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Particle scale modelling of solid flow characteristics in liquid fluidizations of ellipsoidal particles

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ABSTRACT

Particle shape is one of the most important parameters that can cause significant changes of flow characteristics in liquid fluidized beds, which however has not been well studied in the past. In this work, CFD-DEM approach is used to investigate the hydrodynamics of ellipsoidal particles in liquid fluidizations. The non-uniformity distributions of pressure gradient and porosity with bed height are successfully captured for ellipsoids at high liquid superficial velocities, consistent with those reported in literature. The results also show that ellipsoids intend to enter the freeboard region and entrainment may occur. Disc-shape particles expand more significantly than spherical and elongated particles. The force analysis indicates that with particle aspect ratio deviating from 1.0, the drag force acting on ellipsoids increases while pressure gradient force reduces. Particle shape effects shown above are closely related to particle orientations which can significantly affect particle-fluid interaction force and particle terminal velocities.

1. Introduction

The applications of liquid fluidization can be observed in many parts of industries such as particle classification, backwashing of granular filters, leaching and washing, and bioreactors due to the substantial liquid–solid surface contact, high heat and mass transfer rate, high operation flexibilities, and reduced backmixing of fluid and solid phases [1, 2]. In most of these multiphase operations, particle properties such as size, density and shape may experience significant changes because of attrition, coalescence, comminution or chemical reactions, which may affect flow behaviour of particles and hence process performance.

In the past, many studies, either experimentally or numerically, have been conducted on the flow behaviour in liquid fluidizations with mono-sized particles or mixtures. Mono-sized spherical particles often make homogenous fluidized beds [3, 4], and the bed expansion can be described by Richardson and Zaki correlation [5]. Apart from homogenous/particulate flow regimes, other flow regimes such as wavy [6], aggregative/turbulent [3, 6], slugging [7], and bubbly [6] regimes can also be observed in liquid fluidized beds. Moreover, introducing a second or third components with different sizes or densities causes more complicated flow structures. Extensive efforts have been made in this direction to understand the principles of liquid fluidized beds of multicomponent mixtures of spherical particles [1, 6, 8–11]. As a result, various models have been proposed to quantify the solid-liquid fluidized bed characteristics [8, 9, 12].

In spite of substantial studies as mentioned above, the effects of particle shape on the solid-liquid flow behaviour have still less been reported. Except for two physical experimental studies [13, 14], the previous work mainly considered particles as spheres. In practice, particles are generally non-spherical in most of processes [13] such as ore beneficiations using liquid-solid fluidized beds separator [15]. Barghi et al. [14] observed that cylindrical particles with the length/diameter ratio $L/D = 1$ were mixed well with spherical particles, but elongated cylindrical particles with $L/D = 2$ segregated from spherical particles. Escudie et al. [13] reported that differences in particle shape can result in segregation for binary mixtures of particles with the same volume and density. Epstein et al. [16] demonstrated that the serial model [16] was able to predict bed expansions for binary and ternary mixtures of different particle shapes. These observations show that particle shape can cause different flow behaviour in liquid fluidizations rather than that observed for ideal spherical particles. However, the answers to some fundamental questions such as how and why particle shape affects flow phenomena are not clear, and hence still poorly understood.

In recent years, computational modelling, typically based on the CFD-DEM approach, has increasingly become an efficient tool to study fluidisations. CFD-DEM has been verified as one of the most effective approaches to study granular materials [17–19], and it provides microscopic information of flow dynamics in fluidized beds. Therefore, in this work, CFD-DEM is used to examine the effects of particle shape on the flow characteristics in liquid fluidizations. In the simulations, ellipsoids are used as they can represent a wide range of particle shapes from oblate to prolate particles. Different aspect ratios varying from 0.28 to 5.33 are employed, and results are analysed mainly in terms of particle

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flow patterns, pressure drop, and bed expansion. In addition, force and particle orientation analysis is also conducted to explain the occurrence of entrainment phenomenon for different shaped particles.

2. Model description

In the CFD-DEM approach, particle motions are determined by Newton's second law of motion at a particle scale, and the continuum fluid flow is described on the basis of local-averaged Navier-Stokes equations at a computational cell level. The CFD-DEM approach has been well developed and documented in the literature [20–22], and its extension to coarse [23, 24] and fine [25, 26] ellipsoidal particles has been presented for gas fluidizations. In this work, it is further extended to liquid fluidizations. For convenience, the model is briefly given below.

2.1. CFD-DEM governing equations

The particle phase in the particle-fluid flow is considered as a discrete phase. The motion of particles is determined by Newton's second law of motion [27],. 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:

$$\frac{m_i d\mathrm{v}_i}{dt} = \sum_{j=1}^{k_i} \left(\mathbf{f}_{c,ij} + \mathbf{f}_{d,ij}\right) + \mathbf{f}_{pf,i} + m_i\mathbf{g} \tag{1}$$

and

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

where v_i and $\boldsymbol{w}_i$ are translational and angular velocities of the particle i, k_i is the number of particles interacting with the particle i, $\mathbf{f}_{c,ij}$ and $\mathbf{f}_{d,ij}$ are elastic contact force and damping force, respectively. $\mathbf{f}_{pf,i}$ is the interaction force between particle and fluid, and $m_i\mathbf{g}$ is the gravitational force. I_i is the moment of inertia of particle i, and the torque acting on particle i by particle j includes three components: $\mathbf{M}_{t,ij}$ which is generated by tangential force and causes particle i to rotate, $\mathbf{M}_{r,ij}$ commonly known as the rolling friction torque, and $\mathbf{M}_{n,ij}$ is the torque generated by normal force when the normal force does not pass through the particle centre.

The liquid flow field is described on the basis of locally-averaged Navier-Stokes equations [28, 29]. Therefore, the mass and momentum conservation equations governing the liquid phase are respectively described as:

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

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

where $\mathbf{u}$, ρ_f, p, and $\mathbf{F}_{pf}$ are the fluid velocity, fluid density, pressure, and volumetric fluid-particle interaction force, respectively; τ and ε_f are the fluid viscous stress tensor and porosity which are given as $\tau = \mu_e[(\nabla\mathbf{u}) + (\nabla\mathbf{u})^{-1}]$ and $\varepsilon_f = 1 - \sum_{i=1}^{k_i} V_i/\Delta V$, where V_i is the volume of particle i (or part of the volume if particle is not fully in the CFD cell), k_i is the number of particles in the CFD cell. μ_e is the fluid effective viscosity determined by $k-\varepsilon$ model [30] which has been used in our previous work [23, 24, 26]. The volumetric fluid-particle interaction force in a computational cell volume of ΔV is calculated by $\mathrm{F}_{pf} = (\sum_{i=1}^{k_i}\mathrm{f}_{pf,i})/\Delta V$, where $\mathbf{f}_{pf,i}$ is the particle-fluid interaction force on the particle i.

2.2. Particle-particle and particle-fluid interaction forces

The equations to calculate contact forces and torques between two spheres have been well established [17], and also extended to ellipsoidal particles [23, 25]. Zheng et al. [31] proved that the normal and tangential contact force models used for spheres are valid for ellipsoids. In addition, since ellipsoids provide smooth/continuous surfaces, the same Coulomb condition or sliding/rolling friction models as used for spheres can also be applied. The equations used in this work to calculate the inter-particle forces and torques are listed in Table 1.

Various forces have been identified to determine interactions between particles and liquid, including the drag force, the pressure gradient force, the virtual mass force, the Basset force, the Saffman force, and the Magnus force [17]. Comprehensive discussions have been made by Di Renzo et al. [32] that except for the drag force and the pressure gradient force, other types of particle-fluid interaction forces can be ignored in the simulations of liquid fluidizations. This is due to the fact that the equations of these forces were developed mainly based on single-particle/dilute systems or under simplified fluid flow conditions, hence their applicability is questionable [33]. Moreover, such forces have been ignored in many studies in the literature, demonstrating that the reliable and consistent results with experiments can be generated [7, 32, 34–40]. Hence, in this work, only the drag force $\mathbf{f}_{d,i}$ and the pressure gradient force ($\mathbf{f}_{pg,\,i} = -V_i\nabla p$) are considered in the present CFD-DEM model.

Different models have been proposed to calculate the drag force on spheres [17]. In particular, the approach proposed by Di Felice [41] is one of the most popular ones [21–23], and also suitable for ellipsoids as demonstrated in our previous work [23]. Therefore, this method is still used, and the equation is written as [41]:

$$\mathbf{f}_{d,i} = 0.5\times C_D\rho_f A_\perp {\varepsilon_f}^2|\mathbf{u}_i - \mathbf{v}_i|(\mathbf{u}_i - \mathbf{v}_i)\varepsilon_f^{-\gamma} \tag{5}$$

where $\gamma = 3.7 - 0.65\exp[-(1.5 - \log_{10}\mathrm{Re}_i)^2/2]$, $A_\perp$ is the cross-sectional area perpendicular to the fluid flow, Re_i is the relative Reynolds number, which is defined as $\mathrm{Re}_i = \rho_f d_v \varepsilon_f \mid \mathbf{u}_i - \mathrm{v}_i \mid /\mu_f$, where d_v is the equivalent diameter defined as the diameter of a sphere with the same volume as the ellipsoid particle. C_D is the drag coefficient, which can be calculated by different models as briefly discussed below.

Considerable investigations have been made to determine the drag coefficient C_D for non-spherical particles, with shapes varying from cubes and cylinders to ellipsoids and more generally irregular shapes [42–48]. Based on the work by Sommerfeld and Lain [49] that Ganser's [44] correlation over-predicts the particle average velocity, Hölzer and Sommerfeld [46] used a large amount of literature experimental data and propose a correlation for C_D which is applicable over a wide range of Re numbers, and also considers the effects of both particle shape and orientation. Its validity were further verified by Hilton et al. [50],

Table 1
Equations to calculate inter-particle forces and torques acting on particle i.

Forces or torques	Equations
Normal elastic force, $\mathbf{f}_{cn,ij}$	$-4/3E^*\sqrt{R^*}\delta_n^{3/2}\mathbf{n}$
Normal damping force, $\mathbf{f}_{dn,ij}$	$-c_n\left(8m_{ij}E^*\sqrt{R^*\delta_n}\right)^{1/2}\mathbf{v}_{\mathrm{n,ij}}$
Tangential elastic force, $\mathbf{f}_{ct,ij}$	$-\mu_s\mid\mathbf{f}_{cn,ij}\mid(1-(\delta_t/\delta_{t,\,\max})^{3/2})\hat{\boldsymbol{\delta}}_t$
Tangential damping force, $\mathbf{f}_{dt,ij}$	$-c_t\left(6\mu_s m_{ij}\lvert\mathbf{f}_{cn,ij}\rvert\sqrt{1-\delta_t/\delta_{t,\,\max}}/\delta_{t,\,\max}\right)^{1/2}\mathbf{v}_{t,ij}$
Coulomb friction force, $\mathbf{f}_{t,ij}$	$-\mu_s\lvert\mathbf{f}_{cn,ij}\rvert\hat{\boldsymbol{\delta}}_t$
Torque by tangential forces, $\mathbf{M}_{t,ij}$	$\mathbf{R}_{\mathbf{c},\boldsymbol{ij}}\times(\mathbf{f}_{ct,ij}+\mathbf{f}_{dt,ij})$
Torque by normal forces, $\mathbf{M}_{n,ij}$	$\mathbf{R}_{\mathbf{c},\boldsymbol{ij}}\times(\mathbf{f}_{cn,ij}+\mathbf{f}_{dn,ij})$
Rolling friction torque, $\mathbf{M}_{r,ij}$	$\mu_{r,ij}\lvert\mathbf{f}_{n,ij}\rvert\hat{\boldsymbol{\omega}}_{ij}^n$

where $1/m_{ij} = 1/m_i + 1/m_j$, $R^* = 1/(2\sqrt{A'B'})$, $E^* = E/(2(1-v^2))$, $\hat{\boldsymbol{\omega}}_{ij}^n = \boldsymbol{\omega}_{ij}^n/\mid\boldsymbol{\omega}_{ij}^n\mid$, $\hat{\boldsymbol{\delta}}_t = \boldsymbol{\delta}_t/\lvert\boldsymbol{\delta}_t\rvert$, $\delta_{t,\,\max} = \mu_s(2-\nu)/2(1-\nu)\delta_n$, $\mathrm{v}_{ij} = \mathrm{v}_j - \mathrm{v}_i + \boldsymbol{\omega}_j\mathrm{R}_{c,ji} - \boldsymbol{\omega}_i\mathrm{R}_{c,ij}$, $\mathrm{v}_{n,ij} = (\mathrm{v}_{ij}\cdot\mathbf{n})\cdot\mathbf{n}$, $\mathrm{v}_{t,ij} = (\mathrm{v}_{ij}\times\mathbf{n})\times\mathbf{n}$. Note that tangential force ($\mathbf{f}_{ct,ij} + \mathbf{f}_{dt,ij}$) should be replaced by $\mathbf{f}_{t,ij}$ when $\delta_t \geq \delta_{t,\,\max}$.