Shock-to-detonation transition of RDX, HMX and NTO based composite high explosives: experiments and modelling

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Abstract. HMX, RDX and NTO based cast-cured plastic bounded explosive (PBX) are widely used in insensitive ammunitions. Designing modern warheads needs robust and reliable models to compute shock ignition and detonation propagation inside PBX. Comparing to a pressed PBX, a cast-cured PBX is not porous and the hot-spots are mainly located at the grain-binder interface leading to a different burning behavior during shock-to-detonation transition. Here, we review the shock-to-detonation transition (SDT) and its modeling for cast-cured PBX containing HMX, RDX and NTO. Future direction is given in conclusion.

1. Introduction
HMX, RDX and NTO based cast-cured PBX are widely used in insensitive ammunitions. Designing modern warheads needs robust and reliable models to compute the PBX shock-to-detonation transition (SDT). Comparing to a pressed PBX, a cast-cured PBX is not porous. The MEB observation of a cast-cured PBX illustrates this difference figure 1.

Figure 1. RDX-AP-Al-HTPB cast-cured PBX microstructure.

For pressed PBX, the common hypothesis of ignition is at hot spots created by the pore collapse. For cast-cured PBX, we expected that hot-spots are mainly located at the grain-binder interface and lead to a different ignition behavior during SDT. An investigation of how SDT occurs inside cast-cured PBX containing HMX, RDX and NTO is proposed. Two cast cured PBX have been studied. The
first one (B2238) is composed of RDX and HTPB 85:15. Its mean density measured on 34 samples is 1577kg/m$^3$ comparing to the theoretical density of 1573 up to 1578kg/m$^3$ depending of pure RDX data (Cheetah 2.0 or LASL handbook). The second one (B2214) is composed of HMX, NTO and polyurethane 12:72:16. Its measured density is 1634kg/m$^3$ comparing to the theoretical density of 1607 up to 1657kg/m$^3$. The NTO theoretical density is 1930kg/m$^3$ whereas the observed value is 1840kg/m$^3$. The measured densities of these compositions confirm a quasi non porosity.

2. Experimental observations
The two cast-cured PBX have been submitted to a plane sustained shock wave at different pressure levels using a laboratory powder gun of 98mm bore diameter. The configuration is the impact of a 15mm plate (82mm diameter) on a target composed of a 5mm buffer plate (100mm diameter) and 30mm of PBX (80mm diameter). Experimental setups are given figure 2. For B2238 the impactor and the buffer plate are in aluminum. For B2214, the impactor is in copper and the buffer plate in aluminum; the thickness of the buffer plate is enough to avoid the back release wave influence on SDT. The pressure signals are measured using 13m$\Omega$ manganin gauges (manufactured by SEDAD France, thickness 330$\mu$m) inserted at several distances inside the PBX. In each experiment, a gauge measures the pressure at the PBX-buffer plate interface and one gauge is inserted inside the PBX. The calibration has been performed on plane sustained shock Hugoniot data. The corresponding run-distances to detonation are determined using wedge test experiments where the plate impact is performed using the same powder gun and impact configurations (figure 3). The distance-time trajectories are measured using piezoelectric pins and optical fibers on an angle of 30°. In each configuration, the shock wave generated inside the PBX is plane and sustained during the time to detonation transition.

**Figure 2.** Plate impact experiment with manganin gauges inserted at several distances.

**Figure 3.** Wedge test experiment.
The distance-time trajectories obtained for the different initiation pressures are compared by shifting the origin to correspond to the transition to detonation point. We observe that the measured trajectories lie on top of each other. The shock velocity at the PBX entrance depends on the shock input condition. The detonation velocity obtained after transition does not depend on the shock input condition according to a Zeldovich-Von Neuman-Doering model. This led to the conclusion that the distance-time trajectory is independent of the starting pressure for SDT. It is the hypothesis known as the single-curve buildup principle. This behavior seems to be a common property for cast cured PBX, opposite to pressed PBX for which this hypothesis is not valid. Figures 4 and 5 illustrate this behavior for B2238 and B2214. It will be exploited to determine the reaction rate at different shock pressure levels. B2214 is very insensitive compared to B2238 and is clearly in the class of insensitive PBX. The run-distance to detonation versus pressure is linear in a log-log scale and known as a Pop Plot (named after its originator Alphonse Popolato).

Submitted to a plane double shock wave, B2238 exhibit no desensitization. The double shock wave is generated using an impactor composed of a 15mm plate and 3mm of polymethyl methacrylate (82mm diameter). The target is a B2238 cylinder of 30mm thickness and 80mm diameter. The gauge is inserted at 3mm from the impacted face of the PBX. The impactor velocity is chosen to obtain successively 2.5 and 6GPa. The measured pressure signal is compared to the single 6GPa shock input condition at the same distance on figure 6. This behavior is opposite to the desensitization behavior of HMX and TATB pressed PBX. Another experiment performed on a HMX-PU binder 86:14 cast-cured PBX leads to a sensitization by the first shock wave. This sensitization seems to be correlated with the grains cracks observed in recovering samples submitted to a plane sustained shock waves at pressures lower than ignition and in absence of lateral release waves [1]. The reactive behavior of the B2238 and
B2214 cast-cured PBX is clearly different compared to the pressed PBX ones, and leads to conclude to an ignition at the grain-binder interface.

3. Modeling

The shock-to-detonation transition is simulated using the Euler equations plus an equation for the reaction coordinate (mass fraction of products)

$$\frac{\partial (\rho \lambda)}{\partial t} + \frac{\partial (\rho u \lambda)}{\partial x} = \rho R(\lambda, \rho, p)$$

(1)

where $\rho$ is the density, $p$ the pressure, $u$ the particle velocity, $\lambda$ the reaction coordinate and $R(\lambda, \rho, p)$ the reaction rate.

The high explosive (HE) is assumed to be a mixture of reactants (1) and products (2) with a simple chemistry $1 \rightarrow 2$. The HE thermodynamics is based on mechanical equilibrium of the components (1 and 2) and additive volumes, masses and internal energies. Another closure relation is necessary. The classical ones are temperature equilibrium or no heat transfer to the reactants, or constant $\rho_2/\rho_1$ [2]. At early time of SDT the temperature equilibrium assumption is not valid; it is attained when $\lambda \rightarrow 1$. No heat transfer to the reactants is only valid at early time of SDT. Constant $\rho_2/\rho_1$ finds a justification in the reduction to mechanical equilibrium limit of the Baer and Nunziato two-phase model [3].

This reduced model is composed of the reactive Euler equations, additive volumes, masses and internal energies, plus an equation for the products volume fraction. This last equation can be express as an equation for the specific volume and, after some algebra, one obtains:

$$dv_2/dt = \phi dv_1/dt \quad \text{with} \quad \phi = \frac{(\rho_2^2/c_2^2)}{\rho_1^2 c_1^2}$$

(2)

During SDT the value of the ratio $\phi$ lies in the range $0.85 - 0.95$. This suggests a simpler closure model using $\phi = \text{cste}$. In this range, the pressure profiles sensitivity to its value is slight. The choice of its value can be constrained by reasonable temperature profiles inside the reaction zone. A non dependant temperature reaction rate leads to a non dependant temperature reactive flow; the value of $\phi$ is not critical and $\phi = 1$ is a good approximation of the relation closure. Reactants and products equations of state (EOS) read under the Mie-Gruneisen formulation with a 0K isotherm reference curve fitted on the shock Hugoniot for reactants and a CJ isentrope reference curve (JWL) fitted on thermochemical computations for products. The Gruneisen coefficients and heat capacities are assumed constant. EOS improvements can be obtained considering Gruneisen coefficients function of volume.

Dimensional considerations of HE hot spot ignition (see Damamme [4], Menikoff [5]) lead to a factorized form for the reaction rate expressed as

$$R(\lambda, \rho, p) = N^{1/3} h(\alpha) D_f(p)$$

(3)

$N$ being the hot spots number per unit volume, $h(\alpha)$ a function of the products volume fraction and $D_f(p)$ the propagation velocity of quasi-stationary flames from hot spots. In the particular case of hot spots assimilated to a distribution of ignition points without correlation, the function $h(\alpha)$ is the following

$$h(\alpha) = (36\pi)^{1/3}(1-\alpha)\log^{2/3}(1-\alpha)$$

(4)

For a reaction growth starting from the grains boundaries, the factorized form of the reaction rate is the following
\[ R(\lambda, \rho, p) = N^{1/3} h(\lambda) D_f(p) \]  
\[(5)\]

In the particular case of spherical grains of unique size,

\[ h(\lambda) = (36\pi)^{1/3} (1 - \lambda)^{2/3} \]  
\[(6)\]

Generally, the grains are not spherical and a good approximation is \( h(\lambda) \approx (1 - \lambda) \).

Coupled to an ignition model, this approach allows SDT computing. Considering reaction growth starting from the grain-binder interface, one obtains the simple reaction rate

\[ R = (1 - \lambda) D_f(p) \]  
\[(7)\]

A useful way to determine the function \( D_f(p) \) is an inversion method using the run-distance to detonation versus the shock pressure and the shock-change equation, considering no reaction and pressure gradients at the shock front (see the equations (11)-(13) of reference [6]). The method is initialized by zero gradients to compute a first evaluation of the reaction rate at different pressure levels. The gradients, determined from SDT computing, are then taking into account. This method allows determining the reaction rate at shock front where \( R = D_f(p) \). It is represented by

\[ D_f(p) = A p^n \left( 1 + B p^{-7-n} \right) \]  
\[(8)\]

Computed pressure histories are compared to experimental data on figure 7 for B2238 and figure 8 for B2214. This comparison shows a correct model experiment agreement which validates our approach. The model also well compute the double shock input condition response of B2238 (see figure 6). Noisy signals are usually observed for cast-cured PBX comparing to pressed PBX. It seems due to the high heterogeneity and difference in acoustic impedances; 15% of binder is present in cast cured PBX whereas a few percent is present in pressed PBX.

![Figure 7](image1.png)  
**Figure 7.** Pressure histories at 3 distances inside B2238 shocked at 6GPa.

![Figure 8](image2.png)  
**Figure 8.** Pressure histories at 3 distances inside B2214 shocked at 16.2GPa.

Our inversion method requires only the single-curve buildup to detonation. If this curve is measured continuously, the instantaneous shock velocity could be determined and this method allows obtaining the reaction rate with only one pop-plot experiment.

4. Conclusion and future direction
Cast-cured PBX containing HMX, RDX and NTO exhibit no desensitization when submitted to double shock waves and distance-time trajectories independent of the starting pressure for SDT. This
hypothesis, known as the single-curve buildup principle, has been exploited to determine the reaction rate at the shock front.

**Figure 9.** Experimental setup using the RIF.

**Figure 10.** Pop-plot RIF signal and deduced shock velocity.

Pressure histories recorded at different distances inside PBX are successfully computed using a growth reaction model based on this reaction rate. This model is robust and allows numerical simulations of modern insensitive warheads.

Measurement of shock trajectories using piezoelectric pins is a robust metrology, but its accuracy is less than the streak-camera ones to detect the transition point to detonation. Today, the better accuracy is obtained using a radio interferometer technique (RIF) which offers the interest of continuously measuring the shock trajectories from the early time of SDT up to the stationary detonation. Associated with a shock-change equation inversion method, this technique will allow a better determination of the reaction rate at shock front. A first attempt of this technique applied for cast TNT, in the B2214 test configuration, successfully records the SDT distance-time buildup. The deduced shock wave velocity exhibit the influence of the back release wave from the copper-aluminum interface (see figure 6).

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