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Eulerian–Eulerian simulation of irregular particles in dense gas–solid fluidized beds

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ABSTRACT

As an important and essential physical property, particle shape affects fluidization characteristics of dense gas–solid fluidized beds greatly. However, numerical studies of irregular particles in gas–solid fluidization, especially using Eulerian–Eulerian model, are relatively scarce, primarily due to the lack of an appropriate inter-phase drag model. To this end, a simple and effective drag model was proposed in this work to address the critical role of particle shape in determining the inter-phase drag force. This drag model features the usage of Ganser correlation and Ergun correlation, respectively, in dilute and dense solid concentration conditions. Moreover, particle sphericity is introduced as a concise shape descriptor, and can be calibrated by experimentally measured minimum fluidization velocity and the corresponding voidage. To verify the established numerical model, experimental study was also conducted in a lab-scale three-dimensional rectangular bed filled with irregular Geldart group B particles. Other two kinds of irregular bed materials from open literature were investigated as well to provide further validation. The predicted results using the proposed drag model are overall in relatively better quantitative agreement with the experimental data or available empirical correlations, in terms of both macro-scale and micro-scale behavior. In contrast, the numerical model with the drag force assuming perfectly spherical particles completely fails to reproduce the experimental hydrodynamics of the gas–solid fluidized bed. In addition, sensitivity analysis of the proposed drag model demonstrated its weak sensitivity to the minimum fluidization characteristics of particles. The sufficient comparison and analysis indicated that the proposed drag model together with the estimation method of particle sphericity is quite reasonable and convenient for Eulerian–Eulerian simulation of irregular particles behavior in lab-scale dense gas–solid fluidized beds.

1. Introduction

Understanding the behavior of particles in dense gas–solid flows is vital for the successful and effective design, operation, optimization and scale-up of fluidized bed reactor in many important industrial applications, such as drying of solids, numerous synthesis reactors and pulverized coal combustors [1]. In most of practical powder applications, however, both of artificial and natural solid particles frequently have various shapes, ranging from roughly spherical glass beads to strongly irregular mineral particles, fibers or biomass materials. Different shapes of particles result in a large difference in gas–solid drag force [2–4], which in turn affects particle behavior greatly due to the crucial role of drag force in fluidization [5,6] and then the performance of equipment. Thus the effect of particle shape needs an appropriate estimation and consideration for the better utilization of practical powder processes and equipment.

Although it has been widely recognized that the form of particles involved in practical engineering applications is seldom perfectly spherical, so far the majority of efforts in gas–solid flows have been devoted to the completely spherical particles. This oversimplified assumption is prevailing dominantly in numerical simulations. For example in Computational Fluid Dynamics (CFD) simulations of dense gas–solid flows, a vast number of works using Eulerian–Eulerian model [5] or even Eulerian–Lagrangian model [7,8] which can describe flow behavior of particles more elaborately (at a particle scale), have ignored the effect of particle shape totally. This apparently cannot provide reasonable results for irregular particles, in spite of model simplicity and fast computation. Actually in contrast to spheres, the irregular or non-spherical (see Table 1 of Mandø and Rosendahl [9] for specific categorization of particle shapes) shape of particles often makes the flow around single particle or bulk particles much more complicated. As far as the single regular non-spherical particle is concerned, the discrepancy of drag force or lift force becomes more significant as compared to a sphere, due to particle shape (i.e. aspect ratio) and orientation with respect to the flow [4,10]. Generally, the more irregular the particle is, the greater the drag is. This effect of particle shape is

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Table 1
Physical and fluidization properties of IPE experimental particles.

Property	Value	Measure method
Particle composition	Calcium carbonate	X ray fluorescence (Panalytical, Axios max)
Particle density (ρ_s)	3135 kg/m^3	Pycnometer test method
Bulk particle density (Random dense packing)	1429 kg/m^3	Powder flow tester (BrookField, PFT)
Sauter mean particle diameter	341 μm	Laser diffraction particle size analyzer (Beckman Counter, KS-13320)
Wall friction angle	16.1°–20.8°	Powder flow tester (BrookField, PFT)
Internal friction angle of particles (φ_f)	34.3°–35.2°	Powder flow tester (BrookField, PFT)
Particle terminal velocity	1.1677 m/s	Calculated
U_{mf}	0.095 m/s	Pressure drop versus superficial gas velocity diagram
H_{mf}	0.125 m	Ruler
Δp_{mf}	1420 pa	Pressure transducers
ε_{mf}	0.6305	Estimated from Δp_{mf} and H_{mf}
Sphericity (ψ)	0.36	Calculated by Eq. (2) in this work
Superficial gas velocity (U_g)	0.3, 0.4 and 0.45 m/s	Rotary flowmeter (Yuyao yinhuan flowmeter Co. Ltd., LZB-15)

particularly pronounced in Newton's flow regime [11]. Further as for the macroscopic behavior of bulk particles in fluidization, non-spherical particles have a lower minimum fluidization velocity than spherical particles [12] and give poor fluidization quality in terms of pressure drop [13,14].

Through using the improved gas–solid drag model which considers the effect of particle shape, some CFD simulation works [12,14–19] have been conducted for an isolated particle or dense particles with non-spherical shape in gas–solid systems, especially in recent years. The majority of those works used Eulerian–Lagrangian model as the simulation tool. However, in spite of its widespread applications, Eulerian–Lagrangian model at present is largely limited to the simulations of small fluidized beds [14,20], due to the complexity in representing irregular shape and heavy computational demand. Comparatively, Eulerian–Eulerian model shows an outstanding advantage in this aspect, particularly in the systems where the mass-loading of particles is considerable or the system size is quite large. So far, however, very few Eulerian–Eulerian works on fluidization characteristics of irregular particles have been reported, primarily because of the lack of appropriate and efficient inter-phase drag models. To reach better agreement with the measured bed height, Peirano et al. [19] considered the non-spherical effect of particles through modifying two parameters in their three-dimensional Eulerian–Eulerian model: the maximum solid volume fraction and particle relaxation time. Although the aim of their study was to show significant differences between two- and three-dimensional simulations for a bubbling fluidized bed, they also demonstrated clearly the necessary consideration of particle shape. But how to incorporate the shape factor (i.e. the sphericity) into the drag model and estimate particle sphericity was not presented.

One natural and general idea of formulating inter-phase drag model of irregular particles, both in experimental [21–24] and relatively few numerical studies [3,10], is to make use of the framework of the existing correlations of spheres, but take into account some effective shape factors. The determination of unambiguous shape factors is still extremely challenging for real particles at present, despite the fact that many shape factors have been proposed and used widely [25,26]. Even though other shape factors may describe particle shape more sophisticatedly, sphericity may be the most appropriate single measure for characterizing the shape, particularly for isometric non-spherical particles [26,27]. The sphericity is defined as the ratio of the surface area of the equivalent-volume-sphere to the actual surface area of the particle. So this factor provides a much generalized description of the shape, and can make the parameters with respect to particle shape in gas–solid interaction models as few as possible. This undoubtedly reduces the computation cost and simplifies the models. Although some useful drag models on irregular particles using the sphericity as shape factor have been proposed [28], most of them primarily directed at the situation of an isolated particle in an infinite flow field. While in a multi-particle suspension system, such as a gas–solid fluidized bed, the drag force acting on the particle is surely affected by the surrounding particles. On the other hand, the drag models for multi-particle systems used widely by Eulerian–Lagrangian model often require detailed information on the drag acting on particles [23,24,26], such as the orientation area of particles perpendicular or parallel to the flow along the trajectory, in order to obtain the accurate Lagrangian properties of particles. However, these over-rigorous drag models cannot be applied appropriately in Eulerian–Eulerian model, because Eulerian–Eulerian model regards particles as a pseudo-fluid phase, and consequently cannot determine some required input parameters.

The primary objective of this work is to establish an Eulerian–Eulerian CFD model to predict hydrodynamics of particles with irregular shape in dense gas–solid fluidized beds. An effective gas–solid drag model was proposed, accounting for the influence of particle shape by the sphericity, to capture the basic inter-phase momentum transfer feature of an irregular particle system. The drag model combines Ganser correlation and Ergun correlation together. The sphericity of particles, introduced in both of Ganser and Ergun correlations, can be estimated through the experimentally measured fluidization characteristics at the minimum fluidization condition (i.e. U_{mf} and ε_{mf}). To examine the established CFD model, fluidization experiments of irregular particles in a lab-scale three-dimensional rectangular bed were conducted to provide the sufficient data for comparison. In the experiments, the detailed information, such as axial distributions of pressure drop, radial distributions of solid volume fraction and so on, was measured carefully. In addition, another two kinds of irregular bed materials from Reuge et al. [29]'s work were also simulated by the established CFD model to provide further numerical validation. Meanwhile, Syamlal and O'Brien drag model which can modify two constants through U_{mf} and ε_{mf} was investigated to explore its possibility of modeling irregular particles in gas–solid systems. Then sensitivity analysis of above two drag models to U_{mf} and ε_{mf} was further conducted to examine if they are robust enough, since they both use U_{mf} and ε_{mf} to calibrate important parameters and the accurate measurements of U_{mf} and ε_{mf} are usually difficult in practice.

2. Experimental setup

2.1. IPE experiments

2.1.1. Bed materials

Experiments were conducted in Institute of Process Engineering, Chinese Academy of Sciences, China (IPE) to investigate the behavior of irregular particles and supply the adequate data for numerical validation. In the experiments, the calcium carbonate particle was used as bed materials for fluidization. Both physical and fluidization properties of the particle were carefully measured, as summarized in Table 1. The measured particle size distribution is shown in Fig. 1. Most of the particles belong clearly to group B within Geldart's classification system [30]