Simplified pressure calculation of reacting explosives

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Abstract

In numerical simulations of shock initiation process of condensed explosive, state variables in reaction zone are regarded as simple mixture phase of the unreacted and the reacted components. The relations of the specific volumes of the unreacted and the reacted component were investigated under the four types of assumptions. From the numerical results, it was indicated that the specific volume of the unreacted component can be described by the specific volume of the reacted component under the certain assumptions. This relation can be applied as the simpslified pressure calculations of the reacting explosive. The reason why there is such relation is that the unreacted and the reacted components approximately pass two types of single lines in pressure and specific volume plane, respectively. It has been found that the compression processes of reacted component in reaction zone have the path close to Hugoniot line for reacted component under isentropic solid assumption.

1. Introduction

In numerical simulation of initiation process on high explosive it is necessary to determine the pressure of intermediate phase. Due to lack of the knowledge of the intermediate composition during the reaction process, a simple mixture theory has been often used to determine the pressure [1]. In this theory, intermediate states is regarded as simple mixture phase of the unreacted and the reacted phases and is calculated by using individual equations of state for both components and the reaction rate of the detonation products. Therefore, in the numerical simulation, important factors are the equations of state for the unreacted and the reacted components, the reaction rate model and the pressure calculation during reaction process. There have been much studies on the individual equations of state and the reaction rate law of high explosive, in contrast there are few studies relating the calculation method for intermediate component.

We have found that the relation between the specific volumes of unreacted and reacted components show very little dependence on the decomposition degree under a certain assumption [2]. Utilizing this relation we have pro-

posed a new method on the pressure calculation of reacting explosive. In this study four types of the assumptions that are the fourth assumption for the pressure calculation of mixture phase are employed to discuss the intermediate phase. The relations between the unreacted and the reacted state variables extracted from the numerical simulations of shock initiation problems are investigated.

2. Mixture rule of reacting explosive

In order to calculate the pressure of the intermediate phase $P(V, E)$, we have to obtain the solutions of the four unknown variables, specific volumes (V_1, V_2) and internal energies (E_1, E_2) for unreacted and reacted components. Subscript 1 and 2 indicate the unreacted and reacted components, respectively. The internal energy and specific volume of the intermediate components have been represented by a linear combination of individual internal energies and specific volumes,

$$(1 - \lambda)V_1 + \lambda V_2 - V = 0 \tag{1}$$

$$(1 - \lambda)E_1 + \lambda E_2 - E = 0 \tag{2}$$

where λ is the reaction rate; $\lambda = 0$ is un-reacted state and $\lambda = 1$ completely reacted state. The condition of mechanical equilibrium $P = P_1 (V_1, E_1) = P_2 (V_2, E_2)$ is usually used to obtain these solutions. Since we have above three conditions, another physical assumption is needed to obtain the four solutions.

There are many assumptions as fourth condition. Many researchers have adopted the thermal equilibrium condition,

$$T = T_1 (V_1, E_1) = T_2 (V_2, E_2), \tag{3}$$

as the remaining assumption.

The pressure-volume relation along the isentropic line for unreacted component can be obtained by solving following linear first-order ordinary differential equation under the assumption of $\Gamma / V_1 = \text{const.} = a$.

$$\frac{dP_{1S}}{dV} + a\, P_{1S} = P_{1H}\left(1 - \frac{a}{2}\left(V_0 - V_1\right)\right) \tag{4}$$

The assumption of the isentropic solid can be described as follow.

$$E_1 = E_{1S} = \frac{\left(P_{1S} - P_{1H}\right)}{a\rho_0} + \frac{P_{1H}}{2}\left(V_0 - V_1\right) \tag{5}$$

where the subscripts S and H indicate the isentrope and Hugoniot line, respectively. In this case the E_2 is calculated by equation (2) after the E_1 is calculated by equation (5).

Because the Hugoniot and isentropic lines of unreacted components are close each other on pressure vs. volume $(P - V)$ plane, Hugoniot line may be able to be used like isentropic line for modeling the behavior of unreacted component of reacting explosive. The fourth assumption becomes as follow.

$$E_1 = E_{1H} = \frac{P_{1H}}{2}\left(V_0 - V_1\right) \tag{6}$$

In the previous paper [2] we had used the next relation as fourth assumption.

$$\frac{E_1}{E_2} = \frac{E_{1H}}{E_{2S}} \tag{7}$$

We found that the relationship of specific volumes between the unreacted and reacted components can be approximately expressed with one curve regardless decomposition degree of high explosive under the above assumption. The relation of those specific volumes was fitted as $V_1 = f(V_2)$ by non-linear curve fitting method [3].

In this report, for the above mentioned four types of fourth assumptions, $T_1 = T_2$, $E_1 = E_{1S}$, $E_1 = E_{1H}$ and $E_1 / E_2 = E_{1H} / E_{2S}$, were employed in the numerical simulation of shock initiation process, and the state quantities were extracted to investigate the relations of V_1 and V_2 components.

3. Numerical simulation and extraction of state quantities in reaction zone
3.1 Numerical procedure

The one-dimensional Lagrangian code was used for solving the shock initiation phenomena. The governing equations are mass, momentum and energy conservation law and are solved by finite difference method [4].
Reaction rate model is necessary to estimate the degree of the decomposition of explosive. Ignition and growth model is one of the most useful models. In this study, original ignition and growth model [5)-7)] was used.

In addition, the equations of state for unreacted and reacted phases are required to carry out the numerical simulation. For both phases, JWL equation of state [8)-10)] is employed. The JWL parameters of PETN($1.75\ \text{g}\cdot\text{cm}^{-3}$) were taken as the same values as reference (5). In order to examine the assumption of temperature equilibrium, we also used temperature dependent form JWL equation of state [11],

Impact problem PMMA vs. PETN 1.75

Impact velocity $0.6\ \text{km s}^{-1}$
3.5, 4.5, 5.5 μs
——— $T_1 = T_2$
-------- $E_1 = E_{1S}$
— — — $E_1 = E_{1H}$
— · — · $E_1 / E_2 = E_{1H} / E_{2S}$

(a) Impact velocity; $0.6\ \text{km s}^{-1}$

Impact problem PMMA vs. PETN 1.75

Impact velocity $1.2\ \text{km s}^{-1}$
0.2, 0.4, 0.6 μs
——— $T_1 = T_2$
-------- $E_1 = E_{1S}$
— — — $E_1 = E_{1H}$
— · — · $E_1 / E_2 = E_{1H} / E_{2S}$

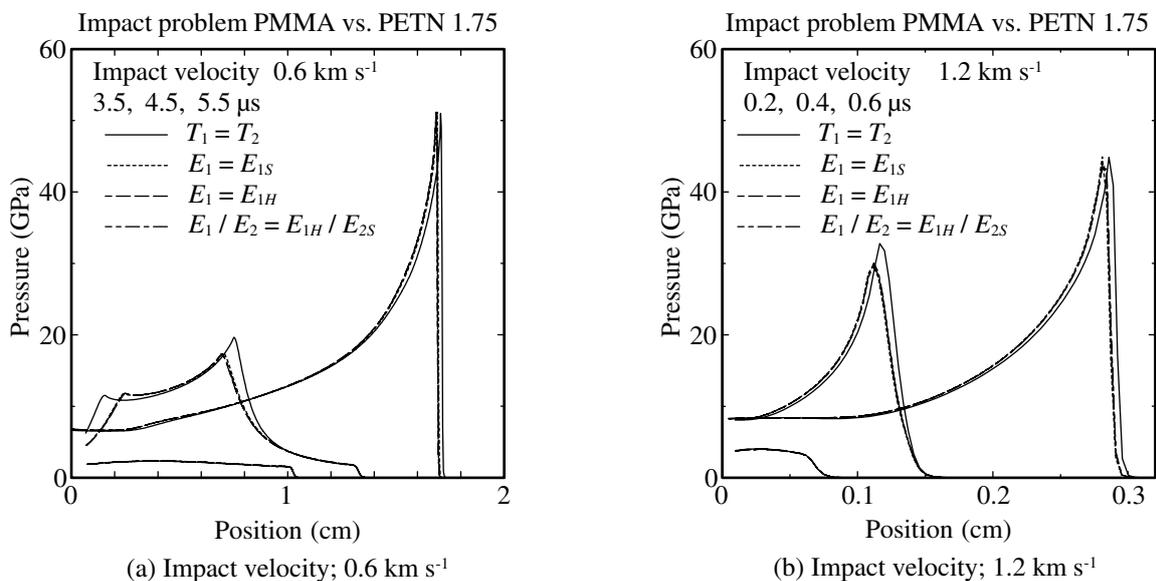(b) Impact velocity; $1.2\ \text{km s}^{-1}$

Fig. 1   Numerical results of shock to detonation transition (SDT) process in PETN.
The position is counted from the initial interface between the PMMA and PETN.

(a) $T_1 = T_2$, and $E_1 = E_{1S}$

(b) $E_1 = E_{1H}$, and $E_1 = E_{1S}$

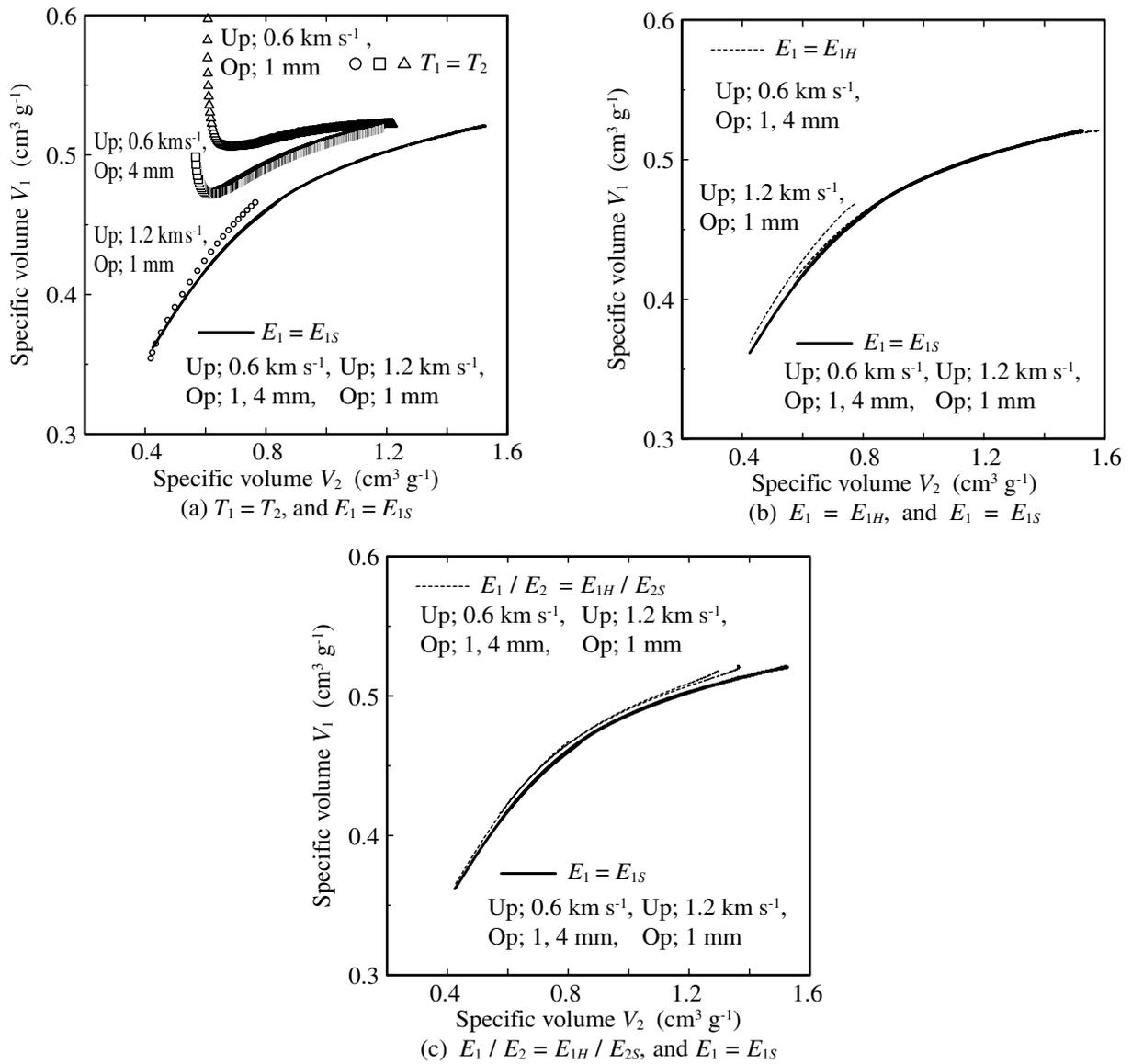(c) $E_1 / E_2 = E_{1H} / E_{2S}$, and $E_1 = E_{1S}$

Fig. 2   Relation of the specific volumes of the unreacted and the reacted component in reaction zone of PETN, the state quantities are extracted from the numerical simulation of shock initiation process, impact problems PMMA vs. PETN. Up; impact velocity, Op; Distance from interface of PMMA and PETN to the observation point.

$$P = A \exp(-R_1 \zeta) + B \exp(-R_2 \zeta) + \frac{\omega\, Cv}{V} T \qquad (8)$$

where ζ is V / V_0, subscript 0 indicate initial state of condensed explosive. A, B, R_1, R_2 and ω are the constants, Cv is the average heat capacity. From thermodynamic relation,

$$dE = Cv\, dT + \left[T \left(\frac{\partial P}{\partial T} \right)_V - P \right] dV \qquad (9),$$

$T(E, V)$ function can be obtained.

3.2 One dimensional impact problems of PMMA vs. PETN

In order to extract the state quantities in reacting explosive, the one-dimensional impact problems of PMMA vs. PETN were carried out using each fourth assumption. Figure 1 shows the shock to detonation transition (SDT) process in PETN with the pressure distributions of three different times. It can be seen that those simulation results are insensitive to the fourth assumption. The aim of this
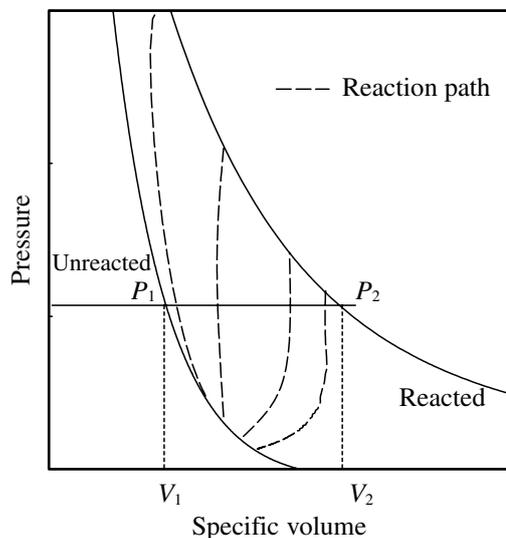

Fig. 3   Conceptual diagram for explanation of the relation of V_1 and V_2.

study is to investigate the relation of the specific volumes of unreacted and reacted components. Therefore we will not consider the reason why the numerical results of shock initiation are insensitive to the assumption adopted. In this paper we take notice of the state quantities in reacting explosive, especially the relation of the specific volumes of each component.

4. Discussion

The relations of specific volumes of V_1 and V_2 obtained under each fourth assumption are shown in Figs. 2 (a)-(c) in V_1 - V_2 plane. Under the assumptions of $T_1 = T_2$ and $E_1 = E_{1H}$, relation of V_1 and V_2 does not pass along the single line in V_1 - V_2 plane. While in the cases of the assumptions, $E_1 = E_{1S}$ and $E_1 / E_2 = E_{1H} / E_{2S}$, the both specific volumes approximately exist on the single line in V_1 - V_2 plane. We have proposed a new method for pressure calculation in reacting explosive under the $E_1 / E_2 = E_{1H} / E_{2S}$ assumption [2]. Because the relation of V_1 and V_2 can be fitted by the

simple function, the V_1 and V_2 can be solved using such function and equation (1). At the same time E_{1H} (V_1) and E_{2S} (V_2) are obtained to solve the solutions of E_1 and E_2. Finally, the pressure in reaction zone is solved without complex iteration which includes the complex form equations of state. In this paper we will try to answer the question why the relation of V_1 and V_2 could be approximately described by the single line in V_1 - V_2 plane.

For explanation we introduce the following assumption. Both components pass along the single line P - V plane, such as Hugoniot, Isentrope. Although the assumption is not acceptable thermodynamically, for simple consideration we consider following situation. The unreacted component follows on Hugoniot line and reacted component changes along the isentrope which pass through the C-J point. Figure 3 is the conceptual diagram for explanation of the relation of V_1 and V_2. The certain state of mixed phase, dotted lines, exists between two lines. Mechanical equilibrium, $P_1 = P_2$ determine the unique combination
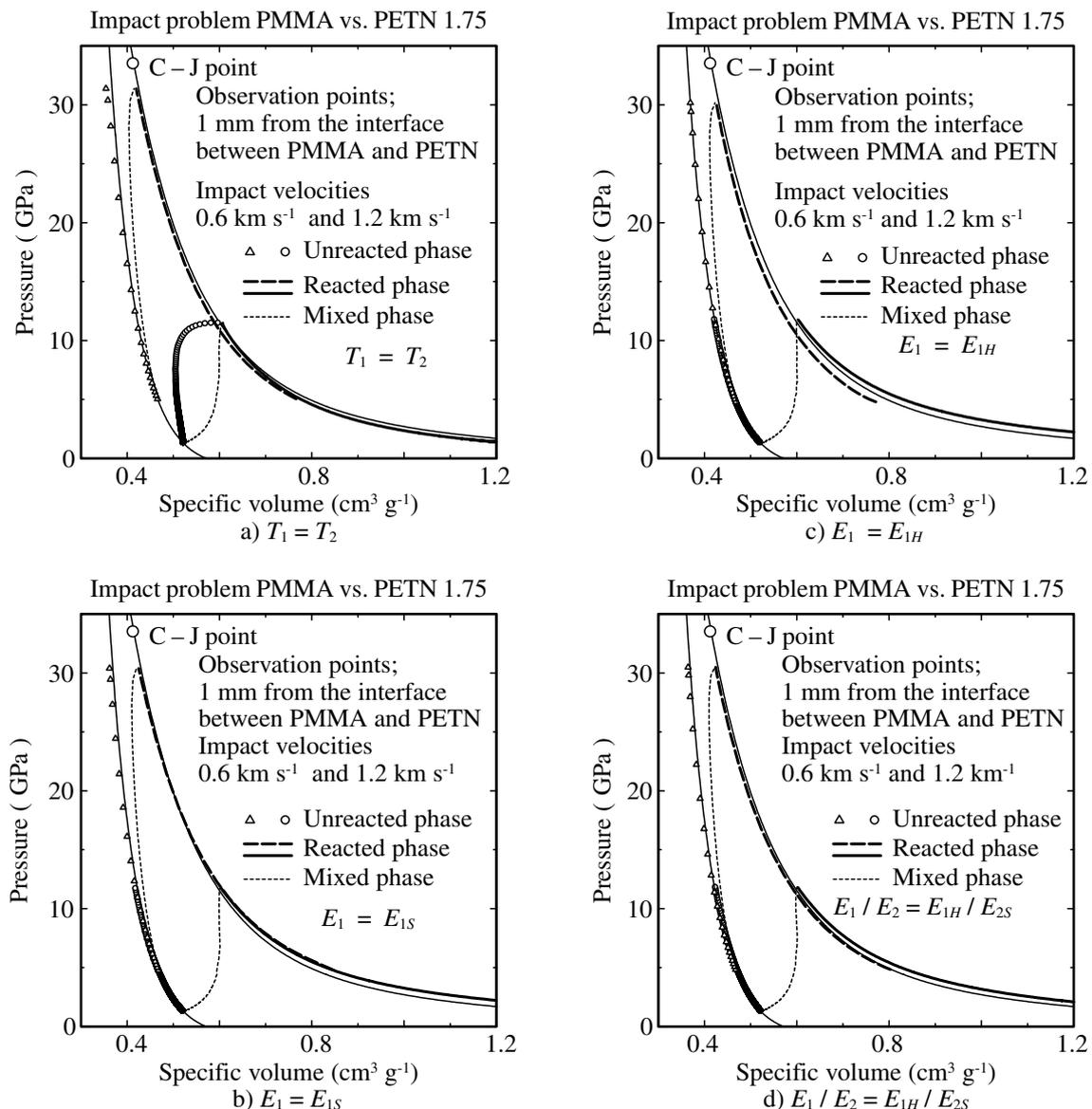

Fig. 4 Loci of the unreacted and the reacted components on *P-V* plane during shock initiation process, the state quantities are extracted from the numerical simulation of shock initiation process, impact problems PMMA vs. PETN.
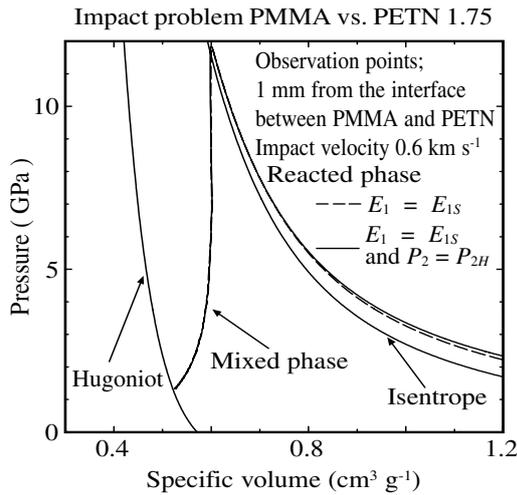
Impact problem PMMA vs. PETN 1.75

Fig. 5 Loci of the reacted component on *P-V* plane during the shock initiation process with the Hugoniot line for reacted component.

of the V_1 and V_2 which is independent on reaction pass. Because two lines are monotonic and single-valued function, the relation of the V_1 and V_2 can be expressed a continuous single-valued function in V_1 - V_2 plane.

Loci of the unreacted and reacted components on P - V plane during shock initiation process which was extracted one dimensional impact problems of PMMA vs. PETN are shown in Fig. 4. In those figure Hugoniot line for unreacted component and isentrope line for reacted component are drawn as reference line. In the case of 1.2 km s⁻¹ impact velocity, the reacted component has the similar path which is very close to the isentrope line except for $E_1 = E_{1H}$ case. The unreacted component also has similar path which is close to the isentrope solid or Hugoniot line. When the decomposition proceeds with high reaction rate as 1.2 km s⁻¹ impact velocity, the Hugoniot for unreacted and isentrope for reacted components probably be able to approximately be used the pressure calculation of the reacting explosive without equation (2). In the cases of 0.6 km s⁻¹ impact velocity, the reacted phases for all cases are deviating from its isentrope line which passes through the C-J point so that above assumption of Hugoniot and isentrope can not be used. Under the $E_1 = E_{1S}$, isentropic solid assumption, the unreacted component is fixed on the isentrope line, and from Fig. 4 (b) the reacted phase approximately pass a single line in P - V plane. This is an answer of the question why both specific volumes could be approximately described by single line in V_1 - V_2 plane. In this case our proposed method for pressure calculation of reacting explosive can be applied.

The single line exist above the isentrope line which pass through C-J point, and the upper limit of this type of shock initiation problems is the Hugoniot line for the reacted component. The pass for the reacted component obtained by isentropic solid assumption is compared with Hugoniot for the reacted component in Fig. 5. It has been found that the compression processes of reacted component of react-

Impact problem PMMA vs. PETN 1.75

(a) Impact velocity; 0.6km s⁻¹

Impact problem PMMA vs. PETN 1.75
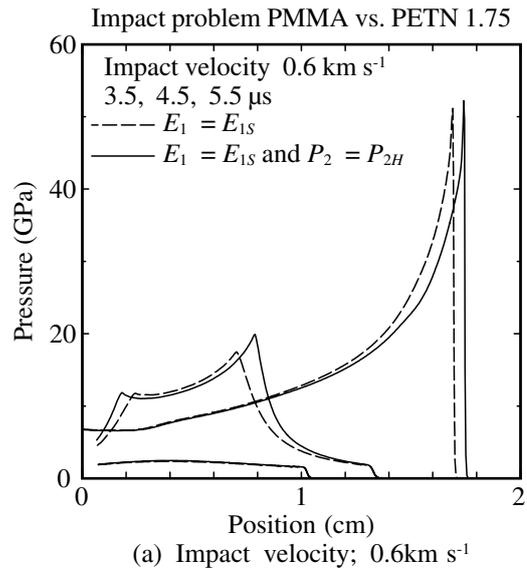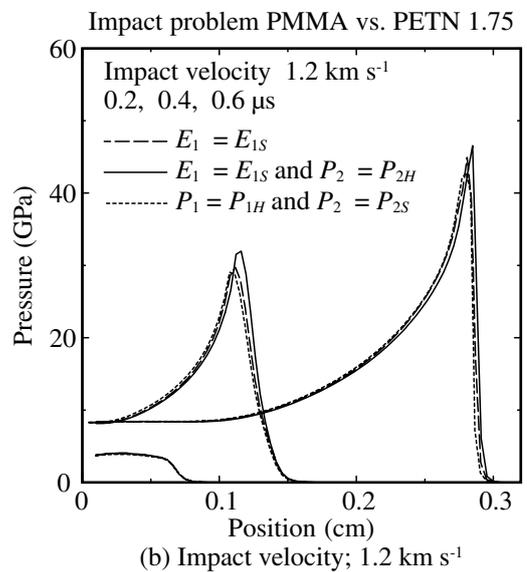
(b) Impact velocity; 1.2 km s⁻¹

Fig. 6 Comparison of the results of isentropic solid assumption and Hugoniot for the reacted component. The position is counted from the initial interface between the PMMA and PETN.

ing explosive have the path very close to Hugoniot line for reacted component under isentropic solid assumption. The assumption of isentropic solid and Hugoniot for reacted component was employed the pressure calculation without equation (2) in the numerical simulations. Figure 6 shows the comparison of the results from the assumption of isentropic solid, and isentoropic solid and Hugoniot for reacted component. Figure 7 is the x-t diagram on shock propagation process in PETN. The inflection points of those lines indicate the SDT point. The difference of those points is about 0.25 mm and is small comparison with the experimental error. Hugoniot for unreacted component and isentropic solid can reasonably be used the shock to detonation process.
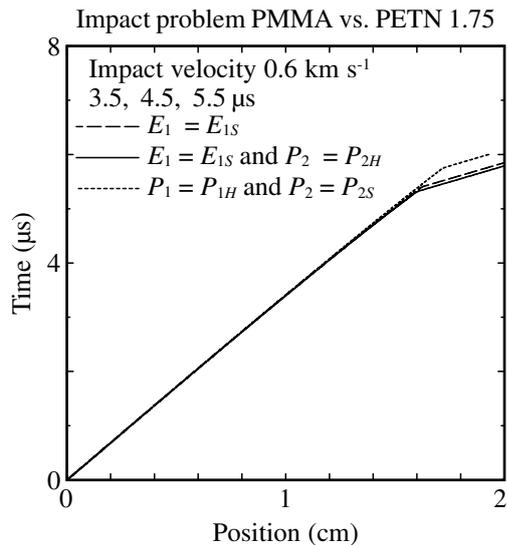
Impact problem PMMA vs. PETN 1.75

Impact velocity 0.6 km s^{-1}
3.5, 4.5, 5.5 μs
$---$ $E_1 = E_{1S}$
$——$ $E_1 = E_{1S}$ and $P_2 = P_{2H}$
$\cdots\cdots$ $P_1 = P_{1H}$ and $P_2 = P_{2S}$

Time (μs) — Position (cm)

Fig. 7 The x-t diagram on shock propagation process in PETN.

5. Conclusion

The state quantities for the unreacted and the reacted components were extracted during the numerical simulations of the shock initiation process under four types of assumptions to investigate its relations. The conclusions are as follows. The specific volumes for the unreacted component can be approximately described by the function of the specific volumes for reacted component without the internal energy and reaction rate in the cases of the assumptions of isentropic solid and $E_1 / E_2 = E_{1H} / E_{2S}$.

When the specific volumes of both components pass two types of single line in P-V plane, respectively, the above relation of the specific volumes is formed. Under the assumption of isentropic solid the reacted component has close path to the Hugoniot for reacted component.

References

1) J. N. Johnson, P. K. Tang, and C. A. Forest, J. Appl. Phys., 57, 4323 (1985).
2) S. Kubota, H. Shimada, K. Matsui, and K. Nagayama, Kayaku Gakkaishi (Sci. Tech. Energetic Materials), 62, 155 (2001).
3) P. R. Bervington, "Data redaction and error analysis for the physical science" (1969), McGraw Hill.
4) C. L. Mader, "Numerical Modeling of Detonations", (1979), University of California Press.
5) E. L. Lee and C. M. Tarver, Phys. Fluids, 23, 2362 (1980).
6) C. M. Tarver and J. O. Hallquist, 7th Symposium (International) on Detonation, pp. 488-497 (1981), Annapolis MD.
7) M. J. Murphy, E. L. Lee, A. M. Weston, and A. E. Williams, 10th Symposium (International) on Detonation, pp. 963-970 (1993), Boston MA.
8) J. W. Kury, H. C. Hornig, E. L. Lee, J. L. McDonnell, D. L. Ornellas, M. Finger, F. M. Strange, and M. L. Wilkins, 4th Symposium (International) on Detonation, pp. 3-13 (1965), White Oak MD.
9) E. Lee, M. Finger, W. Collins, LLNL report, UCID-16189 (1973).
10) H. Hornberg and F. Volk, Prop., Explos., Pyrotech., 14, 199 (1989).
11) C. M. Tarver, R. D. Breithaupt, and J. W. Kury, J. Appl. Phys., 81, 7193 (1997).

反応中の爆薬における簡略化された圧力計算法

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凝縮系爆薬の衝撃起爆の数値解析において，多くの場合，反応領域の状態量はその未反応成分と反応成分との単純な混合相として取り扱われる。この報告では，異なる4通りの仮定のもとで，求められる未反応成分と反応成分との比体積の関係について調べた。数値計算結果から次のことが分かった。ある条件のもとで，未反応成分の比体積は近似的に内部エネルギーや反応率に依存しない反応成分の比体積の関数として表せる。この関係は反応領域の圧力計算簡略化に応用できる。この関係が成立する条件は，未反応成分と反応成分との状態量が，圧力－体積面においてどちらも単一の線に沿って変化することである。未反応成分が等エントロピー的に変化すると仮定した場合，その反応成分は爆轟生成ガスの Hugoniot に近い状態変化を示す。

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