Numerical Prediction on the Dispersion of Inert Solid Particles under the Explosion of Nitromethane

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1 Introduction

Solid particles are widely used for explosives due to their enhancement of impulsive loading. Increment of impulse can be achieved from high pressure explosion and afterburning of explosive product. During the initial stage of explosion, explosion gas momentum is transferred to solid particle. Solid particles have higher inertia than the explosion gas and they maintain momentum for a longer time. Figure 1 shows the wave diagram of the typical explosives with solid particles. After the chemical explosion from a high explosive, a blast wave propagates outward and a rarefaction wave inward. Overexpanded rarefaction wave creates secondary shock near the core. Solid particles overtake and interact with the contact surface. The secondary shock interacts with contact surface and solid particles. It is known that there are two kinds of instabilities in such flow fields--Rayleigh-Taylor and Richtmyer-Meshkov instabilities [1]

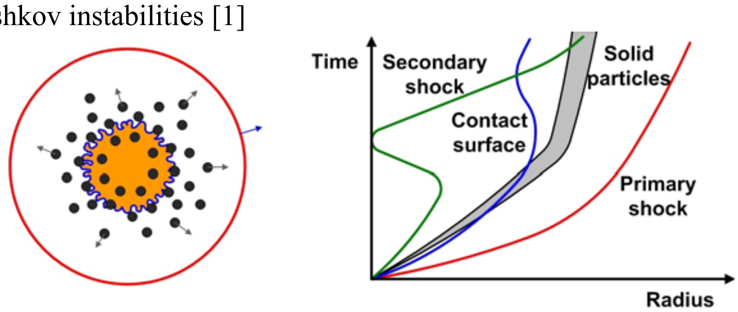

Figure 1. Wave diagram of typical explosives with solid particles.

Zhang et al. [2] reported experimental and numerical studies of nitromethane (NM) explosion with steel particles. They presented trajectories of the primary shock and particle cloud front. They also carried out numerical studies with Eulerian two-phase fluid model and their results provide useful understandings for explosive flow fields with solid particle. In this study, the equation of motion and transport of the solid particles are solved separately. Lagrangian equations are solved for the time history of a stochastically significant sample of individual particles. The numerical results are compared with the experimental results of Zhang at el.

2 Numerical Methods

Gas Phase Solver

The simples approach for the explosion wave propagation is one-dimensional numerical simulation with the assumption of spherical symmetry. The source vectors $\mathbf{S}_{\mathrm{geom}}$ and $\mathbf{S}_{\mathrm{par}}$ represent the geometric source vector and solid particle source vector, respectively.

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_t = \mathbf{S}_{geom}(\mathbf{U}) + \mathbf{S}_{par} \ ,$$

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}, \ \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \end{bmatrix}, \ \mathbf{S}_{geom} = \frac{2}{r}\begin{bmatrix} \rho u \\ \rho u^2 \\ u(E+p) \end{bmatrix}, \ \mathbf{S}_{par} = \frac{1}{\mathrm{V}}\begin{bmatrix} 0 \\ \sum_p -\frac{4\pi}{3}\rho_p r_p^3 n_p \frac{du_p}{dt} \\ \sum_p -4\pi r_p^2 n_p \bar{h}\, \Delta T \end{bmatrix}.$$

The solution is updated including all the intercell fluxes in a single step. At each cell, the local Riemann problem--HLLC approximate Riemann solver--is applied. The HLLC scheme is a modification of the HLL scheme wherein the missing contacts and shear waves are restored. The second-order upwind scheme is achieved using the WAF approach [3].

During the initial stage after explosion, equation-of-state (EOS) correction--real gas EOS--is required due to dense gases at high pressure and temperature. In this study, Noble-Abel EOS [4] and its thermodynamic relations are applied. Thermodynamic coefficients are assumed to be a function of temperature and obtained from polynomial functions.

Solid Particle Motion Equations

The liquid particles are treated by solving Lagrangian equations of motion and transport for the life histories of a statistically significant sample of individual particles. The Lagrangian equations governing the particle motion are

$$\frac{dx_p}{dt} = u_p \ , \ \frac{du_p}{dt} = \frac{3}{16}\frac{C_D \mu_g \mathrm{Re}_p}{\rho_p r_p^2}\left(u - u_p\right) ,$$

where x_p, u_p, C_D, Re_p, ρ_p, r_p represent particle position, velocity, drag coefficient, Reynolds number, density and radius respectively. Internal temperature change of the particle is assumed uniform and obtained from the energy balance at the surface. The second-order accuracy is achieved using the operator splitting method--Strang splitting. The procedure of the operator splitting is:

$$\mathbf{U}^{n+1} = C^{(\Delta t/2)}\ S^{(\Delta t)}\ C^{(\Delta t/2)}(\mathbf{U}^n) \ ,$$

where $C^{(\Delta t/2)}$ represents the convection operator during the time interval $\Delta t/2$and $S^{(\Delta t/2)}$ the particle source operator, respectively.

Drag Coefficient for Solid Particle Motion

The drag coefficient, C_D, is an important parameter to estimate the trajectory of particle motion. There is no universally applicable expression for C_D. From the numerical study of the sphere in detonation flow field as shown in Figure 2, authors found resulting C_Ds have higher values than commonly used empirical expressions as a function of Reynolds number.[5] The following model [6] developed for rocket nozzle flows and its results are similar with the results of sphere flows in detonation products:

$$C_{D0} = \begin{cases} C_1 & , \quad \alpha_2 \le 0.08 \\ \dfrac{(\alpha_2 - 0.08)C_2 + (0.45 - \alpha_2)C_1}{0.37} & , \quad 0.08 \le \alpha_2 \le 0.45 \\ C_2 & , \quad \alpha_2 \ge 0.45 \end{cases} ,$$

where α_1 and α_2 are volume fraction of gas and particle respectively.

The final value of C_D is obtained from following Mach number correction:

$$C_D = C_{D0}\left[1.0 + \exp\left(-\frac{0.427}{M^{4.63}}\right)\right] \qquad \text{where} \quad M = \frac{\left|u_{gas} - u_p\right|}{a_{gas}} \ .$$

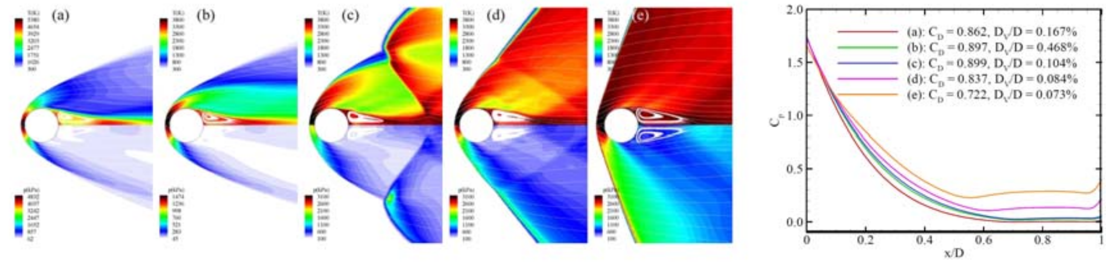

Figure 2. Drag coefficient estimation of sphere in detonation flow fields: (a) C_D=0.862; (b) C_D=0.897; (c) C_D=0.899; (d) C_D=0.837; (e) C_D=0.722.[5]

3 Results and Discussion

The simulation conditions are selected from Zhang's experiments [2]. NM is charged into a spherical glass with diameter of 11.8 cm. Steel particles with diameter of 463 µm are saturated with NM. In this study, initial pressure and temperature profiles if NM explosion are given from NM reaction simulation result. Explosion products are assumed as CO, H_2O, H_2, and N_2. Total mass of steel particles is 4.3 kg. Each particle position is randomly chosen within the radial location of r= 2.95±2.5 cm. Afterburing of explosion product and collision of steel particles are not considered here.

The initial flow development is sensitive to the type of EOS and initial pressure and temperature values. Ideal EOS underestimates the propagation distance of explosion products. With author's numerical methods, averaged initial pressure or assumed pressure of 4.5 GPa [2] did not presented corresponding result with experimental data [2]. In addition, commonly used C_D model highly underestimated the particle propagation distance and its transferred momentum. Thus the initial detonation profile at condensed phase was obtained using the commercial AUTODYN package.

Figure 3 shows the numerical wave diagram results of NM explosion flow field with steel particles (diameter of 463µm). Red and blue circles represent the experimental results [2] of radial position of the primary shock and particle cloud front, respectively. Application of Noble-Abel EOS makes the suitable prediction of the primary shock wave propagation and secondary shock reflection point. The red dashed line presents the numerical result of particle front propagation. The present C_D model [5] shows good agreement with experimental result. Figure 4 shows the extended numerical result. Within 10 m, the particle front velocity varies from 1300 m/s to 200 m/s. The resulting drag coefficient variation shows similar values with the results of sphere flow fields in detonation products. After initial acceleration, particle drag coefficient reached to 0.8. As shown in Figure 2, sphere in detonation products has the value of drag coefficient from 0.772 to 0.899.

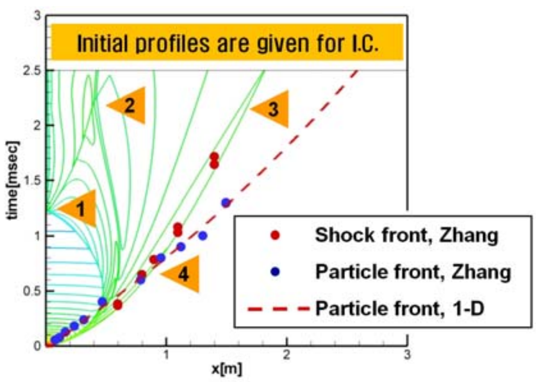

Figure 3. NM explosion with 463µm steel particles: 1 secondary shock reflection point; 2 interaction of secondary shock with contact surface; 3 primary shock wave; 4 overtaking point of shock by particle front.

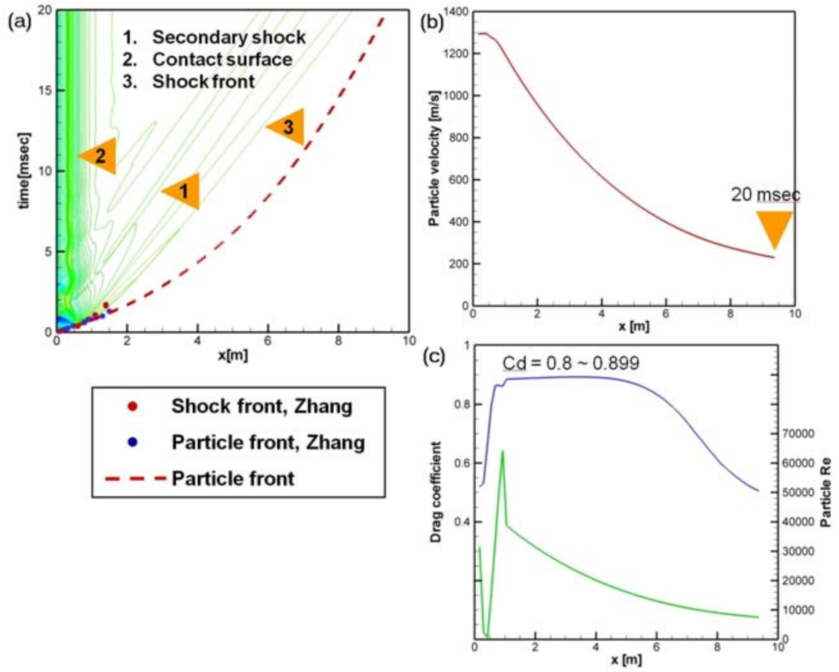

Figure 4. Particle velocity and drag coefficient variations: (a) wave diagram; (b) particle front velocity; (c) drag coefficient (upper blue line) and particle Reynolds number (lower green line).

4 Conclusion

Lagrangian-Eulerian modeling has been carried out to predict the dispersion of inert solid particles under the explosion of high explosive. The application of present modeling to the experimental case of Zhang et al. shows that the present approaches of the initial estimation of explosion profiles, reals gas EOS and the particles tracking with an advanced drag coefficient correlation results in a fairly good agreement with the existing data and gives the interpretation on the physical characteristics of particles dispersion and gas dynamics. The present model has been applied further to find the optimum conditions for the transfer of chemical energy to the mechanical energy by the parametric studies on the particles size, distributions, particle/HE mass ratio with different high explosives, those will be presented in detailed at the meeting.

References

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