Scaling up Bubble Column Reactors with Highly Viscous Liquid Phase

By *R. Krishna** and *J. M. van Baten*

Measurements of gas holdup were made in bubble columns of 0.1, 0.19 and 0.38 m diameter with air as gas phase and Tellus oil as the liquid phase. The gas holdup was found to decrease with increasing column diameter. The reason for this scale dependence is because the strength of the liquid circulations increases with increasing scale. Such circulations accelerate the bubbles travelling upwards in the central core. Computational fluid dynamics (CFD) simulations were carried out using the Eulerian description for both the gas and the liquid phases in order to model the scale dependence of the hydrodynamics. Interactions between the bubbles and the liquid are taken into account in terms of a momentum exchange, or drag, coefficient; this coefficient was estimated from the measured gas holdup data at low superficial gas velocities. The turbulence in the liquid phase is described using the k-ε model. The CFD simulation results are in good agreement with the experimental results for all three columns and provide a reliable strategy for scaling up to reactors of commercial size.

1 Introduction

Bubble columns are widely used in industry for carrying out gas-liquid reactions in a variety of practical applications in industry [1]. They are simple in construction and particularly suited for carrying out relatively slow chemical reactions requiring large liquid holdups in the reactor. The gas-liquid hydrodynamics in bubble columns is, however, quite complex and influenced by several factors, such as (1) physical properties of gas and liquid phases, (2) operating pressure, (3) column diameter, and (4) dispersion height. Traditional methods of scaling up are based on the use of empirical correlations, developed on the basis of laboratory-scale experiments carried out in columns that are usually smaller than about 0.2 m in diameter [1–3]. The extrapolation of such empirical correlations to commercial-scale reactors, that could have diameters up to 6 m, is fraught with uncertainty.

Several recent publications have established the potential of computational fluid dynamics (CFD) for describing the hydrodynamics of bubble columns [4–15]. An important advantage of the CFD approach is that column geometry and scale effects are automatically accounted for. The success of the CFD simulation strategy is, however, crucially dependent on the proper modeling of the momentum exchange, or drag, coefficient between the gas and liquid phases. Though there are several drag correlations for the air-water system, no general guidelines are available for estimating the drag coefficient for systems other than the air-water system.

The focus in this paper is on bubble columns in which the liquid phase is highly viscous; such reactors are encountered in the fermentation industry for example. Our objective is to develop a simple procedure for estimating the drag coefficient for use in CFD models. We demonstrate the validity of our approach by carrying out experimental studies in columns of three different diameters. These results are compared with CFD simulations for the same three column diameters, along with those for a commercial reactor of 6 m diameter.

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2 Experimental Setup and Results

Experiments were performed in polyacrylate columns with inner diameters of 0.1, 0.19 and 0.38 m. The gas distributors used in the three columns were all made of sintered bronze plate (with a mean pore size of 50 μm). The setup is the same as used in earlier studies of our group [3,8–10]. The gas flow rates entering the column were measured with the use of a set of rotameters, placed in parallel, as shown in Fig. 1 for the 0.38 m column. This setup was typical. Air was used as the gas phase in all experiments. Gas holdup measurements were performed with Tellus oil (density, ρ_L = 862 kg m^{-3}; viscosity, μ_L = 0.075 Pa s; surface tension, σ = 0.028 N m^{-1}) as liquid phase. In all experiments the height of the dispersion was kept higher than 2 m.

The measured gas holdup for columns of diameter D_T = 0.1, 0.19 and 0.38 m are shown in Fig. 2. We see that with increasing superficial gas velocity U, the gas holdup ε becomes increasingly scale-dependent. With increasing column diameter, the gas holdup tends to be lower. To emphasize the scale dependence, we plot the bubble swarm velocity V_b = U/ε as a function of U in Fig. 3. For the same U, the swarm velocity V_b increases with increasing column diameter because D_T; this is due to increased liquid recirculations with increasing scale. At low superficial gas velocities the bubble swarm velocity is practically the same for the three columns and V_{b0} = 0.47 m/s; this is indicated by the large filled circle in Fig. 3. The liquid circulations tend to accelerate the bubbles travelling upward in the central core. When the bubbles disengage at the top of

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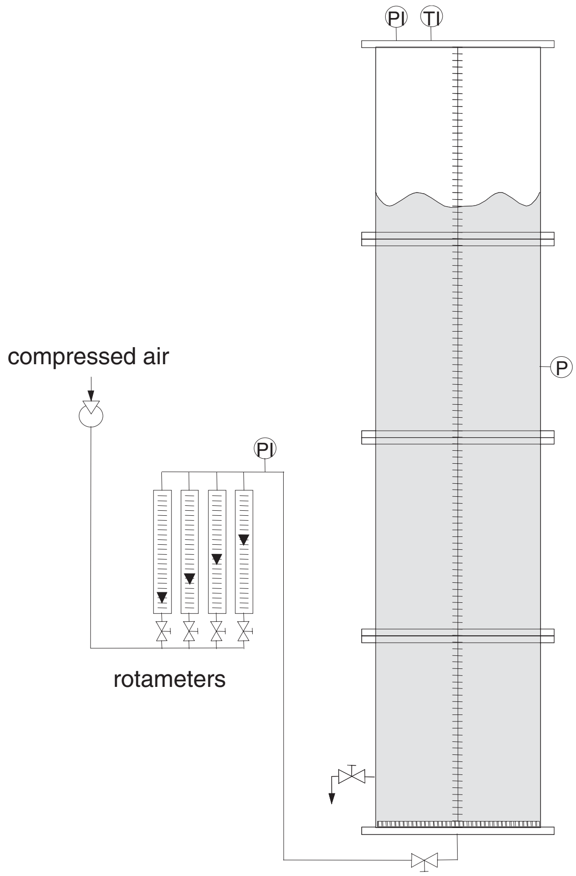

Figure 1. Typical experimental setup for the 0.38 m diameter column.

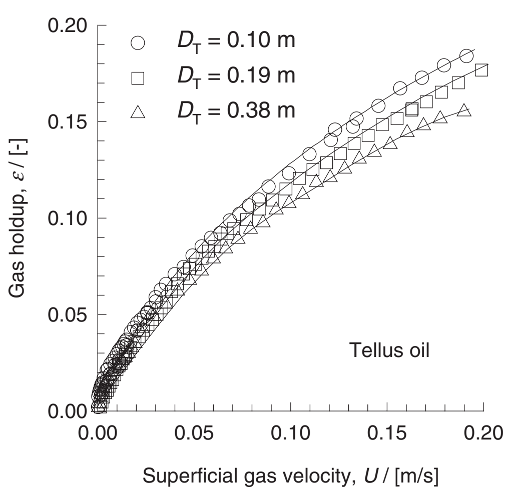

Figure 2. Influence of column diameter on the gas holdup in air/Tellus oil system.

the dispersion, the liquid travels back down the wall region. Clearly, to describe the influence of liquid circulations on the gas holdup, we need to be able to predict the liquid circulation velocity as a function of U and D_T. To enable such a prediction, we resort to Eulerian simulations of the bubble column hydrodynamics.

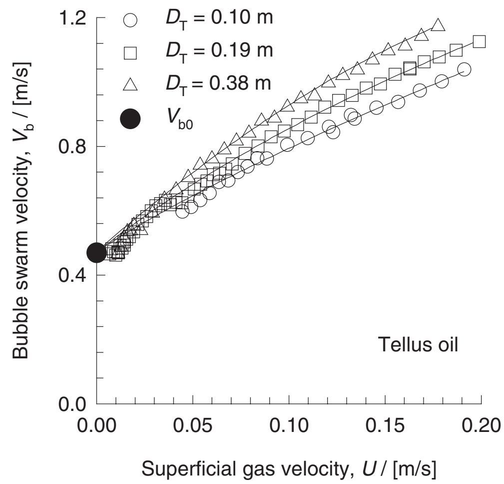

Figure 3. Influence of column diameter on the average bubble swarm velocity air/Tellus oil system.

3 Development of Eulerian Simulation Model

For either gas or liquid phase the volume-averaged mass and momentum conservation equations in the Eulerian framework are given by[1)]:

$$\frac{\partial\left(\varepsilon_k \rho_k\right)}{\partial t} + \nabla \bullet \left(\rho_k \varepsilon_k \mathbf{u}_k\right) = 0 \tag{1}$$

$$\frac{\partial\left(\rho_k \varepsilon_k \mathbf{u}_k\right)}{\partial t} + \nabla \bullet \left(\rho_k \varepsilon_k \mathbf{u}_k \mathbf{u}_k - \mu_k \varepsilon_k \left(\nabla \mathbf{u}_k + \left(\nabla \mathbf{u}_k\right)^T\right)\right) = -\varepsilon_k \nabla p + \mathbf{M}_{kl} + \rho_k \mathbf{g} \tag{2}$$

Here, ρ_k, $\mathbf{u}_k$, ε_k and μ_k represent, respectively, the macroscopic density, velocity, volume fraction and viscosity of phase k, p is the pressure, $\mathbf{M}_{kl}$, the interphase momentum exchange between phase k and phase l and $\mathbf{g}$ is the gravitational force.

The momentum exchange between the gas phase (subscript G) and liquid phase (subscript L) phases is given by:

$$\mathbf{M}_{L,G} = \left[\frac{3}{4}\frac{C_D}{d_b}\rho_L\right]\varepsilon_G \varepsilon_L \left(\mathbf{u}_G - \mathbf{u}_L\right)\left|\mathbf{u}_G - \mathbf{u}_L\right| \tag{3}$$

where we follow the formulation given by Pan *et al.* [5]. We have only included the drag force contribution to $\mathbf{M}_{L,G}$, in keeping with the works of Sanyal *et al.* [6] and Sokolichin & Eigenberger [7]. The added mass and lift force contributions were both ignored in the present analysis. We propose the

1) List of symbols at the end of the paper.

following relation for estimation of the square-bracketed term in Eq. (3) containing the drag coefficient C_D:

$$\frac{3}{4}\frac{C_D}{d_b}\rho_L = \left(\rho_L - \rho_G\right) g \frac{1}{V_{b0}^2} \tag{4}$$

where V_{b0} is the rise velocity of the bubble swarm at low superficial gas velocities (as indicated by the large filled circle in Fig. 3). When the superficial gas velocity U is increased, liquid circulations tend to kick in and Eq. (3) will properly take account of the slip between the gas and liquid phases. Our approach is valid when the bubble size does not increase significantly with increasing U; this is a good approximation for noncoalescing systems, but will not hold for air-water. It is important to note that we do not need to know the bubble diameter d_b in order to calculate the momentum exchange $\mathbf{M}_{L,G}$.

For the continuous, liquid, phase, the turbulent contribution to the stress tensor is evaluated by means of the k-ε model, using standard single-phase parameters $C_\mu = 0.09$, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $\sigma_k = 1$ and $\sigma_\varepsilon = 1.3$. The applicability of the k-ε model has been considered in detail by Sokolichin and Eigenberger [7]. No turbulence model is used for calculating the velocity fields of the dispersed bubble phases.

A commercial CFD package CFX, versions 4.2 and 4.4, of AEA Technology, Harwell, UK, was used to solve the equations of continuity and momentum. This package is a finite volume solver, using body-fitted grids. The grids are nonstaggered and all variables are evaluated at the cell centers. An improved version of the Rhie-Chow algorithm [16] is used to calculate the velocity at the cell faces. The pressure-velocity coupling is obtained using the SIMPLEC algorithm [17]. For the convective terms in Eqs. (1) and (2) hybrid differencing was used. A fully implicit backward differencing scheme was used for the time integration.

All simulations were carried out using axi-symmetric 2D grids. Simulations were run in columns with diameters of 0.1, 0.19, 0.38 m and 6 m, with superficial gas velocities U ranging up to 0.20 m/s. The total column height used in the simulations in the 0.1, 0.19 and 0.38 m is 1.3 m. For the 6 m diameter column the total column height is taken to be 35 m. The grids used for the simulations are uniform in both directions, see Figs. 4 (a) and (b). The total number of cells for the 0.1, 0.19 and 0.38 m diameter columns is 2600. The total number of cells for the 6 m diameter column is 26880.

To prevent a circulation pattern in which the liquid flows up near the wall and comes down in the core, the gas was not injected homogeneously over the full bottom area. Instead, the injection of gas was performed on the inner 75 % of the radius (15 out of 20 grid cells in the 0.1, 0.19 and 0.38 m diameter columns and 36 out of the 48 cells in the 6 m diameter column).

A pressure boundary condition was applied to the top of the column. A standard no-slip boundary condition was applied at the wall. The 0.1, 0.19 and 0.38 m diameter columns were

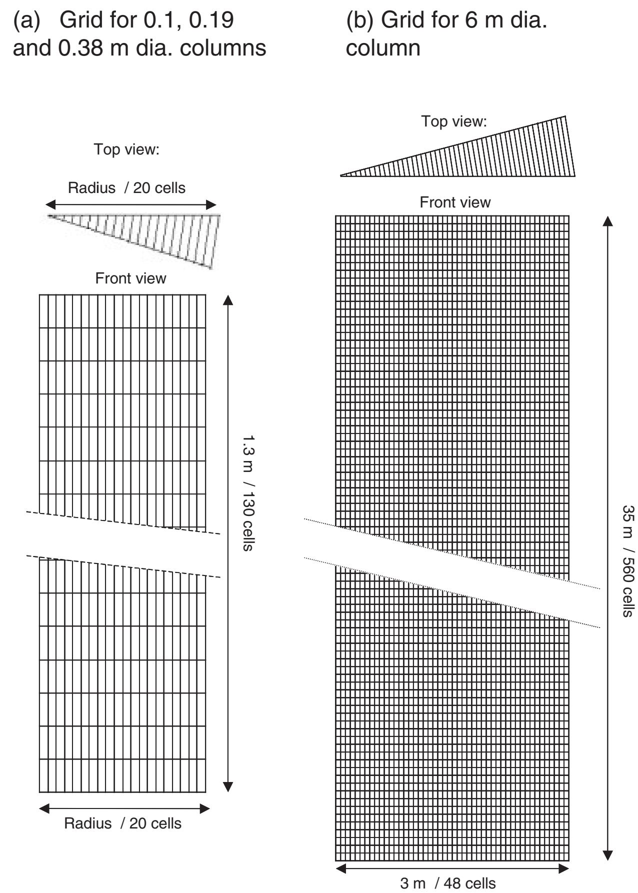

Figure 4. Grid used in the 2-D cylindrical axi-symmetric Eulerian simulations.

initially filled only with liquid, up to a height of 0.8–1 m, depending on the superficial gas velocity. The initial liquid height for the 6 m diameter columns was 25 m. Transient simulations of the column hydrodynamics were then carried out by imposing a constant superficial gas velocity at the bottom inlet. The time stepping strategy used in the transient simulations was 100 steps at 5×10^{-5} s, 100 steps at 1×10^{-4} s, 100 steps at 5×10^{-4} s, 100 steps at 1×10^{-3} s, 200 steps at 3×10^{-3} s, 1400 steps at 5×10^{-3} s, and 8000 steps at 1×10^{-2} s. Steady state was obtained when none of the state variables in the system were subject to change.

The simulations were carried out on Silicon Graphics Power Indigo workstation with a 75 MHz R8000 processors. Each simulation was completed in about 24 hours for the three smaller column diameters. Each of the 6 m column simulations took 4 weeks to complete. When steady state is established, the cumulative gas holdup can be determined along the column height. All the gas holdup data reported in this paper correspond to the cumulative gas holdup at a height of 0.9 m above the distributor for the smaller diameter column and 23 m for the 6 m diameter column.

Further details of the simulations, including animations of column start-up dynamics are available on our web site: http://ct-cr4.chem.uva.nl/viscousbc/.

4 Simulation Results for Scale Influence

The Eulerian simulations for the total gas holdup are compared with the experimental data in Fig. 5. The agreement is seen to be very good. Clearly, the CFD simulations are able to model the scale effects on the gas holdup. In order to understand this further, we examine the radial distribution of the liquid and gas (bubble) velocities, $V_L(r)$ and $V_b(r)$ in Fig. 6 (a) and (b) respectively for $U = 0.02$ m/s. We see from Fig. 6 (a) that the liquid circulation velocities increase strongly with column diameter. At the center of the column, for example the axial component of the liquid velocity $V_L(0)$ is 0.125 m/s in the 0.1 m diameter column; this value increases to 0.20 m/s in the 0.19 m column and to 0.27 m/s in the 0.38 m column. Since the drag between the gas bubbles and the liquid is the same for all three column diameters, the rise velocity of the bubbles has to increase with increasing column diameter. This is reflected in the axial component of the gas (bubble) velocity, $V_b(r)$, shown in Fig. 6 (b). At the center of the column, for example the bubble rise velocity $V_b(0)$ is 0.60 m/s in the 0.1 m diameter column; this value increases to 0.68 m/s in the 0.19 m column and to 0.74 m/s in the 0.38 m column.

The strong influence of column diameter on the gas holdup and the bubble swarm velocity is emphasized in Fig. 7 (a) and (b). We note that the scale effect becomes stronger with increasing superficial gas velocities. Consider operation of the bubble column at $U = 0.15$ m/s. In the 0.38 m diameter column the gas holdup is 0.138; this reduces to a value $\varepsilon = 0.079$ in the 6 m diameter column which amounts to a 40 % reduction.

5 Conclusions

In this paper we have put forward a scale-up strategy for bubble column reactors, with a highly viscous liquid phase, using CFD as a pivotal tool. In such columns, the dispersion consists almost exclusively of fast-rising large bubbles. By extrapolating the bubble swarm velocity data to low superficial gas velocities, the slip velocity between the bubbles and the slurry phase can be determined. For the Tellus oil system used in the experiments a value $V_{b0} = 0.47$ m/s is obtained, see Fig. 3. This value of V_{b0} is used to estimate the drag coefficient C_D (or actually $\frac{3}{4}\frac{C_D}{d_b}\rho_L$) between the gas and the slurry phase using Eq. (4). Eulerian simulations of the slurry bubble column with varying diameters are then carried out to capture the scale effects.

The CFD simulations are in very good agreement with the experimental results for gas holdup in 0.1, 0.19 and 0.38 m diameter columns. Simulations for a 6 m diameter column show the extremely strong scale dependence, especially for increasing superficial gas velocities.

Once the bubble hydrodynamics have been determined for the commercial-scale reactor of say 6 m, more reliable estimates can be made of the axial dispersion coefficients and heat transfer coefficients.

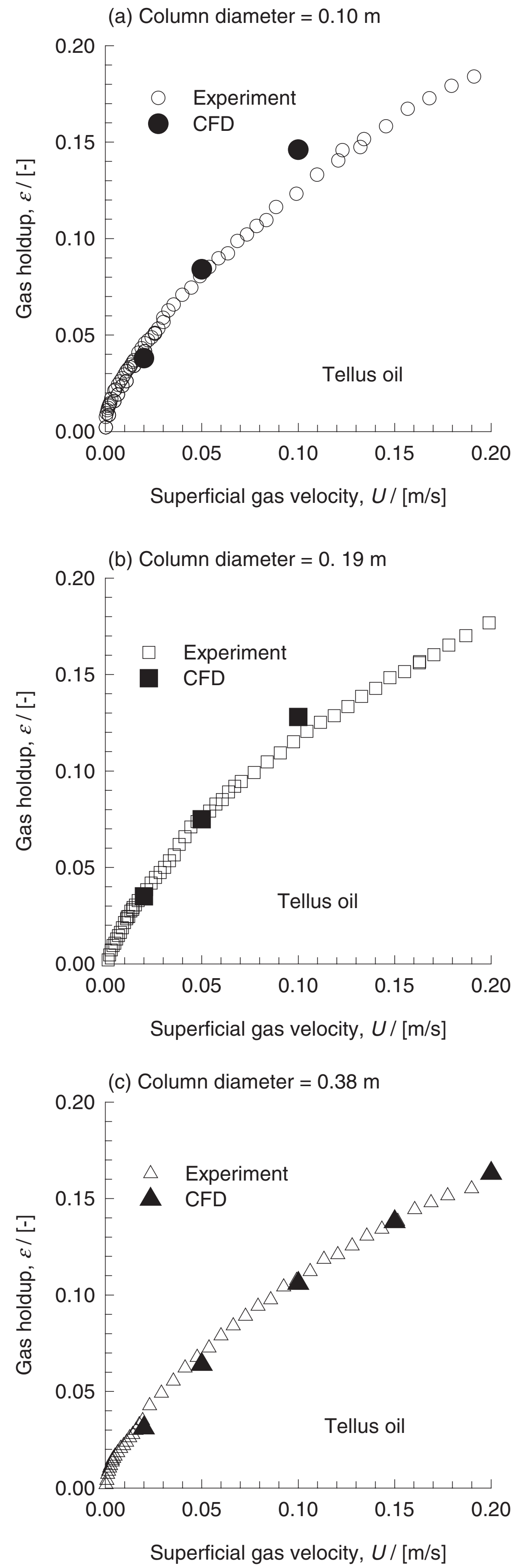

Figure 5. Experimental data on gas holdup as function of the superficial gas velocity U for columns of diameter $D_T = 0.1$, 0.19 and 0.38 m. Comparison with CFD simulations.

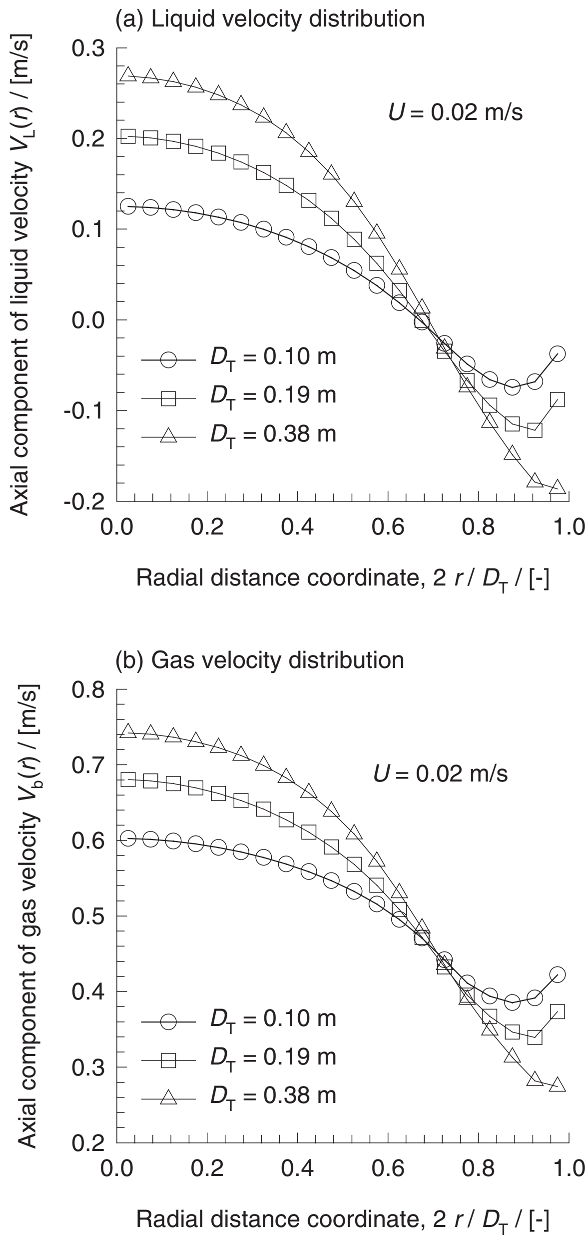

Figure 6. Radial distribution of (a) liquid velocity $V_L(r)$ and (b) gas velocity $V_b(r)$ for varying column diameters for a superficial gas velocity $U = 0.02$ m/s.

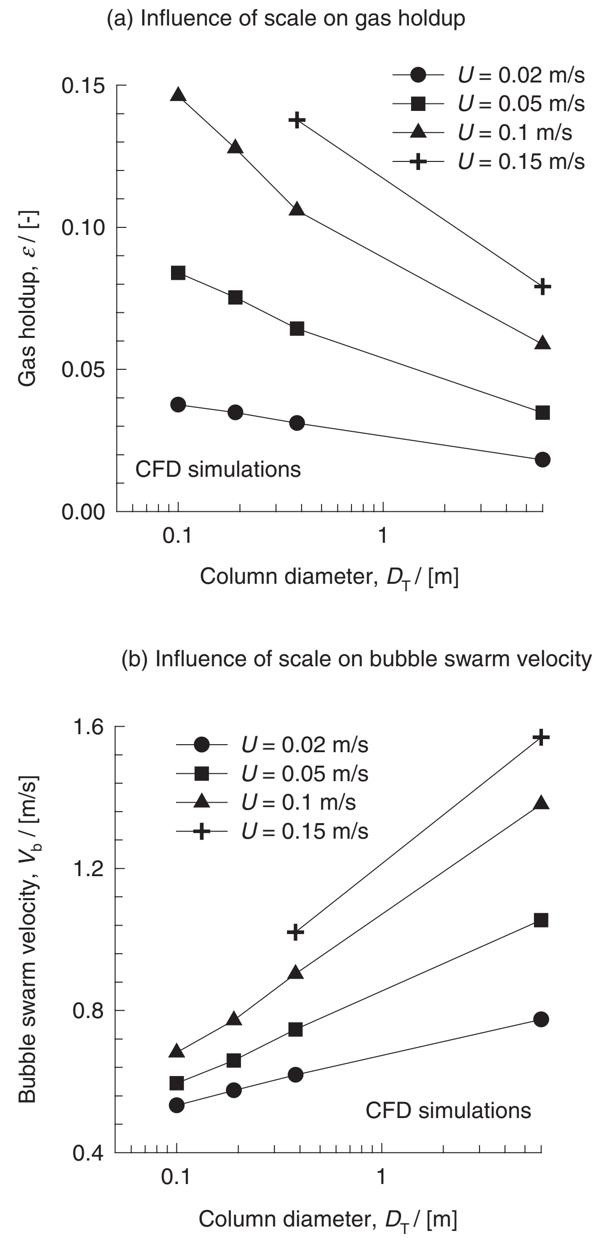

Figure 7. Influence of column diameter on (a) gas holdup and (b) average bubble swarm velocity predicted by CFD simulations.

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Symbols used

C_D	[–]	drag coefficient, dimensionless
d_b	[m]	diameter of bubble
D_T	[m]	column diameter
g	[m s^{-2}]	gravitational acceleration, 9.81 m s^{-2}
$\boldsymbol{g}$	[–]	gravitational vector
$\mathbf{M}$	[N/m^3]	interphase momentum exchange term
p	[Pa]	system pressure
r	[m]	radial coordinate
t	[s]	time
$\mathbf{u}$	[m/s]	velocity vector

U	[m/s^{-1}]	superficial gas velocity
$V_b(r)$	[m/s^{-1}]	radial distribution of bubble velocity
$V_L(r)$	[m/s^{-1}]	radial distribution of liquid velocity
V_b	[m/s^{-1}]	cross-sectional area average rise velocity of bubble swarm
V_{b0}	[m/s^{-1}]	bubble rise velocity at low superficial gas velocities
$V_L(0)$	[m/s^{-1}]	centre-line liquid velocity

Greek symbols

ε	[–]	total gas holdup, dimensionless
μ	[Pa s]	viscosity of fluid phase
ρ	[kg m^{-3}]	density of phase
σ	[N m^{-1}]	surface tension of liquid phase

Subscripts

b	referring to bubbles
G	referring to gas
L	referring to liquid
T	tower or column
k,l	referring to phase k and l respectively

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