Equation of state for detonation product gases

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Abstract. Based on the empirical linear relationship between detonation velocity and loading density, an approximate description for the Chapman-Jouguet (*CJ*) state for detonation product gases has been presented. Assuming that the Grüneisen parameter is a function only of volume, we obtained the Grüneisen parameter along *CJ* states. Thermodynamic identity between the Grüneisen parameter and another non-dimensional material parameter *R* used in the Rice-Walsh type equation of state introduced by Wu and Jing can be used to derive the enthalpy-pressure-volume equation of state for detonation gases. Behavior of this parameter *R* as a function of pressure is calculated and revealed that their change with pressure is very gradual and seems to approach a finite value with decreasing pressure. Release isentropes from *CJ* states of several initial density detonation of PETN is shown.

1. Introduction

It is well known that detonation velocity and loading density of high explosive exhibits linear relationship for various explosives. Authors have proposed an approximate theory of predicting Chapman-Jouguet (*CJ*) parameters based on this empirical law. We have shown that Grüneisen parameter for detonation product gases can be estimated as a function of *CJ*-volume by combining the approximate theory with pressure measurement, etc. [1, 2].

Wu and Jing and their group have proposed a simple theoretical model to predict shock Hugoniot for porous solids [3]. Their model was based on an equation of state (EOS) in terms of pressure, volume and enthalpy, i.e., the Rice-Walsh type EOS [4]. In their EOS discussions, a new non-dimensional material parameter *R* is defined instead of the Grüneisen parameter in the Grüneisen EOS.

We are developing enthalpy-based EOS in order to apply it to numerical simulations of detonation wave propagation, where EOSes of reactant and reacted products are described by Rice-Walsh type EOS, and reactant-reacted products are described by simple mixture rule with pressure equilibration. Use of pressure as an independent variable instead of volume or density together with pressure-based reaction modelling may speed up the calculation.

In this paper, formulation using the parameter *R* for detonation product gases to transform the independent variable from specific volume to pressure.

2. Envelope Approximation and the Grüneisen Equation of State

Empirical relationship between detonation velocity of condensed phase high explosive and initial density can be expressed as

$$D = j + k\rho_0, \tag{1}$$

where D, ρ_0, j, and k denote the detonation velocity, the initial density, material parameters obtained empirically. Since the detonation velocity determines the slope of Rayleigh line, equation (1) gives a group of Rayleigh lines for an explosive. Figure 1 shows several Rayleigh lines for PETN with different initial density states together with measured detonation pressure. Figure 1 shows that an envelope function for group of Rayleigh lines may give good approximation of *CJ*-state parameters, since detonation velocity can be measured in high precision and *CJ* state must be on the Rayleigh line [1, 2].

Envelope function can easily be obtained by combining equation (1) with conservation conditions, and is given by

$$p_{CJ} = \frac{\rho_0 D^2}{2(1+\phi)}, \tag{2}$$

and

$$v = v_0 - \frac{v_0}{2(1+\phi)}, \tag{3}$$

where a parameter ϕ denotes a material parameter relating to the slope in equation (1).

$$\phi = \left(\frac{\partial \ln D}{\partial \ln \rho_0}\right)_{\varepsilon_0} = -\left(\frac{\partial \ln D}{\partial \ln v_0}\right)_{\varepsilon_0} = \frac{k\rho_0}{D}. \tag{4}$$

where the derivative is defined by assuming the initial internal energy being constant.

Figure 2 shows the detonation pressure as a function of initial density calculated by envelope function. Detailed analysis showed that envelope function slightly underestimates the real detonation pressure. Authors reached the conclusion that the difference between the real *CJ* state and the envelope approximation are found from the analytical investigation, and it is shown by using the Jones-Stanyukovich-Manson (*JSM*) relation [5]

$$\Gamma = \frac{\gamma(\gamma - 1 - 2\phi)}{\gamma - \phi}, \tag{5}$$

This equation is derived by the discussion of detonation velocity dependence on initial density, initial internal energy and initial pressure [5]. In Eq.(5), Γ and γ denote Grüneisen parameter and adiabatic index, respectively, and are defined by

$$\Gamma = v\left(\frac{\partial p}{\partial \varepsilon}\right)_v, \tag{6}$$

$$\gamma = -\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_S, \tag{7}$$

Further analysis showed that envelope approximation is reproduced by neglecting the contribution of the Grüneisen parameter to the EOS and gives a system of differential equations for the Grüneisen parameter. This system of equations can be solved by combining Grüneisen EOS with *JSM* relation and with one cylinder expansion data in JWL form for giving release isentrope from *CJ* state [1]. This calculation procedure has been published elsewhere [1].

Figure 3 shows the calculated *CJ* volume dependence of the Grüneisen parameter and adiabatic index. In this calculation, the Grüneisen parameter or other parameters are assumed to be a function only of the specific volume.

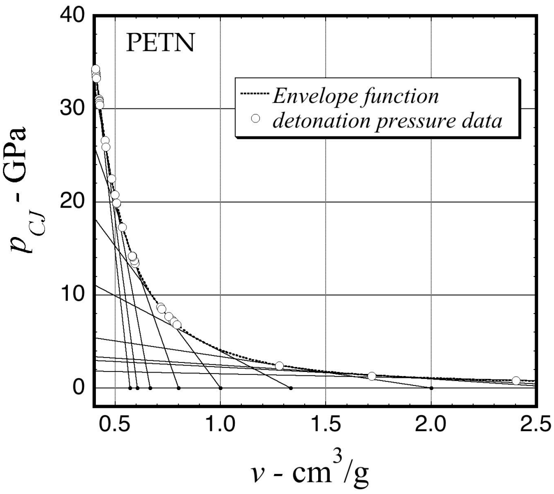

Figure 1 Group of Rayleigh lines and envelope function for PETN high explosive.

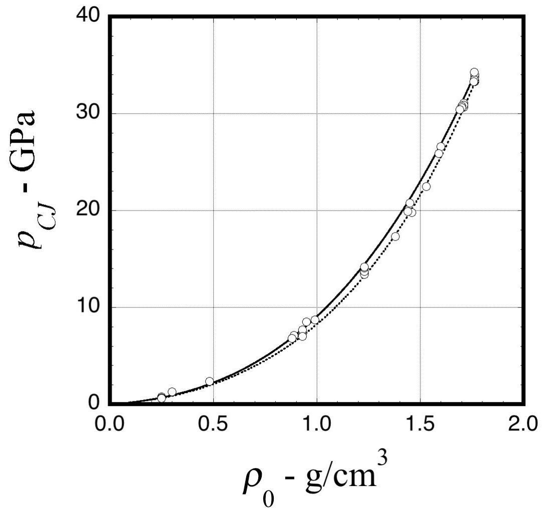

Figure 2 P_{CJ}-ϱ_0 plot for PETN. Dotted line shows the envelope approximation while solid line the Γ-corrected CJ state curve.

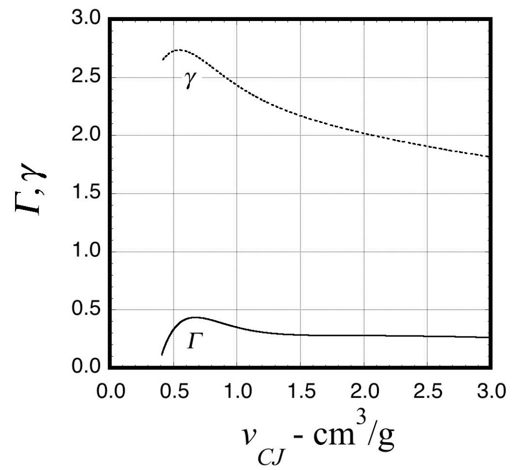

Figure 3 Grüneisen parameter and adiabatic index as a function of volume for PETN.

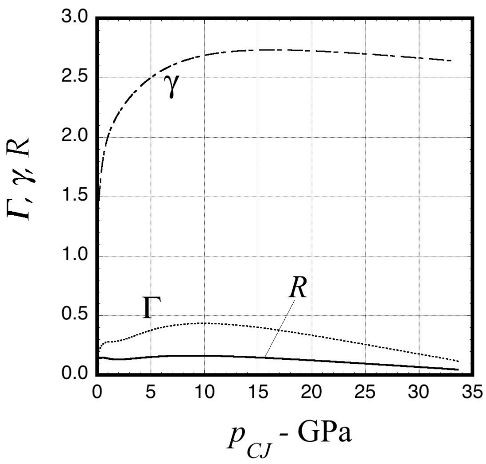

Figure 4 Pressure dependence of the Grüneisen parameter, adiabatic index and the Rice-Walsh parameter for PETN.

3. Formulation of the Rice-Walsh type EOS

In this section, we will try to reform detonation gas EOS of the Grüneisen form to Rice-Walsh EOS [4]. In the Rice-Walsh EOS, a non-dimensional parameter R is related to the Grüneisen parameter as

$$\left(\frac{\partial v}{\partial h}\right)_p = \frac{R}{p} = -\frac{\Gamma}{v\left(\frac{\partial p}{\partial v}\right)_S}\ , \tag{8}$$

or

$$R = -\frac{p\Gamma}{v\left(\frac{\partial p}{\partial v}\right)_S} = -\frac{\Gamma}{\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_S} = \frac{\Gamma}{\gamma} \ . \tag{9}$$

From equation (9), the parameter R is simply the ratio of the Grüneisen parameter and adiabatic index.

Figure 4 shows calculated R as a function of pressure with the Grüneisen parameter and the adiabatic index for PETN. It must, however, be very careful that the R is assumed to be a function only of pressure and not of volume. In figure 4, horizontal axis is not pressure but *CJ* pressure, since R must be evaluated at each *CJ* state. One may also note that the relation between the low-pressure value of Γ and γ does not approach to the value of ideal gas relationship. This calculation will contain errors for extremely low pressure region, since detonation of condensed phase explosive for very low density may not be described by Eq.(1).

In order to formulate the Rice-Walsh type EOS, an isentrope releasing from the *CJ* state reached by the detonation of TMD of PETN is selected as a reference compression curve. In this case, Rice-Walsh EOS can be written as

$$v = v_r(p) + \frac{R(p)}{p}\left[h - h_r(p)\right], \tag{10}$$

where $v_r(p)$ and $h_r(p)$ are an isentrope function released from the *CJ* state by the detonation of TMD of PETN.

4. Calculation of Release Isentropes by Rice-Walsh EOS

We will start the discussion by rewriting equation (10) in the form

$$\left(\frac{\partial h}{\partial p}\right)_S - \frac{R(p)}{p}h = v_r(p) - \frac{R(p)}{p}h_r(p) = F(p), \tag{11}$$

where volume is replaced by the partial derivative of enthalpy. Since the differentiation is made with isentropic condition, any isentrope, $v(p,S)$ satisfy the same differential equation. Difference in this isentrope from reference isentrope satisfy the following equation

$$\left(\frac{\partial \Delta h}{\partial p}\right)_S - \frac{R(p)}{p}\Delta h = 0\ , \tag{12}$$

where

$$\Delta h = h - h_r(p)\ . \tag{13}$$

Equation (12) has a formal but general solution

$$\Delta h = C(S)\Theta(p), \tag{14}$$

with

$$\Theta(p) = \Theta(p_0)\exp\left[\int_{p_0}^{p}\frac{R(p)}{p}dp\right], \tag{15}$$

where entropy function $C(S)$ is an integration function. Equation (10) is now written as

$$v = v_r(p) + \frac{R(p)}{p}\Theta(p)C(S). \tag{16}$$

We have calculated three release isentropes for PETN with three different initial density, since JWL parameters for these isentropes are available by cylinder test. We already have function $R(p)$ in figure 4, and can be integrated with pressure to give $\Theta(p)$. Strategy to calculate an isentrope is, (i) determine $C(S)$ for the starting CJ state data, and (ii) with decreasing pressure, equation (16) gives the volume at that pressure. Figure 5 shows calculated release isentropes for PETN from 22, 14 and 6.2 GPa detonation. Value of $C(S)$ for each detonation increases with decreasing detonation pressure indicating larger entropy production for lower detonation pressure.

Discrepancy between theory and well-collimated cylinder test results indicate the precision that parameter R is a function of pressure but has slight entropy dependence. However, it must be safely said that the entropic dependence of the parameter is not very large.

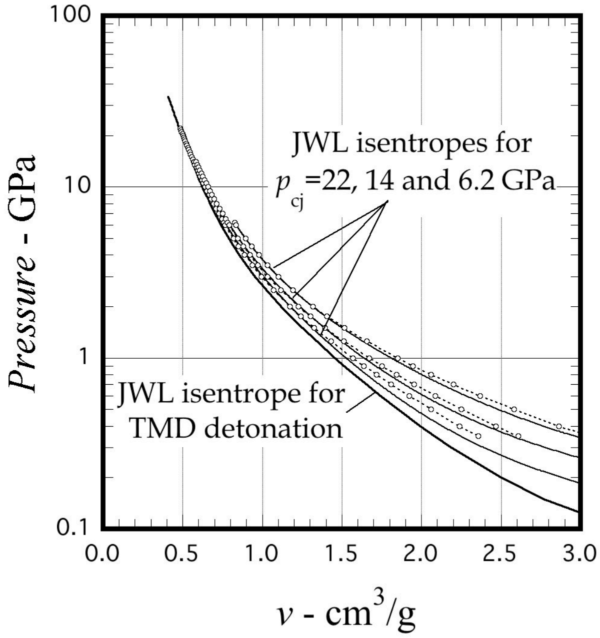

Figure 5 Release isentropes for low initial density detonation of PETN. Isentropes are calculated by equation (16).

5. Conclusion

We have formulated Rice-Walsh type equation of state for detonation gases in terms of volume and enthalpy with pressure as an independent variable. This is made by using envelope approximation based on the initial density dependence of the detonation velocity. Release isentropes have been calculated and compared with available data for PETN.

References

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