Development of new detonation rate model for selective energetic materials

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1 Introduction

The shock to detonation transition (SDT) within a short time scale (~10^{-5}sec) is observed in the reactive response of high explosives subject to an impact. The rate of reaction of certain high explosives and solid propellants under a deflagration to detonation transition (DDT) is normally slower than SDT phenomena, being approximately 10^{-3}~10^{-2}sec. Since in most SDT events, the response time for high explosives to undergo any sort of thermal response such as dissociation or dissipation is slow. Instead, the pressure or compression dependence of initiation is most dominant in the developing detonation waves observed in the impact initiated detonation phenomena.

For numerically capturing of such SDT event that is dominantly pressure sensitive, Lee-Tarver model[1] and JWL++(Jones-Wilkins-Lee++) model[2] have been widely in use. Lee-Tarver considers generation of hotspots and their effect on initiation, and it consists of the equations of states for both product and reactant. The model requires predetermination of excessive number of parameters (12 unknowns) to both empirically and ad hoc, and thus makes it difficult to be universal for general choice of energetic materials. JWL++ model shows simplification to Lee-Tarver, neglecting the initiation step and using only a single growth step for detonating an explosive. Despite the need for better model that combines the strengths of these approaches, methodology to determine the unknowns of such SDT rate laws has yet been accomplished to date. Further the present state of free parameter determination in the context of either Lee-Tarver or JWL++ is cumbersome and quite qualitative.

The present study aims at developing an improved reactive flow model including both ignition and growth steps of a detonation transition due to the mechanical (pressure) stimulus. The suggested model can overcome certain limitations of aforementioned models for SDT simulation. In addition, the free unknown parameters of the model are analyzed theoretically for minimizing ambiguity of numerical iterations. The procedure involves quantitative and accurate determination of model parameters. A list of common high explosives is used in this paper to address their pressure sensitivities that are calibrated quantitatively.

2 Pressured-based detonation rate law

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The production rate of reacted mass fraction consists of initiation and growth [1]

$$\frac{d\lambda}{dt} = I(1-\lambda)^a\left(\frac{\rho}{\rho_0}-1-a\right)^x + G_1(1-\lambda)^c\lambda^d P^y + G_2(1-\lambda)^e\lambda^g P^z \tag{1}$$

Here λ is the burned mass fraction, and constants I, b, a, x, G_1, c, d, y, G_2, e, g, z are the unknown free parameters of the rate model. P is the pressure, t is time, ρ_0 and ρ are the initial and current densities, respectively. The Murnaghan EOS which is expressed in (2) is employed for the unreacted solid-state energetic materials, and the JWL EOS given by (3) is used for the reacted gaseous product.

$$P_{unreacted} = \frac{1}{n\kappa}\left(\frac{1}{v^n}-1\right) \tag{2}$$

$$P_{reacted} = Ae^{-R_1 v} + Be^{-R_2 v} + \frac{C}{v^{1+\omega}} \tag{3}$$

where v is the relative volume ratio given by $v=\rho_0/\rho$. n, κ in (2) are the Murnaghan model parameters, and A, B, C, R_1, R_2 are the material dependent JWL model parameters with ω being the Gruneisen coefficient. Equations (2) and (3) are integrated into a single expression (4) using the product mass fraction, λ and reactant depletion (1-λ).

$$P_{total} = (1-\lambda)P_{unreacted} + \lambda P_{reacted} \tag{4}$$

Lee-Tarver model is comprised of *i*) ignition term that represents formation of the hotspots by the rapid compression, and *ii*) first growth term that describes the effect of the propagation of the reacting waves in the substance and second growth term that represents completion due to detonation transition. For determination of 12 unknowns of Lee-Tarver mode, curve fitting method with optimization technique is used.

If the ignition term involving the initial density ratio is omitted, a JWL++ model[2] is recovered, and it is

$$\frac{d\lambda}{dt} = G(1-\lambda)P^b \tag{5}$$

Here G is the growth constant, b is the pressure sensitivity. The determination of the unknowns is relatively easier and thus the usability of a simplified form of the rate law is wider for applications involving only the fast growths or pressure-dependent process.

An alternative to these two limiting form of the rate law can be casted into a basic form such as

$$\frac{d\lambda}{dt} = I(1-\lambda)\eta^a + G(1-\lambda)P^b \qquad \left(\eta = \frac{\rho}{\rho_0}-1\right) \tag{6}$$

We named the form given in (6) as KYP model (Kim-Yoh-Park). The model consists of an ignition and a growth term. The pressure is defined from the EOS. Four unknown parameters, b, G, a, I are left for determination via the theoretical arguments and available empirical data.

The initiation step requires defining the ignition constant, I, while the reactant depletion (1-λ) is time-resolved in the governing law with a compression term η as given by $\eta=\rho/\rho_0$-1. The ignition of energetic materials is induced by the compression because of the shock wave propagation. The hotspot is formed in a shocked high explosive. So, the void collapse due to shock propagation gives rise to the hot spot forming. Further, any voids and gas bubbles that existed in the high explosive provide potential sites for local adiabatic compression leading to a localized heating beyond the activation energy for the onset of detonation. Such mechanism gives rise to the ignition.

Wackerle et al. [3] reported that the hotspot formation due to void collapse depends on the shock pressure, P_s and the reaction rate is proportional to P^2 experimentally. To investigate the shock-

pressure-squared dependence of ignition process, compression sensitivity, *a*, needs to bet 4 in the ignition calculations because the relationship between pressure and density is parabolic based on the Rankine-Hugoniot relationship. Once again, the pressure squared term is dominant in the shock induced ignition, and pressure is proportional to the compression squared. So, *a* being 4 is the best choice for the most applications including SDT.

Souers et al. [4] provided a useful approach to determine the unknown parameters of JWL++ model. They analytically linked the growth term with unconfined rate stick data. The rate stick test provides detonation velocity versus the inverse radius of a cylindrical charge. With available size effect data from experiment, the unknowns of the growth term can be determined. That is, the relationship between non-dimensional detonation velocity and a non-dimensional inverse radius is derived using a detonation velocity equation of unconfined rate stick from Eyring *et al*. [5] as

$$\frac{U_s}{D} = 1 - \frac{tU_s}{\sigma R_0} \tag{7}$$

where U_s is the detonation velocity for radius R_0, and D is the detonation velocity at infinite radius. t is the time to cross the reaction zone. The parameter σ is empirically described by [5].

$$\sigma = \frac{0.4}{\left[1-(U_s/D)^2\right]^{0.8}} \tag{8}$$

Now all λ are collected on the left of the growth term of KYP model and the equation is integrated to obtain the result

$$\int \frac{1}{(1-\lambda)} d\lambda = \int GP^b dt \quad \rightarrow \quad -\ln(1-\lambda) = GP^b t \tag{9}$$

Here the burn fraction λ is defined in terms of the non-dimensional detonation velocity squared, and the dimensionless radius and growth constant (G) are given by

$$\lambda = (U_s/D)^2 \tag{10}$$

$$R_D = \frac{D}{GP^b} \quad \rightarrow \quad G = \frac{D}{R_D P^b} \tag{11}$$

Finally, equation (12) specifies the relationship between dimensionless detonation velocity and inverse radius.

$$\frac{R_D}{R_0} = -\frac{\sigma}{\ln\left(1-(U_s/D)^2\right)}\left(\frac{U_s}{D}\right)^{2b-1}\left(1-\frac{U_s}{D}\right) \tag{12}$$

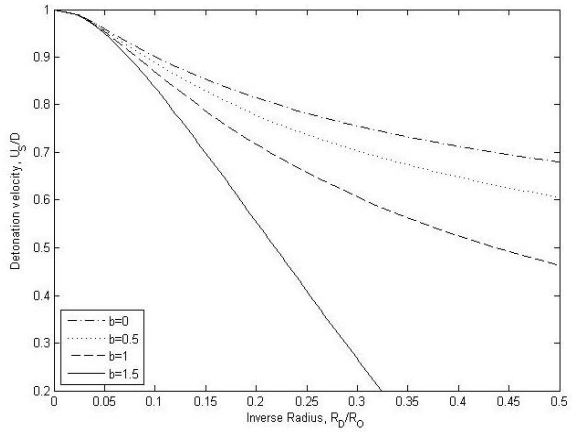

Figure 1. Solutions of analytical approach depending on pressure sensitivity *b*

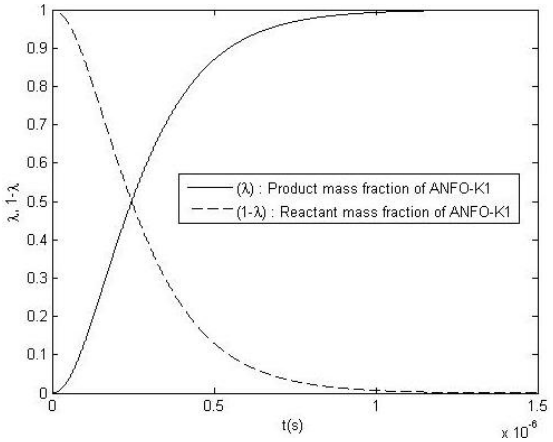

Figure 2. Time trace of product and reactant mass fraction of ANFO-K1 explosive from KYP model

Figure 1 shows the dimensionless detonation velocity change depending on the inverse radius of a cylindrical charge. This figure indicates that size effect curves are concave-up when the power of pressure, b is less than 1. The curve is concave-down with b being higher than 1. The shape is an important factor when it comes to design the charge performance and its size. As the charge diameter decreases, the detonation velocity decreases rapidly in the case of a concave-down. So when b is higher than 1, a larger sized explosive would be needed to generate a strong explosion. This suggests that a concave-up is more desirable since the detonation velocity of this type does not significantly depend on the size.

Figure 2 shows time trajectory of the product and reactant mass fraction of ANFO-K1. The constants of ignition I and growth G are set to $8.37556\text{X}10^{8}$ s^{-1} and $7.0\text{X}10^{-8}$ $s^{-1}Pa^{-b}$, respectively. The pressure sensitivity of ANFO-K1 is 1.38, and the compression sensitivity is 4.0. The C-J (Chapman-Jouguet) pressure and density are $0.1017\text{X}10^{11}$ Pa and 1.33672 g/cm^3, respectively. The growth constant is calculated by (11) using R_D=1.30 mm and D=5865 m/s. The ignition constant is estimated from (13).

$$\frac{I\eta^{a}}{GP^{b}} \sim 0.1 \quad \rightarrow \quad I \cong 0.1GP^{b}\eta^{-a} \tag{13}$$

Table 1: Comparison of the pressure sensitivity parameter for selective energetic materials

Energetic materials	b - Present	b - Others	Concavity
LX-17	1.7	0.6667[6]	down
ANFO-K1	1.38	1.3[2]	down
ANFO emulsion with 30% HMX	1.7	1.5[7]	down
Creamed TNT	1.0	1.75[7]	straight
Urea nitrate (0.69 g/cm^3)	1.0	1.0[7]	straight
HANFO	0.95	0.8[4]	up
TNT	1.0	-	straight
HMX emulsion	1.7	-	down
Non-ideal AN emulsion k1a	1.45	1.5[4]	down
Extremely non-ideal AN	0.8	0.8[4]	up
ANFO prill	1.65	1.5[4]	down
Potassium chlorate/sugar	1.05	0.8[4]	down

Table 1 shows comparison of pressure sensitivities obtained from the present method of analytical approach versus the values from the literature. For example, LX-17, ANFO series, and HMX emulsion have shown strongly down concavity when plotted against the inverse radius. HANFO and extremely non-ideal AN are both concave-up. Urea nitrate and TNT series are shown straight. In the case of LX-17, the literature value was 0.6667 as being concave-up, while the present study provided 1.7 with the shape being concave-down. The sensitivity value of each energetic material was derived by theoretical arguments without any speculations based on numerical trials.

Figures 3-6 show analytical trajectory lines for HANFO, potassium, chlorate/sugar, ANFO prill, and extremely non-ideal AN data. Data for each case are fit quite easily with proper b values shown in Table 1. In the case of HANFO, for instance, the lines of b=0.9 and b=1.0 work as the lower and upper limits, respectively. Thus b=0.95 line emerges as the best fit for the HANFO data.

In order to validate the model parameters, we performed a full hydrocode simulation [8] and constructed the size effect curve that shows the change of fully developed detonation velocity, U_s, with the radius, R_0. The detonation velocities are plotted as a function of 4 sample inverse radius, 1/ R_0=0mm^{-1}, 0.05mm^{-1}, 0.10mm^{-1}, 0.15mm^{-1}. The fully developed detonation velocities were measured when the von Neumann spikes emerged steady for each simulation.

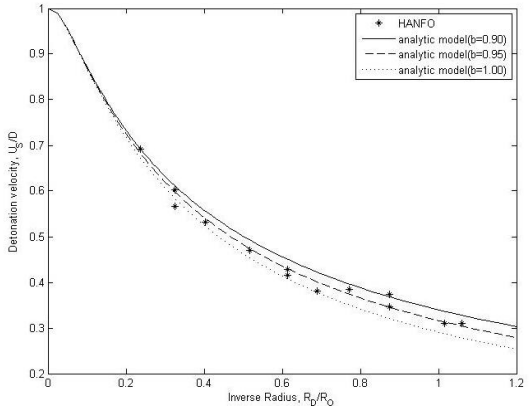

Figure 3. Analytical trajectory lines for HANFO experimental data[4]

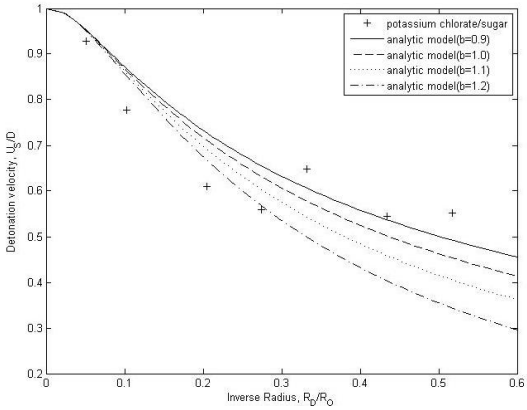

Figure 4. Analytical trajectory lines for potassium chlorate/sugar experimental data[4]

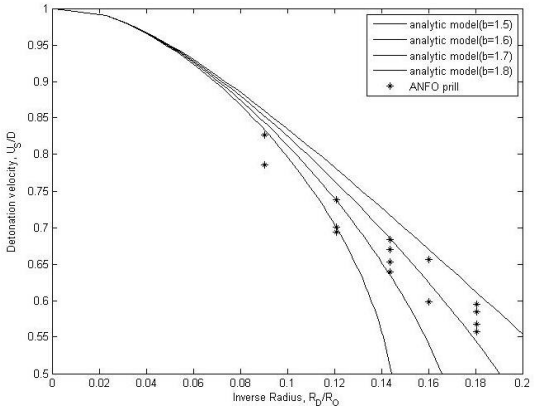

Figure 5. Analytical trajectory lines for ANFO prill experimental data[4]

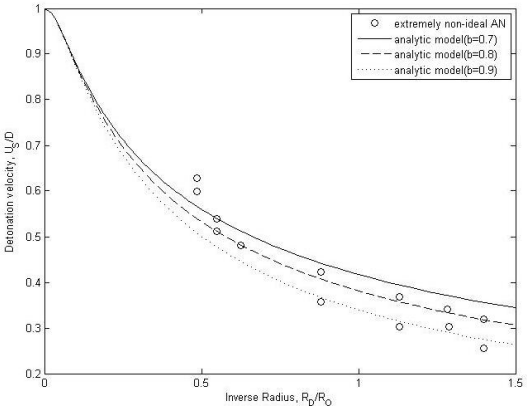

Figure 6. Analytical trajectory lines for extremely non-ideal AN experimental data[4]

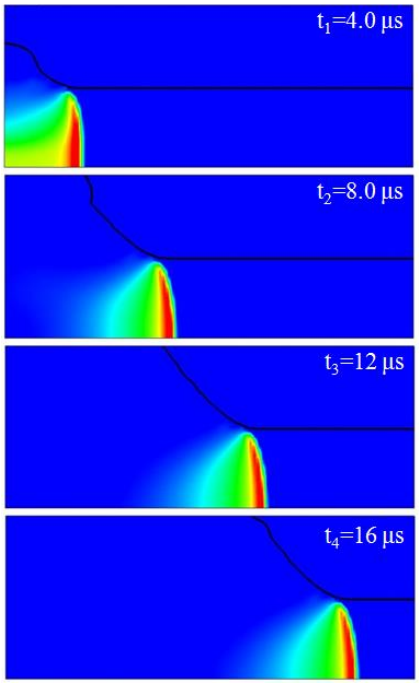

Figure 7. Pressure contours for unconfined rate stick stimulations with 0.05 mm^{-1} inverse radius

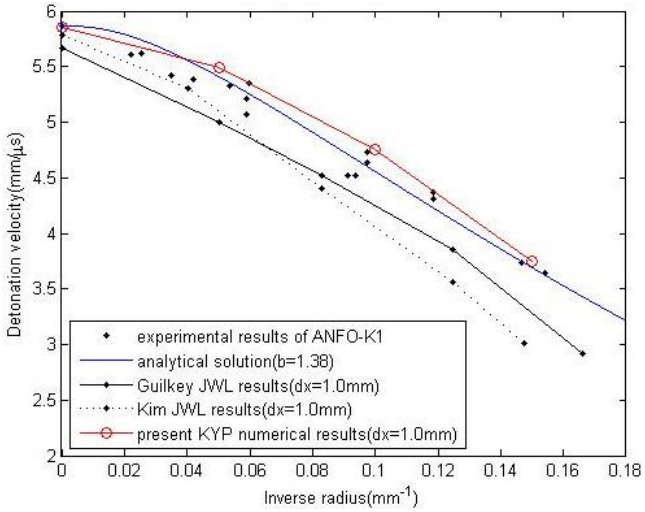

Figure 8. Size effect curve for ANFO-K1 explosive. Experimental(dot), analytical(line), and numerical(present : KYP, Kim[8], Guilkey[9]) data are presented.

A cylindrical chare of ANFO-K1 with 10 cm in length was impacted on one end at 300 m/s. The subsequent pressure rise exceeded the threshold of initiation of a reaction. Figure 7 shows pressure profile showing the curvature of detonation front that expands outward into the voids. The pressure range is from 1 (blue) to 10 (red) GPa. Detonation wave accelerates until t_2, and it reached steady state afterwards. Figure 8 depicts the size effect showing detonation velocity versus inverse radius. Here, KYP model is shown a good agreement with both experimental and analytical data, and preferably a better agreement than the JWL results [8,9] when mesh size of 1.0 mm is used.

3 Conclusions

A pressure-based reaction rate model aimed at accurately simulating the detonation response of high explosives and propellants subjected to an external impact are proposed. Physical approach for determining the free parameters of a KYP model is also discussed. The proposed reaction rate model preserves the physical meaning of conservation law, and has potential to overcome limitations set by other reactive flow models. A step by step approach to pre-determine the four unknowns of the model, namely *b, G, a, I*, is presented before conducting a full simulation of a complex SDT process involving a rate stick test of ANFO-K1.

4 Acknowledgment

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