Modelling of Detonation in PBX 9502 using a Mixture Model Stiffened-Gas Equation of State

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1 Introduction

Numerous experiments in the last 60 years have shown the existence of inherent three-dimensioanl structures in gaseous detonation waves and the idealized structure of detonation waves, in gaseous mixtures, is thus known to be unstable. [1] Comparatively, very little is known about the structure of detonation waves in solid explosives. Experimentations are rendered extremely difficult by the high pressures (30–60 GPa) and fast timescales ($\ll$ 1ns) in such systems. It is thus of interest to try to infer some of the properties of solid explosives, in this case PBX-9502, from mathematical models.

The linear stability analysis can give an indication of the stability of the wave. Until now, simple models have been employed, such as single-phase perfect gas models with $\gamma = 3$. The perfect gas model has the disadvantage of predicting a very low sound speed in the solid reactants, which leads to unphysical detonation wave Mach numbers. More recently, Short et al. [2] looked at the stability of a single-phase, stiffened-gas equation of state, model. Both models suffer from a limited number of free fitting parameters, thus limiting the number of different parameters that can be matched, such as the von Neumann state, the detonation velocity and detonation pressure and shock Hugoniot data.

In the present study, we expand on this work to look at the characteristic of a two phase mixture model where each phase is represented by a stiffened-gas equation of state. The chemical model used is a two step reaction mechanism with varying timescales, to mimic the two heat release timescales present in PBX-9502.

2 Equation of State and Chemical Model

An incomplete equation of state consisting of a mixture of two stiffened-gas phases is used. Each phase's incomplete equation of state is given by

$$e(P, v_i) = \frac{(P + A_i)v_i}{\Gamma_i} \tag{1}$$

where v_i represents the specific volume of the particular phase. One phase represents the solid reactants, while the other represents the high pressure and high density gaseous products. The closure condition used is that of pressure and temperature equilibrium. Using this closure condition, one can derive an incomplete equation of state in terms of the mixture-averaged pressure, P, and specific volume, v. The global heat release, Q, is substituted in place of initial energy parameters akin to enthalpies of formation. Also, as a consequence of the temperature equilibrium, the specific heat at constant volume has to be introduced for both phases. The total number of free parameters is then 6, namely $A_g, A_s, \Gamma_g, \Gamma_s, Q$ and $C_{v,g}/C_{v,s}$, as only the ratio of the specific heats is required.

All the parameters are constants. The parameters of the solid phase, Γ_s, A_s, are selected to match:

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1. the quasi-linear slope of the reactant's shock Hugoniot curve;
2. the initial sound speed of the reactants.

The parameters of the gas phase, Γ_g, A_g and Q, are selected to approximate:

1. CJ velocity for a planar 1-D steady wave;
2. CJ pressure for a planar 1-D steady wave;
3. overdriven shock Hugoniot curve.

Two possible sets of fitting parameters are calculated. One enforces the CJ velocity and pressure to match exactly, at the expense of the overdriven shock Hugoniot data, which can only be approximated, but not matched exactly. The second set of fitting parameters match the shock Hugoniot data much more closely, but produce errors in CJ velocity and pressure of the order of 12% and 20% respectively. Possible fitting parameters are shown in table 3. The shock Hugoniot data is shown in figure 1 along with the fits to that data from the present model.

The ratio of specific heats is estimated by an educated guess. We use the high temperature Debye limit (Dulong-Petit law) and approximations of the specific heats of different gases at different temperatures to estimate the ratio of the two specific heats. Estimates from previous studies were used as reference, for example [3]. The final selected value is

$$\frac{C_{v,g}}{C_{v,s}} = 0.6. \tag{2}$$

While it has recently become popular to use the ignition and growth (IG&G) model or a close derivative thereof, as a chemical model for solid explosives, we select here a simpler choice. We forego the capacity of the IG&G kinetics to model hot spot contributions to the propagation of the wave for a bulk burn model. We employ a two-step kinetic model with both steps releasing a certain fraction of the total heat release on different timescales,

$$\begin{aligned} A &\rightarrow B \\ B &\rightarrow C \end{aligned} \tag{3}$$

with A representing the solid explosive reactants, B representing some intermediate mixture and C representing the final gaseous products. The first rate is pressure dependent while the second rate is state independent. Note that both species B and C are assumed to have the same thermodynamic properties.

The two step mechanism mimics the kinetics of PBX 9502, in which most of the energy is released rapidly and thus close to the front, while a small portion of the energy is released on a longer time scale, associated with the clustering of carbon particles. [4] The complete model thus consists of the incomplete equation of state

$$\begin{aligned} e(P,v,Y_i) - e_0 - \left[1 - Y_A - f_q Y_B\right] Q = (1-Y_a)\frac{(P+A_g)v}{\Gamma_g}\frac{1}{\xi} + \frac{Y_a}{\xi} v \times \\ \times \frac{P + P\Gamma_g + A_g}{P + P\Gamma_s + A_s}(P + A_s)\frac{C_{v,s}(1+\Gamma_s)}{C_{v,g}\Gamma_g(1+\Gamma_g)}, \end{aligned} \tag{4}$$

where

$$\xi = (1 - Y_A) + \left(\frac{P(1+\Gamma_g) + A_g}{P(1+\Gamma_s) + A_s}\right)\frac{C_{v,s}}{C_{v,g}}(Y_A)\frac{(\Gamma_s+1)\Gamma_s}{(\Gamma_g+1)\Gamma_g}, \tag{5}$$

	Γ_s	A_s(GPa)	$Gamma_g$	A_g(GPa)	Q(MJ/kg)	$C_{v,g}/C_{v,s}$
CJ State Enforced	1.62	6.51	1.938	0	1.76	0.6
Overdriven Hugoniot Enforced	1.62	6.51	3.035	27.3	4.18	0.6

Table 1: Thermodynamic parameters used in the mixture model of PBX 9502.

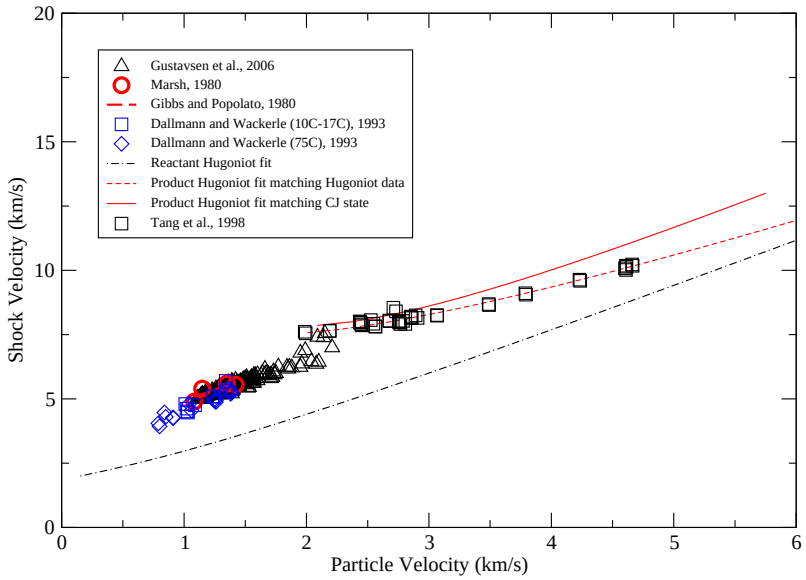

Figure 1: Shock Hugoniot data for PBX 9502 and the corresponding fits of the present model.

and of the chemical model

$$r_1 = k_A Y_A^{\mu} (P/P_{ref})^n, r_2 = f_r k_A Y_B^4 \quad (6)$$

$$\frac{DY_A}{Dt} = -r_1, \frac{DY_B}{Dt} = r_1 - r_2, \frac{DY_C}{Dt} = r_2. \quad (7)$$

The parameters in the chemical model, k_A, μ, n, f_r and f_q, are fitted against VISAR and wave velocity vs̀curvature data. Note that P_{ref} is an arbitrary constant used only for scaling.

3 Analysis

The linear stability analysis is performed to determine the characteristics of the present model and the influence of the different parameters. This model is also integrated in a CFD code to validate the results.

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