Fully Resolved Direct Numerical Simulation of a Liquid Fluidized Bed

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Fully Resolved Direct Numerical Simulation of a Liquid Fluidized Bed


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Keywords: finite size particle DNS, liquid-solid fluidized bed, fictitious domain method, sub-grid lubrication, augmented Lagrangian method

Abstract

We present some results issued from the fully resolved direct numerical simulations of a 3-D liquid-solid fluidized bed, experimentally investigated by Aguilar Corona (2008). In these simulations, the flow is solved by a one-fluid formulation of the incompressible Navier-Stokes equations, where the pressure-velocity coupling is provided by an algebraic augmented Lagrangian method and particles presence is modeled by an implicit penalty fictitious domain method, a sub-grid scale lubrication force and soft-sphere collision model. The simulated fluidized bed is a 8 cm diameter, 64 cm height cylindrical column containing 2133 6 mm glass particles fluidized by a low viscosity liquid (3.8x10⁻³ Pa.s). Particle Reynolds and Stokes number based on terminal velocity are 530 and 7.7 respectively. Simulation results show that homogeneous fluidization regime is obtained for all fluidization velocities investigated, and exhibit large-scale coherent structures in the particle motion. Main features of the Lagrangian velocity signal of the particles are well reproduced by the simulations. Predicted fluidization law nicely fits the experimental curve. Despite the limited time of simulation runs, particle velocity variance is also well predicted as well as the value of the anisotropy coefficient, which is found to be independent of bed concentration. The fluid velocity variance is larger than that of the particles at all bed concentration investigated, following the same trend as Aguilar Corona’s data (2008).

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( U_F )</td>
<td>Fluidization velocity (m/s)</td>
</tr>
<tr>
<td>( U_{fr} )</td>
<td>Terminal velocity of particle (m/s)</td>
</tr>
<tr>
<td>( V_f )</td>
<td>Measured terminal velocity (m/s)</td>
</tr>
<tr>
<td>( \text{Re}_f )</td>
<td>Particle Reynolds number</td>
</tr>
<tr>
<td>( \text{St}_f )</td>
<td>Particle Stokes number</td>
</tr>
<tr>
<td>( C_{Dr} )</td>
<td>Drag coefficient</td>
</tr>
<tr>
<td>( \rho_f )</td>
<td>Fluid density (kg/m³)</td>
</tr>
<tr>
<td>( \mu_f )</td>
<td>Fluid viscosity (Pa.s)</td>
</tr>
<tr>
<td>( \rho_p )</td>
<td>Particle density (kg/m³)</td>
</tr>
<tr>
<td>( d_p )</td>
<td>Particle diameter (m)</td>
</tr>
<tr>
<td>( \chi_p )</td>
<td>Particle indicator function</td>
</tr>
<tr>
<td>(&lt;\alpha_p&gt;_{b})</td>
<td>Bed solid concentration</td>
</tr>
</tbody>
</table>

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. For practical applications, two-phase continuum models are generally used to carry out numerical simulations. However, two-phase continuum modeling of liquid-solid fluidization is still an open research topic and particular developments are needed to correctly represent the particle-particle and particle-fluid interactions. One major issue is to predict the right level of particulate phase fluctuations as a function of solid phase fraction (or fluidization velocity) in the bed.

Fully resolved direct numerical simulation (DNS) of particulate flows has been developing last two decades. These simulations can provide the particulate phase fluctuations characteristics in a liquid-solid fluidized bed in order to develop appropriate two-phase continuum models. Many of these simulations have been carried out on fixed structured grids to take advantage of parallelization and avoid the complexity of mesh reconstruction. Pan et al. (2002) carried out DNS of the fluidization of 1204 finite
size spheres in 2-D bed using the method of distributed Lagrange multipliers and as simulation results, the fluidization velocity versus fluid fraction is found to be a power law which exponent well compares with that predicted by the correlation of Richardson and Zaki (1954). Zhang et al. (2006) performed a fully resolved DNS of 1024 particles settling under gravity in a periodic domain accounting for elastic collisions of particles and they showed that the mean settling velocity and velocity fluctuations were affected by the formation of particle pairs. Uhllmann (2005) simulated the sedimentation of 1000 spherical finite particles and the accuracy of the method was demonstrated by comparison of the results with reference values from experiments and numerical simulations. Corre et al. (2010) first used a fictitious domain approach to perform DNS of the liquid-fluidized bed experimentally studied by Aguilar Corona (2008). Instantaneous and average 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. 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 Penalty Fictitious Domain Method. They are tracked by using a hybrid Eulerian-Lagrangian Volume of Fluid approach which accounts for collisions and lubrication effects.

The aim of the this study is to accurately predict the particulate phase fluctuations by performing direct numerical simulations of a liquid-solid fluidized bed involving finite size particles, with large particle Reynolds and moderate Stokes numbers. The bed geometry, particle size and number and flow parameters used in these simulations are the same as in Aguilar’s experiments, allowing a quantitative comparison between experiments and numerical data. In this article, we first show that homogeneous fluidization of particles is obtained for all fluidization velocities tested. Fluidization law and particle velocity fluctuations predicted by the simulations are then compared to experimental data obtained by Aguilar-Corona (2008).

Flow Configuration

The fluidized bed chosen for the simulations is taken from the experiments of Aguilar-Corona (2008). The experiment technique is based on a 3-D particle tracking in a matched refractive index medium. 2133 Pyrex particles with a diameter of 0.006 m are fluidized by the circulation of a concentrated potassium thiocyanate (KSCN) solution in a glass cylinder of 0.64 m height and 0.08 m diameter at various fluidization velocities. The density of Pyrex is \( \rho_f = 2230 \text{ kg/m}^3 \), the density \( \rho_p \) and the dynamic viscosity \( \mu_f \) of the liquid phase are 1400 kg/m\(^3\) and 3.8\times10\(^3\) Pa.s, respectively. The particle Reynolds number \( Re_p = d_p \rho_p \mu_f U_f \) is equal to 530 and the Stokes number based on the terminal velocity \( V_t \) is 7.7. Terminal velocity of a single particle \( V_t \) was measured by trajectory in the same geometry and was found equal to 0.24 m/s. Stokes number is defined as:

\[
St = \frac{\rho_p}{\rho_f} \frac{8}{3C_{Df}}
\]

where \( C_{Df} \) is the drag coefficient given by Schiller and Naumann (1935). Fluidization law determined by Aguilar Corona (2008) is well described by the Richardson and Zaki’s correlation which reads:

\[
U_f = U_{i0}(1-\alpha_f)^n
\]

where \( n \) is a function of \( Re_p \), \( U_f = \frac{U_f}{U_{i0}} \) is the fluidized velocity, \( \alpha_f \) is the bed-averaged solid concentration, and \( U_{i0} \) is the fluidization velocity leading to particles entrainment. Experimental value of \( U_{i0} \) was found equal to 0.22 m/s, close to the terminal velocity \( V_t \). Main findings of Aguilar Corona (2008) for the fluidization of the 6 mm particles can be summarized as follows:

1. Fluidization is homogeneous with unsteady large-scale recirculation patterns whose size is around the column diameter. Fluidization law is well fitted by Richardson-Zaki correlation.
2. Bed-averaged velocity fluctuations are decreasing with increasing bed global concentration in particles. They also are significantly anisotropic and the anisotropy coefficient is found independent of the fluidization velocity (bed concentration).
3. At all fluidization velocities (bed concentration), fluctuating kinetic energy of the carrier fluid \( E_f \) is larger than that of particles \( E_p \), and the ratio \( E_f/E_p \) increases as the particle concentration in the bed increases.

Physical properties of the phases and the fluidization parameters of the experiments are summarized in Table 1.

<table>
<thead>
<tr>
<th>Liquid Phase</th>
<th>( \rho_f )</th>
<th>1400 kg/m(^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \mu_f )</td>
<td>3.8\times10^3 \text{ Pa.s}</td>
</tr>
<tr>
<td>Fluidiz. velocity</td>
<td>( U_f )</td>
<td>0.17/0.15/0.12/0.09/0.073 m/s</td>
</tr>
<tr>
<td>Particles</td>
<td>( \rho_p )</td>
<td>2230 kg/m(^3)</td>
</tr>
<tr>
<td></td>
<td>( d_p )</td>
<td>6 mm</td>
</tr>
<tr>
<td></td>
<td>( V_t )</td>
<td>0.24 m/s</td>
</tr>
<tr>
<td></td>
<td>( Re_p )</td>
<td>530</td>
</tr>
<tr>
<td></td>
<td>( St )</td>
<td>7.7</td>
</tr>
<tr>
<td>Fluidization law</td>
<td>( U_f = U_{i0}(1-\alpha_f)^n )</td>
<td>( n=2.41 )</td>
</tr>
<tr>
<td></td>
<td>( U_{i0} )</td>
<td>0.224 m/s</td>
</tr>
</tbody>
</table>

Table 1: Physical properties of phases and fluidization parameters of the experiments by Aguilar Corona (2008).

Mathematical Modelling

The numerical approach is based on a one-fluid formalism of the incompressible Navier Stokes equations where an Implicit Tensorial Penalty Method ensures the solid behavior in the framework of Eulerian fixed grids. An algebraic adaptive augmented Lagrangian method is used for pressure-velocity coupling. A Lagrangian Volume OF Fluid (VOF) method enables particle tracking. This approach provides a second order convergence in space and time. The soft collision model for multiple particle-particle and particle-wall interactions integrated in the Navier-Stokes equations for the disperse phase, is based upon an extrapolation of the position of the particle from
previous time step (For details of numerical approach, see Vincent et al. (2012)). Motta et al. (2011) studied the particle-particle and particle-wall collisions in a highly viscous flow at different impact velocities. Fully resolved lubrication fluid layer between a particle and a wall was obtained with an Eulerian grid highly refined at the scale of the particle (~150 grid points/particle). However, such a refinement level is not affordable for the present liquid-solid fluidized bed and a more appropriate sub-grid lubrication force model proposed by Breugem (2010) was used instead. This choice was motivated by the fact that normal restitution coefficient derived from this model, follows the scaling law of Legendre et al. (2006), as shown by Motta et al. (2011).

The computation domain exactly reproduces the experimental column. It is composed of a parallelepiped box of dimensions 0.08x0.08x0.64 m discretized with a uniform grid composed of 160x160x1280 cells. This grid resolution corresponds to 12 cells per particle diameter. The cylindrical tank is represented numerically with a Darcy penalty method (Khadra et al., 2000). The method consists in adding a Darcy term ($\mu_v u/K$) in the momentum equations and the numerical parameters used are a penalty solid viscosity 100 times larger than $\mu_f$ and $K=100$. Taking a permeability that tends towards zero in the cells located outside the cylindrical tank, the velocity is set to zero. The computational domain is shown in Figure 1. For the tensorial penalty of the particles, a reduced diameter of the spheres $d_p-\Delta x$ is considered in order to obtain a correct effective drag force exerted by the fluid on the particles (Vincent et al., 2012). The real particle shape is considered for the definition of the solid density and the treatment of the collisions between the particles. The rebound of particles on the walls of the cylindrical tank is treated as a rebound between two particles.

simulate 20 s of physical time of the flow. The particles are randomly distributed with an average solid fraction of 0.1 in the first half of the bed (0.47$h_b$) and the phase velocities were set to zero as initial conditions. A uniform distribution of fluid velocity was imposed at the bottom of the bed and a free exit boundary condition was used at the top of the bed.

Results and Discussions

Two-Phase Flow field

In figure 2, 3-D snapshots of particle distribution in the bed illustrate the transient stage of the calculation after 5, 10 and 20 seconds ($U_f=0.12$m/s). It can be seen that the bed settles down after 5 s and particle packing takes place within a steady volume. Figure 3 shows the time evolution of the maximum axial particle positions that indicates the beginning of the fluidization regime for each case. It can be seen in figure 3 that this regime is reached in all cases and is stable. Time signals of figure 3 also show that as the fluidization velocity decreases, the fluctuations level of the bed height decreases, as a result of the decrease of granular temperature in the whole bed, as further discussed.

![Figure 2: Three-dimensional views of the particles inside the bed (from left to right: initial condition, t=5, 10, 20 s).](image)

![Figure 3: Particle circulation patterns in the bed for different fluidization velocities: $U_f=0.17, 0.15, 0.12, 0.09, 0.073$ m/s.](image)
Projections of 16 particle trajectories in the radial and vertical planes of the bed have been reported in figure 4, for two different fluidization velocities. It can be seen that particle trajectories are quite sensitive to the global concentration in the bed. At high fluidization velocity (low concentration), trajectories path occupies all the bed space, with an apparent slight deficit of particle presence in the bed bottom sections (close to the fluid inlet). For the same recording time (10 s), the space covered by trajectories tends to reduce at higher concentration (lower fluidization velocity). This confinement effect can be clearly observed on the trajectory envelopes projection in the cross section ((x, y) plane), with the development of dark spots near the bed wall, typical of particle trapping over long-time periods. Also, the shape of the paths becomes more and more angular as the bed is compacted, as a consequence of the increase of inter-particle collisions.

![Figure 4a](image1.png) **Figure 4a**: Projections of particle trajectories in (x, z) plane (left) and (x, y) plane (right). Top: Numerical, Bottom: Experimental data ($U_F=0.15$ m/s, $<\alpha_p>_b=0.15$)

Qualitatively, these features are very similar to those observed in Aguilar Corona’s experiments (12 particle trajectories recorded during more than 3 minutes). For these particles, no clear steady recirculation pattern can be detected from the simulated trajectories envelopes, whereas the shape of the experimental trajectories in the bottom part of the bed could be interpreted as the trace of a toroidal motion (figure 4a bottom left). Note however, that due to the limited time of observation of the numerical signal (10 s) no firm conclusion can be drawn from that observation. Overall, the multi-scale diffusive-like motion of the particles in the bed as calculated by the numerical simulations exhibits remarkable similarities with the experimental signal, suggesting that the physics of the fluid-particle and particle-particle interactions are reasonably well captured by the numerical model, in both dilute and concentrated regimes.

In order to visualize both phases random motion in the bed snapshots of particle and fluid velocities were taken in a vertical median plane of the bed (x, z). Instant field of particle velocity vectors in this plane was superimposed on the instantaneous signal of velocity axial component following one particle trajectory is composed of large scale, low frequency and small scale, higher frequency fluctuations, as in the corresponding experimental signal (figure 6b). On both numerical and experimental signals, the amplitude of

![Figure 5](image2.png) **Figure 5**: Instant particle velocity field (vectors) and liquid velocity contour plot in (x, z) plane. (a) $U_F=0.15$ m/s ($<\alpha_p>_b=0.14$) – (b) $U_F=0.073$ m/s ($<\alpha_p>_b=0.38$)

The instantaneous signal of velocity axial and radial component following one particle trajectory is illustrated in figure 6 for the case ($<\alpha_p>_b=0.3$, $U_F=0.09$ m/s). Qualitatively, numerical and experimental signals look pretty much the same. The numerical Lagrangian velocity signal of the particles is composed of large scale, low frequency and small scale, higher frequency fluctuations, as in the corresponding experimental signal (figure 6b). On both numerical and experimental signals, the amplitude of
fluctuations is more pronounced on the axial $U_{px}$ than on the transverse component $U_{px}$, with a lower frequency on $U_{px}$ than on $U_{px}$. However, modes of high frequency (30 Hz) can be observed in the numerical signal, which is not the case of the experimental signal. This difference might be due to the effect of the sub-grid collisional model used in the numerical simulations or to a filtering effect in the experimental signal, resulting from the spatial resolution of the particle position, the maximum error being estimated of the order of $10^{-3}$ m/s for a sampling frequency of 30Hz of the velocity signal.

Particle velocity histograms following their trajectory (not shown in this paper) have been determined. They are centered on a zero mean value for all components and well fitted by a Gaussian distribution, similarly to experimental velocity pdf. In Aguilar Corona’s experiments, it was noticed that a small positive peak around zero velocity was developing as the bed concentration was increased. It was argued by Aguilar et al. (2011) that this peak could result from the increase of inelastic or soft collisions in the bed, due to the decrease of particle agitation at higher concentration (which involves the notion of critical Stokes number below which restitution coefficient is zero). Interestingly, the numerical simulations exhibit the same trend.

In following sections, for all quantity averaged at the scale of the bed, statistics were calculated over a period of 10 s after the first 10 s of transient.

**Fluidization law**

The steady bed height was determined by averaging in time (over 10 s) and space (over the bed volume) a particle phase indicator function $x_p(x, t)$ defined at each mesh node, equal to 1 if the node is inside the particle and 0 if not. The vertical profile of the time-section average of the particle phase indicator function (or phase fraction) $\langle x_p \rangle$ is displayed in Figure 7. It can be seen that the phase fraction is rather homogeneous along the bed height. For the two highest velocities studied (0.17 and 0.15 m/s), compared to the averaged value, the profiles show a slight excess of particles in the freeboard region and a lack of particles in the bottom part. At lower fluidization velocity, the particle concentration in the bed is quite homogeneous. Note that at the bed freeboard, a gradient of the phase fraction develops which becomes stiffer as the fluidization velocity is decreased. In order to determine an averaged bed height (or a global concentration), a linear regression with a high order polynomial interpolation was applied on the phase fraction profile in the free-board region and the abscissa of the inflection point of that function was defined as the bed height $h_b$. The bed solid concentration $\langle \alpha_p \rangle$ is then calculated by:

$$\langle \alpha_p \rangle_b = \frac{2 n_p D^2}{3 h_b}$$

where $n_p$ is the total number of fluidized particles ($n_p = 2133$) and $D$ is the column diameter ($D = 0.08$ m).

Figure 7: (a) Axial profile of time-section average ($x$, $y$) of the particle phase fraction. (b) Fluidization law.

Figure 8: Fluidization velocity with respect to the bed solid concentration. ©: Aguilar-Corona (2008), ---: Richardson & Zaki’s law with $n = 2.41$ and •: simulations.

Once bed height is determined, plotting the fluidization velocity as a function of $\langle \alpha_p \rangle_b$ gives the fluidization law. Figure 8 shows this plot together with the experimental data of Aguilar Corona (2008) and the agreement is remarkably good. Based upon that result, it can be concluded that numerical calculations faithfully reproduce the macroscopic momentum balance in the whole bed, which reduces to equilibrium between the averaged drag and the buoyancy forces and an extra-term, which is equal to the inter-correlation between the fluctuations of pressure gradient and concentration. It can be shown that this term is scaled by the variance of the concentration in the bed and is
two or three orders of magnitude smaller than the buoyancy term, and can be neglected in the averaged momentum balance in fully fluidized regimes.

Particle and Fluid phase fluctuations

Variance of particle velocity components has been plotted as a function of global concentration and compared to the experimental data in figures 9a and 9b (axial and transverse components, respectively). It is important to mention that experimental data are calculated on a much smaller number of particle trajectories (only 12) but on a much longer time (3 minutes) than numerical statistics (2133 particles during 10 seconds). However, predicted data show a reasonable good agreement with experiments, except for the case at the largest fluidization velocity, for which calculated particle fluctuations level is twice as large as the experimental data. The behavior of particle velocity variance at low fluidization velocity issued from the simulations also differs from the experimental trend, which suggests the existence of a maximum of particle agitation around a concentration of 10%.

For the other test cases, the decay with the global concentration is well captured in both vertical and transverse direction.

Figure 10: Anisotropy coefficient as a function of global concentration in the bed.

Figure 11 reports the evolution with global concentration of the average fluctuating kinetic energy in the bed, for both phases, $E_f$ and $E_p$. Both quantities decrease with respect to the global bed concentration $<\alpha_p>$. Fluid agitation level is always higher than that of the particles. Same trend can be observed with experimental data, but the numerical data underestimate them significantly. Note however that the fluid velocity variance is calculated from PIV measurements performed in the top part of the bed in a median vertical plane, whereas it is averaged on the whole bed volume in the numerical experiments, so the comparison is not quantitatively accurate. The ratio $E_f/E_p$ is a growing function of the bed concentration in both cases, which tends to validate the relevance of the present numerical modeling. At low concentration (highest fluidization velocities), the discrepancy between numerical prediction and experimental data is maximum, as a probable consequence of insufficient computation time.

A remarkable result is obtained with the evolution of the anisotropy coefficient $k_{anis} = 2 <U_{xf}'^2> / (<U_{x}'^2> + <U_{y}'^2>)$ in figure 10, which is close to the experimental value (around 1.5) and is also found to be independent of the solid concentration in the bed. This result suggests that even if the intensity of large-scale motion in vertical direction is decreasing as the concentration is increased, its redistribution on transverse components is probably driven the same mechanism at all concentrations.

Figure 9: Variance of particle velocity versus global concentration in the bed. (a) transverse component, (b) axial component. •: Aguilar-Corona (2008) and ○: simulations.

Figure 11: Fluctuating kinetic energy of fluid phase $E_f$ and of particle phase $E_p$. Black symbols: numerical data. Open symbols: experimental data.
Conclusions

Direct numerical simulations of a liquid-solid fluidized bed were performed using a one-fluid formulation of the incompressible Navier-Stokes equations, where the pressure-velocity coupling is provided by an algebraic augmented Lagrangian method and particles presence is modeled with an implicit penalty fictitious domain method, sub-grid scale lubrication force and soft-sphere collision models. We carried out the simulations in a fluidized bed experimentally investigated by Aguilar-Corona (2008) on a structured uniform Eulerian grid for various fluidization velocities. Simulations results show the ability of the numerical code to reproduce a steady regime of fluidization, and perfectly reproduce the fluidization law identified in Aguilar Corona’s experiments. The instantaneous flow field exhibits small and large-scale motion in both phases. This behavior is observed in all range of fluidization velocity investigated, from dilute (10%) to concentrated regimes (38%). As the concentration is increased, the agitation of both phases is decreased, and the experimental trend is well reproduced except in the case of the lowest global concentration (highest fluidization velocity). However, the anisotropy of the agitation of particles is well predicted and is shown to be independent of the bed global concentration, reproducing the experimental trend. Fluid velocity variance in the bed is larger than that of the particle phase up to an order of magnitude at high concentration, in agreement with the experimental data. Overall, comparison between numerical and experimental instantaneous fields and averaged quantities tend to demonstrate that the physics of particle-fluid and inter-particle interactions are well captured by the present numerical approach.

Future work will focus on particle fluctuating motion statistics at longer time (self-diffusion), collisions statistics and inter-correlation of fluctuating quantities (particle velocity-concentration, pressure gradient-concentration, fluid-particle velocities).

Acknowledgements

This work was granted access to the HPC resources of CINES under the allocation x2012026115 made by GENCI (Grand Equipement National de Calcul Intensif) and of CALMIP under the allocation p0633 (Calcul en Midi-Pyrénées). This work has been supported by the research federation FERMaT (FR CNRS 3089).

References


