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Investigation of causes of layer inversion and prediction of inversion velocity in liquid fluidizations of binary particle mixtures

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ABSTRACT

Liquid fluidization plays an important role in mineral processing such as solid classifiers and biological reactors. When particle properties differ in size, density or shape, segregation can occur. Typically, a segregation phenomenon so-called layer inversion in two-phase solid-liquid fluidization of binary mixtures has been reported in the literature. At low liquid velocities, the two species form distinct layers with the denser smaller particles at the bottom and the lighter larger particles at the top. At high liquid velocities, however, the two layers are inverted with smaller particles being at the top while larger ones at the bottom. In this work, glass beads (193 μm) and activated carbon (778 μm) are used in the simulation as those in Jean and Fan (1986), and the layer inversion is successfully reproduced by CFD-DEM. The underlying segregation mechanism is analyzed in terms of particle-fluid interaction forces. The results reveal that the layer inversion is caused by the relative change of particle-fluid interaction forces on particles. For large particles, the reduction of the pressure gradient force cannot be compensated by the increased drag force, resulting in the downward flow. Meanwhile, small particles tend to move upward because the increased drag force exceeds the decreased pressure gradient force. In addition, the effects of particle and liquid properties on layer inversion are examined, and different drag force models in predicting the layer inversion are also assessed. It indicates that Rong et al.'s drag model represents the layer inversion with the best accuracy. Finally, a model based on the force balance criterion is proposed to predict the inversion velocity showing a better accuracy.

1. Introduction

Segregation is a popular phenomenon for granular materials, and can be observed in various particulate systems due to property differences of particles in size, density, shape, and/or other characteristics such as surface roughness, resilience, and electrostatic properties [1–3]. Segregation can significantly affect the quality of manufactured products, but it can also be used to separate materials. It represents a challenging research area in granular research, and many efforts have been made either experimentally [4] or theoretically [5]. This paper is focused on an important segregation phenomenon called layer inversion in two-phase solid-liquid fluidizations, which plays an important role in fluidized beds solid classifiers or biological reactors [6].

In layer inversion, the fluidization system contains a binary mixture of particles in which small particles are denser than large particles. At low liquid velocities, the two species form distinct layers with the smaller and denser particles at the bottom while the larger and lighter particles at the top. At high liquid velocities, however, the two layers are inverted. Smaller particles move to the top, and larger particles are located at the bottom. This peculiar phenomenon plays an important role in fluidized bed solid classifiers or biological reactors [6]. Layer inversion was reported for the first time by Hancock [7], then it quickly attracted extensive investigations [8–14]. Substantial studies have revealed that the inversion velocity depends on many variables such as mixture compositions, size/density ratio, and fluid properties [8]. Some investigators [7,15] assumed that for a specific binary, the inversion velocity did not depend on the overall compositions of the two species. However, Moritomi et al. [10] experimentally found that the layer inversion can be achieved by not only varying liquid velocity but also changing proportions of a binary mixture. These observations have made a clear picture of layer inversion for later investigators [9,11].

More than 20 models have been proposed in the literature to predict the layer inversion phenomenon in liquid-solid fluidized beds (for example, [9,11,12,16–18]). Escudié et al. [8] compared these models using available experimental data, and classified the models into five distinct groups based on mechanisms and approaches adopted. It was found that there were uncertainties in their comparisons because in some experimental cases the temperature had not been reported or specified exactly. Nonetheless, the best model could calculate the inversion phenomenon properties within ±14% error. Some studies provided some data in large liquid fluidized bed (210 mm semi-cylindrical

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column [19] and 190 mm cylindrical column [20]). Layer inversion phenomenon in three-phase gas-liquid-solid fluidized beds was also studied experimentally by Rim et al. [21,22].

Despite a large number of experimental investigations on layer inversion in two-phase solid-liquid fluidized beds, only a few researchers have put their efforts to study this phenomenon numerically. Generally speaking, there are two approaches to model liquid fluidized beds: continuum approach (e.g. so called Eulerian-Eulerian approach or two-fluid model [14,23,24]) and discrete approach (e.g. so called Lagrangian-Eulerian or discrete element method [6,20,25–27]). Particularly, as discrete approach such as CFD-DEM can provide some fundamental concepts of the flow at a particle scale, it has been verified as one of the most effective approaches to study fundamental behaviour of particle-fluid flow systems [28,29]. Such an approach has been used by some investigators to study layer inversion phenomenon (for example, [6,20,25–27]).

Mukherjee and Mishra [25] combined DEM approach with a simplified fluid model to investigate the layer inversion, but they just qualitatively observed this phenomenon. Zhou and Yu [26] used the combined CFD-DEM approach and reproduced the layer inversion behaviour, but they applied a method to adapt the monodisperse [30] drag force model for the binary mixtures. Di Renzo et al. [6] utilized a new drag force model which was developed for polydisperse systems [31], and found that the comparison between experimental data from literature and their simulation results were satisfactory. Experimental and numerical studies were also conducted by Vivacqua et al. [20] to analyze the factors such as temperature and bed aspect ratio on layer inversion in liquid fluidized beds. The simulated results were in a reasonable agreement with experimental measurements.

Even though substantial studies conducted, limited efforts have been made to explain the segregation mechanisms behind this peculiar phenomenon. Therefore, there is a need to elucidate the fundamentals for the occurrence of layer inversion. In principle, the motion of particles is governed by forces acting on them, including particle-particle, particle-wall, and particle-fluid interaction forces [28,29]. Thus, the layer inversion must be controlled by these interactions, and quantifying these interaction forces is crucial to reveal the segregation mechanism. Unfortunately, these interaction forces are difficult to measure experimentally. This difficulty, however, can be overcome by the CFD-DEM. Therefore, the aim of this paper is to use this approach to address what causes layer inversion in the two-phase solid-liquid fluidized beds and provide an explanation. Different drag models are also compared to examine their applicability in generating layer inversion phenomenon. In addition, parametric studies are conducted to figure out the impacts of particle and liquid properties on the inversion velocity. Finally, a mathematical model based on the force balance criterion is proposed to predict the inversion velocity.

2. Model description

The combined CFD-DEM has been well developed and documented in the literature (for example, [32–34]). Here, it is extended to liquid fluidizations with some modifications in the calculation of particle-fluid interaction force. For convenience, the model is briefly described below.

2.1. Governing equations for particle phase

Particles in particle-fluid flow systems generally have two motions: translational and rotational. According to Newton's second law of motion, the governing equations are given by:

$$\frac{m_i d\boldsymbol{v}_i}{dt} = \sum_j \left(\mathbf{f}_{e,ij} + \mathbf{f}_{d,ij}\right) + \mathbf{f}_{pf,i} + m_i\boldsymbol{g} \tag{1}$$

and

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_j \left(\mathbf{T}_{t,ij} + \mathbf{T}_{r,ij}\right) \tag{2}$$

where m_i is the mass of particle i, $\boldsymbol{v}_i$ and $\boldsymbol{\omega}_i$ are the translational and angular velocities of particle i, I_i is the moment of inertia of particle i, $\mathbf{f}_{e,\ ij}$ and $\mathbf{f}_{d,\ ij}$ are the elastic contact force and damping force, respectively, $\mathbf{f}_{pf,\ i}$is the interaction force between particle and fluid, and $m_i\boldsymbol{g}$ is the gravitational force. The torque acting on the particle i by particle j includes two components: $\mathbf{T}_{t,\ ij}$which is generated by tangential force and causes particle i to rotate, and $\mathbf{T}_{r,\ ij}$ commonly known as the rolling friction torque. The required equations to calculate these forces have been well established and can be found elsewhere [28]. Table 1 lists the equations used to calculate the particle-particle, particle-wall, and particle-fluid interaction forces and torques.

Note that the particle-fluid interaction force consists of many types of forces, including drag force, pressure gradient force, virtual mass force, Basset force, Saffman force, and Magnus force [28]. According to Di Renzo et al. [35], the drag force and the pressure gradient force are two dominant forces, and other types of particle-fluid interaction forces can be ignored in the CFD-DEM simulations of liquid fluidizations. Further efforts are required to justify the importance of other forces such as lubricant force in liquid fluidization. But in this work, only the drag force and the pressure gradient force are considered and included in the present CFD-DEM model.

Drag force can be calculated by different drag models (for example see [14,30,36–38]). Note that the drag models developed for monosized particles should not be employed for multi-sized systems. Therefore, some investigators attempted to propose new correlations for multicomponent systems (for example, [26,31,39–41]). In this work, Rong et al.'s drag model [41] is applied, but the applicability of other

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

Forces or torques	Equations
Normal elastic force, $\mathbf{f}_{en,\ ij}$	$-(\frac{4}{3})E^*\sqrt{R^*}\delta_n^{3/2}\mathbf{n}$
Normal damping force, $\mathbf{f}_{dn,\ ij}$	$-c_n(6m_{ij}E^*\sqrt{R^*\delta_n})^{\frac{1}{2}}\mathbf{v}_{n,ij}$
Tangential elastic force, $\mathbf{f}_{et,\ ij}$	$-\mu_s\lvert\mathbf{f}_{cn,\ ij}\rvert[1-(1-\min\{\lvert\delta_{t,\ ij}\rvert,\delta_{t,\ ij,\ \max}\}/\delta_{t,\ ij,\ \max})^{3/2}]\boldsymbol{\delta}_t$
Tangential damping force, $\mathbf{f}_{dt,\ ij}$	$-\gamma_t(6\mu_s m_{ij}\lvert\mathbf{f}_{cn,ij}\rvert\sqrt{1-\delta_{t,ij}/\delta_{t,ij,\ \max}}/\delta_{t,ij,\ \max})^{1/2}\mathbf{v}_{t,ij}(\delta_{t,ij}/\delta_{t,ij,\ \max})$
Coulomb friction force, $\mathbf{f}_{t,\ ij}$	$-\mu_s\lvert\mathbf{f}_{en,\ ij}\rvert\boldsymbol{\delta}_t$
Torque by tangential forces, $\mathbf{T}_{t,\ ij}$	$\boldsymbol{R_{ij}}\times(\mathbf{f}_{et,\ ij}+\mathbf{f}_{dt,\ ij})$
Rolling friction torque, $\mathbf{T}_{r,\ ij}$	$\mu_{r,\ ij}\lvert\mathbf{f}_{en,\ ij}\rvert\boldsymbol{\omega}_{ij}^n$
Drag force, $\mathbf{f}_{d,\ i}$	Rong et al.'s model [36] (see Table 2)
Pressure gradient force, $\mathbf{f}_{pg,\ i}$	$-V_i\nabla p$

where $\frac{1}{m_{ij}}=\frac{1}{m_i}+\frac{1}{m_j}$, $\frac{1}{R^*}=\frac{1}{R_i}+\frac{1}{R_j}$, $E^*=\frac{E}{2(1-\nu^2)}$, $\mathbf{n}=\frac{\boldsymbol{R}_i}{\lvert\boldsymbol{R}_i\rvert}$, $\boldsymbol{\omega}_{ij}^n=\frac{\boldsymbol{\omega}_{ij}^n}{\lvert\boldsymbol{\omega}_{ij}^n\rvert}$, $\boldsymbol{\delta}_t=\frac{\delta_t}{\lvert\boldsymbol{\delta}_t\rvert}$,$\boldsymbol{\delta}_{t,ij,\ \max}=\mu_s\frac{2-\nu}{2(1-\nu)}\boldsymbol{\delta}_n$, $R_{ij}=\frac{R_i(r_i-r_j)}{R_i+R_j}$, $\boldsymbol{v}_{n,\ ij}=(\boldsymbol{v}_{ij}.\ \mathbf{n}).\mathbf{n}$, $\boldsymbol{v}_{t,\ ij}=v_{ij}-\boldsymbol{v}_{n,\ ij}$. Note that the tangential force $(\mathbf{f}_{ct,\ ij}+\mathbf{f}_{dt,\ ij})$ should be replaced by $\mathbf{f}_{t,\ ij}$when $\delta_t\geq\delta_{t,\ \max}$.