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Conservative particle weighting scheme for particle collision in gas-solid flows

Yongxiang He, Haibo Zhao*

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China

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ABSTRACT

Even though the particle volume fraction is small in gas-solid flows, the particle-particle collision plays an important role due to the turbulent transport effect and the preferential concentration effect. The direct simulation Monte Carlo (DSMC) method coupled with Eulerian-Lagrangian models for hydrodynamics has been proposed for describing particle-particle collision in gas-solid flows for decades. Huge statistical noise occurs in some less-populated regions (e.g., two edges of log-normal size spectrum of particles) where there are insufficient simulation particle numbers for the DSMC method that tracks the equally weighted simulation particles. To circumvent this difficulty, a new differentially weighted (i.e., conservative particle weighting, CPW) scheme that explicitly conserves mass, momentum and energy during collisions is proposed in the framework of the DSMC method, and a limiting case of high inertia particle flow is simulated to demonstrate its utility in terms of computational precision. Then simulation strategy of coupled DSMC method for particle collision and Lattice Boltzmann-cellular automatic (LB-CA) probabilistic model for hydrodynamics (LB-CA-DSMC) is proposed. The resultant two-phase gas-solid flow model with the consideration of four-way coupling is then used to simulate the gas-solid flows over a backward-facing step. By comparing with the results of LB-CA method (without particle collision) and the experimental measurement, good agreements can be found between the LB-CA method and LB-CA-DSMC method for the case of small mass loading (=0.1), in such a way that the coupling strategy of LB-CA and DSMC is effectively verified. Finally, a “fictitious” gas solid flow over a backward-facing step with bidisperse copper particles injected is calculated, where each simulation particle is represented by variable number weight and the proposed CPW scheme is used to handle collision between differentially-weighted particles. Compared to the results from the conventional equally-weighted DSMC method for particle collision, improved resolution of particle field can be obtained simultaneously by the CPW method for less-populated particles.

Introduction

Gas-solid two phase flows are common in the industrial fields and atmospheric environment such as pulverized-coal particle transport, pneumatic conveying of granular material, separating of solid particles from the flue gas, and diffusion and sedimentation in atmospheric environment (Hunt, 1991). Two critical parameters that determine the level of interaction between the phases are fractional volume ϕ_v and mass loading ϕ_m, defined as ratio of volume or mass of the dispersed to continuous phase respectively (Balachandar and Eaton, 2010). With the increase of ϕ_v and ϕ_m, the level of interaction between the phases varies from one-way coupling (influence of the dispersed phase on the continuous phase can be neglected) to two-way coupling (the back influence of the dispersed phase on the continuous phase is considered), and further to four-way coupling (considering the interactions between particles, typically collision). Since particle-particle collisions will modify the particle phase properties and eventually the gas phase, the consideration of the four-way coupling effect is essential to the simulation precision of gas-solid flows. Lain and Garcia (2006) simulated a particle-laden flow in a free turbulent round jet with the consideration of four-way coupling and found that the collisions tend to isotropise the particle turbulence and flatten the profile of particle mean axial velocity in a mass loading of 1.8. However, the average loading is not the only measure for the importance of collisions because the particle may be drawn into dense clusters by turbulence. This phenomenon is called preferential accumulation and is one of the key features in turbulent gas-solid flow (Elghobashi and Truesdell, 1992; Maxey, 1987; Squires and Eaton, 1991). Wang et al. (2000) adopted the direct numerical simulation

* Corresponding author. Tel.: +86 27 87545526; fax: +86 27 87545526.
E-mail address: klinsmannzhb@163.com (H. Zhao).

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(DNS) method to calculate the particle collision rate in the context of a turbulent continuous-phase flow with initial monodisperse solid particles and found that the turbulent transport effect and the preferential concentration effect lead to an increase of particle-particle collision rates by a factor of 30. For the purpose of accurate description and control in continuous and dispersed phase, the particle-particle collision and four-way coupling between the continuous and discrete phases should be processed. In this paper, we focus on the particle-particle collision and four-way coupling.

In traditional computational fluid dynamics (CFD) model, most of simulations for gas-solid flow are based on the hypothesis of a monodispersed solid phase (i.e. all particles have the same size) or on the hypothesis of a constant particle size distribution (PSD) (i.e. no evolution in particle size). But in many practical cases especially in industrial fluidized beds, widely-distributed polydisperse particle population is a typical characteristic. Even if their initial distribution is monodispersed, particle dynamics such as agglomeration and fragmentation leads to dynamic evolution of particle size distribution. Hence, the effects of particle size distribution should be taken into account. Beetstra et al. (2007) performed a discrete particle simulation of a segregating system using drag relations with a polydispersity factor derived on the basis of lattice-Boltzmann (LB) simulations and found that the polydispersity factor has a major effect on the segregation velocity and the final degree of segregation. Chen et al. (2013) coupled the population balance model (PBM) with two-fluid model (TFM) and Energy Minimization Multi-Scale (EMMS) drag model for simulating heterogeneous gas-solid flow, discovering that particle polydispersity has a notable effect on the particle velocity distributions.

As known, the multiphase model can be divided into Eulerian-Eulerian models and Eulerian–Lagragagian models, depending on the simulation methodology of the dispersed phase in an Eulerian reference frame or in a Lagragagian reference frame. The DSMC method, which was initially proposed by Bird (1976) as a stochastic approach for the computation of highly rarefied flows, has been applied to deal with particle collision in the framework of Eulerian-Lagragaian for decades (Tsuji et al., 1998). The conventional DSMC method for particle collision tracks equally-weighted simulation particles, that is to say, each simulation particle represents the same number of real particles. However, in many application of interest, there are insufficient numbers of simulation particles in some less-populated regions (e.g., two edges of log-normal size spectrum) of a polydisperse particle population, leading to huge statistical noise. To circumvent this difficulty, a scheme in which the physical weight is dependent upon its size spectrum is required in the framework of DSMC method. Thus, the weight of the simulation particles in a size spectrum having less real particles would be given a lower value than that in regions having abundant particle numbers. The differentially weighted scheme for particle collision for the first time was proposed by Bird (1994) for rarefied gas dynamic. In the weighted scheme of Bird (1994), when two particles having different particle number weights collide, the properties of simulation particles is changed according to the probability. However, this scheme does not conserve the momentum and energy explicitly at each collision and Bird (1994) recommended against the use of this scheme. Boyd (1996) developed a conservative species weighting (CSW) scheme to deal with trace species involved in some non-reactive physical processes that explicitly conserve both linear momentum and energy during each collision. The CSW scheme has been extended to application in chemical vapor deposition process (Sakiyama et al., 2000; Wu et al., 2003) and reactive re-entry flows (Petkow et al., 2012). Nanbu and Yonemura (1998) used a common Monte Carlo (MC) simulation technique that is similar to the method of Bird (1994) to deal with differentially weighted collisions of plasma with different charges. Vikhansky and Kraft (2005) developed a conservative method based on the redistribution of the statistical weights in a way that does not affect the physical relevant statistical moments for the reduction of the number of particles. The difficulty of this method is to find the optimal distribution of particles and the optimal proportion between number of the groups and number of the moments to be conserved by the transformation.

In solving the particle population equation (PBE) for dynamic evolution (e.g., coagulation) in dispersed systems, we firstly developed a differentially weighted time-driven Monte Carlo (MC) method for particle coagulation to capture the dynamics with low noise and track the size distribution over the full size range simultaneously (Zhao et al., 2009). Subsequently, the concept of differentially weighted scheme is held together with the event-driven constant-volume method (Zhao and Zheng, 2009b), multi-Monte Carlo (MMC) method (Zhao and Zheng, 2009a) and majorant kernel method (Xu et al., 2014). Recently, a new differentially weighted Monte Carlo (DWMC) method is used to simulate two-component coagulation processes (Zhao et al., 2010) and gain insight into the dependence of steady state mixing degree on overall mass fraction (Zhao and Einar Kruis, 2014), and coupled with the Lagragian-Eulerian model for particle coagulation in spatially inhomogeneous systems (Zhao and Zheng, 2013). It should be noted that both coagulation and collision (only binary collision is considered in this paper) involves two discrete particles. Once a coagulation event occurs, two simulation particles will merge together into one simulation particle, reducing the number of total simulation particles. Situation for collision dynamic event is totally different from coagulation dynamic event, as the process of collision mainly focuses on the transfer of momentum and energy without any particle loss. So far, few reports gave study about the use variable particle weight for particle collision in gas-solid flow except for the split-restoration scheme proposed by us recently (He et al., 2014). The scheme can be described in brief as follows: for two simulation particles i and j with number weight w_i and w_j ($w_i > w_j$), the first stage is to split the simulation particle i into two simulation particle 1 and 2 with number weight w_j and w_i - w_j, respectively. Then, collision between simulation particle 1 and j with equal weight w_j is performed. The final stage is to restore the number of simulation particles with some specified schemes that could maintain the mass, momentum or energy of the control volume. Although improved resolution for size spectrum having less simulation particle numbers could be obtained, this split-restoration scheme cannot explicitly conserve mass, momentum and energy simultaneously during each collision. If differentially-weighted simulation particles are tracked in gas-solid flows, the key issues include how to design a rule (model) that could explicitly conserve mass, momentum and energy within a certain number of total particle numbers (N/2-2N) with the use of variable particle weight for particle collision. Therefore, a conservative particle weighting (CPW) scheme that could explicitly conserve these properties during each collision (similar to Boyds CSW scheme for rarefied gas flows) is adopted in the framework of Eulerian–Lagragagian model.

On the other side, the lattice-Boltzmann method has been developed since 1980s and is a very promising numerical approach for gas flows at the mesoscopic level. This methods simulate continuous fluids at the macroscale in terms of the dynamics of discrete fictitious “fluid particles”, and the macroscopic features of flows can be obtained through the statistics of many discrete fluid particles, which transport between regular grid points and collide with each other. Up to now, there are three kinds of gas-solid flow models based on the LB method and it is possible to distinguish them among Lagrangian point-particle tracking approach (Filippova and Hänel, 1997), Lagrangian full-resolution-particle tracking approach (Ladd and Verberg, 2001), and cellular automation probabilistic approach (CA) (Chopard and Masselot, 1999), depending