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DEM-CFD simulations of layer inversion in two-component liquid fluidized beds

F. Cello, A. Di Renzo, F.P. Di Maio
Dipartimento di Ingegneria Chimica e dei Materiali, Università della Calabria
Via Pietro Bucci - Cubo 44A – 87036 Rende (CS), Italy

The inversion phenomenon occurring in liquid-fluidized beds composed of a small but heavier and a large but lighter species has attracted a considerable attention in the scientific literature on fluidization. In particular, a model able to predict its characteristics (i.e. the velocity and voidage at inversion) was sought by a number of researchers with a variable success. However, considerable uncertainties are still present on the true interplay between fluid drag and gravity on the fluidized species. The goal of this work is to simulate the detailed hydrodynamics in such systems by means of an *in-house* developed code based on the DEM-CFD method (Discrete Element Method, DEM, combined with Computational Fluid Dynamics, CFD). As it can be expected, the role of the drag force model adopted is crucial. For this reason, a recently proposed model valid for bi-disperse systems is utilized and tested. A suitable set of experiments on a glass-hollow char binary mixture fluidized by water was selected from the literature. The simulated voidage and particle species concentration profiles at steady state were analyzed and compared against measurements. The model predictions prove the effectiveness of the approach in reproducing the actual system behavior, with the voidage values at different velocities in very good agreement and the inversion velocity in good agreement with experiments.

1. Introduction

In binary beds fluidized with a liquid when a solid species is larger and less dense than the other one, an interesting phenomenon called “layer inversion” can appear. At low liquid velocities gravity exceeds the drag force and buoyancy and, thus, the small but heavy particles will reside in the bottom of the column. At the same time, the larger, less dense particles occupy the top of the bed and form a layer above a mixed one where both phases are present. A progressive increase in liquid velocity causes the layers to invert: the drag force and buoyancy dominate over gravity and the smaller particles will occupy the top section. At the “inversion velocity”, the two phases are completely mixed. This phenomenon was first examined experimentally by Moritomi et al. (1982), who observed that it could be induced by varying the liquid velocity, or by varying the solids composition of the system at fixed velocities.
Several studies have been carried out about this phenomenon, mostly using an experimental approach to determine macroscopic parameters (Gibilaro, 1986, Moritomi,

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1986), although some purely analytical work has been presented based on force balance methods (Funamizu and Takakuwa 1995). These models use the bulk properties and provide good estimates of the critical velocity, but are insufficient in predicting the voidage at inversion point.

In recent years, computational models have provided considerable improvements in characterizing the transient behaviors of these systems. Some simulations of inversion phenomenon using continuum two-fluid models have been reported in literature (Syamlal and O'Brien, 1988, Howley and Glasser, 2002). However the Eulerian/Eulerian methods require a difficult formulation of constitutive equations (e.g. particle–particle drag) which may affect the simulation accuracy.

In this work, the layer-inversion phenomenon in liquid fluidized beds is studied by using the DEM-CFD method, which proved particularly promising (Di Renzo and Di Maio, 2007): the fluid flow is obtained by solving the locally-averaged continuity and Navier-Stokes equations (CFD), while the motion of individual particles is studied by means of the Discrete Elements Method (DEM). This method presents the advantage of the capability to model precisely the fluid properties and the particle sizes and densities. Only one study using a discrete-particle approach is reported in the literature by Malone et al. (2007), but bed voidages and the segregation patterns differ from experimental studies.

The predictions of the inversion velocity are sensitive to the binary system composition and to the liquid viscosity and consequently depend on the exact bed temperature (Escudié et al. 2006); this introduces a significant uncertainty because this parameter was not specified in most of the experimental studies.

To obtain accurate and detailed DEM-CFD simulations, the closure term describing the momentum exchange between the fluid and the particles is of crucial importance. For this reason, a recently proposed model (Di Maio et al., 2008) with significant advantages over previous formulations is used. DEM-CFD simulations are carried out on a liquid-fluidized binary bed to validate the drag formulation and characterize the phenomenon.

2. The drag force model for bidisperse suspension

In DEM-CFD simulations the solid and fluid phase are solved sequentially. The fluid flow field is typically calculated on a computational cell scale that is of the order of a few particle diameters wide, the local flow around and in the interstices among the particles being taken into account only by means of a drag force model. The solid phase motion is evaluated at the particle scale in a Langrangian framework, i.e. the equation of Newton is solved for each particle:

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{c=1}^{N_c} \mathbf{F}_{c,i} + \mathbf{F}_{g,i} + \mathbf{F}_{d,i} \tag{1}$$

In eq. (1) m_i and v_i are the i-th particle mass and velocity; $\mathbf{F}_{g,i}$ takes into account gravity and buoyancy; $\mathbf{F}_{c,i}$ is the resultant of forces arising from the N_c contacts; $\mathbf{F}_{d,i}$ is the drag exerted from the fluid, witch depends on the voidage ε, the Reynolds number and the polydispersion index of the suspension y_i.

Typically a dimensionless modulus of the drag force is usually defined as the ratio of the actual value to that in the Stokes' regime:

$$F(\varepsilon, Re, y_i) = \frac{\left|\mathbf{F}_{d,i}(\varepsilon, Re, y_i)\right|}{\left|\mathbf{F}_{st,i}(1, Re, 1)\right|} \tag{2}$$

Recently, a model for the drag calculation was proposed by Di Maio et al. (2008) to improve the simulations accuracy. For monodisperse systems it reads:

$$\begin{cases} F_{mono}(\varepsilon, Re, 1) = 1 + K_1 \cdot K_3 + K_2 \cdot (1 - 0.44 K_1) \\ \phi = 1 - \varepsilon;\ K_1 = \dfrac{2.5\phi}{1 + 1.5\phi};\ K_2 = \dfrac{1 + 0.13Re + 6.66 \cdot 10^{-4} Re^2}{1 + 3.42 \cdot 10^{-2} Re + 6.92 \cdot 10^{-6} Re^2} - 1 \\ K_3 = \dfrac{387\phi - 964\phi^7 + 0.433 \cdot (1 + 10\phi) \cdot Re + 9.09 \cdot 10^{-5} \cdot Re^2}{1 + \phi \cdot (70 - 81.1 \cdot K_1) + 4.54 \cdot 10^{-6} \cdot Re^2 - 2.87 \cdot 10^{-9} \cdot Re^3} \end{cases} \tag{3}$$

While for polydisperse systems the following formulation holds:

$$\begin{cases} F_i(\varepsilon, Re, y_i) = f_i(\varepsilon, y_i) \cdot \langle F \rangle (\varepsilon, \langle Re \rangle) \\ \langle F \rangle = F_{mono}(\varepsilon, \langle Re \rangle, 1),\ \langle Re \rangle = \dfrac{\rho\, u \langle d_p \rangle}{\mu}, \langle d_p \rangle = \left(\sum_{i=1}^{N_{sp}} \dfrac{x_i}{d_{p,i}} \right)^{-1} \\ f_i(\varepsilon, y_i) = \varepsilon \cdot y_i + (1 - \varepsilon) \cdot y_i^2 + C_i(\varepsilon, y_1, y_2, \cdots, y_{Nsp}),\ y_i = \dfrac{d_{p,i}}{\langle d_p \rangle} \\ C_i(\varepsilon, y_1, y_2, \cdots, y_{Nsp}) = 0.407 \cdot \dfrac{N_{sp}^2}{\sum_j y_j \cdot \sum_j (1/y_j)} (1 - \varepsilon) \cdot (y_i^2 - y_i) \end{cases} \tag{4}$$

Where x_i is the relative volume fraction of two species and $d_{p,i}$ is the diameter of i-th solid species. It is important to remark that all properties appearing in eqs. (3)-(4) are evaluated in the vicinity of the particle considered, thus taking into account all local inhomogeneities that could develop.

3. Simulations

3.1 Simulation setup

In DEM-CFD simulations the column size, the relative volume fractions and the diameters ratio of the two particulate species heavily influence the computational burden of the calculation. For this reason, among the various systems available in literature binary IV from Moritomi et al. (1982) was selected. The bed materials used are glass beads (GB214, ρ_p=2450 kg/m^3, 100 g charged) and porous hollow char (HC775, $\rho_{p,wet}$=1500 kg/m^3, 50 g charged).

Table 1 Simulation data

x_1	d_1 [mm]	d_2 [mm]	Np_1	Np_2	ρ_1 [kg/m^3]	ρ_2 [kg/m^3]	L [mm]	H/L	N_{cell}		
									x	y	z
0.53	0.214	0.776	36138	672	2450	1500	16.8	1.25	14	55	1

u [mm/s]:	8	10	12	15	17	19
Experim. ε (Moritomi et al., 1982):	0.660	0.700	0.750	N/A	N/A	N/A
Calculated ε at steady state:	0.625	0.722	0.761	0.823	0.860	0.883

1 = fine particles, 2 = coarse particles

Table 1 shows the simulation setup data. The original experimental column diameter was 50.8 mm but to reduce the number of particles a 16.8 mm-wide bed was considered. The only other one difference is that a slim portion under 3D periodic condition was simulated, respecting the initial aspect ratio and species fractions of the experiments. The resulting depth is about two coarse particle diameters, but under periodic conditions for the particles (i.e. a particle that exits the domain re-enters it from the opposite side).

3.2 Simulation results

As is shown in Table 1 six simulations were carried out varying the fluid velocity from 8 to 19 mm/s, starting from random initial position of the particles and monitoring the resulting system voidage. Figure 1 shows snapshots of the particles position on increasing fluid velocity: black and white spheres represent coarse and fine solids, respectively.

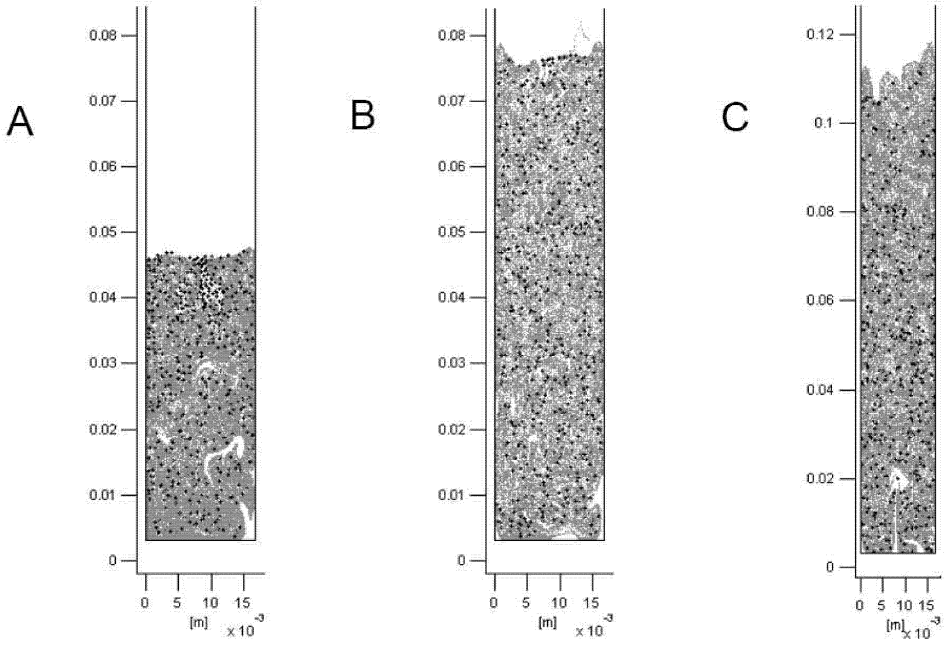

Figure 1: Snapshots of simulations at 10 mm/s after 10 s (A), at 15 mm/s after 12.7 s (B) and at 19 mm/s after 16 s (C).

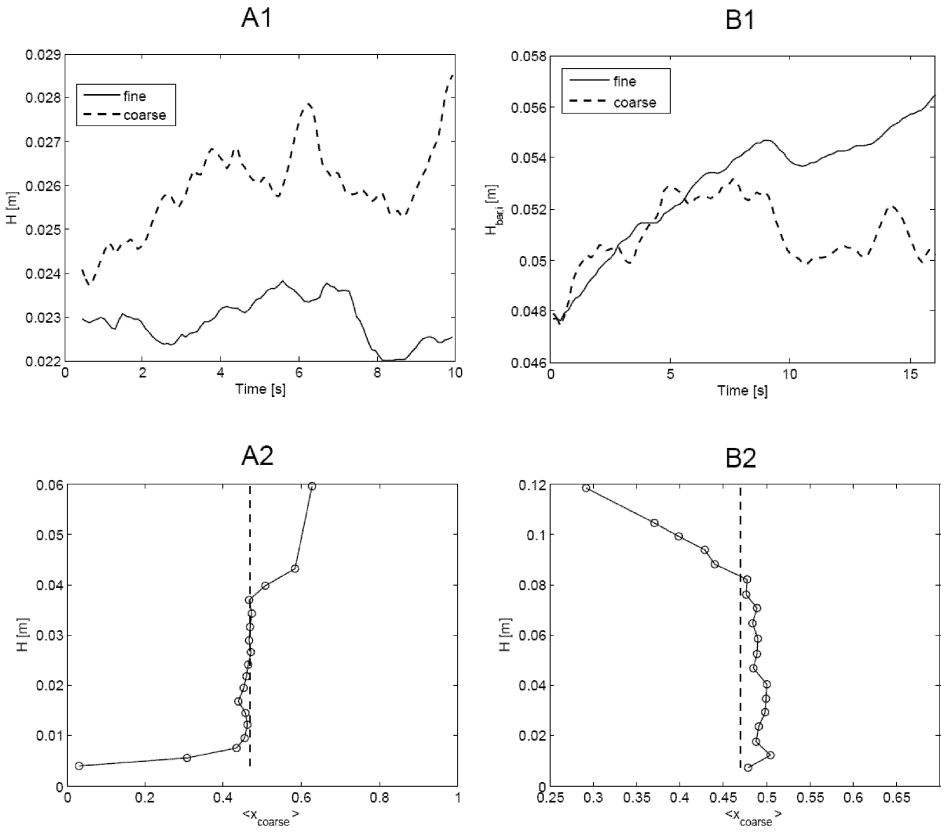

Figure 2: Evolution of the centres of mass of the two species at 10 mm/s (A1) and at 19 mm/s (B1). Variation of relative volume fraction of coarse species with height at 10 mm/s after 10 s (A2) and at 19 mm/s after 16 s (B2).

It was not possible to clearly identify the point of complete mixing because a fully steady state was not reached in the simulation time considered. It is important to remark that these simulations are very CPU-intensive, despite the size considered was reduced compared to the experiments. As an indication, one day of CPU clock time is required to run about 1.5 seconds of simulation.

A simple visual observation of simulations (Figure 1) suggests that the system is mixed at 15 mm/s, while only at 19 mm/s fine particles segregate on top of the column. However, a quantitative analysis is necessary to determine the real system conditions at 12 mm/s. Figure 2 shows the time evolution of the center of mass heights (A1-B1) for the two solid species and the axial concentration profile of the coarse particles (A2-B2). This analysis reveals that at 10 mm/s the coarse particles preferentially reside to the top of the column, something that was not evident in Figure 1. Coupling quantitative and qualitative analysis, it is reasonable to conclude that the simulated system exhibits inversion at 15 mm/s. The experimental inversion velocity is 12 mm/s with $\varepsilon = 0.750$. While the velocity appears only reasonably estimated by the simulations, it shall be remarked that the bed expansion is effectively and quantitatively captured (see Table 1).

A number of factors need be analyzed to further investigate the difference in the velocity. The uncertainty on the real experimental temperature (that in the simulations was assumed 20 °C) is one important aspect (Escudié et al., 2006). The particles size distribution may also have a role and it shall be remarked that fully developed steady state was not reached in the simulations. The inversion phenomenon was qualitatively well reproduced, but further work is needed to check the validity of the entire model. Longer simulations as well as tests on other data from the literature are in progress.

4. Conclusions

An appropriate binary mixture of particles with different diameter and density fluidized by water was selected from the literature to investigate by simulation the inversion phenomenon. Several DEM-CFD simulations with a new drag model were performed at fixed mixture compositions to predict the behavior of this system, for which several fluid velocities below and above the inversion point were considered. From the simulation results, the predicted inversion velocity was overestimated, whilst the voidage, at inversion point, was in good agreement with experimental data.

References

Di Renzo A. and Di Maio F. P., 2007. Homogeneous and bubbling fluidization regimes in DEM-CFD simulations: hydrodynamic stability of gas and liquid fluidized beds. Chem. Eng. Sci. 62, 1-2, 116-130.

Di Maio F. P. , Di Renzo A. and Cello F. , 2008. A new drag force model for detailed simulations of fluid-particle systems. MFIP2008 - 11th International Conference on Multiphase Flow in Industrial Plant, 243-250.

Gibilaro L.G., Di Felice R., Waldram S.P. and Foscolo P.U., 1986. A predictive model for the equilibrium composition and inversion of binary-solid liquid fluidized beds. Chem. Eng. Sci. 41, 379-387.

Escudié R., Epstein N., Grace J.R. and Bi H.T., 2006. Layer inversion phenomenon in binary-solid liquid-fluidized beds: Prediction of the inversion velocity. Chem. Eng. Sci. 61, 6667-6690.

Funamizu N., Takakuwa T., 1995. An improved Richardson–Zaki formula for computing mixed layer composition in binary solid–liquid fluidized beds. Chem. Eng. Sci. 50, 3025-3032.

Howley M.A. and Glasser B. J., 2002. Hydrodynamics of a uniform liquid-fluidized bed containing a binary mixture of particles. Chem. Eng. Sci. 57, 4209-4226.

Malone K.F., Xu B.H. and Fairweather M., 2007. Numerical investigation of the layer-inversion phenomenon in binary solid liquid fluidized beds. Fluidization XII, 295-304. ECI.

Moritomi H., Iwase T. and Chiba T., 1982. A comprehensive interpretation of solid layer inversion in liquid fluidised beds. Chem. Eng. Sci. 37 (12), 1751-1757.

Moritomi H., Yamagishi T. and Chiba T., 1986. Prediction of complete mixing of liquid-fluidized binary solid particles. Chem. Eng. Sci. 41, 297-305.

Syamlal M. and O'Brien T.J., 1988. Simulation of granular layer inversion in liquid fluidized beds. Int. J. of Multiphase Flow 14 (4), 473-481.