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Three-dimensional ghost-fluid large-scale numerical investigation on air explosion

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ABSTRACT

Based on the double shockwave approximation procedure, a local Riemann solver for strongly nonlinear equations of state (EOS) such as the Jones–Wilkins–Lee (JWL) EOS is presented, which has suppressed successfully numerical oscillation caused by high-density ratio and high-pressure ratio across the interface between explosion products and air. The real ghost fluid method (RGFM) and the level set method have been used for converting multi-medium flows into pure flows and for implicitly tracking the interface, respectively. A fifth order finite difference weighted essentially non-oscillatory (WENO) scheme and a third order TVD Runge–Kutta method are utilized for the spatial discretization and the time advance, respectively. An enclosed-type MPI-based parallel methodology for the RGFM procedure on a uniform structured mesh is presented to realize the parallelization of three-dimensional (3D) air explosion. The overall process of 3D air explosion of both TNT and aluminized explosives has been successfully simulated. The overpressures at different locations of 3D air explosion for both explosives mentioned above are monitored and analyzed for revealing the influence of aluminum powder combustion on the overpressure of the explosion wave. Numerical results indicate that, due to aluminum powder afterburning, the attenuation of the explosion wave formed by aluminized explosives is slower than that caused by TNT.

1. Introduction

Air explosion is a typical multi-medium problem, in which the explosion flow field usually consists of many media such as detonation products and air. It is obvious that the sharp medium interface with high-density ratio and high-pressure ratio separates detonation products from air. In the numerical simulation of air explosion, because of the abrupt change of density and pressure close to the interface, unphysical numerical oscillation may easily appear in the neighborhood of the interface. Meanwhile, with the continuous upgrade of explosives, density ratio and pressure ratio increase constantly and significantly. Therefore, tracking and treating the strong nonlinear discontinuous interface in air explosion have received considerable attention.

Many interface tracking techniques have been discussed over the past few decades. The marker-and-cell (MAC) method proposed by Harlow and Welch [1] has often been used to track interface movement and flow field evolution. However, the maintenance of a sharp interface among multi-medium is difficult. Hirt and Nichols [2] presented another interface tracking algorithm known as volume-of-fluid (VOF) method without tracking the motion of the multi-medium interface, in which, as time increases, the volume of each medium in each cell is changing continuously and the new interface is reconstructed from the volume at the current time level. The main drawback of the VOF method is that, for deciding the normal direction of the multi-medium interface, a cluster of eight neighboring cells for the two dimensional case must be taken into consideration [3]. To overcome such drawbacks of the VOF method, the moment of fluid (MOF) method introduced by Ahn and Shashkov [4] and by Dyadechko and Shashkov [5] with second order accuracy employed not only volume fractions but also the position of the centroid, which allows the MOF method to utilize the cell where reconstruction is performed. The well-known particle-in-cell (PIC) algorithm by Amsden [6] is a Lagrangian description of the flows in which particles are explicitly associated with different medium and thus the interface can be tracked easily. The principal drawbacks are a large numerical diffusion and a numerical noise, due to the momentum transfer between grids and particles and the employment of finite particle numbers. The level set method developed by Osher and Sethian [7] is a simple and versatile method for tracking the evolution of a locomotive

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interface. We would like to mention in particular the work of Vahab and Miller [8], which provided a second order front-tracking method by combining the Godunov algorithm with the level-set method, in which global conservation was realized. The level-set method [9–11] generally uses a Hamilton–Jacobi equation to describe the moving interface, which is tracked as the zero level set of a continuous function mimicking the signed distance function instead of an explicit function at the new time level. Thus, cases with complex interfaces, such as crisscross, torsion and separation, etc., can be easily handled by the level-set method.

Fedkiw et al. [12] presented the original ghost fluid method (OGFM), which can address excellently the interaction between a weak shock wave and an interface. To further improve the accuracy of the OGFM method, Liu et al. [13] discussed the modified ghost fluid method (MGFM) procedure, which performed better than OGFM due to a local Riemann solver, where the status of the ghost fluid across the interface for each phase was defined by predicted interfacial status. The accuracy of MGFM for gas-gas Riemann problem performed by Liu et al. in [14] shows that, compared with the exact solution of a Riemann problem, the MGFM solution could reach second order accuracy near multi-medium interface. The key point of the real ghost fluid method (RGFM) procedure, presented by Wang et al. [15] was that, according to the status of the medium across the interface, a local Riemann problem was constructed at first and interfacial status obtained was then used to redefine flow status for not only the real fluid grid points close to the interface but also the ghost fluid grid points, by which smaller error was introduced in the RGFM procedure in comparison to the MGFM procedure. We remark that the RGFM method we adopt in this paper does have conservation errors, like other ghost fluid type methods, but it seems to have smaller conservation errors than OGFM or MGFM in numerical simulation. We refer the readers to [15] for a more detailed discussion on this issue.

Since OGFM, MGFM and RGFM were introduced, an increasing number of numerical simulations combining these methods for multi-medium flows can be found in the literature. However, most of the previous simulations with GFM-based procedures used simple and linear equation of state (EOS) for describing multi-medium flows such as explosion products and air in air explosion, while the complex EOS such as the Jones-Wilkins-Lee (JWL) EOS have seldomly been used. Meanwhile, numerical simulations based on the RGFM procedure splitting a multi-medium problem into pure flows usually require large parallel computer resources. In general, serial computation cannot meet the requirements of multi-dimensional large-scale engineering applications.

In this paper, based on a double shockwave approximation procedure, we first present in detail a technique to construct and solve the local Riemann problem with the complex EOS such as JWL used in air explosion. Our numerical simulation demonstrates that this technique effectively eliminates unphysical oscillation which often occurs at the multi-medium interface in explosion flow fields. Combining the RGFM method, formally transforming multi-medium flow into pure flows with an enclosed-type parallelization module, the mechanisms of 3D air explosion are studied by using a fifth order finite difference WENO scheme on a uniform structured mesh.

2. Governing equations

The governing equations in a conservative form without considering the viscous and thermal diffusion effects for describing a 3D air explosion can be written as

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}+\frac{\partial G(U)}{\partial y}+\frac{\partial H(U)}{\partial z}=0$$

$$U=(\rho,\rho u,\rho v,\rho w,\rho E)^T$$

Table 1
JWL EOS parameters for explosion products of TNT charge.

ρ_0 (kg/m^3)	A (MPa)	B (MPa)	R_1	R_2	ω
1630.0	373800.0	3747.0	4.15	0.9	0.35

$$\begin{aligned}F(U)&=(\rho u,\rho u^2+p,\rho uv,\rho uw,(\rho E+p)u)^T\\G(U)&=(\rho v,\rho uv,\rho v^2+p,\rho vw,(\rho E+p)v)^T\\H(U)&=(\rho w,\rho uw,\rho vw,\rho w^2+p,(\rho E+p)w)^T\end{aligned}\tag{1}$$

where ρ and p denote the density and pressure, respectively. u, v and w are velocity components in the x, y and z directions in Eulerian coordinates, and the total energy E, generally consisting of internal energy and kinetic energy, is given as

$$E=\frac{u^2+v^2+w^2}{2}+e\tag{2}$$

where e is the internal energy per unit mass.

For aluminized explosives, the Miller model [16] describing the combustion and heat release process of aluminum powder can be used to describe the reaction process. By coupling the above 3D Euler equations with the Miller model, the whole process of air explosion for aluminized explosives can be captured numerically. The Miller model given in [16] is

$$\frac{d\lambda}{dt}=\frac{1}{4}(1-\lambda)^{\frac{1}{2}}p^{\frac{1}{6}}\tag{3}$$

where $\frac{d\lambda}{dt}$ is the material derivative and λ is the chemical reaction process variable characterizing the aluminum powder reaction degree. The reaction process parameters $\lambda=0$ and $\lambda=1$ are defined as the initially unreacted and completely burned states, respectively. The material derivative in (3) is first converted to Eulerian derivatives and then (3) is solved together with the governing Eq. (1) using the WENO scheme described below. To close the above governing equations, the respective EOS for air and explosion products should be introduced. The ideal gaseous EOS for air can be presented as

$$p=(\gamma-1)\rho e\tag{4}$$

where $\gamma=1.4$ is a gaseous constant.

Assuming no heat loss to the surroundings, the expansion of explosion products of TNT charge is usually described by the JWL EOS [17], which can be expressed in the following form

$$p=A\left(1-\frac{\omega\rho}{R_1\rho_0}\right)e^{-\frac{R_1\rho_0}{\rho}}+B\left(1-\frac{\omega\rho}{R_2\rho_0}\right)e^{-\frac{R_2\rho_0}{\rho}}+\omega\rho e\tag{5}$$

where the parameters A, B, R_1, R_2, ω and ρ_0 are material constants of detonation products, which are shown in Table 1.

The EOS of detonation products of aluminized explosives should be able to establish the essential relationship among pressure, density, internal energy and the reaction process variable. The JWL-Miller EOS [16] for describing detonation products of aluminized explosives are adopted as

$$p=A\left(1-\frac{\omega\rho}{R_1\rho_0}\right)e^{-\frac{R_1\rho_0}{\rho}}+B\left(1-\frac{\omega\rho}{R_2\rho_0}\right)e^{-\frac{R_2\rho_0}{\rho}}+\frac{\omega\rho(\widetilde{E}+\lambda Q)}{\rho_0}\tag{6}$$

where $\widetilde{E}$ denotes the energy content of aluminized explosives for keeping the so-called CJ condition, which denotes a relationship between the propagating velocity of the detonation wave and the local speed of sound. The constant Q is defined as afterburning energy release after the CJ plane located at the end of the reaction zone. A, B, R_1, R_2, ω and ρ_0 in the above Eq. (6) are material constants of detonation products, which can be found in Table 2.