Development of a 2D eulerian code for reactive shock analysis using CIP scheme

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Eulerian numerical technique is superior to the Lagrangian method in the calculation of problems involving shocks and large deformations. However, the Eulerian method has its own several technical problems that are being improved presently. A major one of those is the numerical diffusion related to the computational scheme; another is the determination of pressures in mixed cells when problems include two or more types of materials. The cubically interpolated polynomial (CIP) scheme exhibits its advantages to the prevention of numerical diffusion. For the pressures in mixed cells, a relatively simple method has recently been proposed for solving the interactions of materials with solid and gaseous phases. The method explicitly solves pressures in mixed cells without use of the iteration procedures. This paper will describe the development of a two-dimensional Eulerian code, MARS2D (Multi-dimensional Analysis Code for Reactive Shocks, 2D vision), that employs the above two technical routines for the purposes of calculating the problems involving strong shocks and reactive media. Problems of high-velocity impact, blast waves in air, and cylinder expansion test will be taken as the computational examples.

1. Introduction

Shock waves and large deformations are often encountered in the processes of high velocity impact of materials and of explosions of explosives in the surrounding media. The propagation of shock wave and the material deformation presented in such phenomena are very complicated and cannot be solved by empirical formulas or analytical methods in practice. So, numerical approaches become major tool in the treatment on those types of problems. Generally there are two kinds of numerical formulations to solve the problems involving shocks and large deformations, Lagranian and Eulerian methods.[1] The Lagrangian method has the advantages in numerical accuracy and also in the tracing of the motion of the material interfaces when a problem involves multiple materials. However, in the cases of strong shocks and large deformations, the Lagrangian formulation exposes its drawbacks in the calculation. Mesh tangling and crashes due to the strongly deformed cells will result in the stagnation of the progress of the calculation unless a very complex procedure, rezoning technique, is introduced to weaken the effect of those shortcomings. The Eulerian formulation does not possess such problems because the mesh used in the calculation is fixed regarding to the space. From this point of view, the Eulerian technique is of great advantage over the Lagrangian method. Even so, the Eulerian method has its own several technical problems that are being improved presently. A major one of those is the numerical diffusion related to the computational scheme; another is the determination of pressures in the mixed cells when problems include two or more types of materials.

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On the computational schemes, the cubically interpolated polynomial (CIP) scheme [2-3] exhibits its advantages to the prevention of numerical diffusion. Employing that scheme, a series of computer programs (MARS1D, MARS2D and MARS3D) have been developed or are still being developed at AIST [4]. On the other hand, for the pressures in mixed cells, the most commonly used method is the iteration procedures by assuming that each component in the mixtures is in thermal and pressure equilibria or only in pressure equilibrium. Recently, Vorobiev and Lomov [5] have tried a relatively simple method on the determination of pressures in mixed cells of materials with solid and gaseous phases. The method explicitly solves pressures in mixed cells without use of the iteration procedures. It demonstrates much superiority both in program coding and in reduction of computing time. This paper will describe the development of a two-dimensional Eulerian code, MARS2D, which employs both technical routines for the purposes of calculating the problems involving strong shocks and reactive media. Problems of high-velocity impact, blast waves in air, and cylinder expansion test are used as the computational examples.

2. CIP Scheme

The basic consideration in the numerical technique of cubically interpolated polynomial (CIP) scheme is to divide a hyperbolic form of partial differential equation into two parts called the non-advection phase and the advection phase, respectively, and the solution to the equation is taken as a consequence of the advection of the temporary solution obtained at the non-advection phase. In order to have a quick understanding to this numerical scheme, a one-dimensional partial differential equation is employed for illustration,

$$\frac{\partial f(x,t)}{\partial t} + u\frac{\partial f(x,t)}{\partial x} = g(x,t), \qquad (1)$$

where, f and g are functions of space coordinate, x, and time, t, u is a positive constant and is usually called the advection velocity. In the CIP scheme, the above equation is divided into two sub-equations such as,

$$\frac{\partial f(x,t)}{\partial t} = g(x,t), \text{ (non-advection phase)} \qquad (2)$$

$$\frac{\partial f(x,t)}{\partial t} + u\frac{\partial f(x,t)}{\partial x} = 0, \text{(advection phase)} \qquad (3)$$

In general, Eq. (1) can be solved by finite difference approach with no difficulty. If denoting the solution at the non-advection phase by f^* and keeping in mind that f^* is a discrete solution with respect to space at new time cycle, then, the solution at the intermediate position between spatial position of x and its immediately left (or right) neighboring spatial position is connected by a cubic polynomial of

$$f^*(\xi,t) = a(\xi - x)^3 + b(\xi - x)^2 + (\xi - x)\frac{\partial f^*(x,t)}{\partial x} + f^*(x,t), \qquad (4)$$

where ξ is the space coordinate at the neighborhood of spatial position of x, $\partial f / \partial x$ is the partial derivative of $f(x,t)$ with respect to x. On the other hand, the solution at the advection phase has the trivial form of $f(x,t+\Delta t)=f(x-u\Delta t, t)$. As a result, the substitution of ξ with $x-u\Delta t$ into Eq. (4) leads to the acquirement of the solution to Eq. (1) at space x and new time cycle, $t+\Delta t$, as

$$f(x,t+\Delta t) = a(-u\Delta t)^3 + b(-u\Delta t)^2 + (-u\Delta t)\frac{\partial f^*(x,t)}{\partial x} + f^*(x,t). \qquad (5)$$

It should be noted that in Eq. (4) the value of partial derivative $\partial f / \partial x$ is used and this quantity, at present, is still unknown. However, it can readily be realized that when a partial differentiation with respect x is performed on both sides of Eq. (1), the following equation may be gained

$$\frac{\partial}{\partial t}\left[\frac{\partial f(x,t)}{\partial x}\right] + u\frac{\partial}{\partial x}\left[\frac{\partial f(x,t)}{\partial x}\right] = \frac{\partial g(x,t)}{\partial x}. \qquad (6)$$

It can be seen that Eq. (6) of $\partial f / \partial x$ has the similar form of Eq. (1). Likely, it is also divided into the non-advection phase and the advection phase. In the non-advection phase, $\partial f / \partial x$ is solved for the use in the cubic polynomial interpolation. In the advection phase, its solution may be found by differentiating Eq. (4) with respect to ξ and substituting ξ with $x-u\Delta t$ subsequently. The detailed illustration is not recited and can be found elsewhere. [2,3]

3. Multi-materials System

The practical problems involving shock and reactive processes usually present the co-existence of multiple materials. Before pursuing numerical solution to such system, the governing equations of mass, momentum and energy should first be

established. For a multi-materials system including N components that can be taken as compressible fluids, one way for doing this is of the following set of equations, [5)6)]

$$\begin{aligned}
&\frac{\partial f_\alpha}{\partial t}+\vec{u}\cdot\nabla f_\alpha = f_\alpha\left(\frac{K}{K_\alpha}-1\right)\nabla\cdot\vec{u}\\
&\frac{\partial f_\alpha\rho_\alpha}{\partial t}+\vec{u}\cdot\nabla(f_\alpha\rho_\alpha) = -f_\alpha\rho_\alpha\nabla\cdot\vec{u}\\
&\frac{\partial\vec{u}}{\partial t}+\vec{u}\cdot\nabla\vec{u} = -\frac{1}{\rho}\nabla p\\
&\frac{\partial f_\alpha\rho_\alpha e_\alpha}{\partial t}+\vec{u}\cdot\nabla(f_\alpha\rho_\alpha e_\alpha) = -f_\alpha\rho_\alpha e_\alpha\nabla\cdot\vec{u}-\eta_\alpha p\nabla\cdot\vec{u}
\end{aligned} \tag{7}$$

where, α denotes a component within 1 to N. f is the volume fraction of one component in total volume, p is the pressure, ρ is the density, e is the specific internal energy, u is the vector of velocity. K_α is the bulk modulus of one component, K is the equivalent bulk modulus of total components, η_α is the mass fraction of one component in a total mass. The expressions for K_α, K and η_α will be given later. Naturally, there are valid that $\Sigma f_\alpha=1$ and $\Sigma\eta_\alpha=1$ from definitions. It is noticeable that Eq. (1) is not written in a conservative form but in a non-conservative type favorable for being divided into the non-advection phase and the advection phase that are required by the CIP scheme.

After the establishment of the governing equations for a multi-materials system, it is still necessary to have knowledge of the equation of state in order to make the system solvable. For a single material system, the equation of state has been known in one way or other ways, however, for a multi-materials system, studies on this aspect seem to be sparse. A general methodology to achieve this goal is to assume that the components of multi-materials system be in thermal and pressure equilibria or only in pressure equilibrium, and then, to perform the iteration procedures to obtain the pressures. Needless to say that such treatment is troublesome in program coding and more is time-consumed in computation. Following Vorobiev and Lomov's point of view, [5)] a simple procedure for the acquirement of pressure in the multi-materials system will be introduced.

For αth component whose equation of state is known, as first approximation, the pressure variation at state (P_α, V_α) may be expressed as

$$\Delta P_\alpha = -K_\alpha\frac{\Delta V_\alpha}{V_\alpha}, \tag{7}$$

where, K_α is the bulk modulus of αth component which is given by $-V_\alpha\partial P_\alpha/\partial V_\alpha$. To the total system, it is able to assume the same expression for the variation of pressure. Hence, it is valid for

$$\frac{\Delta P}{K}=-\frac{\Delta V}{V}=-\frac{\Sigma\Delta V_\alpha}{V}=-\sum\left[\frac{\Delta V_\alpha}{V_\alpha}\cdot\frac{V_\alpha}{V}\right]=\sum\frac{\Delta P_\alpha f_\alpha}{K_\alpha}, \tag{8}$$

where, K is the equivalent bulk modulus for the system. According to the point of pressure equilibrium, the variation of pressure in each component is equal to that for the system, so, there is obtained,

$$K=\left[\sum\frac{f_\alpha}{K_\alpha}\right]^{-1}. \tag{9}$$

On the other hand, owing that the work done by pressure within the change of volume for the system is equal to the sum of the work done for each component with its individual change of volume (in reality, it is the virtual work principle), it leads to the acquirement of pressure as

$$P=K\sum\frac{P_\alpha f_\alpha}{K_\alpha}. \tag{10}$$

For the mass fraction of a component, it is given by

$$\eta_\alpha=\frac{\rho_\alpha f_\alpha}{\rho}, \tag{11}$$

where, ρ represents the density of total components.

4. Computational Examples

4.1 One dimensional impact problem

As a simple test for the application of the present code, one dimensional impact problem is chosen to demonstrate the computational ability of the code. An aluminum block with a length of 25 mm impacts a copper block with the equivalent length at velocity of 2 km s^{-1} from the left. The calculated shock positions and pressures at several times are presented in Fig. 1 (a). Theoretical shock amplitude at the given condition is also plotted for comparison. It is found that the shocks in aluminum and copper steadily propagate with a constant strength corresponding to the theoretical value. At the beginning of the impact, somewhat oscillation appears in the vicinity of the interface during the calculation, however, it soon vanishes and the reasonable pressure is obtained. To further

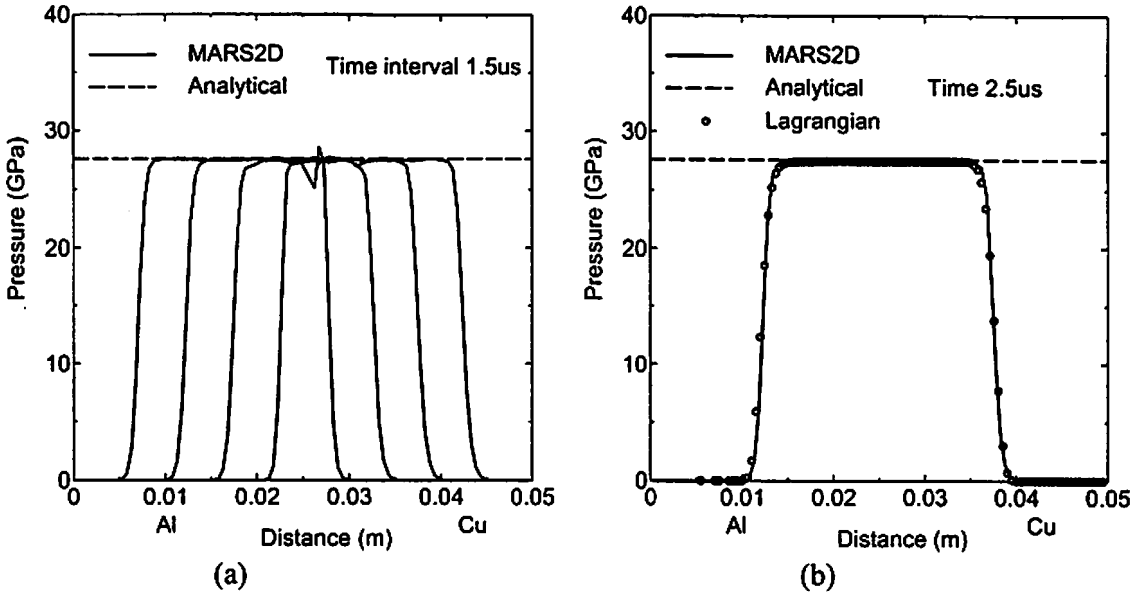

Fig. 1 shock propagations in one dimensional impact of aluminum and copper. (a) shock profiles; (b) comparison with result from Lagrangian code.

examine the shock profile, the same problem was calculated with a Lagrangian code. Two shock profiles at time of 2.5 μs after impact are presented in Fig. 1(b) and can be found in good consistency with each other.

4.2 Two dimensional impact problem

In the two dimensional impact calculation, the case is considered that a rectangular copper 25 mm long and 5 mm wide penetrates a plate of aluminum with the height of 45mm and the thickness of 5 mm. The impact velocity of copper is assumed to be 2 km s^{-1}. The calculation should treat the interactions of various waves as well as the motions of the boundaries. Vacuum is introduced as one material to account for the motions of the free boundaries. Fig. 2 shows the penetration processes at different phases of time in the forms of isopycnics. After short time of impact, as shown in Fig. 2(b), it is clearly seen that shock propagations occur in both copper impactor and aluminum plate. With the increase of time, it is visible that a large rarefaction area at the back of the aluminum plate opposite the impact region appears. This is resulted from the assumption of the materials with fluid-like behavior at present. In practice, the materials are at the state of elastic-plastic flow, so it is the place in which many fragments form due to the spalling appearance. Therefore, the elongation shape of the plate is obtained.

4.3 Blast wave propagation

Using MARS2D, a blast wave problem is computationally performed to demonstrate the calculation on the strong shock propagation. A 10 mm square TNT is exploded in the air with dimensions of 100 mm times 100 mm area. TNT is assumed to be exploded under constant volume model. This implies that the initial TNT gases are with density and specific internal energy equivalent to solid TNT density and its detonation heat. Several typical blast wave images from the calculation are presented in Fig. 3. The high pressure TNT gases cause a strong shock in the surrounding air and subsequently the shock spreads outward to expand its affecting circle. From those graphical results, it can be seen that the calculation is successful to some extent. The interactions of blast waves as well as the propagation of blast wave under complicatedly geometrical condition are left for the future work.

4.4 Cylinder expansion test

Cylinder expansion test is a standard experiment to determine the parameters in Jones-Wilkins-Lee (JWL) equation of state for detonation products, and also is a good measure to assess the

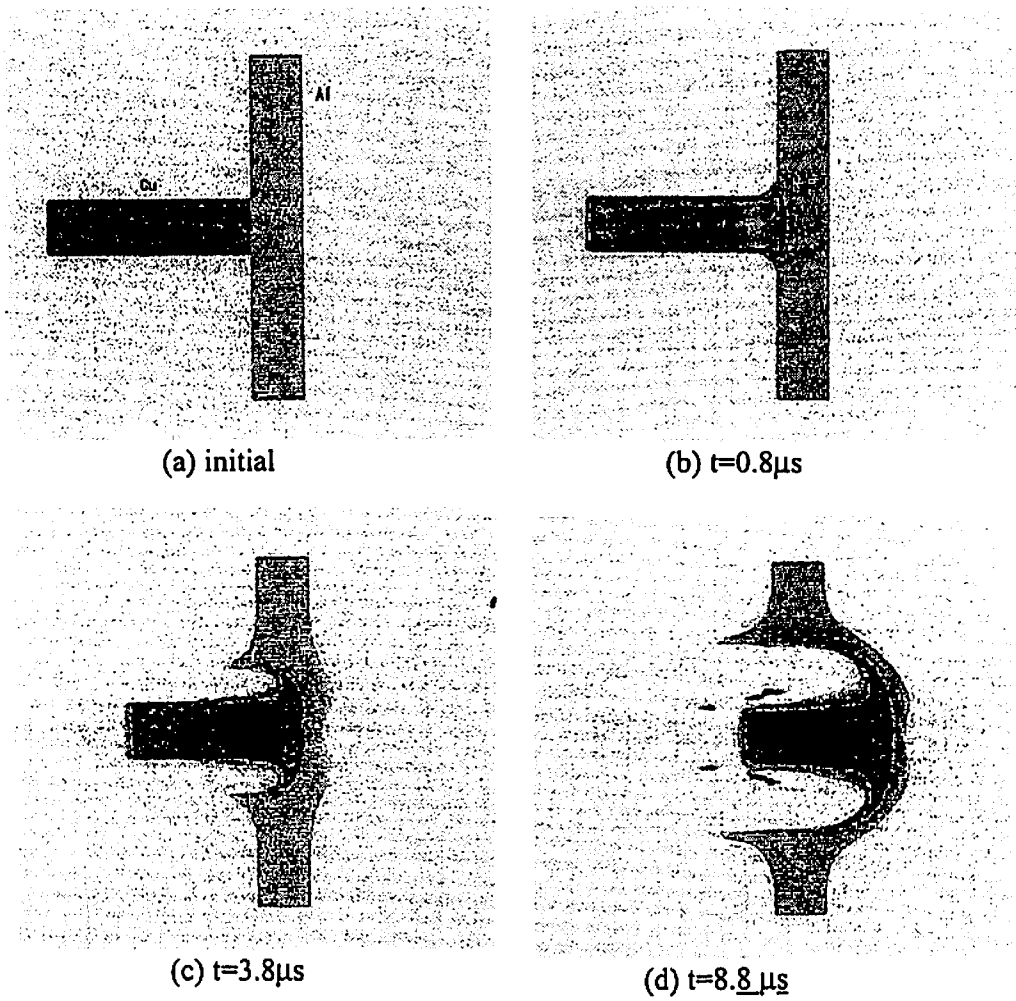

Fig. 2 Calculated processes in two dimensional impact of copper and aluminum.

performance abilities of the explosives. The numerical simulation to such experiments may be a good test to make a code be applicable to reactive materials because the calculation must deal with the detonation of the explosive. In the calculation, the plane geometry is used in place of the axisymmetric shape in experiment for simplicity. The explosive is the nitromethane and the copper is used for the metal confinement. Outside the copper and nitromethane is the vacuum. The detonation process of nitromethane is modeled by a simple burn model called C-J volume burn. The nitromethane is of a width of 50.8 mm and 300 mm long. The copper is 300 mm long and 2.6 mm thick. Fig. 1 shows several snaps obtained from the calculation. The detonation of nitromethane and the expansion of copper are clearly demonstrated. In the area near the initiating end, even the copper deforms to such extent, its shape, however, is completely kept. It illustrates that the CIP scheme indeed has a high capability in the prevention of numerical diffusion. Fig. 5 gives the profiles of pressures in nitromethane detonation products along the centerline at several instants. The propagation of the detonation wave is revealed to be in a steady progress during the calculation although the peaks are slightly lower than its nominal detonation pressure. Some improvements should be expected in the future.

5. Concluding Remarks

Developments of the Eulerian codes are particularly beneficial to the solutions of the problems involving strong shocks and large deformations. However, because of its essential feature of Eulerian formulation, it is desired that Eulerian codes should be less numerically diffusive and be of efficiency in the treatment of multi-

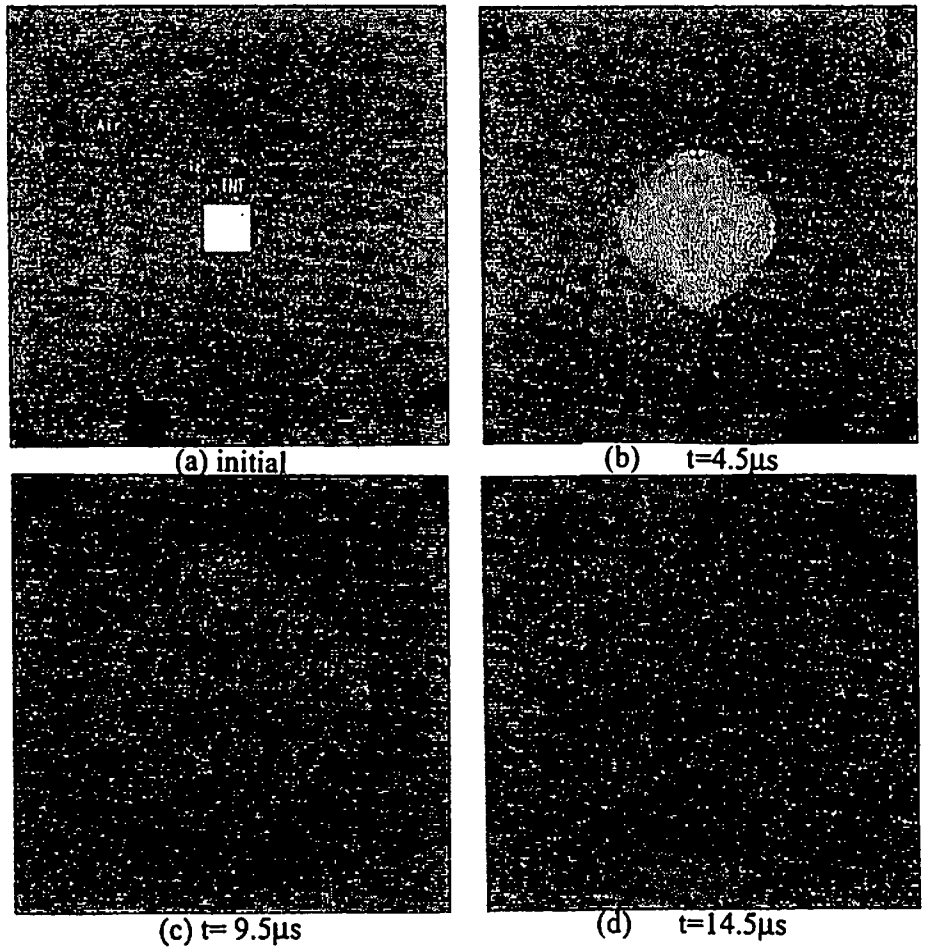

Fig. 3 Typical images of strong shocks in air blast of TNT.

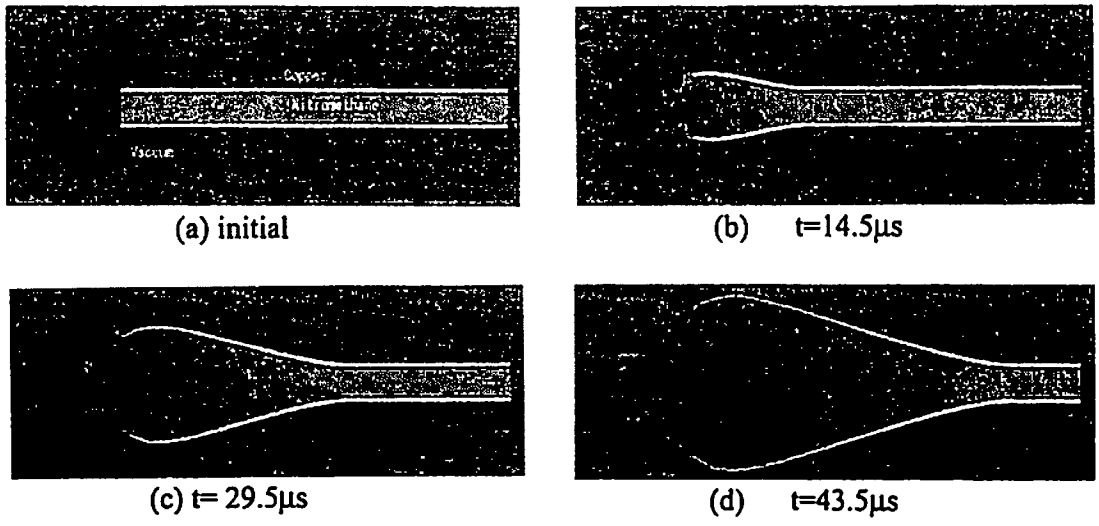

Fig. 4 Calculated snaps of detonation propagation and deformation of metal plate.

materials. The combination of CIP scheme and a simply technical treatment on multi-materials makes MARS2D be a promising code in the family of Eulerian codes. Several examples presented demonstrate the capability of MARS2D in the calculations of problems involving strong shocks and large deformations. Owing to its initial phase in development, much work will still be done in the future in order to make it applicable to the more realistically practical problems.

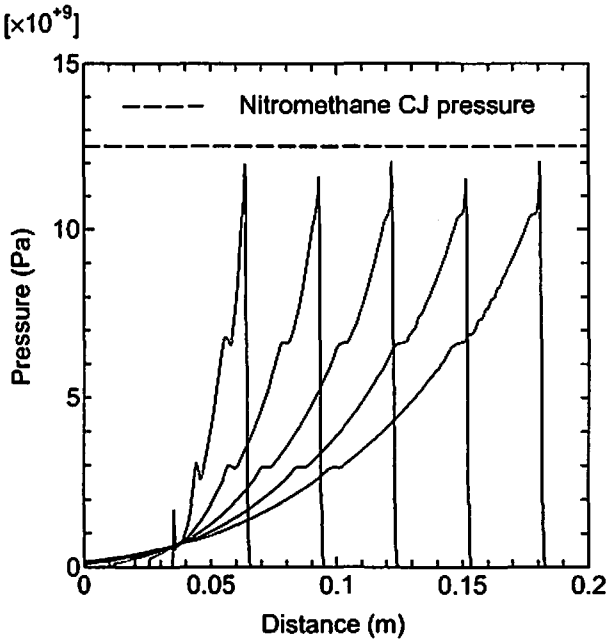

Fig. 5 Calculated pressure profiles in detonation products of Nitromethune.

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References

1) Zukas, J. A., *High Velocity Impact Dynamics*, Wiley Intersciences, New York, 1990.

2) Takewaki, H. and Yabe, T., "The cubic interpolated pseudo particle (CIP) method: application to nonlinear and multi-dimensional hyperbolic equations," *J. Comp. Phys.*, Vol. 70, pp. 355-372, 1987.

3) Yabe, T. and Wang, P., "Unified numerical procedure for compressible and incompressible fluid," *J. the Phys. Soc. of Japan*, Vol. 60, No. 7, pp. 2105-2108, 1991.

4) Reports of the All Japan Association for Security of Explosives.

5) Vorobiev, O. Yu and Lomov, I. N., "Numerical simulation of gas-solid interfaces with large deformations," *Advances in Computational Engineering & Sciences 2000*, Vol. 1, Tech Science Press, pp. 922-927, 2000.

6) Miller, G. H. and Puckett, E. G., "Higher-order Godunov method for multiple condensed phases," *J. Comp. Phys.*, Vol. 128, pp. 134-164, 1996.