Article

Prediction of C-J state for high explosive based on the initial density dependence of detonation velocity

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This paper presents a simpler method to predict the C-J state of high explosive based only on the initial density dependence of detonation velocity. To predict C-J pressure by this method, for example, we need the slope of the detonation velocity as a function of initial density.

We first define a succession of C-J states on a pressure-volume-energy state surface. Available data set of the initial density dependence of the detonation velocity gives a collection of Rayleigh lines. The C-J state curve can be approximated by an envelope function of Rayleigh lines. This envelope function can be given by a simple mathematical function. Present approximation gives an exccelent description of the C-J state curve especially on p-v plane. Since the detonation velocity is a sensitive function of initial density, and the measurements can be made very accurately, this method may serve a handy and relatively easier method to estimate the C-J state for high explosive. The physical meanings of the approximation is discussed in thermodynamic terms, which revealed that it is the approximation that the Grüneisen parameter is set to zero.

1. Introduction

One of the important research topics in the understanding of the detonation processes of the condensed explosive charge is the equation of state (EOS) for the detonation product gases.[1-4] Pressure range treated in this field is several to several tens of GPa depending upon the explosive charge and on the loading density. The high pressure high temperature states attained by the product of detonation gases can be studied both in the microscopic theory[5-8] and in the semi-empirical theory.[9-12] Imporatnce of the macroscopic and phenomenological approaches is recognized, since they provide convenient tool to use in a computer code for the numerical simulation[3] of the detonation phenomena.

There still need a simple closed form EOS function, which is proved to be valid with practical accuracy. For example, to simulate the shock to detonation transition (SDT) process, EOSes of the detonation gases and unreacted material, and a physical model of shock-induced initiation are required. None of these have known precisely for any kind of energetic materials. Among these issues, information of the EOS of the detonation gases may be the most reliable than the other two issues.

This paper presents another way of determining the usable EOS function based on the minimum set of experimental data on the detonation velocity and some others, explained later. The present method gives an EOS, which is fully compatible with the experimental measurement within the experimental error. Based on the close examination of the Jones-Stanyukovich-Manson relation[13, 14], the role of the Grüneisen parameter is discussed. In the course of this process, very simple

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approximation to the C-J states is formulated. Then the error contained in the estimated functional form of EOS is discussed.

2. Envelope function approximation

Detonation velocity is a parameter which can be measured in highest precision among various parameters specifying the detonated thermodynamic state. Emprically, the detonation velocity D is found to be a linear function of loading density ρ_0, namely,

$$D = j + k\rho_0 \,, \qquad (1)$$

where j and k denote material parameters determined for an explosive and for an interval of the initial density.[1, 15] In case of PETN, for example, the value of them are

$j = 2.14,\ k = 2.84 \quad \rho_0 < 0.37,$

$j = 1.82,\ k = 3.7 \quad 0.37<\rho_0<1.65,$

$j = 2.89,\ k = 3.05 \quad 1.65 < \rho_0,$

That is, the relation is given by three linear segments, although the ranges in the initial density of lowest and highest are very small. Kerley[16] has pointed out that at least the deflection at ρ_0 = 1.65 g/cm3 might be explained by the production of HCOOH, but the influence is gradual and has no sharp jump in the slope. Defelction at the lower side may have some problems of measurements and scatter of the data due to the measurement method. It may have a plausible possibility that the relationship between detonation velocity and initial density is almost linear but very complicated.[17] As shown later, the slope k of the relationship plays an important role for the formulation of EOS, and due to the reason explained above, there is no rigid physical reason to adopt a three segment linear relationship given above. Rather we can show that the break in the slope k gives a break in some physical variables, like the detonation pressure. We will adopt the following simple linear relation in the following analysis,

$$j = 1.8482,\ k = 3.6511. \qquad (2)$$

Parameters used here are close to the widest range of the density above. Figure 1 shows the D-ρ_0 relationship described by the parameters in Eq.(2) and several of experimental data.

If one knows the value of the initial density of the high explosive and the correspoding detonation velocity, one can plot the so-called Rayleigh line in the p-v plane. The C-J state should be on this line. Rayleigh line in p-v plane is described as

$$p_{CJ} = -\rho_0^2 D(\rho_0, \varepsilon_0)^2 [v - v_0] \,, \qquad (3)$$

where p, v, and ε denote the pressure, the specific volume and the specific internal energy, respectively, and the suffix 0 denotes the value at the initial state. In Eq.(3), the detonation velocity $D(\rho_0, \varepsilon_0)$ is realized by the initial state specified by the initial density and specific internal energy, (ρ_0, ε_0) or the initial volume and specific internal energy, (v_0, ε_0). According to the C-J hypothesis, Rayleigh line touches the Hugoniot compression curve at the C-J point, and the slope of the Hugoniot curve at the C-J point is equal to that of an isentrope centering the C-J point. If we have a collection of data on the detonation velocity as a function of initial volume or initial density, it is a collection of Rayleigh lines, which covers the accessible thermodynamic states in p-v plane. Since the thermodynamic states on each Rayleigh line has a physical meaning especially on the C-J state, a collection of Rayleigh lines corresponds to a collection of isentropes, which is meaningful only in a narrow region near the C-J states.

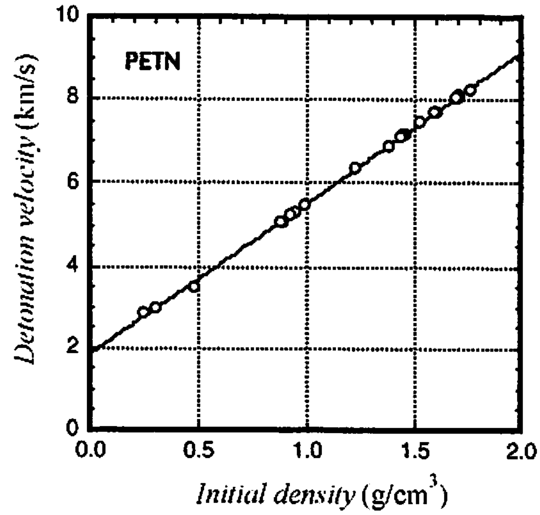

Fig. 1 Initial density dependence of detonation velocity for PETN. Open circles show data with additional data of C-J pressure.

Figure 2 shows the collection of Rayleigh lines on p-v plane drawn by using the experimental

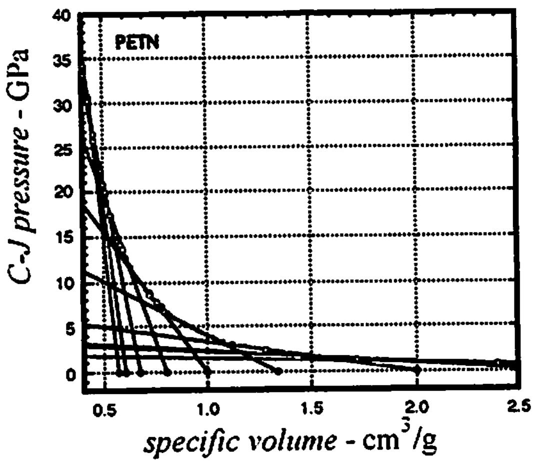

Fig. 2 Rayleigh lines with different initial volume, and the envelope function for PETN. Open circles are experimental data.

values of detonation velocities for PETN. C-J pressure data points given by Hornig et al[18] are also shown in the same plot. As is seen clearly, experimental pressure volume points are naturally on their Rayleigh line, and they seem to be on a curve of the envelope of the collection of Rayleigh lines. This looks a very good approximation for this data. We checked other explosive data and found that the envelope function of Rayleigh lines on *p-v* plane gives an excellent approximation to the C-J states on the plane.

Functional form of the envelope function of Rayleigh lines can be derived easily as

$$v = v_0 - \frac{v_0}{2\left[1+\left(\frac{\partial \ln D}{\partial \ln \rho_0}\right)_{\varepsilon_0}\right]} \tag{4}$$

$$p_{CJ} = \frac{\rho_0 D^2}{2\left[1+\left(\frac{\partial \ln D}{\partial \ln \rho_0}\right)_{\varepsilon_0}\right]} \tag{5}$$

where an important parameter to describe this relationship is the following non-dimensional parameter α

$$\alpha \equiv \left(\frac{\partial \ln D}{\partial \ln \rho_0}\right)_{\varepsilon_0} = \frac{\rho_0}{D}\left(\frac{\partial D}{\partial \rho_0}\right)_{\varepsilon_0} = \frac{k\rho_0}{D} \tag{6}$$

where the last expression is obtained by inserting the empirical linear relation, Eq.(1). We will stress here that this parameter α can be estimated only through the measurement of the detonation velocity. Since this parameter is determined by the slope of the empirical relationship, there still needs a reliable data set of the detonation velocity on different initial densities. Present approximation, therefore, needs a precision of this parameter α. Error from the precision of α is discussed later. Other parameters on the C-J state

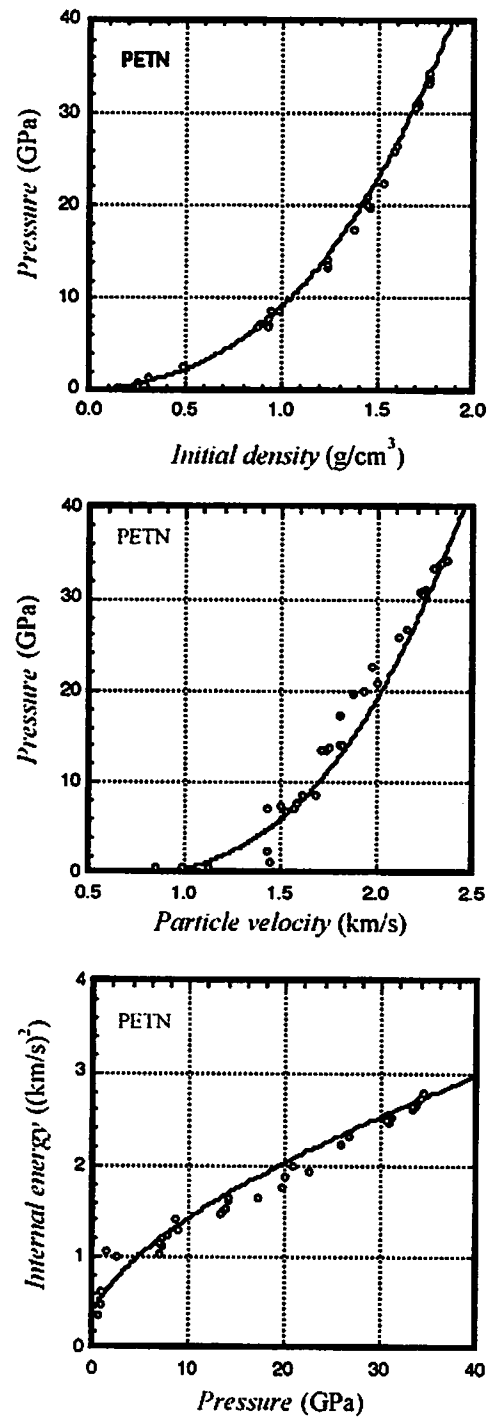

Fig. 3 C-J pressure vs initial density relationship for PETN. Dotted line is an envelope (Γ=0) approximation.

can be obtained through the jump conditions for the detonation wave front, which then gives relationships between other variables on C-J state.

Figure 3 shows the predicted C-J pressure, particle velocity and internal energy for PETN are shown. Agreement of the data with the theory depends on the combination of variables as shown in Fig. 3. Compared with these plots, it is noticeable that the agreement of pressure-volume relationship shown in Fig. 2 is excellent. Data scatter is also dependent upon the variable combination. Even so, the agreement of the theory with the experimental data is good. Small discrepancy between theory and experiment seems to be somewhat systematic. This may have some deep physical reason. We will discuss this later.

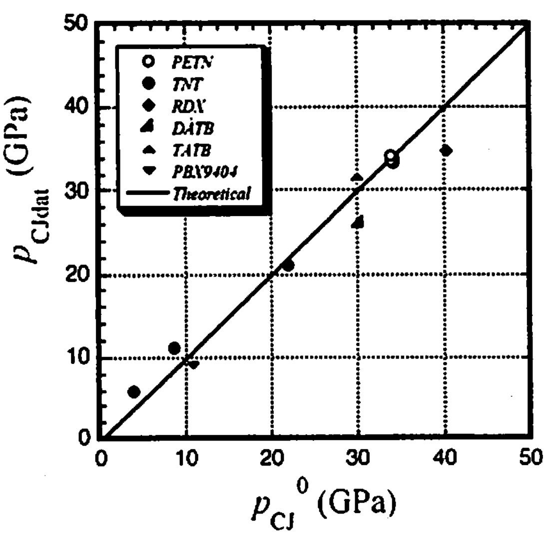

Fig. 4 Comparison of the predicted detonation pressure, p^0_{CJ} with the measured data, p_{CJ}.

Figure 4 shows the comparison of the measured C-J pressure with the present approximation for various condensed explosives. Most of the measured pressure is somewhat lower than the predicted value as seen in Fig. 3. Later consideration shows that some data larger than the prediction can be understood in one of following three possibilities. One is that C-J assumption is violated in the sense that the state at the wave front reaches no complete thermodynamic equilibrium. The other possibility is that chemical reaction does not finished at the front. Experimental error contained in the data is within the difference in the pressure value. In other words, larger data is physically prohibited for C-J states. Precision of the present approximation will be discussed in more detail in a later section.

3. Jones-Stanyukovich-Manson (J-S-M) relation and the Gr・eisen parameter

It is well known that the thermodynamic analysis of the change in the detonation velocity with changing the initial density or the initial internal energy leads to the so-called Jones-Stanyuko-vich-Manson (J-S-M) relation,[13, 14]

$$\Gamma = \frac{\gamma(\gamma - 1 - 2\alpha)}{\gamma - \alpha} \tag{7}$$

where Γ and γ denote the Grüneisen parameter, and the adiabatic index for an isentrope passing through the C-J state. These parameters are defined as

$$\Gamma = v\left(\frac{\partial p}{\partial \varepsilon}\right)_v \tag{8}$$

$$\gamma = \left(\frac{\partial \ln p_{CJ}}{\partial \ln \rho}\right)_S = \frac{\rho_0 D^2}{p_{CJ}} - 1 \tag{9}$$

All of the parameters, Γ, γ, and α are state variables, and a function of initial density ρ_0 or volume v_0. The envelope approximation developed in the previous section is proved to be the approximation that the value of the Grüneisen gamma Γ is equal to zero. This assumption is then proved to be equivlent to the assumption that the slope of the adjacent C-J states with different initial volume is equal to that of an isentrope passing through the state. The difference of the C-J pressure data and that of envelope approximation can be seen in Fig. 4.

The formulae of Eqs.(4) and (5) can be derived by putting Γ=0 in the J-S-M relationship, i.e,

$$\gamma_0 = 1 + 2\alpha \tag{10}$$

Using this result to look at the comparison of the approximation with the experimental data in Fig. 3, one may note that the slight difference stems from the contribution from the Grüneisen parameter. The magnitude of the contribution, however, is relatively small. To achieve higher precision prediction of the detonation properties, we have to include the effects of the Grüneisen gamma to the theoretical analysis or to obtain precise experimental data other than the detonation velocity in very high precision high than a few %. The correction, however, seems modest as is understood by the present analysis.

4. Conclusion

We have developed a simple approximation for the C-J state variables based on the detonation velocity measurement with different initial density. The present model is found to be an approximation of Grüneisen gamma equal to zero.

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