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Computational Modeling of the Impact of Solid Particles on the Gas Hold-Up in Slurry Bubble Columns

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Three-phase bubble column reactors, despite their broad diffusion in chemical process, are often difficult to describe given the intricate mutual phase interactions. Moreover, validation of computational models is likewise complex, since it is considerably challenging to obtain exhaustive and precise experimental data from these systems. The aim of this work is to predict reliably the effect of disperse solid particles on the overall fluid dynamics of a bubble column by computational fluid dynamics.

The small size of particles allowed us to approximate the solid-liquid mixture as a single pseudo-homogeneous phase in the Euler-Euler framework. The simulation settings were tuned on two-phase gas-liquid systems and then extended to the three-phase gas-solid-liquid columns. Experimental data from different setups and correlations for the global gas hold-up in slurry systems were used to validate the model. In particular, what emerges from experiments is that the presence of the solid reduces gas hold-up, as a consequence of the higher density of the slurry in comparison to the pure liquid and the increased coalescence of the bubbles.

Results show that this model is able to predict the reduction of the hold-up with a solid volumetric loading up to 20%, achieving good agreement with experimental data. Moreover, what stands out from the simulations is that the addition of the solid also changes the shape of the flow map curve (global hold-up as a function of the gas superficial velocity), switching to a smoother transition between the behavior at low and high gas superficial velocity.

1. Introduction

Slurry bubble column reactors are intensively used in many of industrial processes involving multiphase systems such as Fischer-Tropsch synthesis, alkylation, fermentation and wastewater treatments (Kantarci et al. 2005). Such broad diffusion is due to their easiness in construction operation and in versatility, together with their excellent performance in mass and heat transfer provided by the motion of gas bubbles without the movement of any mechanical part. In the most common arrangement, a batch solid-liquid dispersion resides in the lower part of the column, while the gas phase is continuously injected from the bottom through the formation of bubbles with size distribution depending on the characteristics of the sparger. The bubbles interact with the surrounding suspension and the other bubbles, undergoing break-up and coalescence and eventually leaving the column from the top section.

When solid particles are added to the gas-liquid system, the overall behavior is strongly influenced by their physical properties and the modeling of such three-phase flows becomes difficult. The key parameter is the particles Stokes number: if it is considerably low, the inertia of the solid particles may be neglected since they follow the liquid streamlines and both gas-solid and gas-liquid interactions may be coupled as a single gas-slurry interaction, being the latter the solid-liquid mixture approximated as a single pseudo-homogeneous phase. On the other hand, when the Stokes number is large the particles have a significant inertia, consequentially the solid phase must be modeled as a new phase.

Furthermore, the solid particles have a substantial impact on the gas hold-up in the column. Although different effects have been reported for hydrophobic and hydrophilic solids, it is generally observed that solid particles

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reduce the gas hold-up. This behavior is a consequence of the larger density of the slurry in comparison with the pure liquid as well as the bubble coalescence promoted by the solid particles.

In this regard, Computational Fluid Dynamics (CFD) simulations reproduced correctly the changed behavior when solid load was introduced; the regimes shift was observed and validated through empirical correlations (Basha et al. 2015).

The main goal of this work is the investigation of the impact of solid particles on the overall and local fluid dynamics of bubble columns and the comparison their behavior to the analogous two-phase systems. With this aim, CFD simulations were performed on different experimental set-up to validate the model with experimental data. However, given the difficulty to obtain exhaustive experimental data from those systems due to their turbidity, a broad and detailed model validation cannot be performed until local experimental distribution of quantities such as velocity or bubble size distribution are detailly sampled.

2. Modeling

In the majority of industrial processes performed in slurry bubble columns the solid particles act as catalyst, therefore they are finely dispersed ($d_p \leq 100$ μm) to maximize the interfacial area. Because of the small size of such particles, the solid-liquid mixture may be modeled as a single pseudo-homogeneous phase, having modified density (ρ) and viscosity (μ) according to the volumetric solid loading (C_s):

$$\rho_{sl} = \rho_l(1 - C_s) + \rho_s C_s \tag{1}$$

$$\mu_{sl} = \mu_l \exp\left(2.5 \frac{C_s}{1 - 0.609 C_s}\right) \tag{2}$$

where the subscripts l, s and sl refer respectively to the liquid, solid and slurry phase.

In this way the original three-phase solid-liquid-gas system is reduced to a two-phase slurry-gas system. If the Euler-Euler framework is adopted, the mass and momentum conservation equations are solved for each phase k:

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

$$\frac{\partial}{\partial t} \alpha_k \rho_k \mathbf{u}_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = -\alpha_k \nabla p + \alpha_k \rho_k \mathbf{g} + \mu_k \nabla^2 (\alpha_k \mathbf{u}_k) + \mathbf{F}_k \tag{4}$$

With α_k and $\mathbf{u}_k$ denoting the volume fraction and velocity of the generic phase k. In particular, in Eq. (4) $\mathbf{F}_k$ denotes the interfacial force per unit volume of system experienced by the phase k. For our case, where a gas phase is dispersed in a liquid medium, we included:

- The drag force, $\mathbf{F}_{Drag}$ which is predominant due to the relative velocity ($\mathbf{u}_r$) between the bubble and the surrounding slurry medium. Indicating the bubble diameter with d_b, it may be expressed as:

  $$\mathbf{F}_{Drag} = \frac{3}{4} C_{Drag} \frac{\alpha_g \rho_{sl}}{d_b} |\mathbf{u}_r| \mathbf{u}_r \tag{5}$$

  Where the drag coefficient C_{Drag} is evaluated on the basis of the correlation proposed by Tomiyama for partially contaminated air-water system (Tomiyama 1998). For an isolated bubble:

  $$C_{Drag}^{\infty} = \max\left[\min\left[\frac{24}{Re}(1 + Re^{0.687}), \frac{72}{Re}\right], \frac{8}{3} \frac{Eo}{Eo + 4}\right] \tag{6}$$

  Being $Re = \rho_{sl} u_r d_b / \mu_{sl}$ and $Eo = g(\rho_{sl} - \rho_g) d_b^2 / \gamma$ respectively the Reynolds and Eötvös number of the bubble (here γ denotes the interfacial tension). However, in bubbly flow bubbles are extremely close together and the drag force experienced by every bubble is influenced by its neighbors. This phenomenon is called swarm effect and is taken into account by adjusting the drag coefficient for a single isolated gas bubble (Simonnet 2007) through the following factor, which is a function of the local value of volume gas fraction α_g:

  $$h = \frac{C_{Drag}}{C_{Drag}^{\infty}} = (1 - \alpha_g)\left((1 - \alpha_g)^{25} + \left(4.8 \frac{\alpha_g}{1 - \alpha_g}\right)^{25}\right)^{-2/25} \tag{7}$$

- Among the secondary interfacial forces, the lift force $\mathbf{F}_{Lift}$ originates from the rotational components of the velocity field and acts perpendicularly to the main direction of the flow, while the wall lubrication force $\mathbf{F}_{WL}$ arises from the presence of the wall:

$$\mathbf{F}_{Lift} = -\,C_{Lift}\rho_{sl}\alpha_g\left(\mathbf{u}_{sl} - \mathbf{u}_g\right) \times \nabla \times \mathbf{u}_g \quad (8)$$

$$\mathbf{F}_{WL} = C_{WL}\rho_{sl}\alpha_g\left|\left(\mathbf{u}_{sl} - \mathbf{u}_g\right)_t\right|^2 \mathbf{n}_w \quad (9)$$

Where C_{Lift} and C_{WL} are the respective forces coefficients. In this work they are evaluated from the relationships proposed by Tomiyama (Tomiyama 1998, Tomiyama 2002). The effective presence of these forces has not been deeply understood yet and it is still subject of debate in the literature (Tabib et al. 2008, Shiea et al. 2019). However, it is generally agreed that the implementation of the lift force may provide more accurate results in case of non-uniform gas feed, while the wall lubrication force becomes relevant when the column sectional area is small. Moreover, additional interfacial forces that are hardly taken into account are the turbulent dispersion and the virtual mass forces, the former being caused by the motion of turbulent eddies and the second one by the relative acceleration between phases. Nevertheless, they have a negligible impact on the final outcome of the simulation and therefore they have been omitted.

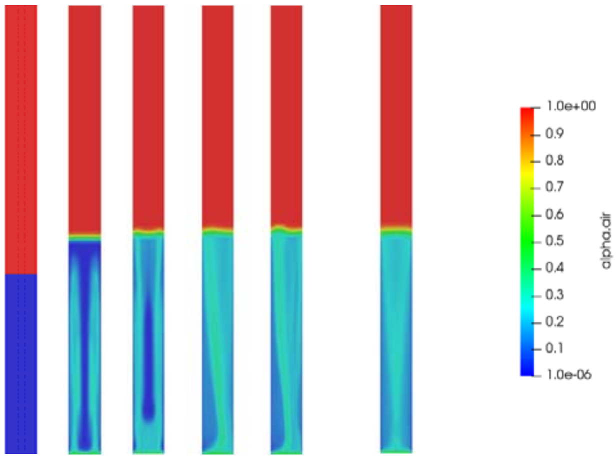
2.1 Experimental and computational set-up

With the aim of maximizing the applicability range of the model, two different experimental set-up were used to validate the model. The former case is based on study by Ojima et al. (2014) and investigated a column of square section with side L = 0.2 m, gas superficial velocities of 0.020 and 0.034 m/s and volumetric solid loading from 0 to 20%; they used particles with average diameter and solid particles equal to 100 μm and 2250 kg m^{-3}. The second set of data refers to the study of Guan et al. (2017) who investigated the behavior of a column with round cross section of diameter D = 0.15 m, by varying gas velocity from 0.02 to 0.16 m/s and solid loading between 0 and 20%; in this set-up, the mean size and viscosity of solid particles were 100 μm and 2354 kg m^{-3}.

Since in bubble columns the flow pattern reaches only a pseudo-stationary state (Figure 1), transient simulations were performed; the results presented in the following section are averaged on a time period equal to 100 s, after having discarded the first 80 s of simulations to exclude the initial transient behavior. Bubble size is fixed according to experimental data: for the square column is 8 mm, for the circular one 6.5 mm. The gas phase was assumed laminar, while the slurry phase was modeled as turbulent accordingly to the k-ε model, being the most suitable for describing bubbly flows (Tabib et al. 2008).

At the inlet section the gas fraction was set to 0.5 and the velocity was set accordingly to the gas superficial velocity considered, while the turbulence intensity and viscosity ratio are equal to 0.05 and 10 respectively.

For both geometries various meshes were tested in order to get grid-independent results: in both cases this was reached with an average cell size of 6 mm.



(a) (b)

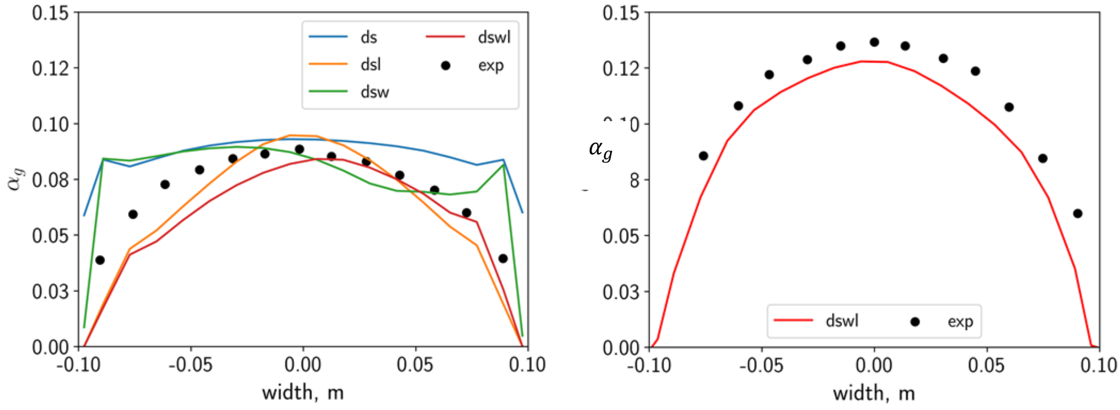
Figure 1: (a) time snapshots of the axial contour plot of the instantaneous gas hold-up at superficial gas velocity 0.08 m/s at times 0, 2, 4, 16 and 80 s. (b) time averaged gas-hold up.

3. Results

3.1 Square column

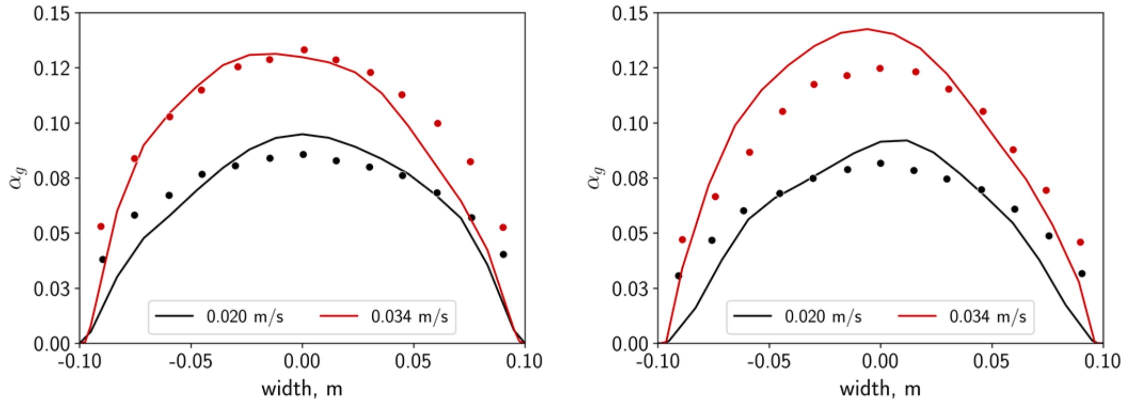
Primarily, simulations were performed for a pure gas-liquid system in order to assess the effective relevance of the various interfacial forces. Local profiles of gas fraction at elevation *z/L* = 3, evaluated with gas superficial velocity equal to 0.02 m/s, are reported in Figure 2a. What emerges is that the most accurate configuration is the combination of the drag (corrected for the swarm effect), lift and wall lubrication forces: if the lift force is neglected (green and blue lines) the gas fraction profile is unrealistically flat, while the wall lubrication allows an enhancement of the prediction. The simulation performed at 0.034 m/s (Figure 2b) confirmed that this set of forces provides a good estimation of the behavior of the system.

Subsequentially, the presence of the solid particles was accounted for by modifying liquid density and viscosity according to Eq. (1) and (2). The results, shown in Figure 3a for solid loading 10% and Figure 3b for solid loading 20% demonstrate how the pseudo-homogeneous model with drag, lift and wall lubrication forces is able to reproduce experimental data.



(a) *(b)*

Figure 2: Square column with gas-liquid flow, (a) Impact of interfacial forces on the local gas hold-up at height z/L = 3 and superficial gas velocity 0.02 m/s (gas-liquid flow). Legend reports the enabled forces for each line: drag (d), swarm correction of the drag (s), lift (l) and wall lubrication (w). (b) Local gas hold-up at height z/L = 3 and superficial gas velocity 0.034 m/s.



(a) *(b)*

Figure 3: Local gas hold-up at height z/L = 3 at superficial gas velocity 0.02 and 0.034 m/s with 10% (a) and 20% (b) solid loading.

The simulations were performed by considering a fixed bubble size and, consequently, the enhancement of coalescence due to the solid particles was neglected. Clearly, we expect that coupling the CFD with a population balance method, capable of predicting locally the mean bubble size, would increase further the quality of the solution.

However, symmetrical profiles were reported for all the variables at any gas superficial velocity and solid loading: as example, Figure 4 reports the contour plots of time averaged gas fraction and liquid axial velocity for superficial gas velocity 0.020 m/s and solid loading 10%. The inlet conditions seem to have a limited impact on the lower part of the system: above a certain height, approximately equal to the hydraulic diameter of the column, the fluid dynamics patterns were assessed and became regular until the free surface of the slurry.

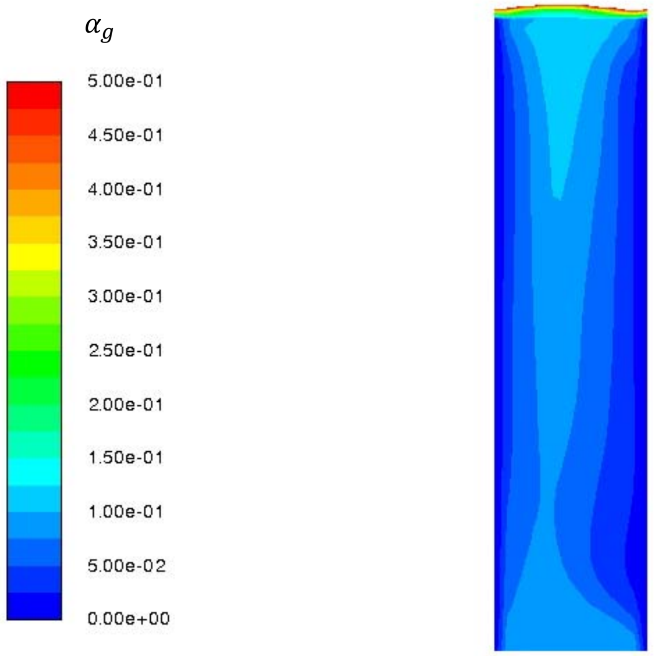
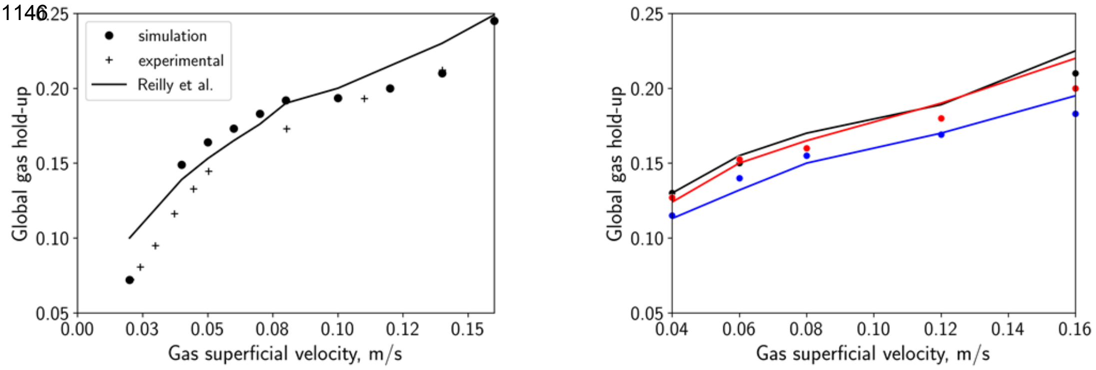


Figure 4: Time averaged gas hold-up for the square column at superficial gas velocity 0.020 m/s and solid loading 10% (region above the free surface is omitted).

3.2 Circular column

The simulations aim was to investigate how global properties changed with solid addition starting from the two-phase system. As done for the square column, simulations and experiments were first matched for the two phase gas-pure liquid system. A remarkable difference between round and circular columns concerns the role of the lift force. Satisfactory agreement between experiments and simulations in circular column is normal obtained neglecting lift effects (Gemello et al. 2018), as confirmed by Figure 5a, where the global gas hold-up is reported. On the contrary, for this type of column, the activation of the lift force has a strong destabilizing effect on the simulation. After the assessment of the fluid dynamics of pure gas-liquid flow slurry simulations were performed with three different solid loadings: 5, 10 and 20% (Figure 5b).

Simulations capture correctly the decrease of gas hold-up caused by the solid, as visible in Figure 5b, where the CFD results are compared with the empirical correlation of Reilly (Lakhdissi et al. 2019). Also, the transition from a double infection curve for pure two-phase system to a single inflection curve at high solid volume fractions, observed by Orvalho et al. (2018) for a system operating under the same conditions as those of the simulation, is reproduced exactly.



(a) *(b)*

Figure 5: (a) Global gas hold-up calculated through CFD for the two-phase system compared with the experiments by Guan et al. (2017); (b) Global gas hold-up calculated through CFD (dots) compared with Reilly correlation (continuous lines) for solid loading 5 % (black), 10% (red) and 20% (blue). Lift and wall lubrication forces were neglected in the simulation.

4. Conclusions

Slurry bubble column reactors of different geometries were simulated using Euler-Euler framework and approximating the solid-liquid mixture as one pseudo-homogeneous phase. The properties of this phase were computed adjusting the liquid density and viscosity according to the solid particle concentration. Results show that the main effect of the solid particles is the reduction of gas hold-up and are consistent with experimental data, proving the validity of the model for particles diameter equal to 100 μm and gas velocity up to 0.16 m s^{-1}. Moreover, the model is capable of well predicting the behavior of the flow up to a solid volumetric loading equal to 20% if the drag term is corrected for the swarm factor. A significant difference is found between square and circular columns regarding the role of lift forces in the simulation: while such interactions must be taken into account to correctly reproduce the operation of square columns, they originate numerical instability and inaccuracy in circular ones.

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