Research paper

Equation of state for detonation product gases compatible with cylinder tests

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Received: February 23, 2018 Accepted: November 21, 2018

Abstract

It is well known that the cylinder tests have been conducted with four different initial densities for PETN (pentaerythritol tetranitrate), and JWL parameters for each test are available, which describe the isentropic release of detonation gases from the estimated C-J (Chapman-Jouguet) state for each initial density. These datasets of $p-v$ isentropes contain information on the equation of state (EOS) of detonation product gases provided that all four detonations can be described by a unique EOS for detonation product gases of the same chemical composition. In this paper, we assumed the Grüneisen type EOS and also the Rice-Walsh type EOS in order to search for the EOS compatible with all the cylinder tests. For this purpose, six different forms of EOSes were tested. It is shown that both the simple Grüneisen type EOS with Grüneisen parameter assumed as a function of volume alone, and the Rice-Walsh EOS with Wu-Jing parameter assumed as a function of pressure alone, were incompatible with the experimental data. Among tested EOSes, it is concluded that the only possible EOS which can describe all the release isentropes obtained by the cylinder tests is the extended Grüneisen EOS with the Grüneisen parameter containing a term of the thermal contribution squared.

Keywords: detonation product gases, JWL parameters, Grüneisen equation of state, Rice-Walsh equation of state

1. Introduction

Jones-Wilkins-Lee (JWL) $p-v$ functional form has been adopted to fit the parameters to describe the isentropic behavior released from the assumed Chapman-Jouguet (C-J) state realized by cylinder expansion tests[1)−4)]. Where p and v denote the pressure and the specific volume, respectively. This procedure has been used as one of the standard tasks to study the fundamental feature of high explosives. For PETN, four JWL function parameters were determined to fit to four different C-J states reached by different initial densities.

Nagayama and Kubota showed that the initial density dependence of the detonation velocity gives approximate description of C-J state parameters other than detonation velocity, if the relationship is available[5)]. In this case, we did not assume the JWL equation of state[6)], but the Grüneisen parameter was assumed to be a function of volume alone. The Grüneisen assumption together with the relationship led to the volume compression behavior of the Grüneisen parameter to provide possible Grüneisen type EOS for detonation product gases[5)].

Nagayama showed that the dimensionless material parameter R introduced by Wu and Jing into the Rice-Walsh equation of state (EOS) deduced from the shock Hugoniot data for porous Al and Cu was shown to be well approximated by a function of pressure alone[7)]. The Rice-Walsh EOS with the Wu-Jing parameter empirically determined from porous shock data gives sufficient description of porous shock Hugoniots of different initial porosities of several metals except for very high porosity Hugoniot[7), 8)]. This EOS can also be assumed as one of the candidates of unreacted and reacted high explosives.

A fundamental assumption of the present investigation is that all the detonation of four different initial densities of

Table 1 JWL parameters for PETN used in the calculations.

Index	Material name	p_{CJ} [GPa]	ρ_0 [g cm^{-3}]	A_i [GPa]	R_{1i}	B_i [GPa]	R_{2i}	C_i [GPa]	ω_i	ε_{00i} [(km s^{-1})^2]
r1	PETN	33.5	1.770	617.0	4.40	16.93	1.20	0.699	0.25	−12.105
r2	PETN	22.0	1.500	625.3	5.25	23.29	1.60	1.152	0.28	−7.220
r3	PETN	14.0	1.260	573.1	6.00	20.16	1.80	1.267	0.28	−4.943
r4	PETN	6.2	0.880	348.6	7.00	11.29	2.00	0.941	0.24	−2.933

Table 2 Types of EOSes tested in this study.

EOS No	EOS type	Material function
EOS I	Grüneisen type	$\gamma(v,\varepsilon) = \Gamma_{00}(v)$
EOS II	Grüneisen type	$\gamma(v,\varepsilon) = \Gamma_{00}(v) + \Gamma_{02}(v)[\varepsilon - \varepsilon_{r1}(v)]$
EOS III	Grüneisen type	$\gamma(v,\varepsilon) = \Gamma_{00}(v) + \Gamma_{03}(v)[\varepsilon - \varepsilon_{r1}(v)]^2$
EOS IV	Rice-Walsh type	$R(p,h) = R_{00}(p)$
EOS V	Rice-Walsh type	$R(p,h) = R_{00}(p) + R_{02}(p)[h - h_{r1}(p)]$
EOS VI	Rice-Walsh type	$R(p,h) = R_{00}(p) + R_{03}(p)[h - h_{r1}(p)]^2$

PETN is the fully detonated gas consisting of the same chemical composition, which is the necessary condition of satisfying unique EOS surface. In this case, all the C-J states should be on a EOS surface of a material, since the chemical composition of the detonated condition for all detonated gases is assumed fixed. Although no clear evidences of this has been obtained. It is known that the estimated C-J state of the detonation of lower initial density is of higher entropy compared with that of theoretical maximum density (TMD) detonation.

Efforts of searching for the EOS to be implemented to the hydrocodes may be important in the sense of convenient engineering model EOS to reproduce the detonation behavior of the condensed phase high explosives. In this paper, we assumed the Grüneisen type EOS and also the Rice-Walsh type EOS in order to search for the EOS compatible with the cylinder tests. For this purpose, six different forms of EOSes were tested in this paper.

2. JWL isentrope functions for PETN of four different initial densities

For PETN, four independent sets of JWL parameters are published by using cylinder tests of PETN samples of four different initial loading densities. Published JWL parameters for these data of PETN are summarized in Table 1.

JWL function for i-th different initial density is written as

$$p_{ri}(v) = A_i e^{-R_{1i} v} + B_i e^{-R_{2i} v} + C_i v^{-1-\omega_i} \tag{1}$$

where A_i, R_{1i}, B_i, R_{2i}, C_i and ω_i are parameters fitted to well describe the experimental streak record trace of cylinder expansion test[1),2)].

Corresponding internal energy vs volume relationship can be obtained by integrating Equation (1) along the release isentrope,

$$\varepsilon_{ri}(v) = \frac{A_i}{R_{1i}} e^{-R_{1i} v} + \frac{B_i}{R_{2i}} e^{-R_{2i} v} + \frac{C_i}{\omega_i} v^{-\omega_i} + \varepsilon_{0i} + \varepsilon_{00i}, \tag{2}$$

where integration constant $\varepsilon_{0i} + \varepsilon_{00i}$ should be chosen to satisfy the Rankine-Hugoniot condition at the C-J state of i-th different initial density,

$$\varepsilon_{ri}(v_{CJi}) - \varepsilon_{0i} = \frac{p_{CJi}}{2}(v_{0i} - v_{CJi}), \tag{3}$$

where suffix CJi denotes the value at the i-th C-J state. In Equation (2) and (3), ε_{0i} denotes the initial internal energy at the unreacted state. Values of ε_{00i} can be determined for each initial density. We assume that the initial internal energy ε_{0i} for each initial density is equal irrespective of initial density. This means that the surface energy of particles in porous medium cannot have a large contribution to the internal energy. The determined values, ε_{00i} are also shown in Table 1.

3. Test EOSes studied

We have tested six different forms of EOSes searching for the EOS compatible with all cases of cylinder tests for PETN. They are summarized in Table 2. Notations and assumed material functions in the table will be explained in the following sections.

3.1 The Grüneisen type EOS

We start with the thermodynamic definition of the Grüneisen parameter given by[9),10)]

$$\gamma(v,\varepsilon) = v\left(\frac{\partial p}{\partial \varepsilon}\right)_v. \tag{4}$$

We use three different form of EOSes with the following Grüneisen functions.

$$\gamma(v,\varepsilon) = \Gamma_{00}(v) + \Gamma_{0i}(v)[\varepsilon - \varepsilon_{r1}(v)]^{i-1}, \tag{5}$$

where $i = 1, 2, 3$, which corresponds to EOS I to EOS III in Table 2. Two material functions, $\Gamma_{00}(v)$ and $\Gamma_{0i}(v)$ are introduced assumed dependent only on specific volume, which will be determined to adjust JWL isentropes. Where $\varepsilon_{r1}(v)$ denotes the release isentrope for TMD detonation assigning index r1 in Table 1. The second term in Equation (5) indicates the possible thermal contribution to the Grüneisen parameter, since the assumption that the Grüneisen parameter is a function of volume alone has no firm physical basis.

The corresponding form of EOS from Equation (5) is obtained by integrating Equation (4) along an isochore as follows :

(i) if the Grüneisen parameter is assumed to be a function of volume alone, i.e., $i=1$, then we have

$$p = p_{r1}(v) + \frac{\Gamma_{00}(v)}{v}[\varepsilon - \varepsilon_{r1}(v)] \text{ with } \Gamma_{01}(v) = 0 \quad (6)$$

(ii) if the Grüneisen parameter is assumed to be of the form of $i=2$, we have

$$\gamma(v,\varepsilon) = \Gamma_{00}(v) + \Gamma_{02}(v)[\varepsilon - \varepsilon_{r1}(v)] \quad (7)$$

By integrating this equation along an isochore, we have

$$p = p_{r1}(v) + \frac{\Gamma_{00}(v)}{v}[\varepsilon - \varepsilon_{r1}(v)] + \frac{\Gamma_{02}(v)}{2v}[\varepsilon - \varepsilon_{r1}(v)]^2 \quad (8)$$

(iii) if the Grüneisen parameter is assumed to be of the form of $i=3$, we have

$$\gamma(v,\varepsilon) = \Gamma_{00}(v) + \Gamma_{03}(v)[\varepsilon - \varepsilon_{r1}(v)]^2 \quad (9)$$

By integrating this equation along an isochore, we have

$$p = p_{r1}(v) + \frac{\Gamma_{00}(v)}{v}[\varepsilon - \varepsilon_{r1}(v)] + \frac{\Gamma_{03}(v)}{3v}[\varepsilon - \varepsilon_{r1}(v)]^3, \quad (10)$$

It is assumed here that $p_{r1}(v)$ and $\varepsilon_{r1}(v)$ can be the release isentrope of the TMD detonation. In later sections, we have tried to estimate other material functions, $\Gamma_{00}(v)$ and $\Gamma_{0i}(v)$ using release isentrope function data.

3.2 The Rice-Walsh type EOS

We restart with the definition of the Wu-Jing parameter given by[11)]

$$R(p,h) = p\left(\frac{\partial v}{\partial h}\right)_p \quad (11)$$

introduced into the Rice-Walsh EOS, where h denotes the specific enthalpy[12)]. We used three different form of EOSes with the following Wu-Jing parameter into the Rice-Walsh EOS given by

$$R(p,h) = R_{00}(p) + R_{01}(p)[h - h_{r1}(p)]^{i-1}, \quad (12)$$

where $i = 1,2,3$, which corresponds to EOS IV to EOS VI in Table 2. Two material functions, $R_{00}(p)$ and $R_{0i}(p)$ are introduced assumed dependent only on pressure, which will be determined to adjust JWL isentropes. The second term in Equation (12) indicates the possible thermal contribution to the Wu-Jing parameter, since the assumption that the Wu-Jing parameter is a function of pressure alone also has no firm physical basis.

The corresponding form of EOS from Equation (12) is obtained by integrating Equation (12) as follows :

(i) if the Wu-Jing parameter is assumed to be a function of pressure alone, i.e. $i=1$, then we have

$$v = v_{r1}(p) + \frac{R_{00}(p)}{p}[h - h_{r1}(p)], \text{ with } R_{01}(p) = 0 \quad (13)$$

where $v_{r1}(p)$ is the reverse function of $p_{r1}(v)$ in Equation (6).

(ii) if the Wu-Jing parameter is assumed to be of the form of $i=2$, we have

$$R(p,h) = R_{00}(p) + R_{02}(p)[h - h_{r1}(p)] \quad (14)$$

Instead of temperature variable, we adopt enthalpy difference. By integrating this equation along an isobaric, we have

$$\nu = v_{r1}(p) + \frac{R_{00}(p)}{p}[h - h_{r1}(p)] + \frac{R_{02}(p)}{2p}[h - h_{r1}(p)]^2 \quad (15)$$

(iii) if the Wu-Jing parameter is assumed to be of the form of $i=3$, we have

$$R(p,h) = R_{00}(p) + R_{03}(p)[h - h_{r1}(p)]^2 \quad (16)$$

By integrating this equation along an isobaric, we have

$$\nu = v_{r1}(p) + \frac{R_{00}(p)}{p}[h - h_{r1}(p)] + \frac{R_{03}(p)}{3p}[h - h_{r1}(p)]^3, \quad (17)$$

where $v_{r1}(p)$ and $h_{r1}(p)$ are reference isentrope functions. It is again assumed here that $v_{r1}(p)$ and $h_{r1}(p)$ can be the release isentrope of the TMD detonation. In later sections, we have tried to estimate the functional forms of other material functions, $R_{00}(p)$ and $R_{0i}(p)$ using release isentrope function data.

3.3 Relationship between the Grüneisen type EOS and the Rice-Walsh type EOS

The assumptions that the parameter R is a function of pressure alone, and that the Grüneisen parameter is a function of volume alone are independent and are incompatible with each other. This is highlighted by the following thermodynamic identities[13)]:

$$\frac{dT}{T} = -\frac{\gamma(v,S)}{v}dv + \frac{dS}{C_v(v,S)}, \quad (18)$$

$$\frac{dT}{T} = \frac{R(p,S)}{p}dp + \frac{dS}{C_p(p,S)}, \quad (19)$$

where T, S, C_v, and C_p denote the temperature, the entropy, the specific heat at constant volume, and the specific heat at constant pressure, respectively.

Important assumptions in the case of $i=1$ for both the Grüneisen and the Rice-Walsh EOS should impose various limitations on the properties of EOS, but they actually have no firm physical basis for the assumptions. This is the motivation for the comparison of EOS which is more preferable to the measured detonation properties.

4. Estimation procedure of the Grüneisen parameter and the Wu-Jing parameter using four different isentropes

4.1 Procedure of deducing the Grüneisen parameter : EOS I

In this case, the averaged value of the Grüneisen parameter can be calculated by comparing two isentropes, $p_{r1}(v)$ and $p_{ri}(v)$ as

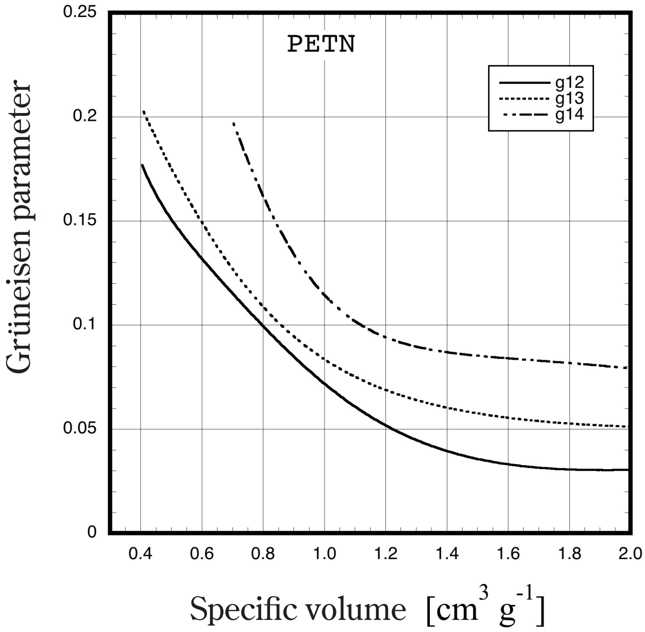

Figure 1 Estimated average Grüneisen parameter between two isentropes. In the figure, the legend, g1i ($i = 2,3,4$) denotes the calculated value of the Grüneisen parameter using the release isentropes $r1$ and ri in Table 1.

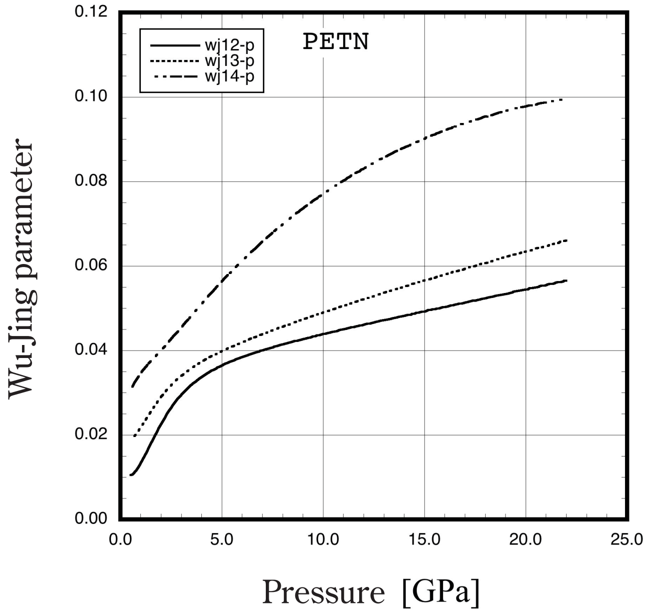

Figure 2 Estimated average Wu-Jing parameter between two isentropes. In the figure, the legend, wj1i (i=2,3,4) denotes the calculated value of the Wu-Jing parameter using the release isentropes $r1$ and ri in Table 1.

$$\left[\frac{\gamma(v)}{v}\right]_{1i} = \frac{\Gamma_{00}(v)}{v} = \frac{p_{r1}(v) - p_{ri}(v)}{\varepsilon_{r1}(v) - \varepsilon_{ri}(v)} \tag{20}$$

Combining two of four isentropes, three different Grüneisen functions were deduced by using the above equation. The result is shown in Figure 1. The Grüneisen parameter decreases with increasing volume. This tendency is opposite of that for solid substances. Furthermore, the Grüneisen parameter increases with increasing entropy, since the value of entropy at the C-J state increases with decreasing initial density. This tendency violates the assumption, Equation (5) with $i = 1$.

At this point, the Grüneisen EOS with $i = 1$ (EOS I) is excluded to describe the release isentropes from four different C-J states. It is therefore necessary to include the thermal effects to the behavior of Grüneisen parameter under compression.

4.2 Procedure of deducing the Wu-Jing parameter : EOS IV

Averaged value of the Wu-Jing parameter between $v_{r1}(p)$ and $v_{ri}(p)$ can be estimated by

$$\left[\frac{R(p)}{p}\right]_{1i} = \frac{R_{00}(p)}{p} = \frac{v_{r1}(p) - v_{ri}(p)}{h_{r1}(p) - h_{ri}(p)} \tag{21}$$

Using two of four isentropes, three different Wu-Jing pressure functions were deduced. The result is shown in Figure 2. The Wu-Jing parameter increases with increasing pressure, which is in harmony with the tendency of solid substances[6)]. Furthermore, the Wu-Jing parameter increases with increasing entropy, since the C-J entropy increases with decreasing initial density. However, this tendency violates the assumption, Equation (16) with $i = 1$.

At this point, the Rice-Walsh EOS with $i = 1$ (EOS IV) is also excluded to describe the release isentropes from four different C-J states. It is therefore necessary to include the thermal effects to the behavior of the Wu-Jing parameter under compression.

5. Extended Grüneisen and Rice-Walsh EOS formulation

5.1 Formulation of EOS with Grüneisen parameter including thermal contribution : EOS II and III

By combining the thermodynamic relationship

$$p - p_{r1}(v) = -\left(\frac{\partial[\varepsilon - \varepsilon_{r1}(v)]}{\partial v}\right)_S, \tag{22}$$

the extended Grüneisen EOSes described in Equation (8) and (10) are both regarded as a differential equation for the internal energy difference given for EOS II and III respectively as

$$\left(\frac{\partial[\varepsilon - \varepsilon_{r1}(v)]}{\partial v}\right)_S + \frac{\Gamma_{00}(v)}{v}[\varepsilon - \varepsilon_{r1}(v)] + \frac{\Gamma_{02}(v)}{2v}[\varepsilon - \varepsilon_{r1}(v)]^2 = 0 \tag{23}$$

$$\left(\frac{\partial[\varepsilon - \varepsilon_{r1}(v)]^2}{\partial v}\right)_S + \frac{2\Gamma_{00}(v)}{v}[\varepsilon - \varepsilon_{r1}(v)]^2 + \frac{2\Gamma_{03}(v)}{3v}[\varepsilon - \varepsilon_{r1}(v)]^4 = 0 \tag{24}$$

These two differential equations can be integrated along an isentrope to obtain the following general solution as

$$\varepsilon - \varepsilon_{r1}(v) = \frac{C(S)\,\Theta_{v2}(v)}{1 - C(S)\displaystyle\int_{v_0}^{v}\frac{\Gamma_{02}(v)}{2v}\Theta_{v2}(v)\,dv}, \tag{25}$$

$$[\varepsilon - \varepsilon_{r1}(v)]^2 = \frac{C(S)\,\Theta_{v3}(v)}{1 - C(S)\displaystyle\int_{v_0}^{v}\frac{2\Gamma_{03}(v)}{3v}\Theta_{v3}(v)\,dv}, \tag{26}$$

where

$$\Theta_{v2}(v)=\exp\left[-\int_{v_{0ref}}^{v}\frac{\Gamma_{00}(v)}{v}dv\right], \tag{27}$$

$$\Theta_{v3}(v)=\exp\left[-\int_{v_{0ref}}^{v}\frac{2\Gamma_{00}(v)}{v}dv\right], \tag{28}$$

where $C(S)$ denotes the integration function. In Equation (27) and (28), v_{0ref} denotes some reference volume. Equations (25) and (26) are a general expression for an isentrope of detonation product gases. Similar procedure of constructing extended Grüneisen EOS has been already discussed previously [14].

5.2 Formulation of EOS with Wu-Jing parameter including thermal contribution : EOS V and VI

It is also possible to construct an extended Rice-Walsh EOS with the Wu-Jing parameter as a function of pressure and enthalpy. The extended Rice-Walsh EOSes described in Equation (15) and (17) both are regarded as a differential equation for the enthalpy difference given for EOS V and VI respectively as

$$\left(\frac{\partial[h-h_{r1}(p)]}{\partial p}\right)_S+\frac{R_{00}(p)}{p}[h-h_{r1}(p)]+\frac{R_{02}(p)}{2p}[h-h_{r1}(p)]^2=0 \tag{29}$$

$$\left(\frac{\partial[h-h_{r1}(p)]^2}{\partial p}\right)_S+\frac{2R_{00}(p)}{p}[h-h_{r1}(p)]^2+\frac{2R_{03}(p)}{3p}[h-h_{r1}(p)]^4=0 \tag{30}$$

These two differential equations can be integrated along an isentrope to obtain the following general solution as

$$h-h_{r1}(p)=\frac{C(S)\Theta_{p2}(p)}{1-C(S)\int_{p_0}^{p}\frac{R_{02}(p)}{2p}\Theta_{p2}(p)dp}, \tag{31}$$

$$[h-h_{r1}(p)]^2=\frac{C(S)\Theta_{p3}(p)}{1-C(S)\int_{p_0}^{p}\frac{2R_{03}(p)}{3p}\Theta_{p3}(p)dp}, \tag{32}$$

where

$$\Theta_{p2}(p)=\exp\left[-\int_{p_{0ref}}^{p}\frac{R_{00}(p)}{p}dp\right], \tag{33}$$

$$\Theta_{p3}(p)=\exp\left[-\int_{p_{0ref}}^{p}\frac{2R_{00}(p)}{p}dp\right], \tag{34}$$

where $C(S)$ denotes the integration function. In Equation (33) and (34), p_{0ref} denotes some reference pressure. Equations (31) and (32) are a general expression for an isentrope of detonation product gases.

6. Compatibility of extended EOS

6.1 Determination of Grüneisen parameter including thermal contribution : EOS II and III

In order to determine the concrete EOS formulation, it is necessary to determine two material functions, $\Gamma_{00}(v)$ and $\Gamma_{0i}(v)$ by using the JWL function $p_{r1}(v)$ of TMD detonation.

Three isentropes are necessary to determine these two material functions, and we decided to deduce these material functions by the following formula.

In the case of $i=2$, we have

$$\Gamma_{02}(v)=2v\frac{\left[\frac{p_{r2}(v)-p_{r1}(v)}{\varepsilon_{r2}(v)-\varepsilon_{r1}(v)}-\frac{p_{r3}(v)-p_{r1}(v)}{\varepsilon_{r3}(v)-\varepsilon_{r1}(v)}\right]}{\varepsilon_{r2}(v)-\varepsilon_{r3}(v)} \tag{35}$$

and

$$\Gamma_{00}(v)=v\frac{p_{r2}(v)-p_{r1}(v)}{\varepsilon_{r2}(v)-\varepsilon_{r1}(v)}-\frac{\Gamma_{02}(v)}{2}[\varepsilon_{r2}(v)-\varepsilon_{r1}(v)] \tag{36}$$

In the case of $i=3$, we have

$$\Gamma_{03}(v)=3v\frac{\left[\frac{p_{r2}(v)-p_{r1}(v)}{\varepsilon_{r2}(v)-\varepsilon_{r1}(v)}-\frac{p_{r3}(v)-p_{r1}(v)}{\varepsilon_{r3}(v)-\varepsilon_{r1}(v)}\right]}{(\varepsilon_{r2}(v)-\varepsilon_{r1}(v))^2-(\varepsilon_{r3}(v)-\varepsilon_{r1}(v))^2} \tag{37}$$

and

$$\Gamma_{00}(v)=v\frac{p_{r2}(v)-p_{r1}(v)}{\varepsilon_{r2}(v)-\varepsilon_{r1}(v)}-\frac{\Gamma_{03}(v)}{3}[\varepsilon_{r2}(v)-\varepsilon_{r1}(v)]^2 \tag{38}$$

These two equations can be solved easily to determine the material functions for each volume. Exclusion of the last 4 th isentrope in this procedure is simply because the C-J pressure is the lowest of other isentropes. JWL function can be calculated for the states of higher pressure over C-J states, but the precision will degrade with pressure.

The resultant material functions, $\Gamma_{00}(v)$ and $\Gamma_{0i}(v)$ as obtained in this procedure is shown in Figure 3. Material function, $\Gamma_{00}(v)$ for both $i=2$ and $i=3$ is now the Grüneisen parameter along the TMD isentrope. Therefore, negative region for some large volume values in the case of $i=2$ should be unphysical. Furthermore, derivative of the Grüneisen parameter, $\Gamma_{02}(v)$ and $\Gamma_{03}(v)$ are found to be positive value over entire volume. At this point, case $i=3$ is preferable to describe isentropes with arbitrary value of entropy. Release isentropes can be evaluated by Equation (26).

6.2 Determination of Wu-Jing parameter including thermal contribution : EOS V and VI

In order to determine the concrete EOS formulation, it is necessary to determine two material functions, $R_{00}(p)$ and $R_{0i}(p)$ together with JWL function $v_{r1}(p)$ of TMD detonation. By using three isentropes, we decided to deduce these material functions by the following formula.

In the case of $i=2$, we have

$$R_{02}(p)=2p\frac{\left[\frac{v_{r2}(p)-v_{r1}(p)}{h_{r2}(p)-h_{r1}(p)}-\frac{v_{r3}(p)-v_{r1}(p)}{h_{r3}(p)-h_{r1}(p)}\right]}{h_{r2}(p)-h_{r3}(p)} \tag{39}$$

and

$$R_{00}(p)=p\frac{v_{r2}(p)-v_{r1}(p)}{h_{r2}(p)-h_{r1}(p)}-\frac{R_{02}(p)}{2}[h_{r2}(p)-h_{r1}(p)] \tag{40}$$

In the case of $i=3$, we have

$$R_{03}(p)=3p\frac{\left[\frac{v_{r2}(p)-v_{r1}(p)}{h_{r2}(p)-h_{r1}(p)}-\frac{v_{r3}(p)-v_{r1}(p)}{h_{r3}(p)-h_{r1}(p)}\right]}{(h_{r2}(p)-h_{r1}(p))^2-(h_{r3}(p)-h_{r1}(p))^2} \tag{41}$$

and

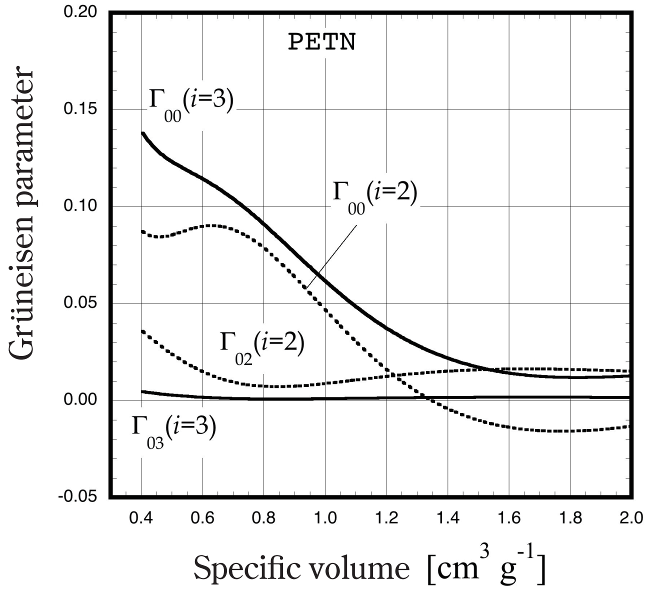

Figure 3 The Grüneisen parameter coefficients estimated using release isentropes of index numbers r1 to r3.

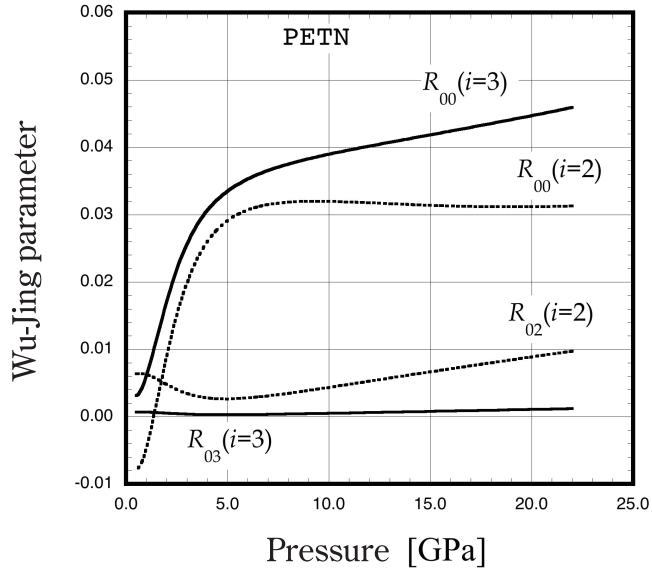

Figure 4 The Wu-Jing parameter coefficients estimated using release isentropes of index numbers r1 to r3.

$$R_{00}(p) = p\frac{v_{r2}(p) - v_{r1}(p)}{h_{r2}(p) - h_{r1}(p)} - \frac{R_{03}(p)}{3}[h_{r2}(p) - h_{r1}(p)]^2 \quad (42)$$

These two equations can be solved easily to determine the material functions for each volume. The reason why the last fourth isentrope in the above procedure is excluded is the same as explained in the last section to determine the Grüneisen parameter. JWL function can be calculated for the states of higher pressure over C-J states, but the precision will degrade with pressure.

The resultant material functions, $R_{00}(p)$ and $R_{0i}(p)$ as obtained in this procedure are shown in Figure 4. Material function, $R_{00}(p)$ for both $i=2$ and $i=3$ is now the Wu-Jing parameter along the TMD isentrope. Therefore, negative region for some low pressure values in the case of $i=2$, $R_{02}(p)$ should be unphysical. Furthermore, derivative of the Wu-Jing parameter, $R_{02}(v)$ and $R_{03}(v)$ are found to be positive value over entire volume. At this

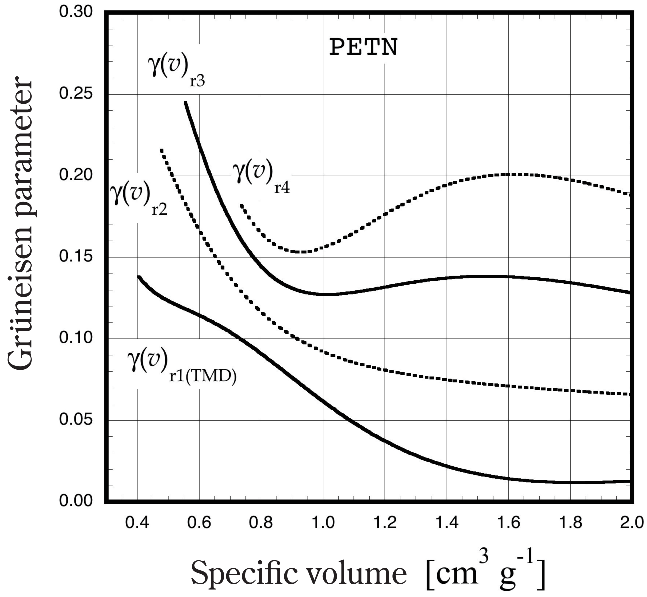

Figure 5 Volume dependence of the Grüneisen parameter along each release isentropes. (EOS III) Symbols attached to each curve, i.e. $\gamma(v)_{ri}$ indicates the calculated Grüneisen parameter along the release isentrope ri in Table 1.

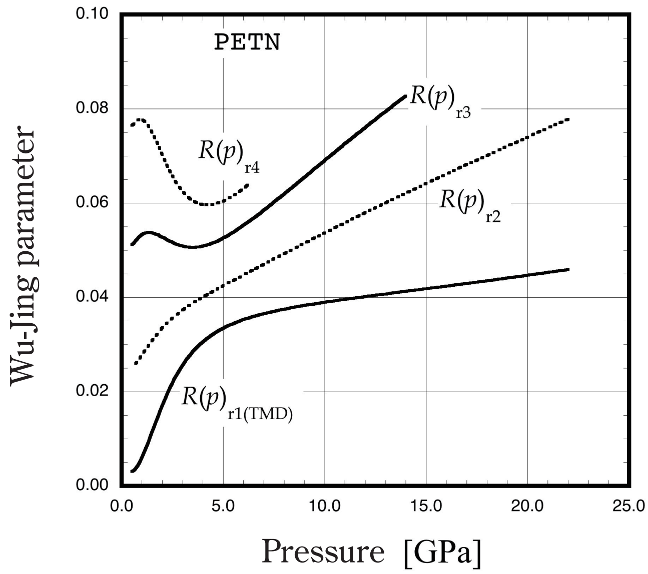

Figure 6 Pressure dependence of the Wu-Jing parameter along each release isentropes. (EOS VI) Symbols attached to each curve, i.e. $R(p)_{ri}$ indicates the calculated Wu-Jing parameter along the release isentrope ri in Table 1.

point, case $i=3$ is preferable to describe isentropes with arbitrary value of entropy. Release isentropes can be evaluated by Equation (32).

7. Reproduction of release isentropes by the extended Grüneisen EOS : EOS III

We have calculated the Grüneisen and Wu-Jing parameter along each isentropes in the case of two extended Grüneisen and Rice-Walsh EOSes and are shown in Figure 5 and Figure 6. From Figure 5 and from Figure 6, both the extended Grüneisen EOS and the extended Rice-Walsh EOS nicely represent the material parameters along release isentropes of TMD detonation. However, we

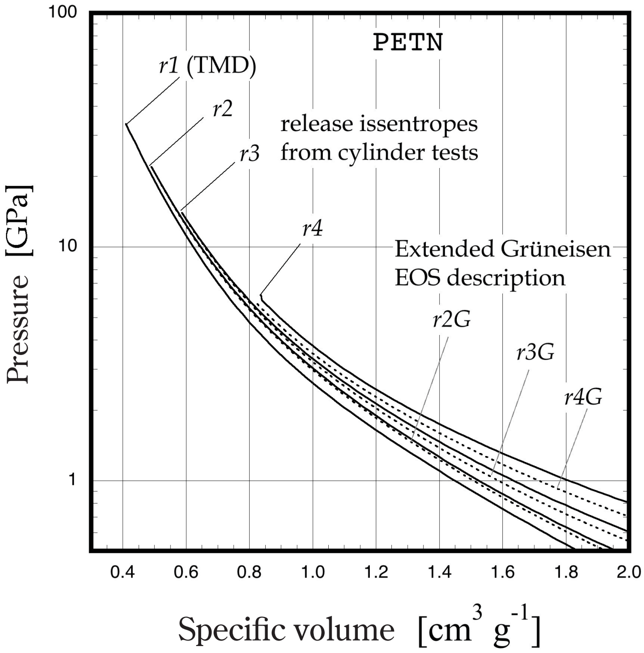

Figure 7 Release isentropes from four different C-J states for PETN. Labels on each curve for release isentrope obtained from cylinder tests are indexes defined in Table 1. Calculated isentropes using extended Grüneisen EOS of $i = 2$ in Equation (10) are labeled as $r2G$ to $r4G$. Differences between JWL function and the Grüneisen EOS calculation increases with decreasing C-J pressure. As explained in the text, calculations does not include the information on r4 isentropes, so that the discrepancy between r4 JWL function and the Grüneisen EOS calculation is large as shown in the figure.

need to consider the limiting condition of using Rice-Walsh EOS with Wu-Jing parameter. That is, the Wu-Jing parameter along any isentropes should tend to zero at zero pressure. As shown in Figure 6, however, Wu-Jing parameter along release isentropes except for the TMD detonation does not seem to tend to zero. In this sense, both of the extended Rice-Walsh EOS is excluded to describe release isentropes other than TMD detonation.

We finally chose the extended Grüneisen EOS with the Grüneisen parameter containing thermal contribution $i = 3$. We have calculated the release isentropes from four different C-J states for PETN by using Equation (26) combined with Equation (10), and the result is compared with JWL functions. These plots are shown in Figure 7.

8. Conclusion

Published JWL isentrope functions for PETN were used to search for the EOS for detonation product gases fully compatible for the cylinder tests. The Grüneisen type and the Rice-Walsh type EOSes were used as a candidate of the EOS compatible with cylinder tests.

For this purpose, both the Grüneisen and the Rice-Wlah type EOSes were extended by introducing material parameters containing thermal contribution. One of the extended Grüneisen type EOS was shown to be compatible with all the cylinder test results.

Further investigation, however, is necessary to improve the accuracy of reproduction of the release isentropes.

References

1) E. L. Lee, H. C. Hornig, and J. W. Kury, University of California Report, No. UCRL-50422 (1968).
2) E. Lee, M. Finger, and W. Collins, Lawrence Livermore Laboratory Report, No. UCID-16189 (1973).
3) P. W. Cooper, "Introduction to Detonation Physics in Explosive Effects and Applications", ed. J. A. Zukas, and W. P. Walters, Springer, 2002.
4) A. L. Kuhl, LLNL-CONF-425882, Proc. 14th Int. Detonation Symp. 2010.
5) K. Nagayama and S. Kubota, J. Appl. Phys., 93, 2583-2589 (2003).
6) R. Menikoff, Los Alamos Report, LA-UR-15-29536 (2017).
7) K. Nagayama, J. Appl. Phys., 119, 195901-1-11 (2016).
8) K. Nagayama, J. Appl. Phys., 121, 175902-1-9 (2017).
9) R. G. McQueen, S. P. Marsh, J. W. Taylor, J. N. Fritz, and W. J. Carter: "High Velocity Impact Phenomena", ed. R. Kinslow, Academic Press, New York, 1970.
10) K. Nagayama, "Introduction to the Grüneisen EOS and Shock Thermodynamics", Kindle ebook, Amazon, 2011.
11) Q. Wu and F. Jing, J. Appl. Phys., 80, 4343−4349 (1996).
12) M. H. Rice and J. M. Walsh, J. Chem. Phys., 26, 824−830 (1957).
13) K. Nagayama and S. Kubota, Shock Compression of Condensed Matter−2013, 052032 (2014).
14) K. Nagayama, J. Phys. Soc. Japan, 63, 3729−3736 (1994).