Modeling of Interior Ballistic Gas-Solid Flow Using a Coupled Computational Fluid Dynamics-Discrete Element Method

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In conventional models for two-phase reactive flow of interior ballistic, the dynamic collision phenomenon of particles is neglected or empirically simplified. However, the particle collision between particles may play an important role in dilute two-phase flow because the distribution of particles is extremely nonuniform. The collision force may be one of the key factors to influence the particle movement. This paper presents the CFD-DEM approach for simulation of interior ballistic two-phase flow considering the dynamic collision process. The gas phase is treated as a Eulerian continuum and described by a computational fluid dynamic method (CFD). The solid phase is modeled by discrete element method (DEM) using a soft sphere approach for the particle collision dynamic. The model takes into account grain combustion, particle-particle collisions, particle-wall collisions, interphase drag and heat transfer between gas and solid phases. The continuous gas phase equations are discretized in finite volume form and solved by the AUSM+ scheme with the higher order accurate reconstruction method. Translational and rotational motions of discrete particles are solved by explicit time integrations. The direct mapping contact detection algorithm is used. The multigrid method is applied in the void fraction calculation, the contact detection procedure, and CFD solving procedure. Several verification tests demonstrate the accuracy and reliability of this approach. The simulation of an experimental igniter device in open air shows good agreement between the model and experimental measurements. This paper has implications for improving the ability to capture the complex physics phenomena of two-phase flow during the interior ballistic cycle and to predict dynamic collision phenomena at the individual particle scale. [DOI: 10.1115/1.4023313]

1 Introduction

The physical and chemical reactions in the interior ballistic process occurring in a few milliseconds are very complex. In the past decades, one of the most important objectives in the field of interior ballistic is to understand the entire phenomena more clearly and describe the mathematical models more accurately.

There are two numerical approaches to solve the two-phase flow problems, i.e., the Eulerian-Eulerian approach and Eulerian-Lagrangian approach. The Eulerian-Eulerian approach is also known as a two-fluid model [1-4]. This model considers the gas and solid (propellant) phase as two continuum flow phases, with each having its mass, momentum, and energy equations, respectively. This model is very popular in the numerical simulation of interior ballistics and has advantages in those cases where the number density of solid particles is high and the volume fraction of solid phase could be a dominating flow parameter. However, this two-fluid model cannot describe the practical situation in the chamber and cannot recognize the discrete character of the solid phase. It only provides a macroscopic two-phase description of flow in the gun chamber. Also each burning particle size is different and this model has not yet provided a quantitative analysis to assess multiparticle microstructures.

In the Eulerian-Lagrangian approach, the fluid phase is treated as a continuum and the solid phase is treated as an individual particle. In this model the trajectory and the state of each individual particle are tracked in space and time, and the fluid phase is mod-

eled by the local averaged equations at the macroscopic scale. This Eulerian-Lagrangian approach has been used in the development of the next generation interior ballistic code named as NGEN [5,6]. The three-dimensional NGEN code is developed by Nusca and Gough [7] and applied in different interior ballistic processes, such as the telescoped-ammunition propelling charge, modular artillery charge system [8,9]. Matsuo [10,11] also used this approach to simulate the interior ballistic process of the tubular solid propellant. Recently Jang [12] investigated the effect of the position of the charge on interior ballistics using the Eulerian-Lagrangian approach. Our group also simulated the interior ballistics of different systems by using the Eulerian-Lagrangian approach [13-17]. This approach has advantages for predicting two-phase flows in which large particle accelerations occur and also can handle poly-dispersed particle size distributions [18].

In all Eulerian-Lagrangian approaches mentioned above which have been used in the two-phase flow of the interior ballistic, each particle is tracked individually and the particle-fluid interaction is considered as two-way coupling. But in practice the dispersed phase particles not only affect the fluid flow but also affect each other by way of collisions (often called four-way coupling). In general, methods assume either (a) the interphase drag is the only force on the particle and collisions are neglected, or (b) an empirical-based intergranular stress is used to calculate the collision force between particles, and the trajectory of particles are independent of each other. For a better understanding of the two-phase interior ballistic flow, the basic physical model of the gas-particle, particle-particle, and particle-wall interactions should be fully considered at the microscale. In particular, collisions between particles may play an important role in dilute two-phase

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flow because the distribution of particles is extremely nonuniform. The collision force may be one of the key factors influencing the particle movement.

For this purpose, a discrete element method (DEM), designed to satisfy these specific requirements, provides a full insight into particle positions, velocities and forces during the whole simulation process. In the combined computational fluid dynamics and discrete element method (CFD-DEM), particles are modeled as a discrete phase, described by Newton's laws of motion on an individual particle scale, while the gas phase is treated as a continuum, described by the local averaged Navier–Stokes equations on a computational cell scale. Interphase interaction terms or detailed submodels are used to model interactions between the two phases, such as interphase drag and heat transfer.

In this paper, an efficient CFD-DEM method is developed for the gas-solid reacting flow in the interior ballistic process. The objective of the present work is to understand the entire interior ballistic phenomena more clearly and describe the mathematical models more accurately. A distinct advantage of the CFD-DEM method is that the particle motion and distribution in the interior ballistic two-phase flow can be accurately determined at an individual particle scale, especially dynamic collision phenomena.

2 Theoretical Models

In this study, the gas flow field is described by the continuum model, and the motion of a particle is determined by the DEM. The two phases are coupled with the interaction terms, such as interphase drag, heat transfer, etc.

2.1 Gas Phase. The gas phase is modeled as a continuum, which is described by a set of volume averaged Euler equations with source terms. The governing equations for the gas-phase flow consist of mass, momentum, and energy conservation equations.

The mass conservation equation of the gas phase,

$$\frac{\partial(\phi \rho_g)}{\partial t} + \nabla \cdot (\phi \rho_g \mathbf{V}_g) = m_c \quad (1)$$

The momentum conservation equation of gas phase,

$$\frac{\partial(\phi \rho_g \mathbf{V}_g)}{\partial t} + \nabla \cdot (\phi \rho_g \mathbf{V}_g \mathbf{V}_g) = -\phi \nabla p - \mathbf{F}_{pg} + \mathbf{M}_{cp} \quad (2)$$

The energy conservation equation of the gas phase,

$$\begin{aligned} \frac{\partial(\phi \rho_g E_g)}{\partial t} + \nabla \cdot \left(\phi \rho_g \mathbf{V}_g \left(E_g + \frac{p}{\rho_g} \right) \right) + p \frac{\partial \phi}{\partial t} \\ = -Q_p - W_{F_{pg}} + E_{cp} \end{aligned} \quad (3)$$

In the above equations, ϕ is the volume fraction of the gas phase, ρ_g is the gas density, $\mathbf{V}_g$ is the gas velocity, p is the gas pressure, E_g is the total energy of the gas phase, m_c is the mass generation rate of gas due to propellant combustion, $\mathbf{F}_{pg}$ is the interphase drag per unit volume, $\mathbf{M}_{cp}$ is the added momentum due to the gas production, Q_p is the interphase heat transfer due to conduction and radiation per unit volume, $W_{F_{pg}}$ is the work done by the interphase drag, and E_{cp} is the added energy due to the decomposition of the solid phase.

2.2 Solid Phase. The solid phase is treated as a discrete phase which is modeled by the discrete element method. The DEM is an approach for predicting the movement of particles by

solving equations of motion, taking account of contact forces between particles or between a particle and a wall.

2.2.1 Particle Movement. The particle movement in a gas flow is caused not only by particle-particle or particle-wall contact forces, but also by interphase forces, such as the drag force, Saffman lift force, Magnus force, Basset force, etc. In this study, only contact forces and the drag force are considered. The translational and the rotational motion of a particle are described by Newton's second law, and given by

$$m_p \frac{d\mathbf{V}_p}{dt} = \sum_{i=1}^{k_c} \mathbf{F}_c + \mathbf{f}_s \quad (4)$$

$$I \frac{d\boldsymbol{\omega}}{dt} = \sum T_{ij} \quad (5)$$

where m_p is the mass of particle, $\mathbf{F}_c$ is the contact force, k_c is the number of contacting particles, $\mathbf{f}_s$ is the particle-fluid interphase drag, $\mathbf{V}_p$ and $\boldsymbol{\omega}$ are the translational and rotational velocities of the particle, I is the moment of inertial, T_{ij} is the torque between particles i and j .

2.2.2 Contact Forces. The simulation of the actual mechanical behavior of the propellant is difficult because, for example, black powder is not completely spherical and maybe an ellipsoid especially during combustion. To simplify the model, we assume all particles are spherical. This approximation was also used in other models for black powder or ball propellant. Contact information is derived from the spherical geometry.

The contact forces between two particles can be obtained by the linear spring-damper model proposed by Cundall and Strack [19]. The particle-particle contact forces, namely, the normal, damping, and sliding forces, act on the two particles. Particle-wall contact forces are modeled in the soft sphere model using mechanical elements like springs, dashpots, and sliders.

The contact force $\mathbf{F}_c$ acting on a particle j due to contact with particle i is expressed as

$$\mathbf{F}_c = \mathbf{F}_{cn,ij} + \mathbf{F}_{ct,ij} \quad (6)$$

The normal component of the contact force $\mathbf{F}_{cn,ij}$ is given as

$$\mathbf{F}_{cn,ij} = -k_n \delta_n \mathbf{n} - c_n (\mathbf{V}_{ij} \bullet \mathbf{n}) \mathbf{n} \quad (7)$$

The tangential component of the contact force $\mathbf{F}_{ct,ij}$ is given as

$$\mathbf{F}_{ct,ij} = -k_t \delta_t \mathbf{n} - c_t (\mathbf{V}_{ij} \times \mathbf{n}) \times \mathbf{n} \quad (8)$$

The sliding condition is provided by Coulomb's friction law, and the tangential force is given by

$$|\mathbf{F}_{ct,ij}| = \begin{cases} |\mathbf{F}_{ct,ij}|, & |\mathbf{F}_{ct,ij}| < \mu_s |\mathbf{F}_{cn,ij}| \\ \mu_s |\mathbf{F}_{cn,ij}|, & |\mathbf{F}_{ct,ij}| \geq \mu_s |\mathbf{F}_{cn,ij}| \end{cases} \quad (9)$$

where k_n , k_t , c_n , c_t are the spring and dashpot coefficients in the normal and tangential directions, δ_n , δ_t are the particle displacements in the normal and tangential directions, $\mathbf{V}_{ij}$ is the slip velocity, μ_s is the maximum static friction coefficient, $\mathbf{n}$ is the unit vector from the center of particle i to particle j .

Also, the torque acting on a particle due to particle-particle contacts is expressed as

$$T_{ij} = r_{ij} \mathbf{n} \times \mathbf{F}_{ct,ij} \quad (10)$$

2.3 Source Terms. The CFD model provides the gas information in a fluid cell and the DEM model describes individual particles. Since the gas phase cell is much larger than the particle size, the individual particle information cannot be used in the

continuum gas phase model directly. Also, in order to close the governing equations above, some constitutive relations or detailed submodels are used to model the interaction between the two phases, such as interphase drag, heat transfer, etc.

2.3.1 Interphase Drag. A drag force model based on the Anderssen law for the fluidized bed is used to calculate the interphase drag. However, as the drag force model describes the fluid-particle interaction forces per unit volume, the expression must be modified for calculation of the drag acting on a single particle.

The drag $\mathbf{f}_s$ on a particle is given by

$$\mathbf{f}_s = V_i \frac{1-\varphi}{d_p} |\mathbf{V}_g - \mathbf{V}_p| (\mathbf{V}_g - \mathbf{V}_p) \rho_g C_f \quad (11)$$

where V_i is the volume of each particle, d_p is the equivalent diameter, φ is the porosity, and C_f is the empirical coefficient.

The interphase drag between the gas-solid phases obeys Newton's third law, the fluid-particle interphase drag $\mathbf{F}_{pg}$ for gas phase per unit volume is obtained by summing up the interaction forces acting on all particles in a fluid cell, and dividing by the volume of the fluid cell,

$$\mathbf{F}_{pg} = \sum_{i=1}^{k_c} \mathbf{f}_s / V_{\text{cell}} \quad (12)$$

where k_c is the number of particles in a fluid cell, and V_{cell} is the volume of a fluid cell.

Thus the work done by the interphase drag per unit volume can be written as

$$W_{F_{pg}} = \sum_{i=1}^{k_c} \mathbf{f}_s \cdot \mathbf{V}_p / V_{\text{cell}} \quad (13)$$

2.3.2 Propellant Combustion. When the solid propellant temperature reaches the assumed ignition temperature, the propellant starts to burn. An empirical burning law is used in the associated burning rate calculations. The production rate of gases per unit fluid cell is shown as the following:

$$m_c = \sum_{i=1}^{k_c} b p^n \rho_p S_p / V_{\text{cell}} \quad (14)$$

where b , n are constants for a given propellant material and S_p is the current surface area of the grain.

Similarly, the added momentum $\mathbf{M}_{cp}$ due to the gas production and the added energy E_{cp} due to the decomposition of solid phase can be calculated.

2.3.3 Interphase Heat. The interphase heat transfer Q_p due to the conduction and radiation per unit volume can be given as

$$Q_p = \sum_{i=1}^{k_c} (q_c + q_r) S_p / V_{\text{cell}} \quad (15)$$

where q_c , q_r are the heat flux due to convection and radiation per unit surface area.

3 Numerical Methods

The continuous gas phase equations are discretized using a finite volume method and solved by the AUSM+-up scheme [20] with the higher order accurate reconstruction method. Previous work has shown that this method can compute a very strong shock wave propagating across the two-phase interface [21]. The translational and rotational motions of discrete particles are solved by explicit time integrations [22].

The DEM solver is first solved to obtain the position and velocity of particles. Then the void fraction in each computational grid is estimated based on the particle positions. Also, mass, momentum, and energy source terms are added to the discrete control volume in which the particle resides. Next, the flow field of the gas-phase is solved by the CFD solver. This procedure will be iterated until the calculation is finished.

It is important to note that generating a neighbor list for each particle is necessary at every time step to compute the contact force. This is one of the most time-consuming processes in DEM using the soft sphere model. In this work the direct mapping contact detection algorithm is used [22]. This algorithm is performed in two steps: (1) map discrete elements onto cells, and (2) find discrete elements that may be in contact. It is worth noting that two discrete elements mapped onto cells that share either nodes or edges (neighboring cells) can be in contact. Hence the direct mapping contact detection algorithm is simple and efficient.

The multigrid technique is used in this work. As mentioned above, one grid called the DEM-grid is used in the contact detection procedure. Of course the CFD procedure needs a second grid called CFD-grid. Also, a third grid called the porosity-grid is set up to compute the void fraction. The small cells in the porosity-grid are mapped onto a cell in the CFD-grid; the porosity of each cell in the CFD-grid is calculated by summing the relevant cells in the porosity-grid.

4 Results and Discussions

4.1 Validations and Test Cases. During the code developing process, several particular validations were used to test the CFD code and DEM code. In this section some particular verification tests are discussed in detail.

Test 1: Double Mach Reflection of a Strong Shock. This test problem is a classic example and widely used to test CFD codes. It has been extensively studied by Woodward and Colella, and the same setup as in Ref. [23] is used in our test case. Considering the reflection of a planar Mach shock in air from a wedge, the setup is of a Mach 10 shock, which initially makes a 60° angle with a reflecting wall. When the shock hits the sloping wall, a complicated shock reflection occurs. The wave pattern consists of two Mach stems with two contact discontinuities.

The simulation result on a grid of 1200 × 300 at time 0.2 is shown in Fig. 1. Obviously, the density contour result agrees well with the figures in the paper by Woodward and Colella [23]. This good agreement shows that the CFD code has enough accuracy to capture the strong shock.

Test 2: Validation Tests for DEM Code. Some special cases were examined during the code developing process. These cases tested the implementation of the force behavior in isolation, in free motion, single contact, and multiple contacts, etc. [24]. In this section, we only show the results of the normal force test in the vertical direction using our DEM code.

In Fig. 2, a free falling particle under gravity hits the base, and the tangential forces are set to zero. The stiffness constant is set as 800 N/m, the damping coefficient is 0.5, and the particle radius is 0.002 m. The vertical position of the particle is shown in Figs. 2(a) and 2(b). We can see that particle fails to reach the original height and its height decays due to the damping force. All of

Fig. 1 Density contour of double Mach reflection of a strong shock

Fig. 2 Normal force test in the vertical direction under gravity (a) position of particle with elastic force and (b) position of particle with elastic and damping force

Fig. 3 Schematic diagram of igniter test device in open air

Table 1 Structural parameters of the igniter test device

L0 (mm)	L1 (mm)	L2 (mm)	L3 (mm)	D (mm)	d0 (mm)
210	25	53	28	15	3

Fig. 4 Comparison between the calculated and measured pressure-time traces at the P3 location

the tests indicate that the DEM code is working correctly for the collision problem.

4.2 Application to the Igniter Test Device in Open Air. In this section, an igniter test device in open air is simulated. Experimental measurements can be obtained by this test device. The schematic diagram of this test device is shown in Fig. 3 and the main dimensions of the test device are listed in Table 1. The average diameter of black powder is 4 mm. The stiffness constant is set as 800 N/m, the damping coefficient is 0.5, and the friction coefficient is set as 0.3.

Calculated and experimental pressure-time traces in the igniter are compared in Fig. 4. The calculated results show good agreement with the measured data. The pressure distributions in the

(a) 0 ms (b) 1 ms (c) 1.5 ms (d) 2 ms (e) 2.5 ms (f) 3 ms
(g) 4 ms (h) 4.5ms (i) 6 ms (j) 7 ms (k) 8 ms

Fig. 5 Pressure distributions at different times

igniter at different times are shown in Fig. 5. It shows the detailed pressure phenomena during the whole combustion process. Figures 5(a)–5(d) show the early phase pressure wave distributions. The pressure waves travel from the burned region towards the unburned region. With the propagation of the pressure wave, a rarefaction wave is formed and travels towards the bottom of the igniter, which is shown in Fig. 5(e). At about $t = 3.0$ ms, the vent holes start to rupture and the pressure in the region of the vent holes has a slight drop, which is shown in Fig. 5(f). In Fig. 5(g), the overall trend of the pressure gradient continues to increase. At about $t = 4.5$ ms, the pressure starts to decay gradually and the pressure distributions in the igniter are approximately uniform except in the region of the vent holes.

The particle distributions at different times are shown in Fig. 6. With the flame propagation, the particles are ignited by the heat transfer between the two phases. At about $t = 2$ ms, all particles are ignited completely. Figure 6 also shows the detailed flame propagation process and it also has similar distributions to the pressure distributions shown in Fig. 5.

Fig. 6 Particle temperature distributions at different times

Fig. 7 Porosity distributions at different times

The porosity distributions at different times are shown in Fig. 7. Nonuniform porosity distributions are clearly evident; this is because the gas porosity is calculated using the position of each particle and all particle positions are both randomly distributed and constantly changing. This is one of the biggest differences between our CFD-DEM approach and other interior ballistic two-phase models.

Figures 8 and 9 present the distributions of the gas velocity vector at different times. The gas velocity vector distributions before the vent holes open are shown in Fig. 8 and the gas velocity vector

Fig. 8 Gas velocity vector distributions before vent holes open

Fig. 9 Gas velocity vector distributions after vent holes open

distributions after vent holes open are shown in Fig. 9. It shows a strong 2D effect and the gas flow field is described clearly.

The particle velocity vector distributions at different times are shown in Fig. 10. It shows not only the velocity vector of each particle but also the size and position of each particle. In the beginning of the combustion process, the particles move from the bottom of the igniter towards the top of the igniter. Some particles near the top of the igniter rebound due to collisions between the particles and the wall. Collisions between particles are constantly occurring. After the vent holes open, particles start to cluster gradually near the region of the vent holes because of the discharging of combustion products through the vent holes. These collisions and clustering are another big difference between our CFD-DEM approach and other interior ballistic two-phase flow models.

(a) 1ms (b) 2ms (c) 3ms (d) 4ms (e) 6ms (f) 7ms (g) 8ms

Fig. 10 Particle velocity vector distributions at different times

5 Conclusions

This paper developed a two-phase flow model considering the dynamic collision process of particles to study the complex interior ballistic process. The main conclusions are summarized as follows:

- (1) The CFD approach is used to describe the continuum flow, taking into account detailed grain combustion, particle-particle collisions, particle-wall collisions, interphase drag and heat transfer between the gas and solid phases.
- (2) The DEM approach is provided to track the dynamic collision process of particles and predict dynamic collision phenomena at the individual particle scale.
- (3) Verifications of the theoretical model and code demonstrate the accuracy and reliability of this approach. Simulation of an igniter test device in open air shows excellent agreement between numerical simulation and experimental measurements. The numerical results show nonuniform porosity distributions and clustering of particles after the vent holes open.
- (4) This approach is taken to understand the entire interior ballistic phenomena more clearly and to describe the mathematical models more accurately. It is reliable as a prediction tool for the understanding of the physical phenomenon and can therefore be used as an assessment tool for future interior ballistics studies.

The future direction for this work will address the description of the particle geometry. We plan to apply this model to different

geometries of propellants. Additionally, the code also needs to be extended to three dimensions.

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