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Simulation of shock-powder interaction using kinetic theory of granular flow

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ABSTRACT

Numerical simulation of the shock-powder interaction in a shock tube is carried out using the Eulerian-Eulerian approach, and special emphasis is placed on the particle phase behavior responding to the shock wave. The kinetic theory of granular flow is incorporated into the mathematical model of the compressible gas-particle flow. Since the particle phase pressure is provided by the kinetic theory, characteristics analysis demonstrates that the set of particle phase governing equations is a well-posed system, and the Roe scheme is then used in the numerical simulation process. The predicted results show that the particle phase is compressed by the shock wave, and the accumulation of particles increases the pressure of the particle phase. While, the reflected and transmitted shock waves are generated after the shock-powder interaction, the expansion waves in the particle powder show a decrease trend in the gas phase pressure. In addition, the passage of the shock wave gives rise to a sharp increase of the velocity slip between the gas phase and the particle phase. Performance of the particle kinetic theory in the present model is examined by the experimental data, which provides the numerical basis for implementing the particle kinetic theory in compressible multiphase flow problems.

1. Introduction

Shock-powder interaction is an important process encountered in many technological and engineering applications, including detonations of multiphase explosives, solid-propellant rocket motors and shock-induced powder compaction [1–3]. As implied by previous researches [4–8], a complicated system consisting of regular and irregular shock-wave reflection, diffraction and focusing can be observed when a shock wave propagates over a particle sphere. However, for practice applications involving the propagation of a shock wave in a powder or dispersal of particles, it is of great importance to understand the physical interaction process, especially under the dense particle conditions.

Pioneering investigations have been conducted including fundamental experiments as well as theoretical and numerical studies. Boiko et al. [9] considered the process of a shock wave passing through a cloud of particles experimentally, and found the shock waves interfering with each other when passing over individual particles, and overlapping to form a collective leading shock. The corresponding numerical simulation also revealed the formation mechanism of the reflected shock wave ahead of the cloud of particles. Experiment and numerical work were carried out by Rogue et al. [10] to investigate the motion of particle beds induced by a shock wave. The strength of the reflected and transmitted shock waves was measured in the experiment, and shadowgraph images were recorded to show the particle layer movement. In their numerical simulation, the drag coefficient from the investigation of a single particle was applied and a particle interaction tensor accounted for the collisions between particles. It is found that the particle collisions are essential during the initial shock-bed interaction. Ilea et al. [11] studied dust lifting behind shock waves numerically with log-normal distribution of particle sizes, and found that particles with smaller sizes than the mean value of the distribution contributed the most to the lifting effect. Furthermore, particle collisions showed to be the main cause for change in particle kinetic energy. Through the previous investigations, it is shown that the particle powder in a dense state will exhibit integral rather than individual particles when responding to a shock wave, and the particle collisions become important in the shock-powder interaction.

On the basis of the preceding efforts, a comprehensive knowledge about the shock-powder interaction is acquired. Given the high speed of the shock wave and limitations of the experimental measurements, the transient time scale of the shock-powder interaction make it difficult to describe the particle phase response behavior, in particular, the variations of particle acceleration and concentration. Therefore, numerical approach is recommended for further understanding the physical process in the particle powder.

Two main modeling techniques are commonly used in the simulations of gas-particle flow [12–17]. One is the Eulerian–Lagrangian method, where particles are considered as point masses, and are traced individually during the simulations according to the Newton's second law of motion. The other one is the Eulerian-Eulerian method, where the particle phase is treated as continuous media, and governed by a

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set of Euler equations as in the gas phase. In the Eulerian–Lagrangian method, in order to get the information of the particles distribution, additional statistical procedure [18] should be carried out. However, the concentration of the particle phase can be obtained directly by solving the continuity equation in the Eulerian-Eulerian method. Moreover, by introducing the particle phase pressure, collisions between particles can be taken into consideration in a simple way, while the virtual particle concept as in the Direct Simulation Monte Carlo (DSMC) technique [19–21] is usually employed for collision modeling in the Eulerian–Lagrangian method, which demands expensive computation cost especially when particles are in dense state. From this point of view, the Eulerian-Eulerian technique possesses advantages for the shock-dense particle powder interaction in contrast with the Eulerian–Lagrangian method.

The particle kinetic theory is a continuum concept which has been applied in the Eulerian-Eulerian method, and has been widely used to model the granular flow in circulating fluidized bed in the last decades [22–30]. In the present study, the particle kinetic theory is extended into the compressible gas-particle flow for the first time as far as the authors know. For a brief introduction, the particle kinetic theory is deduced by analogy from the dense-gas kinetic theory as described by Chapman and Cowling [31]. The starting point is the Boltzmann integral-differential equation used to derive the governing equations of the particle phase. The particle random motion and collisions are analogous to the thermal motion of molecules in the gas phase, which contribute to the transfer of particle momentum and produce pressure and viscosity of the particle phase. Based on the Maxwellian velocity distribution for a single particle, a conservation equation for the so-called granular temperature is derived by Jenkins and Savage [32], which characterizes the random motion and collisions in the particle phase. In a similar manner, the granular temperature is related to the particle phase pressure by an equation of state as in the gas phase. Sinclair and Jackson [33] were the first to apply this theory to model the fully developed gas-particle flow in a vertical pipe, and the results have demonstrated the applicability of this theory in gas-particle flow. Pita and Sundaresan [34] studied the steady developing flow of gas-particle suspensions in a vertical riser numerically, and the results revealed remarkable rich varieties of behavior over a wide range of flow conditions. In addition, several investigators such as Lu et al. [35], Ding and Gidaspow [36], Nieuwland et al. [37], Samuelsberg and Hjertager [38], have carried out numerical simulations on bubbling fluidization, circulating fluidization and pneumatic transport, and contribute to the development of the particle kinetic theory. Gidaspow [39] and Enwald et al. [40] gave comprehensive reviews about the applications of the kinetic theory. Though the Eulerian-Eulerian method has been employed in the simulations of compressible multiphase flow [41,42], the application of particle kinetic theory into the shock-particle interaction problem is rarely to be seen in the open sources. In view of a dense powder condition, an evaluation of the performance of the kinetic theory in the compressible multiphase flow is needed.

The main objective of this paper is to present numerical simulations of the shock-powder interaction based on the particle kinetic theory, and gives a close inspection to the particle phase response behavior to the passage of a shock wave within the dense particle powder. The simulations were carried out using own developed codes compiled with Fortran. The main point that distinguished the present codes from the commercial or open-source codes is the application of kinetic theory of the particle phase into the Eulerian-Eulerian method. As a result, a well-posed governing equation system of the particle phase is obtained and the numerical technique for simulations is then discussed in the present study. In order to verify the particle kinetic theory in modeling the particle phase in the shock-powder interaction problems, simulation was conducted under specific conditions with respect to a multiphase shock tube (MST) experiment. The experiment has been carried out by Ling et al. [43] at Sandia National Laboratories recently, in which a planar incident shock wave travels through a particle curtain, and trajectories of the particles are recorded by high-speed schlieren images. The particle curtain is formed in the MST with a volume fraction about 21%, and makes it a dense particle powder. Comparisons between the numerical results and experimental data will be shown in Section 3.2. After that, attentions will be focused on the response behavior of the gas and particle phases within the particle curtain when the shock wave passes by. It is noted that the particle phase is compressed by the shock wave, resulting in un-uniform distribution of the particle concentration. The evolutions of the particle phase pressure and granular temperature provide an approach to study the particle collisions affected by the passage of the shock wave. Furthermore, the velocity slip between the two phases has been examined, and appears to violate the zero limit assumption of the particle Mach number [44], which indicates the standard-drag correlation is not adequate for applications in the shock-particle interaction. Improved drag coefficient correlation based on Mach number correction given by Parmar et al. [45] is therefore employed in the modeling of the interaction force between the two phases, and plays the role in evaluation of the shock effect on the interaction process. In addition, the reflected and transmitted shock waves are presented in the simulation results, and expansion waves obtained within the particle curtain imply the decreasing strength of the transmitted shock wave. The influence of the particle size and volume fraction on the shock-powder interaction process will be discussed in Section 4.4.

2. Mathematical model

In this paper, both the gas phase and particle phase governing equations are expressed in Eulerian frame of reference. Inter-phase interaction is realized through the source terms in the equations. For the shock tube problem, the gas is taken to follow the ideal-gas law, and is regarded as inviscid, except in the modeling of the inter-phase interaction. The particles are taken to be inert, rigid and spherical. The numerical study of shock-powder interaction in the shock tube is taken as a one-dimensional problem. Due to the well-designed experimental facility [46], the center of the shock tube remains nearly one-dimensional, and the influence of the dimensionality is supposed to be small. In addition, the deviation resulting from the experimental measurement has been discussed by Ling et al. [43] and Wagner et al. [46], which shows that the one dimensional model of multiphase shock tube is qualified for the present numerical investigation.

2.1. Governing equations of gas phase

The compressible conservative form governing equations for the gas phase are given as follows:

Gas phase continuity equation

$$\frac{\partial\left(\alpha_g\rho_g\right)}{\partial t}+\nabla\cdot\left(\alpha_g\rho_g\mathbf{u}_g\right)=0, \tag{1}$$

Gas phase momentum equation

$$\frac{\partial\left(\alpha_g\rho_g\mathbf{u}_g\right)}{\partial t}+\nabla\cdot\left(\alpha_g\rho_g\mathbf{u}_g\mathbf{u}_g\right)=-\alpha_g\nabla P_g+\mathbf{S}_I, \tag{2}$$

Gas phase energy equation

$$\frac{\partial\left(\alpha_g\rho_gE_g\right)}{\partial t}+\nabla\cdot\left[\alpha_g\mathbf{u}_g\left(\rho_gE_g+P_g\right)\right]=S_{II}. \tag{3}$$

In the above expressions, α_g is the volume fraction, and ρ_g, u_g and E_g are the density, velocity and total energy, respectively, with the subscript “g” representing the gas phase. It should be mentioned that the nozzling term [47] in Eq. (2) and the corresponding contribution