Simulation of sympathetic detonation by a CIP Eulerian code

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Abstract

We have developed the two-dimensional Eulerian hydrodynamic code to estimate various explosion phenomena which include large deformation, multi-material flow and the shock initiation process. The CIP method has been adopted to reduce numerical diffusion caused by calculation of the advection term in the Euler equations. To solve the initiation process of energetic material, an ignition and growth model has been employed. In this study numerical simulations of sympathetic detonation in the gap test were carried out. The charge diameter and gap length were varied to understand the size effect on the sympathetic detonation. We found that the critical gap length and the charge weight approximately have a linear relationship with a logarithmic scale.

Keywords: Eulerian hydrodynamic code, CIP method, ignition and growth model, gap test, sympathetic detonation.

1 Introduction

The practical problems for the risk assessment of the energetic materials include various complicated phenomena, large deformation of the materials, multi-material flows and the chemical reaction of energetic materials. For the problems that include the materials interfaces, the Lagrangian coordinate system is suitable to simulate the phenomena. However for solving the large deformation process of material the Lagrangian method encounter the difficulty because of the mesh crashes, and therefore we have selected the Eulerian coordinate system in our CFD code [1, 2]. In this case the two major problems remain. One is how to prevent the large numerical diffusion occurred by calculation of advection term.
in Euler equations, another is how to estimate the pressure in multi-material cell. CIP method [3, 4] has been adopted to reduce the numerical diffusion. In the cell in which the multi-material coexists, the iterative methods have been often adopted to calculate the pressure under the equilibrium assumption. In such cases, iterative calculation consumes the calculating time and frequently does not converge to solve the solutions. In the problems which include the reaction of the energetic materials, such us impact problem for metal vs. energetic material the cells near the impact surface will become multi-material cell of the metal and the energetic materials, at the same time the decomposition of the energetic material will begin after the impact. Therefore at the multi-material cell near the impact surface, we have to consider not only the mixing rule of metal and energetic material but also that reactant and detonation products components of energetic material to calculate the pressure. Those complicated cases frequently appear in the calculations of shock initiation phenomena. To avoid those difficulties of the pressure calculation the governing equations are constructed for all materials components in calculation field, and without iterative calculation the pressure of mixing phase is calculated by using the pressures of each components which are calculated by the volumes and internal specific energies for each components.

We have carried out the risk assessment of the energetic materials by the experiments and the numerical simulations. One of the most important items for the explosion risk is sympathetic detonation of energetic materials. Therefore we have to understand the sympathetic detonation phenomena under the various scales. The gap test is one of the most typical and simple technique to understand the sympathetic detonation phenomena for various scales explosions. In this study, we carried out the numerical simulations of gap test for various scales and examined the effect of size on the sympathetic detonation.

2 Numerical techniques and calculation model of the gap test

The governing equations in our CFD code are

\[
\frac{\partial f_{u}}{\partial t} + \vec{u} \cdot \nabla f_{u} = f_{u} \left( \frac{K}{K_{a}} - 1 \right) \nabla \cdot \vec{u} \tag{1}
\]

\[
\frac{\partial f_{\rho}}{\partial t} + \vec{u} \cdot \nabla (f_{\rho} \rho) = -f_{\rho} \rho \nabla \cdot \vec{u} \tag{2}
\]

\[
\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{1}{\rho} \nabla p \tag{3}
\]

\[
\frac{\partial f_{\rho e_{a}}}{\partial t} + \vec{u} \cdot \nabla (f_{\rho e_{a}}) = -f_{\rho e_{a}} \rho e_{a} \nabla \cdot \vec{u} - \eta_{a} p \nabla \cdot \vec{u} \tag{4}
\]

where \( \vec{u} \) is the velocity vector for \( x \) and radial directions, \( f_{\rho} \), \( \rho \) and \( e_{a} \) are the volume fraction, density and internal specific energy of the component \( \alpha \). In order to reduce the numerical diffusion caused by calculation of advection term
in Euler equations, cubic interpolated polynomial (CIP) scheme has been adopted. This method has been developed for solving general hyperbolic equations and for solving advection terms of flow equations applied after the non-advection phase is solved by finite difference method.

The pressure in multi-materials cell can be briefly calculated using following equation without iteration [5].

\[ P = K \sum \frac{P_a f_a}{K_a} \quad (5) \]

\( K \) is average bulk modulus for mixture cell and described as follows.

\[ K = \left\{ \sum \frac{f_a}{K_a} \right\}^{-1} \quad (6) \]

In addition, the reaction rate model is necessary to calculate the degree of decomposition of energetic materials. The ignition and growth model [6] was applied, and expressed as

\[ \frac{d\lambda}{dt} = I(1 - \lambda)^{2/9} \eta^4 + G(1 - \lambda)^{2/9} \lambda^{2/3} P^z, \quad (7) \]

where \( \lambda \) is the mass fraction of detonation products; \( \lambda = 0 \) corresponds to the unreacted state and \( \lambda = 1 \) to the completely reacted state, and \( \eta = \rho/\rho_0 - 1 \). The parameters \( z, G, I \) depend on the explosive properties and are chosen as giving the best agreement with shock initiation experimental data. The advection term of eqn.(7) is also solved by CIP method. In order to calculate the pressure of reacting explosive, the simple mixture theory, in which the reacting explosive is regarded to be a simple mixture phase of reactant and product components, has been adopted. The equations of state for materials are also necessary. For unreacted and reacted phases, Jones, Wilkins and Lee (JWL) equation of state [7] [8] is employed. The expression is given in the below,

\[ P = A\left[1 - \omega/(R_1 \zeta)\right]\exp(-R_1 \zeta) + B\left[1 - \omega/(R_2 \zeta)\right]\exp(-R_2 \zeta) + \frac{\omega}{\zeta} \rho_0 e \quad (8) \]

where \( \zeta \) is \( \rho_0/\rho \), subscript 0 indicates initial state of condensed explosive. A, B, \( R_1, R_2 \), are constants, \( \omega \) is the Gruneisen coefficient. The JWL parameters of Composition B are shown in table 1 [9]. For air and PMMA, ideal gas and Mie Gruneisen form equations of state are employed, respectively.

The calculation model of the gap test is shown in fig.1. There are five materials in this calculation model. Both of the donor and the acceptor charges are composition B, and the substance of gap material and explosive holder is PMMA. A witness plate is made by steel and the surroundings of equipment are air. The ratio of length and diameter of both charges is set to 1, and size of
charge diameters was varied to understand size effect in sympathetic detonation phenomena.

![Calculation model for gap test.](image)

Figure 1: Calculation model for gap test.

Table 1: JWL parameters for Composition B.

<table>
<thead>
<tr>
<th>Explosive</th>
<th>Phase</th>
<th>A (GPa)</th>
<th>B (GPa)</th>
<th>R₁</th>
<th>R₂</th>
<th>ω</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composition B</td>
<td>Reacted</td>
<td>524</td>
<td>7.678</td>
<td>4.2</td>
<td>1.1</td>
<td>0.34</td>
</tr>
<tr>
<td></td>
<td>Unreacted</td>
<td>788</td>
<td>-5.03</td>
<td>11.3</td>
<td>1.13</td>
<td>0.894</td>
</tr>
</tbody>
</table>

3 The parameters of ignition and growth model

In order to obtain the parameters of the ignition and growth model for Composition B we calculated the one-dimensional shock initiation problem. Those parameters were chosen as giving the best agreement with the experimental data. We compared the numerical results and the published experimental data, and the parameters were adjusted by trial and error method. Figure 2 indicates the plots for Run distance to detonation versus initial pressure for Composition B. In this figure the good agreement between the experimental [10] and the numerical results can be confirmed. The parameters of ignition and growth model were I = 44, G = 1200 and z = 2.54, respectively. The numerical results of one-dimensional impact problems are shown in fig. 3 to compare the
results of Lagrangian and CIP Euler. Although the Lagrangian is more advantageous than Euler method in this calculation, the good agreement can be confirmed. Those results demonstrate that the CIP Euler method well represents the shock initiation phenomenon.

Figure 2: Run distance to detonation versus initial pressure for Composition B.

Figure 3: Numerical results of one-dimensional impact problems of Aluminum versus Composition B. Original point of the shock front is the initial contact surface between aluminum and the composition B, and time is measured from the moment of a collision.
Figure 4: The propagation process of shock wave in half cross section of the calculation model with density distributions. Charge diameter; 260 mm, Gap length; 500mm

Figure 5: Relationship of the critical gap length and the charge weight obtained by CIP Euler code.

Charge weight: 10 g, 36 g, 300 g, 2.2 kg and 20 kg
Comp. B ($\rho_o=1.712$ g/cc)

Gap length (mm)

no detonation

Critical gap length
Gap material: PMMA

Charge weight (kg)
4 Discussion

Figure 4 shows the propagation process of shock wave with density distributions. The ignition point of donor charge is the origin. The ignition and growth model is employed for both charges. Time is counted from the ignition of donor charge. In this case the shock to detonation transition (SDT) occurs at the middle points in acceptor charge at 230 $\mu$s. When the SDT occur before the shock front arrives at the interface of witness plate and acceptor charge, we regarded such situation as the sympathetic detonation. The critical gap length in which the sympathetic detonation does not occur was estimate by varying the gap length. The relationship of the critical gap length and the charge weight are shown in fig. 5.

The calculation results have indicated that the relationship of critical gap length and the charge weight approximately have linear relationship with logarithmic scale.

5 Summary

Numerical simulations of sympathetic detonation in gap test were carried out by a CIP Eulerian code. Both of the donor and the acceptor charges are Composition B, the ratio of length and diameter of both charges is set to 1 and gap material is PMMA. Both of the gap length and the charge weight are varied to understand the size effect in sympathetic detonation. The calculations results show that the critical gap length and the charge weight approximately have linear relationship with logarithmic scale.

References


