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MP-PIC simulation of CFB riser with EMMS-based drag model

Fei Li [a,*], Feifei Song [a], Sofiane Benyahia [b], Wei Wang [a], Jinghai Li [a]

[a] State Key Laboratory of Multi-phase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China
[b] National Energy Technology Laboratory, Morgantown, WV 26507, USA

HIGHLIGHTS

- Combination of the MP-PIC method with the EMMS drag force model.
- Dense flows in CFB risers were accurately simulated with this method.
- We examine the effects of the number of particles per parcel (n_p) on simulations.
- There exists a critical n_p, below which, the stable solid flux can be achieved.
- Below another critical n_p, decreasing n_p will increases the simulation time.

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ABSTRACT

MP-PIC (multi-phase particle in cell) method combined with the EMMS (energy minimization multi-scale) drag force model was implemented with the open source program MFIX to simulate the gas–solid flows in CFB (circulating fluidized bed) risers. Calculated solid flux by the EMMS drag agrees well with the experimental value; while the traditional homogeneous drag over-predicts this value. EMMS drag force model can also predict the macro- and meso-scale structures. Quantitative comparison of the results by the EMMS drag force model and the experimental measurements show high accuracy of the model. The effects of the number of particles per parcel and wall conditions on the simulation results have also been investigated in the paper. This work proved that MP-PIC combined with the EMMS drag model can successfully simulate the fluidized flows in CFB risers and it serves as a candidate to realize real-time simulation of industrial processes in the future.

1. Introduction

Numerical simulation is a powerful tool in the investigation of fluidization engineering, which can aid in the optimization of design and operation of the real processes. Reports show that virtual experiments that are full-loop simulation of industrial scale reactors can be achieved using large scale parallel computing (Zhang et al., 2008, 2010). However, tens of hours are needed to simulate even one second real process, which is far from the demand of rapid simulation or even the real-time simulation. Recently, the rapid development in computer hardware, specifically the graphic process unit (GPU) which can efficiently handle the parallel computing of independent data, has promoted the dream of rapid simulation of real processes come true (Ge et al., 2011). For fluidization engineering, rapid simulation requires not only efficient but also accurate simulation of fluidization phenomenon in fluidized beds. In our group, a EMMS based drag force model was developed and this model has been coupled with the two-fluid model (TFM) to successfully simulate the gas–solid flow field in risers (Yang et al., 2003; Wang and Li, 2007; Wang et al., 2008a,b; Li, 2009; Lu, 2009). Reported results show that simulation with the EMMS based drag force model can give a much higher accuracy than simulation with the traditional homogeneous drag force model (Jiradilok et al., 2006; Qi et al., 2007; Nikolopoulos et al., 2010; Benyahia, 2011; Lu et al., 2011). So the EMMS based drag force model fulfills the accuracy requirement for rapid simulation. As mentioned above, the development of high performance computing in recent years has provided the hardware foundation for rapid simulation. Specifically, a large computer system (mole-8.5) with hybrid computing structure which consists of CPU and GPU and reaches Petaflops range is available in our group (Chen et al., 2009; Ge et al., 2011). Finally, a proper computing method is required to fulfill efficiency demand to realize rapid simulation.

* Corresponding author. Tel.: +86 10 82544843; fax: +86 10 62558065.
E-mail address: lifei@home.ipe.ac.cn (F. Li).

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There are three main suitable computing methods for the dense gas–solid fluidization, including two-fluid model (TFM) simulation (Ishii, 1975; Gidaspow, 1994; Neri and Gidaspow, 2000), discrete element method (DEM) (Tsuji et al., 1992, 1993; Deen et al., 2007; Chu and Yu, 2008) and multi-phase particle-in-cell (MP-PIC) method (Andrews and O'Rourke, 1996; Snider, 2001; Benyahia and Galvin, 2010; Pirker et al., 2010).

For TFM method, particle phase is assumed to be a pseudo fluid and the two phases interpenetrating with each other. Partial differential equations describing the two-phase hydrodynamics are always discretized to form linear equations and variables of neighbor cells are interrelated, thus these equations are not suitable to be solved with CPU–GPU hybrid computing. On the other hand, when the number of solid phase increases that is to say with poly-dispersed particles, the equation set becomes very large and the computing load will increase dramatically.

For DEM, particles are treated as real spheres with different diameters, and particle interaction is treated as particle collision. Thus, particles are interrelated with each other, which is also not suitable for CPU–GPU hybrid computing.

For MP-PIC method, particles are treated as parcels and each parcel contains a certain number of real particles of the same diameter (Snider, 2001). The particle interaction is considered through the solid phase normal stress but not directly through particle collision, thus particles move independently from the view of numerical computing whose computation speed can be remarkably accelerated on CPU–GPU hybrid computing platform (Xiong et al., 2010). In addition, MP-PIC method needs not to take the particle collisions implicitly, hence a much bigger time step can be adopted, specifically the time step for particle calculation is the same with that for fluid calculation, which can further accelerate the calculation. In MP-PIC method, it is the "parcel" that has to be tracked but not the real particle, which can also reduce the computing effort greatly. All these advantages make MP-PIC simulation of the large scale particle fluidization system much faster. And with this calculation mode, it is expected to satisfy the efficiency demand of rapid simulation.

Other coarse grained simulation methods have also been reported, just like the similar-particle-assembly (SPA) model (Kuwagi et al., 2004; Mokhtar et al., 2011), DEM simulation based on particle cluster (Liu et al., 2006) and so on. Generally, those methods assume a representative particle with much larger diameter instead of original fine particle and the soft sphere model is used to describe particle collision. However, a criterion to determine the representative particle diameter is still absent as well as the collision parameters.

Since the homogeneous drag force model used in the present MP-PIC method is inaccurate when simulating complex flows with coarse mesh, and as a first step to realize rapid simulation, the primary goal of this study is to integrate MP-PIC and the EMMS based drag force model with the open source multi-phase simulation program MFIX (Syamlal et al., 1993). Subsequently, the gas–solid flow in a CFB riser is simulated to verify the accuracy of the EMMS modified MP-PIC method. Finally, the effects of different model parameters, including the parcel–wall interaction conditions and the number of particles per parcel are investigated.

2. Numerical models and simulation settings

2.1. MP-PIC method

MP-PIC method was first developed by Andrews and O'Rourke to simulate dense particulate flows (1996). In this method, the gas phase is described with the Eulerian type equations which are very similar to the equations in the TFM method. While for the solid phase, a certain number of particles with the same diameter and velocity are represented by a parcel, and the parcels are tracked with the Newton's Law. Particles do not collide with each other, but take effect through solid phase normal stress (Patankar and Joseph, 2001; Snider, 2001; Benyahia and Galvin, 2010). In practice, all the parcels in a fluid cell are responsible for the solid phase normal stress on the cell grid. The solid phase normal stress is first calculated on the fluid grid point, and then it is interpolated to the parcel location. The governing equations of the MP-PIC method are as follows (Snider, 2001):

Gas phase continuity equations:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{u}_g) = 0 \tag{1}$$

where the subscript g represents the gas phase.

Gas phase momentum equations:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \vec{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{u}_g \vec{u}_g) = -\varepsilon_g \nabla p + \nabla \cdot \bar{\bar{\tau}}_g + \varepsilon_g \rho_g \vec{g} - \sum_{p=1}^{n_T} n_p \frac{V_p}{V_c} \beta_p (\vec{U}_g(\vec{x}_p) - \vec{U}_p) \tag{2}$$

where n_T is the parcel number in the fluid cell and n_p is the number of particles per parcel. V_p and V_c are the volumes of particle and fluid cell, respectively. β_p is the drag force coefficient, $\vec{U}_g(\vec{x}_p)$ is the gas velocity at parcel location, $\vec{x}_p$, and $\vec{U}_p$ is the parcel velocity. $\bar{\bar{\tau}}_g$ is the gas phase stress tensor

$$\bar{\bar{\tau}}_g = 2\mu_g \bar{\bar{S}}_g, \quad \bar{\bar{S}}_g = \frac{1}{2}\left[\nabla \vec{u}_g + (\nabla \vec{u}_g)^T\right] - \frac{1}{3}\nabla \cdot \vec{u}_g \bar{\bar{I}} \tag{3}$$

Parcel motion equations:

$$\frac{d\vec{x}_p}{dt} = \vec{U}_p \tag{4}$$

$$\frac{d\vec{U}_p}{dt} = -\frac{\nabla p}{\rho_s} - \frac{\nabla p_s}{\varepsilon_s \rho_s} + \vec{g} + \frac{\beta_p}{\rho_s}(\vec{U}_g(\vec{x}_p) - \vec{U}_p) \tag{5}$$

where p_s is the particle pressure, which can be expressed as (Snider, 2001; Benyahia and Sundaresan, 2011)

$$p_s = \frac{P_s^* \varepsilon_s^\alpha}{\varepsilon_{s,\max} - \varepsilon_s} \tag{6}$$

where P_s^*, α, are model parameters, $\varepsilon_{s,\max}$ is the solid volume fraction at close pack. Their values are summarized in Table 1.

2.2. Drag force model

Drag force modeling is of great importance to accurately simulate the solid distribution in CFB risers with two-fluid model. Most recently, Benyahia and Sundaresan also indicated that homogeneous drag force model is insufficient to capture complex gas–solid flow structures with discrete particle models when using coarse mesh (Benyahia and Sundaresan, 2011). Here, homogeneous drag model describes the drag force exerted on particles which are homogeneously distributed in gas flows. Particles in CFB risers usually aggregate to form clusters, which lead to local heterogeneous solid distributions. Specifically, particle cluster diameter has been found to be a function of a lots parameters, including particle diameter, gas and solid velocities, etc. (Li and Kwauk, 1994; Breault, 2012). EMMS theory does not describe clusters directly, but it uses flow field decomposition and energy minimization to characterize local heterogeneous solid distributions. Then the decomposed field parameters are used to formulate the EMMS drag (Wang and Li, 2007). In this study, a traditional homogeneous drag force model (Ergun, 1952;