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Particle resolved direct numerical simulation of a liquid–solid fluidized bed: Comparison with experimental data

A. Ozel[a,e], J.C. Brändle de Motta[a], M. Abbas[b,*], P. Fede[a], O. Masbernat[b], S. Vincent[c,d], J.-L. Estivalezes[a], O. Simonin[a]

[a] Institut de Mécanique des Fluides de Toulouse (IMFT), Université de Toulouse, CNRS, INPT, UPS, Toulouse, France
[b] Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INPT, UPS, Toulouse, France
[c] Université Paris-Est Marne-La-Vallée, UMR 8208, Laboratoire de Modélisation et Simulation Multi Echelle (MSME), Marne-La-Valle F-77454, France
[d] Université de Bordeaux, Institut Polytechnique de Bordeaux (IPB), Institut de Mécanique et Ingénierie (I2M), Bordeaux F-33000, France
[e] FERMaT, Université de Toulouse, CNRS, INPT, INSA, UPS, Toulouse, France

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ABSTRACT

Particle-resolved direct numerical simulations of a 3-D liquid–solid fluidized bed experimentally investigated by Aguilar-Corona (2008) have been performed at different fluidization velocities (corresponding to a range of bed solid volume fraction between 0.1 and 0.4), using Implicit Tensorial Penalty Method. Particle Reynolds number and Stokes number are $O(100)$ and $O(10)$, respectively. In this paper, we compare the statistical quantities computed from numerical results with the experimental data obtained with 3-D trajectography and High Frequency PIV. Fluidization law predicted by the numerical simulations is in very good agreement with the experimental curve and the main features of trajectories and Lagrangian velocity signal of the particles are well reproduced by the simulations. The evolution of particle and flow velocity variances as a function of bed solid volume fraction is also well captured by the simulations. In particular, the numerical simulations predict the right level of anisotropy of the dispersed phase fluctuations and its independence of bed solid volume fraction. They also confirm the high value of the ratio between the fluid and the particle phase fluctuating kinetic energy. A quick analysis suggests that the fluid velocity fluctuations are mainly driven by fluid–particle wake interactions (pseudo-turbulence) whereas the particle velocity fluctuations derive essentially from the large scale flow motion (recirculation). Lagrangian autocorrelation function of particle fluctuating velocity exhibits large-scale oscillations, which are not observed in the corresponding experimental curves, a difference probably due to a statistical averaging effect. Evolution as a function of the bed solid volume fraction and the collision frequency based upon transverse component of particle kinetic energy correctly matches the experimental trend and is well fitted by a theoretical expression derived from Kinetic Theory of Granular Flows.

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1. Introduction

Liquid fluidization is used in various industrial application involving biochemical, catalytic reactions and crystallization processes. The flow in a liquid fluidized bed lies within an intermediate regime between the settling of particles controlled by the hydrodynamic interactions and the rapid granular flow controlled by the collisions between particles, where the particle Reynolds number is in a range of $O(100)$ and the particle Stokes number is in a range of $O(10)$, both based on particle settling velocity. In this sense, liquid fluidization is a challenging problem for two-phase modeling. For practical applications, two-phase continuum models are generally used to carry out numerical simulations, based upon two-fluid or statistical models (Gevrin et al., 2008; Zhang et al., 2013). However, modeling of liquid–solid fluidization is still an open research topic and multi-scale modeling developments are still needed to correctly predict inter-particle and particle–fluid interactions. One major issue is to predict the right level of particulate and carrying flow phase fluctuations as a function of bed solid phase fraction (or fluidization velocity).

Resolved particle direct numerical simulations of particulate flows have been developing last two decades (see the review of Tenetti and Subramanian, 2014). These simulations can provide the particulate phase fluctuation characteristics in order to develop appropriate two-phase continuum models. Many of particle resolved simulations have been carried out on fixed structured grids to take

* Corresponding author.
E-mail address: micheline.abbas@ensiacet.fr (M. Abbas).

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advantage of parallelization and avoid the complexity of mesh reconstruction.

Pan et al. (2002) carried out resolved simulations of fluidization of 1204 finite size spheres in a 2-D bed using the method of distributed Lagrange multipliers and as simulation results, the fluidization velocity versus fluid fraction was found to be a power law which exponent well compared with that predicted by the correlation of Richardson and Zaki (1954). Zhang et al. (2006) performed a 3-D fully resolved simulation of 1024 particles settling under gravity in a periodic domain accounting for elastic collisions of particles. Their method is based on a linearization of Navier–Stokes equations in the vicinity of particle interface (Zhang and Prosperetti, 2005). In their study, Particle Reynolds number was $O(10-50)$ and the solid volume fraction equal to 10%. They have shown that the settling velocity was matching (Richardson and Zaki, 1954) correlation and evidenced the relation between the velocity fluctuations and particles micro-structuration. Bagchi and Balachandar (2003), Burton and Eaton (2005) and then Vreman (2016) used body-fitted methods to study turbulent homogeneous isotropic turbulence (steady or decaying in time) in the presence of fixed spheres of finite size compared to the smallest turbulent length scale.

Using a Lattice Boltzmann Method to solve the interstitial flow and an equation of motion accounting for lubrication and collisions between particles, Derksen and Sundaresan (2007) have simulated in limited size domains the propagation of concentration waves in liquid–solid fluidized beds with large bed solid fraction (close to maximum packing) and particle Reynolds number of order of $O(10)$. Their results were in qualitative agreement with an experimental study of Duru and Guazzelli (2002). Based on the same method, Derksen (2014) performed the simulation of the mixing of a passive scalar in a fluidized bed with periodical boundaries in a wide range of bed solid volume fraction (0.2–0.5) and particle Reynolds numbers of order 10. Derksen's results first show a good agreement with Richardson and Zaki (1954) exponent dependence with Reynolds number. Interestingly, Derksen (2014) showed that the diffusion of the passive scalar in the bed is similar to the auto-diffusion of particles, scaling of which is close to what was experimentally observed in sedimentation by Nicolai et al. (1995).

Uhlmann (2005) developed an Immersed Boundary Method to simulate the sedimentation of 1000 spherical finite particles at high Reynolds number (400) and highly dilute limit, but no quantitative comparison with existing data was provided. More recently, Uhlmann and Dušek (2014) evaluated the accuracy of their method as a function of the spatial resolution (number of meshes per particle diameter) for the case of a single sphere settling in an infinite stagnant fluid, in a wide range of Reynolds and Archimedes (or Galileo) numbers. The higher the latter number, the higher spatial resolution is required, up to 48 mesh points per particle diameter at high Galileo number. Then Chouippe and Uhlmann (2015) and Fornari et al. (2016) used this method to study particle settling in turbulent flow conditions.

Corre et al. (2010) used a fictitious domain approach to perform particle-resolved simulations of the liquid-fluidized bed experimentally studied by Aguilar-Corona (2008). Instantaneous and averaged flow characteristics of the fluidized bed were qualitatively in good agreement with experimental trends. Since then, this method was improved and has been applied in the present study with a higher level of accuracy (Vincent et al., 2014). The numerical technique is a four-way coupling method, based on a one-fluid formulation of the incompressible Navier–Stokes equations solved on a structured Cartesian grid. The resolved-scale particles are modeled by an Implicit Tensorial Penalty Fictitious Domain Method (ITPM). They are tracked by using a hybrid Eulerian–Lagrangian Volume of Fluid approach, which accounts for collisions and lubrication effects.

Table 1
Phase properties and fluidization parameters.

Liquid phase	ρ_f	1400 kg/m^3
	μ_f	3.8×10^{-3} Pa s
Fluidization velocity	U_F	0.17/0.15/0.12/0.09/0.073 m/s
Particles	ρ_p	2230 kg/m^3
	d_p	6×10^{-3} m
	V_t	0.24 m/s
	Re_t	530
	St_t	5.3
Fluidization law	$U_{F0}(1-\phi_b)^n$	$n = 2.41,\ U_{F0} = 0.226$ m/s

This study has two scopes. The first one is to evaluate the effective ability of ITPM to predict two-phase flow behavior by performing particle resolved simulations of a liquid–solid fluidized bed involving finite size particles, with large particle Reynolds and moderate Stokes numbers. The second one is to analyze velocity fluctuations of both phases in this regime. The bed geometry, particle size and number and flow parameters used in these simulations are the same as in Aguilar's experiments, allowing a direct quantitative comparison between experiments and numerical data.

The paper is structured as follows: flow parameters and numerical model (detailed in other references) are briefly presented in Sections 2 and 3, respectively. Statistical quantities (as defined in Appendix A) computed from the numerical results are compared with experimental data obtained by Aguilar Corona with same flow parameters and geometry. Fluidization law and particle velocity fluctuations predicted by the simulations are also compared in Section 4.

2. Flow parameters

Flow parameters chosen for the simulation of the fluidized bed are taken from the experimental study of Aguilar-Corona (2008) in a cylindrical column of 8 cm inner diameter. Phase material properties and fluidization parameters are reported in Table 1. Monodisperse spherical beads of Pyrex ($d_p = 6$ mm, $\rho_p = 2230$ kg/m^3) have been fluidized in a concentrated aqueous solution (65% w/w) of potassium thiocyanate (KSCN) of density $\rho_f = 1400$ kg/m^3 and viscosity $\mu_f = 3.8 \times 10^{-3}$ Pa s at $T = 20\,^\circ$C. At this temperature, refractive indices of both phases are matched, allowing the implementation of optical techniques such as high-speed video for the 3-D Lagrangian tracking of colored particles or high frequency Particle Image Velocimetry for the measurement of the velocity field in the liquid phase (Aguilar-Corona, 2008). Particle terminal velocity, V_t, is 0.24 m/s and Reynolds number based on V_t is $Re_t = 530$. Inertia of the particles is characterized by a Stokes number here defined as $St_t = \frac{8\rho_p}{3\rho_f C_{Dt}} = 5.3$ (C_{Dt} is the drag coefficient of a single particle at V_t, here equal to 0.8). Fluidization law and fluctuating motion of both phases have been measured by Aguilar-Corona (2008) in a range of fluidization velocities ranging between 0.17 and 0.05 m/s, corresponding respectively to be solid volume fraction ranging between 0.1 and 0.5. Details of the measurement techniques can be found in Aguilar-Corona (2008).

3. Numerical model

Details of numerical approach and validation test cases are given in Vincent et al. (2014). The DNS approach is based on a one-fluid formalism of the incompressible Navier–Stokes equations with an algebraic adaptive augmented Lagrangian method used for pressure-velocity coupling (Implicit Tensorial Penalty Method, ITPM). The particles are considered as a fluid with specific rheological properties whose evolutions are modeled by the Navier–Stokes equations. This method enforces the solid behavior of the parti-

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