Chemical Engineering Science 163 (2017) 11–26

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Micromechanical analysis of flow behaviour of fine ellipsoids in gas fluidization

J.Q. Gan, Z.Y. Zhou *, A.B. Yu

Laboratory for Simulation and Modeling of Particulate Systems, Department of Chemical Engineering, Monash University, Clayton, VIC 3800, Australia

HIGHLIGHTS

- Microscopic structures of fine ellipsoids in gas fluidisation are investigated.
- Fine ellipsoids have a large bed expansion ratio and bed porosity.
- Orientation order of ellipsoids varies significantly with gas velocity and particle size.
- The bed expansion criterion based on force balance is confirmed valid for ellipsoids.

ARTICLE INFO

Article history:
Received 15 September 2016
Received in revised form 1 December 2016
Accepted 9 January 2017
Available online 10 January 2017

Keywords:
CFD-DEM
Flow structure
Fluidization
Fine ellipsoids
Interparticle forces
Orientation

ABSTRACT

The macro-scale flow behaviour of granular materials in gas fluidization is governed by particle-particle and gas-particle interactions, which are affected significantly by particle size and shape. Understanding the micro-scale flow structure of fine non-spherical particles is essential for process design, optimisation and control. In this work, the combined approach of computational fluid dynamics for gas phase and discrete element method for particles is used to study flow and force structures of fine ellipsoids in gas fluidization. The results reveal that fine particles have vortex flow structure in fluidized beds, and the vortex flow becomes more significant particularly for oblate particles. The microscopic structure analysis demonstrates that when aspect ratio deviates from 1.0, the packed beds could experience compaction, and in expanded beds, the bed expansion ratio increases. The effect of particle size is investigated, showing that with the decrease of particle size, the mean coordination number decreases due to more significant role of van der Waals force. Ellipsoids exhibit higher orientation order which varies greatly with gas velocity and particle size. In fluidized beds, ellipsoids tend to flow in small projected area to the fluid flow direction to reduce the flow resistance. The bed expansion criteria established in the literature are confirmed still valid for ellipsoids, but the gas velocity range for expanded bed interval is much wider than spheres.

1. Introduction

Fluidization is widely used in many processes such as fluidized catalysis cracking and combustors due to its unique advantages in mixing and heat transfer performance. Understanding the fluidization fundamentals is of paramount importance to the formulation of strategies for process development and control. A number of factors can affect fluidization characteristics, among which particle size and shape are two important variables. For example, for fine particles, it is generally agreed that there is an interval starting from the minimum fluidization point (notated by U_{mf} – minimum fluidization velocity) and terminated at the minimum bubbling point (notated by U_{mb} – minimum bubbling velocity). The two critical points of U_{mf} and U_{mb} demarcate fine particle beds into three flow regimes: fixed beds ($U_g < U_{mf}$, where U_g is the gas superficial velocity), expanded beds ($U_{mf} < U_g < U_{mb}$), and fluidized beds ($U_g > U_{mb}$). In fixed bed regime, particles are quiescent and gas flows through interstices. In expanded bed regime, the bed expands smoothly and homogeneously, and finally reaches stable state with negligible particle motions and well defined bed surface. In fluidized beds, gas bubbles form, coalesce and grow, and particles move vigorously. In this flow regime, the inhomogeneous flow which takes the form of clusters/agglomerates/streamers due to the existence of van der Waals force has drawn great interests of researchers (Sonnenberg and Schmidt, 2005); and different shapes of clusters have been reported (Horio and Kuroki, 1994; Davidson, 2000). These three macroscopic flow regimes and their behaviour

* Corresponding author.
E-mail address: zongyan.zhou@monash.edu (Z.Y. Zhou).

http://dx.doi.org/10.1016/j.ces.2017.01.020
0009-2509/

can be addressed by microscopic properties such as particle-particle and particle-fluid interactions achieved from physical and numerical experiments. For example, the stability of expanded bed is attributed to hydrodynamic interactions between solid and fluid phases (Jackson, 1963; Foscolo and Gibilaro, 1984; Batchelor, 1988), inter-particle forces (Rietema, 1973; Mutsers and Rietema, 1977; Tsinontides and Jackson, 1993; Lee et al., 1999), or the combined effect of both particle-fluid and inter-particle forces (Xu and Yu, 2002; Valverde et al., 2003; Hou et al., 2012). A bed expansion criterion was formulated in terms of the balance of particle-particle and particle-fluid interaction forces (Xu and Yu, 2002; Valverde et al., 2003; Hou et al., 2012). Correlations between bed porosity and gas velocity (Girimonte and Formisani, 2009) and phase diagrams between particle coordination number and porosity were also used to predict the demarcation of flow regimes (Hou et al., 2012).

However, majority of the studies above assume that the shape of fine particles is spherical, not considering the effect of particle shape. As reported in the literature, non-spherical particles give poor fluidizing quality, and minimum fluidization velocity changes markedly with particle shape (Liu et al., 2008; Zhou et al., 2011b). Long 'neck-laces' and particle strings or agglomerates are observed in the flow direction for elongated particles (Gunes et al., 2008). Similar "chain" phenomenon is also observed in our recent work for ellipsoidal particles (Gan et al., 2016a). The earlier onset of fluidization of non-spherical particles is explained by an increase in mean projected area which increases the magnitude of particle drag term for a given superficial velocity (Hilton et al., 2010). Moreover, coarse non-spherical particles were found to have the preference to orient in mean flow direction (Zhang et al., 2001a; Mortensen et al., 2008; Zhou et al., 2011b). The formation of shear-induced clusters in viscoelastic fluid of micron-sized (2.4–3.7 μm) and prolate particles is attributed to that the neighbour particles tend to remain parallel and pack with an angle of about 30° between the lines joining their centres and their principal axis (Gunes et al., 2008).

As demonstrated above, both particle size and shape show significant influence on fluidization characteristics, which however are, in essence, governed by the micro-scale inter-particle interactions and particle-fluid interactions. The combined effect of particle size and shape on fluidization has not been well studied yet. In our recent work (Gan et al., 2016a), the effect of these two factors on the flow pattern and several macroscopic fluidization parameters (e.g., pressure drop, U_{mf} and U_{mb}) were analysed for fine ellipsoids, demonstrating the significant effect. Still, many fundamental questions remain unknown for flow structures of cohesive ellipsoidal particles. For example, how does particle orientation preference change when particle size reduces from millimetres to microns in gas fluidization? How does particle shape affect the inter-particle forces and the interval of expanded beds? To address these questions, in this work, the combined method of computational fluid dynamics and discrete element method (CFD-DEM) is still used, which has been illustrated a promising approach to understand underlying flow mechanisms (Xu and Yu, 2002; Ye et al., 2004, 2005; Zhou et al., 2011b; Hou et al., 2012).

Thus, following up our previous work on the macroscopic flow behaviour (Gan et al., 2016a), the micro-scale flow structure (for example, particle velocity, bed porosity, coordination number, and particle orientation), and force structure for fine non-spherical particles are generated by CFD-DEM, and then analysed in this work. Particularly, ellipsoidal particles are still used as they can represent a large number of shapes from platy to elongated that are practically applied in industry fluidized bed reactors. Ellipsoids with aspect ratio from 0.25 to 3.5, and sizes from 50 μm to 10 mm are used.

2. Simulation models for ellipsoids

2.1. CFD-DEM governing equations

In CFD-DEM simulation, the solid phase is based on DEM, and gas phase is treated as a continuum phase in a similar way to the two fluid model (TFM). CFD-DEM has its unique advantages in studying the micromechanical properties of particles. In particular, it can track the motion of each particle in the system, and generate extensive flow and force structures for analysis and understanding. CFD-DEM has been well established for particle-fluid flow systems (Zhou et al., 2010). Note that in this approach, three sets of governing equations exist: type I, type II and type III, with the last two corresponding to the so called model A and model B (Bouillard et al., 1989). Each type of model has its own advantages and disadvantages. Type I is, however, the most rational, and is employed in the present work.

Various attempts have been made to extent DEM from spheres to ellipsoids (Ting, 1992; Lin and Ng, 1995; Džiugys and Peters, 2001; Zhou et al., 2011a; Dong et al., 2015), but only a few efforts have been made to develop a general CFD-DEM model to describe the dynamics of non-spherical particles coupled with fluid flow (Hilton et al., 2010; Zhou et al., 2011b). The present work follows that of Zhou et al. (2011b) and Gan et al. (2016a), but here we focus on fine ellipsoids. For convenience, a brief description of the method is given below.

According to the DEM, a particle in a gas-fluidized bed can have two types of motion: translational and rotational, which are determined by Newton's second law of motion. The governing equations for the translational and rotational motion of particle i with radius R_i, mass m_i, and moment of inertia I_i can be written as

$$m_i \frac{d\mathbf{V}_i}{dt} = \mathbf{f}_{pf,i} + \sum_{j=1}^{k_c} (\mathbf{f}_{c,ij} + \mathbf{f}_{d,ij} + \mathbf{f}_{vdw,ij}) + m_i\mathbf{g} \tag{1}$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{k_c} (\mathbf{M}_{t,ij} + \mathbf{M}_{r,ij} + \mathbf{M}_{n,ij}) \tag{2}$$

where $\mathbf{v}_i$ and $\boldsymbol{\omega}_i$ are the translational and angular velocities of the particle, respectively, and k_c is the number of particles in interaction with the particle. The forces involved are: particle-fluid interaction force $\mathbf{f}_{pf,i}$, the gravitational force $m_i\mathbf{g}$, and inter-particle forces between particles, which include elastic force $\mathbf{f}_{c,ij}$, and viscous damping force $\mathbf{f}_{d,ij}$. For fine particles, the van der Waals force $\mathbf{f}_{vdw,ij}$ need to be considered. These inter-particle forces can be resolved into the normal and tangential components at a contact point. The torque acting on particle i by particle j includes two components: $\mathbf{M}_{t,ij}$ which is generated by tangential force and causes particle i to rotate, and $\mathbf{M}_{r,ij}$ commonly known as the rolling friction torque, is generated by asymmetric normal forces and slows down the relative rotation between particles. Additional torque $\mathbf{M}_{n,ij}$ should be added because the normal contact force and van der Waals force do not necessarily pass through the particle centre. A particle may undergo multiple interactions, so the individual interaction forces and torques are summed over the k_c particles interacting with particle i. The force models used are discussed in Section 2.2.

The continuum fluid phase is calculated from the continuity and Navier-Stokes equations based on the local mean variables over a computational cell, which can be written as

$$\frac{\partial \varepsilon_f}{\partial t} + \nabla \cdot (\varepsilon_f \mathbf{u}) = 0 \tag{3}$$

$$\frac{\partial(\rho_f \varepsilon_f \mathbf{u})}{\partial t} + \nabla \cdot (\rho_f \varepsilon_f \mathbf{u}\mathbf{u}) = -\nabla p - \mathbf{F}_{fp} + \nabla \cdot \varepsilon_f \boldsymbol{\tau} + \rho_f \varepsilon_f \mathbf{g} \tag{4}$$