FIGURE 3. Experiment 2s-750; initial pressure = 15.4 GPa; detonation distance = 9.4 mm; model (left); experiment (right)

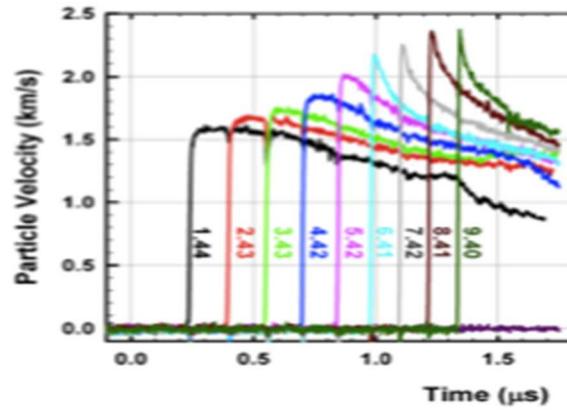
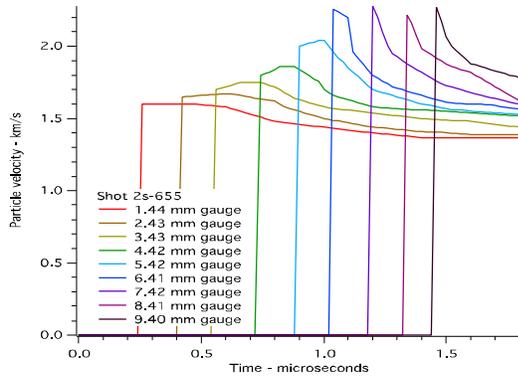


FIGURE 4. Experiment 2s-655; initial pressure = 17.3 GPa; detonation distance = 6.4 mm; model (left); experiment (right)

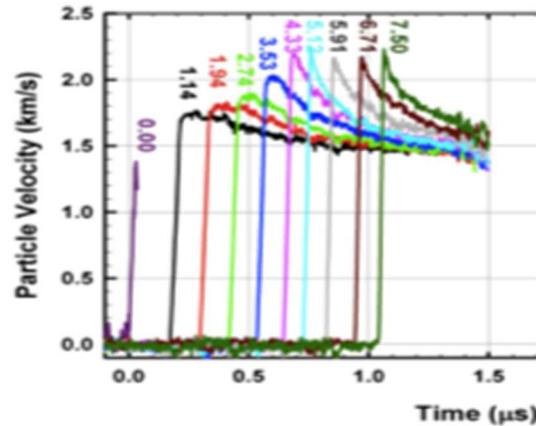
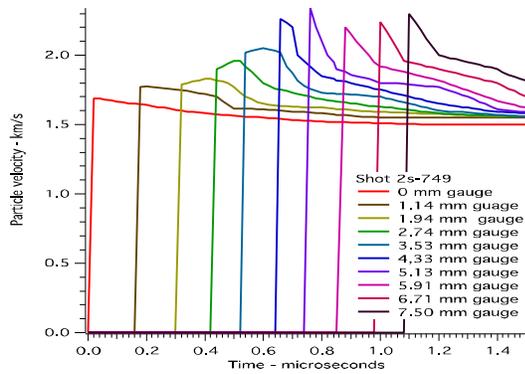


FIGURE 5. Experiment 2s-749; initial pressure = 19.6 GPa; detonation distance = 4.3 mm; model (left); experiment (right)

The experimental and calculated PDV interface particle velocity histories for detonating PBX 9502 and the various window materials (PMMA, Kel-F 800, and LiF) are shown in Fig. 6. The refractive indexes for PMMA and Kel-F are assumed to be equal to one. The known LiF refractive index correction was used. The agreement is excellent.

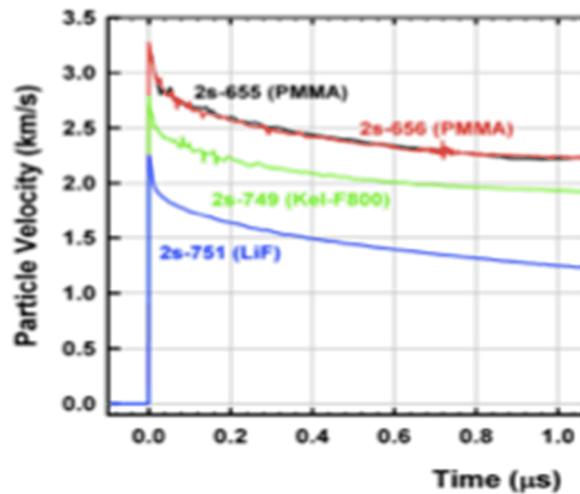
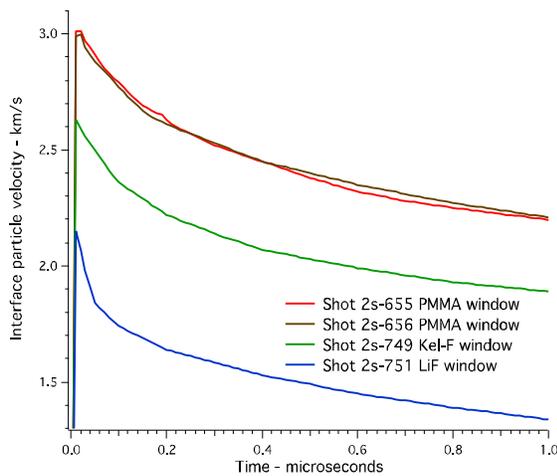


FIGURE 6. Experimental and calculated interface particle velocity histories for detonating PBX 9502 and various windows

CONCLUSIONS

Since the TATB based PBX 9502 detonated at -196°C , other solid explosive (PBX's or pure) pressed to about 98% TMD should also be detonable. This may not be the case for homogeneous liquid or solid explosives. Several liquid explosives have shown rapidly increasing failure diameters as their initial temperatures decrease [8]. To help quantify the effect of this very cold initial temperature on shock initiation, the five shock initiation experiments on PBX 9502 cooled with liquid nitrogen to -196°C ($+ 77\text{K}$) were successfully calculated by the Ignition and Growth model using reaction rate coefficients (I , G_1 and G_2) that were reduced substantially from those previously developed to model -55°C data. This is reasonable, because the very low initial temperature most likely causes a reduced number of effective hot spot sites, slower growth of the reacting hot spot into the cold surrounding particles, and slower coalescence of the expanding and interacting reaction product regions during the completion of the energy release. There is embedded gauge shock initiation experimental data for PBX 9502 and/or LX-17 at eight initial temperatures from -196°C to $+250^{\circ}\text{C}$, a span of 446°C . A future effort is to publish all the data in one paper and overlay the modeling and test results for direct comparisons.

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