Research paper

Numerical simulations of detonation phenomena in PETN by systematic equation of state for detonation products

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Abstract

The general equation of state (EOS) for detonation products of PETN has been constructed using the Gruneisen coefficient as function of density and the isentrope line for the theoretical maximum density of PETN. Although JWL equation of state require each parameter set for initial density, the constructed EOS with one parameter set can be applied for arbitrary initial density. The EOS has been examined by performing numerical simulations of the propagation process of a detonation wave for various initial densities of PETN. The simulations results were in agreement with the wide range of published experimental data for various initial densities. The sensitivities of the numerical results to the Gruneisen coefficient were also investigated. The constructed EOS is expected to a powerful tool, for numerical modeling of the initiation process in PETN-type energetic materials.

Keywords : EOS, DETN, gruneisen coefficient, JWL

1. Introduction

The numerical simulation of detonation phenomena including the initiation process in energetic materials is important from the viewpoints of both the explosive safety and the effective application of detonation energy. In macroscopic hydrodynamic computations, the reacting energetic material is regarded as a mixture of the solid reactants and detonation products ; thus, simulations of the initiation phenomena require at least the initiation model together with the equations of state (EOSs) for both the reactants and the detonation products and a mixture rule for the reacting explosive. We have studied the initiation phenomena of energetic materials and investigated the equation of state and the initiation model to remove the uncertainties encountered in the simulation of the initiation process[1)-6)]. In this paper we have constructed and discussed a very useful EOS for detonation products.

Many types of EOS for detonation products have already been proposed[7)-10)]. One of the most useful EOS for engineering purposes is the Jones-Wilkins-Lee (JWL) EOS [11),12)], which is an empirical EOS. The Gruneisen-type EOS for detonation products is frequently employed in hydrodynamic simulations of detonations and explosion phenomena. One major EOS treatment in the hydrodynamic simulation is performed as follows. The isentropic line, which passes through the Chapman-Jouguet (C-J) point, is selected as the reference line, and the Gruneisen parameter is assumed to be constant. The necessary data can be obtained by a cylinder expansion test [13)], which is employed to estimate the JWL parameters. The advantage of the JWL EOS is that a wide range of detonation properties and parameter sets for the EOS of energetic materials have been published. In addition, because this treatment is convenient, the well-known EOS code for

detonation products, Cheetah, has an option that outputs the above-mentioned JWL EOS parameter set.

Detonation velocity and the sensitivity of initiation for condensed phase energetic materials depend not only on the constituents of material but also the initial density. PETN is a well- known explosive material that has a linear relationship between detonation velocity and initial density and has been studied by many researchers [14)-16)]. Since various published data including the initiation properties of PETN are available, it is meaningful to select a PETN as the object of study when modeling the initiation process. The JWL EOS also requires a specific parameter set for any initial density of PETN. For example, we can find parameter sets for PETN detonation products with densities of 0.88, 1.26, 1.5 and 1.77 g cm^{-3} in Ref. [17)]. On the other hand, with the exception of density of 1.77 g cm^{-3}, EOS parameters for the solid reactants obtained from PETN with the above-mentioned initial densities are not available. This situation indicates that to obtain the parameters for both the solid reactants and the detonation products, new parameters have to be obtained by experiments or by the chemical equilibrium calculation of product species. This problem can be avoided by constructing a systematic EOS in which the parameters are independent of the initial density of PETN. The most important point is that the numerical simulation using this EOS will clarify the effect of the product components on the simulation results of the initiation problem, i.e., one uncertainty can be removed.

If the Gruneisen coefficient, $\Gamma(\varepsilon,v)$ or $\Gamma(v)$, is known together with the reference line, the $\varepsilon-P-v$ surface can be determined as a function of two of the state variables. In a previous paper[1)] we proposed differential equations whose solution gives $\Gamma(v)$ for an EOS of the detonation products of the energetic material. In this paper we have constructed a systematic EOS that only requires $\Gamma(v)$, the isentrope for the detonation products at the theoretical maximum density (TMD), and the current initial density of the energetic material, and we have evaluated the EOS by performing numerical simulations of the propagation of detonation. A similar attempt was performed by Lee and Hornig[18)]. Our approach has following differences. The Gruneisen coefficient is obtained by an original and simpler method, and the applicability of the systematic EOS in the numerical simulations has been consistently evaluated on the basis of the results of numerical simulations.

2. Theory and systematic EOS for detonation products of PETN

The $\varepsilon-P-v$ form of the Gruneisen EOS is expressed as,

$$P=\frac{\Gamma(v)}{v}(\varepsilon-\varepsilon_r)+P_r \tag{1}$$

where the subscript r indicates the reference line, which can be selected any physical reference state. $\Gamma(v)$ is the Gruneisen coefficient. The JWL EOS for the detonation products is constructed by substituting both ε_S and P_s into equation. (1) with ω instead of $\Gamma(v)$. P_s is the isentrope line passing through the C-J point and is expressed as follows ;

Table 1 JWL parameters for PETN of initial density 1.77 g cm^{-3} (Ref. 12).

A(GPa)	B(GPa)	C(GPa)	R1	R2	ω	Eo(MJ/kg)	Pj (GPa)
617	16.93	0.699	4.4	1.2	0.25	5.7	33.5

$$P_S=A\exp(-R_1V)+B\exp(-R_2V)+CV^{-(\omega+1)} \tag{2}$$

V is the ratio of the specific volume of the detonation products to that of the initial energetic material, and the parameters A, B, C, R_1, R_2 and ω are constants determined by the cylinder expansion test and the analysis of data obtained therein. ε_S is also an isentrope line and can be obtained by integrating equation (2). ω corresponds to $\Gamma(v)$, which is assumed to have a constant value that is adjusted to be equal to $\gamma-1$ when $V>10$ in the general JWL treatment. To construct a more powerful EOS and to describe the $\varepsilon-P-v$ surface for the detonation products, $\Gamma(v)$ has to be obtained as a function of the specific volume.

We have developed differential equations that can give $\Gamma(v)$ for an EOS of the detonation products in a previous paper which also gives details of their derivation and a discussion[1)]. When the relationship between the detonation velocity and the initial density of the energetic material is linear, the proposed differential equations require only one C-J pressure value and the pressure-specific volume (P-v) isentrope passing through the corresponding C-J point. At the same time P-v relation at the C-J points are calculated. The following relationship between detonation velocity and initial density has been employed in the integration of the differential equations ;

$$D=1.8482+3.6511\rho_0 \tag{3}$$

$\Gamma(v)$ for the PETN is calculated using the P-v isentrope for the PETN with an initial density of 1.77 g cm^{-3}. Because this density is very close to TMD for PETN, we will call this density the TMD. The parameters for the JWL EOS in this case are shown in Table 1[12)].

Figure 1 shows the relationship between $\Gamma(v)$ and v. In

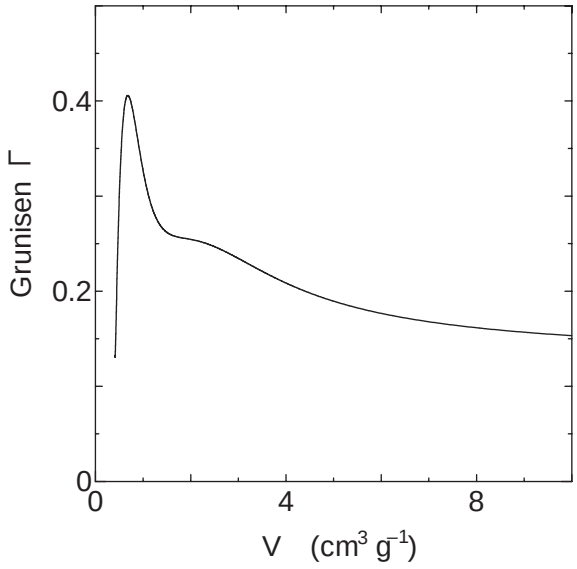


Fig. 1 The relationship between Γ and specific volume for PETN.

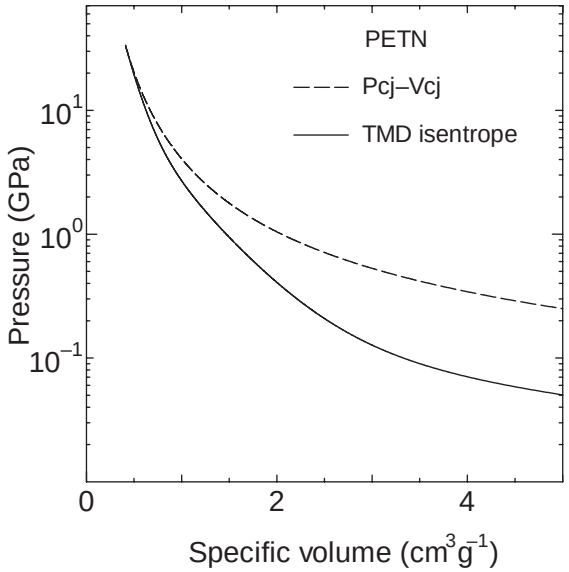


Fig. 2 The p–v line along the C–J points, and TMD isentrope for PETN.

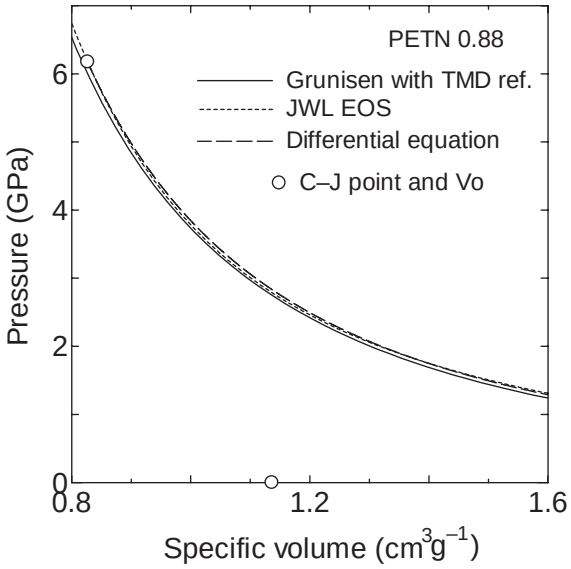


Fig. 3 Isentrope for PETN of 0.88 g cm^{-3} initial density (Parameter of JWL EOS of 0.88 g cm^{-3} PETN ; ref.12).

Table 2 Typical condition for simulation of detonation propagation in PETN.
ρ_0 ; Density of PETN, Vi ; initial velocity, Length of high velocity region ; 1mm
ρ_{i0} ; Density of PETN in initial high velocity region, Length of PETN ; 6cm
*JWL parameter ; Ref. 13, CG1 ; $\Gamma = 0.25$, CG2 ; $\Gamma = 0.45$ in equation (4)

ρ_0 (gcm^{-3})	vj (cm^{3}g^{-1})	ρ_{i0} (gcm^{-3})	Vi (kms^{-1})	Li (mm)	Gruneisen with TMD	JWL*	CG1	CG2
1.77	0.41013	1.77	1	1	○	○		
1.7	0.42708	1.77	1	1	○		○	○
1.65	0.44055	1.77	1	1	○			
1.6	0.45489	1.77	1	1	○			
1.5	0.48632	1.5	1	1	○	○	○	○
1.26	0.57947	1.26	1	1	○	○	○	○
0.88	0.81678	0.88	1	1	○	○	○	○
0.48	1.42718	0.88	0.5	1	○		○	○
0.3	2.20162	0.88	0.5	1	○			
0.25	2.60122	0.88	0.5	1	○		○	○

the numerical simulation by computer code, $\Gamma(v)$ has to be calculated for given v. Instead of the curve fitting, the data set for (v, $\Gamma(v)$) was stored into a same array variable, and the $\Gamma(v)$ was taken from the variable by simple algorithm.

Figure 2 shows the TMD isentrope and the locus of P–v for the C–J points obtained from our differential equations. Because, using this data set for the C–J points and initial densities, the Rayleigh line can be obtained for each initial density, the detonation velocity can be estimated from the slope of the Rayleigh line.

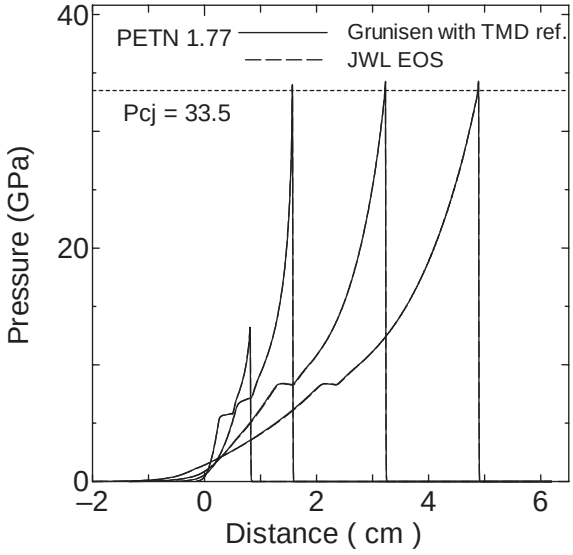
Using the Gruneisen coefficient and the isentrope line for the TMD, the Gruneisen–form EOS can be written as

$$P = \frac{\Gamma(v)}{v}\left(\varepsilon - \varepsilon_S^{TMD}\right) + P_S^{TMD} \qquad (4)$$

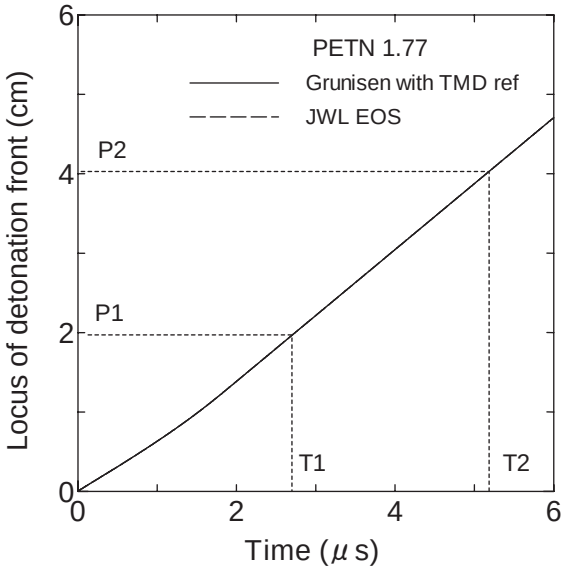
This EOS can be adapted to arbitrary initial density of PETN, and the hydrodynamic code for this EOS requires only the initial density of PETN as the input data. We call this EOS the systematic EOS or the 'Gruneisen with TMD ref.'. Isentrope lines for PETN an initial density of 0.88 g cm^{-3}are shown in Fig. 3. The solid line is obtained by substituting ε_S, which is the JWL isentrope for the 0.88 g cm^{-3} PETN[13], into ε in equation (4).

3. Numerical procedure

The governing equations are the one–dimensional mass, momentum and energy conservation laws, which are solved by the finite difference method. Detonation propagation processes were simulated for various initial densities of PETN using C–J volume burn technique[9]. Because this burn technique employs only the EOS for the detonation products, the results of simulation using this model are suitable for discussing the adaptability of the EOS for detonation processes. The detonation in PETN was triggered by a thin PETN region with high velocity. Typical



(a) Pressure distributions



(b) Locus of detonation front

Fig. 4 The simulations results for TMD case. (P1, P2, T1, and T2 are the points and times for estimating the detonation velocity.)

conditions used in the simulations are summarized in Table 2. Although the simulation of detonation phenomena does not require C−J value, the specific volume at the C−J point is necessary in the C−J volume burn technique. The corresponding C−J volume is also shown in Table 2. All mesh sizes in the calculation were set to 0.05 mm. For comparison, the simulations using JWL EOS were also performed. The sensitivities of the numerical results to Gruneisen coefficient were investigated. To investigate the sensitivity, the cases of constant Γ were simulated by considering the cases Γ= 0.25 and Γ= 0.45, similarly in the study by Lee and Horing[18], but our numerical simulation was employed to confirm not only the detonation velocity but also the waveform of the detonation wave.

Typical results for the TMD case are shown in Fig 4 and Table 3. In the case of the TMD because the simulation results obtained using the systematic EOS are consistent with those with the JWL EOS, the two lines completely overlap. The detonation velocity estimated from the numerical results is shown in Fig. 4 (b) and Table3.

4. Discussion

The relationships between detonation velocity and initial density obtained by the simulations using the systematic EOS and using the JWL EOS are summarized in Table 4. In this table, the detonation velocities estimated using the Rayleigh line and using Equation (3) are also shown. The pressure and specific volume at the C−J points for each initial density are calculated together with $\Gamma(v)$ using the linear relationship between the detonation velocity and initial density. Therefore, detonation velocity, which is obtained using these C−J values and the initial density, must satisfy equation (3). Since the maximum difference between these values was less than 0.04%, the above−mentioned condition is satisfied. In case of the JWL EOS, the detonation velocity was also calculated using the Rayleigh line, and the maximum difference between the simulation results was less than 0.02%. This means that the process of the propagation of detonation wave is precisely simulated by our code. The differences between the velocities obtained by simulations using the systematic EOS and the corresponding Rayleigh line are as follows. For initial densities of 0.88, 1.26 and 1.5 g cm^{-3}, the differences are 1.31, 0.77 and 0.43% respectively. The difference between the detonation velocities for the systematic EOS and the Rayleigh line is slightly greater than that between those obtained using the JWL EOS and the Rayleigh line. It may be considered that even if the relationship between the C−J value and initial density is precisely obtained by the integration of our proposed differential equations, the accurate estimation of the Gruneisen coefficient requires a more precise procedure during numerical integration. As a reference, the differences between the detonation velocities for the systematic EOS and the JWL EOS are 1.6, 1.9 and 2.2% for the above densities, respectively.

Figure 5 shows the relationship between the detonation

Table 3 The estimation of the detonation velocity for numerical simulations of PETN (TMD) P1, P2, T1, and T2 corresponds to those in Fig. 4 (b). Dj is detonation velocity.

EOS	P1(cm)	P2(cm)	T1(μs)	T2(μs)	Dj (m s^{-1})
Systematic EOS	2.002543	4.002594	2.500104	4.91023	0.829853
JWL EOS	2.002544	4.002596	2.471581	4.881707	0.829854

Table 4 The comparisons of detonation velocities among the results obtained by simulation, Rayleigh line and Equation (3) ($D = 1.8482 + 3.6511\ \rho_0$ (3)) unit ; (km s^{-1}), Energetic material is PETN.

EOS	ρ_0 (g cm^{-3})	Simulation	Rayleigh line	Equation (3)
Systematic	0.88	4.995	5.061	5.061
JWL EOS	0.88	5.075	5.074	–
Systematic	1.26	6.397	6.446	6.449
JWL EOS	1.26	6.522	6.524	–
Systematic	1.50	7.293	7.325	7.325
JWL EOS	1.50	7.455	7.454	–

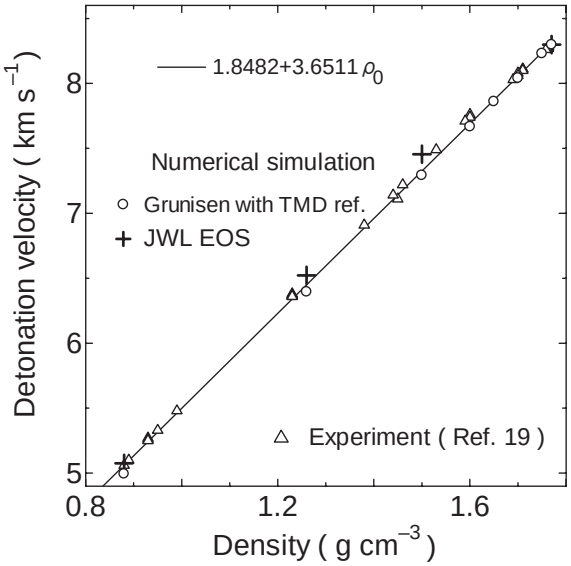


Fig. 5 The relationship between the detonation velocity and Initial density for PETN, (The comparison of systematic EOS, JWL, and published data (Ref.19).)

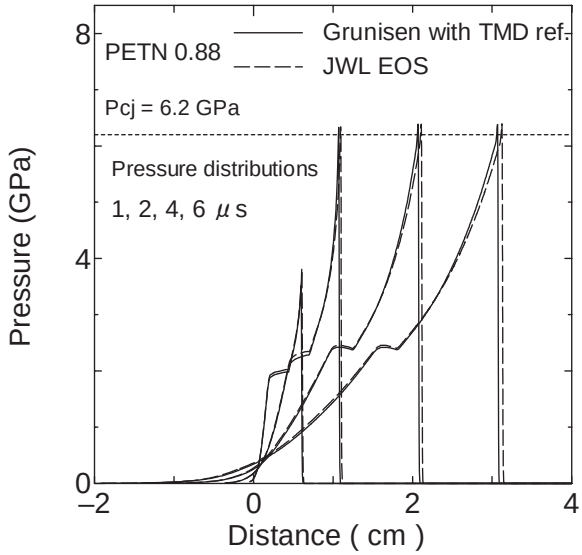


Fig. 6 The comparison of the simulated detonation wave in PETN. (Initial density ; 0.88 g cm^{-3})

velocity and initial density for PETN together with the simulation results. The experimental data obtained by Hornig et al.[19] were also plotted in this figure. Since the result of the JWL EOS for a density of 0.88 lies on the relationship between the detonation velocity and initial density, the result of the systematic EOS at this density has been compared with the JWL EOS result. The propagation processes in PETN with a density of 0.88 g cm^{-3} are presented in Fig. 6. The difference between the detonation fronts obtained from the JWL EOS and the systematic EOS is less than 0.5 mm but the waveforms are almost the same when the detonation front arrived at about 3 cm from the start point. Note that above–mentioned difference of 1.3% is not a serious error in some problems. For initial densities from 0.88 to 1.77g cm^{-3} the results of simulation using the systematic EOS were consistent with the experimental results.

In the case of a low initial density, similar results were also obtained, as summarized in Table5. The detonation velocity obtained using the Rayleigh line was consistent with that obtained by equation (3). As the initial density decreases, the difference between detonation velocities obtained by the simulation and the Rayleigh line increases. At an initial density of 0.25 g cm^{-3},the difference is 1.8 %.

Table 5 The comparisons of detonation velocities in case of low density PETN, simulation (only systematic EOS), Rayleigh line, and Equation (3) ($D = 1.8482 + 3.6511\ \rho_0$ (3)), unit (km s^{-1})

ρ_0 (g cm^{-3})	Simulation	Rayleigh line	Equation (3)
0.48	3.552	3.601	3.601
0.3	2.891	2.944	2.944
0.25	2.710	2.761	2.761

The sensitivity of the numerical results to the Gruneisen coefficient was also investigated. Figure 7 shows the dependence of the detonation velocity of PETN on the initial density. In the case of a high initial density of more than 1.5 g cm^{-3}, the simulation is not sensitive to the Gruneisen coefficient, at least for the detonation velocity and the pressure waveform.

For a density of lower than 1.26 g cm^{-3} the contribution of the Gruneisen coefficient, i.e., the effect of internal energy, increases as density decreases, particularly when Γ= 0.45. In the case of Γ=0.25, for initial densities of 0.88 and 1.26 g cm^{-3} the simulation results were inconsistent with those obtained experimentally however, for initial densities of 0.48 and 0.25 g cm^{-3} the simulation results were consistent with the experiment results. Because Γ is a func-

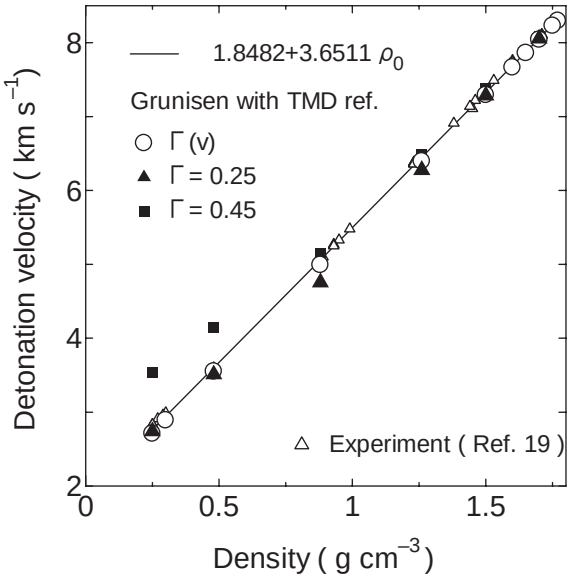


Fig. 7 The dependence of the detonation velocity of PETN on the initial density, (The sensitivity check of the Gruneisen coefficient.)

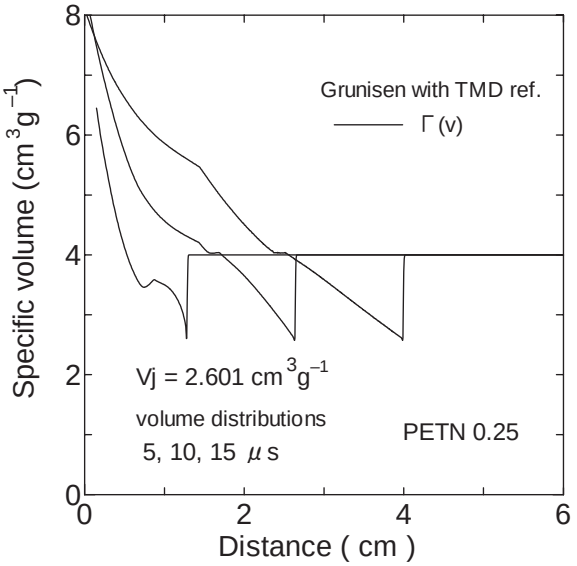


Fig. 8 The simulation result of the propagation of the detonation wave in PETN. (with specific volume distributions, Initial density ; 0.25 g cm^{-3})

tion of specific volume, the propagation process is shown in Fig. 8 in the form of the specific volume distributions. It can be considered that since detonation is a self−sustaining wave, we can only estimate Γ near the detonation front, i.e., the region from the volume at the C−J point to the initial volume. Γ is between 2.6 and 4 in the case of an initial density of 0.25 g cm^{-3}and between 1.4 and 2.1 when the initial density of 0.48 g cm^{-3}. These regions have been plotted in Fig. 9. It can be confirmed that at these regions the calculated value of Γ(v) is about 0.25. The detonation velocities in Table 6 suggest that although the difference is very small, when the initial density of 0.25 g cm^{-3}, Γ= 0.25 may give better results than our calculated Γ(v).

As can be seen in Fig 7 the simulations using the systematic EOS are in agreement with the wide range of experimental results published[19] for various initial densities of PETN. The systematic EOS is expected to a powerful

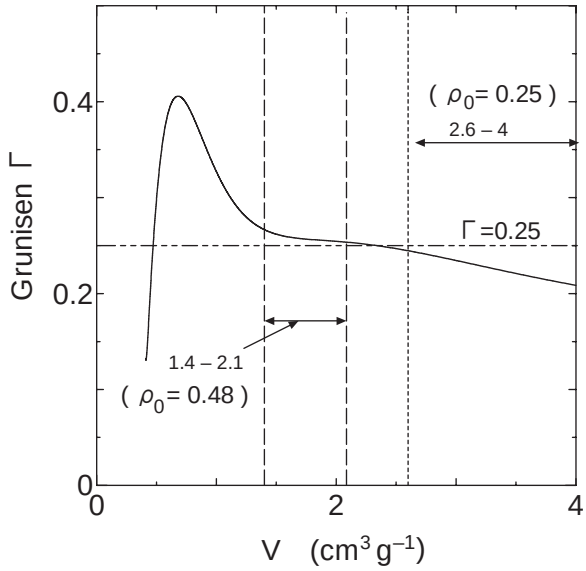


Fig. 9 Function of Gruneisen coefficient for PETN. The regions which have main contribution to calculation results for 0.25 and 0.48 initial density.

Table 6 The detonation velocity obtained by numerical simulations in cases of Γ(v) and Γ= 0.25. (low density region)

ρ_0 (g cm^{-3})	Γ(v)	Γ= 0.25	Equation (3)
0.48	3.552	3.510	3.601
0.25	2.710	2.741	2.761

tool, for numerical modeling of the initiation process in PETN−type energetic materials with a linear relationship between detonation velocity and initial density.

5. Conclusion

An equation of state (EOS) has been constructed for PETN that can be used for an arbitrary initial density. The EOS was evaluated by performing numerical simulations of the propagation of detonation in PETN. The simulations using EOS were in agreement with the wide range of experimental results published for various initial densities of PETN. The constructed EOS is expected to become a powerful tool for numerical modeling of the initiation process in PETN −type energetic materials with a linear relationship between detonation velocity and initial density.

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系統立てられた状態方程式によるPETNの爆轟現象の数値解析

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密度の関数としてのGruneisen係数と理論密度の等エントロピー線を使用して，PETNの爆轟ガスに対する一般的な状態方程式を構築した。JWL状態方程式は初期密度毎にJWLパラメータが必要であるが，本状態方程式は１つのパラメータセットで任意の初期密度に適用可能である。本状態方程式を採用して，種々の初期密度のPETN中の爆轟波が数値解析され，その適用性について調べた。数値計算結果は公表されている種々の初期密度に対する実験結果と比較され，広範囲で一致が確認された。さらにGruneisen係数が計算結果に与える影響が検討された。構築された状態方程式は起爆現象の数値解析的モデリングのための強力なツールになることが期待される。

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