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Scale-up strategy for bubble column slurry reactors using CFD simulations

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Abstract

Bubble column slurry reactors are widely used in industry. Often in practice, high catalyst loadings are used, and the liquid phase is usually an organic liquid. Literature correlations are not reliable enough for commercial scale up. In this paper, we develop a scale-up procedure that relies on the use of computational fluid dynamics (CFD), with Eulerian descriptions of the gas and slurry phases. Interactions between the bubbles and the slurry are taken into account by means of a momentum exchange, or drag, coefficient; this coefficient is estimated from the experimental measurements of gas holdup in a column of 0.051 m diameter. The turbulence in the slurry phase is described using the k–ε model. The CFD model is first validated by comparison with the measured gas holdup data for a range of superficial gas velocities. The validated CFD model is then used to simulate the hydrodynamics of a column of 1 m diameter. The CFD simulations clearly demonstrate the strong influence of scale on the column hydrodynamics.

Keywords: Gas holdup; Bubble columns; Scale effects; Computational fluid dynamics; Liquid circulations; Concentrated slurries

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1. Introduction

Bubble column slurry reactors are widely used in industry for carrying out gas–liquid (solid catalysed) reactions in a variety of practical applications in industry [1], such as hydrogenations and oxidations. An important emerging application of bubble column slurry reactors is for Fischer–Tropsch synthesis [2]. Though bubble column slurry reactors are simple in construction and operation, the hydrodynamics are complex and are a strong function of operating conditions (e.g. pressure, superficial gas velocity), physical properties (e.g. liquid viscosity, surface tension) and scale (reactor diameter and height). Published experimental data in the literature are most commonly restricted to air–water systems at atmospheric pressure in columns that are smaller than 0.3 m in diameter. Available literature correlations [1–3] cannot be used with confidence for scale up.

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 modelling 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 major objective of the present communication is to discuss and develop a scale-up strategy for bubble

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column slurry reactors that relies on the use of CFD. The key inputs to the CFD model are obtained from a set of experimental data in a column of *small* diameter, using the same gas, liquid and catalyst concentrations as envisaged in the commercial scale. After checking the ability of the CFD approach to reproduce the measured data, the model is used to predict the influence of scale on the reactor hydrodynamics.

Nomenclature

C_D	drag coefficient (dimensionless)
d_b	diameter of bubble (m)
D_T	column diameter (m)
g	gravitational acceleration (9.81 m s^{-2})
$\mathbf{g}$	gravitational vector (m s^{-2})
$\mathbf{M}$	interphase momentum exchange term (N m^{-3})
p	system pressure (Pa)
r	radial coordinate (m)
t	time (s)
$\mathbf{u}$	velocity vector (m s^{-1})
U	superficial gas velocity (m s^{-1})
V_b	cross-sectional area average rise velocity of bubble swarm (m s^{-1})
$V_b(r)$	radial distribution of bubble velocity (m s^{-1})
V_{b0}	bubble rise velocity at low superficial gas velocities (m s^{-1})
$V_L(r)$	radial distribution of liquid velocity (m s^{-1})
$V_L(0)$	centre-line liquid velocity (m s^{-1})

Greek letters

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

Subscripts

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

2. Experimental setup and results

To illustrate our scale-up strategy we investigate the hydrodynamics of a bubble column slurry reactor of 0.051 m diameter with air as the gas phase (density, $\rho_G = 1.3\,\mathrm{kg\,m^{-3}}$; viscosity, $\mu_G = 1.7 \times 10^{-5}$ Pa s), ethanol as the liquid phase (density, $\rho_L = 797\,\mathrm{kg\,m^{-3}}$; viscosity, $\mu_L = 0.0012$ Pa s; surface tension, $\sigma = 0.023\,\mathrm{N\,m^{-1}}$) into which cobalt catalyst particles (bulk density $= 1200\,\mathrm{kg\,m^{-3}}$; skeletal density $= 4100\,\mathrm{kg\,m^{-3}}$; mean diameter $= 25\,\mu\mathrm{m}$) are suspended in varying concentrations. The experimental setup is the same as used in our earlier publication [16]. The gas distributor consisted of a sintered glass disk of 5 mm thickness with pore sizes of 10–16 μm. In all the experiments, the total liquid height was held constant at 1 m. The gas holdup was measured by visual reading of the dispersion height.

The measured gas holdup for pure ethanol and for slurries of 4.4, 8.5, 12.4 and 16 wt.% are shown in Fig. 1. We note that with increasing slurry concentrations, the gas holdup decreases; this is in line with our previous measurements with paraffin oil–silica catalyst experiments [16]. Also noteworthy is the fact that the sharp maximum in the holdup curve for pure ethanol vanishes with increases slurry concentrations. This sharp maximum denotes a shift in the regime

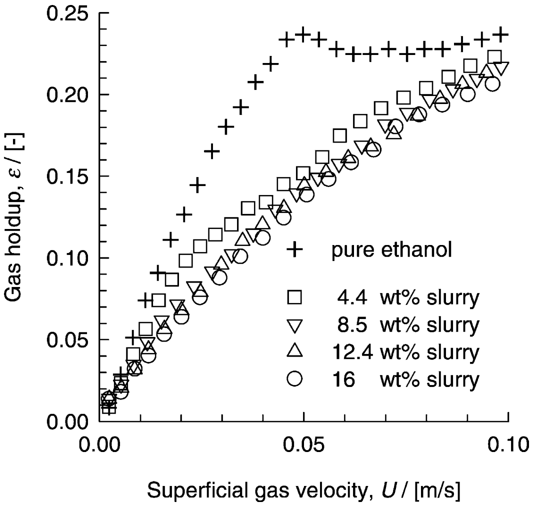


Fig. 1. Experimental data on gas holdup in 0.051 m diameter column. Air is the gas phase. The liquid phase consists of ethanol with varying catalyst concentrations.

from homogeneous bubbly flow to churn-turbulent flow. With the addition of catalyst particles, the coalescence of small bubbles is promoted and the dispersion becomes more homogeneous and consists predominantly of large sized bubbles. The gas holdup data for 12.4 and 16 wt.% slurries are practically the same, indicating that the bubble size is not further increased with catalyst addition beyond 12.4 wt.%. In this paper, we focus our attention on developing a scale-up strategy for a reactor operating with air–ethanol containing 16 wt.% catalyst. In particular, we demonstrate how the holdup in a column of 1 m diameter can be estimated on the basis of the information shown in Fig. 1, obtained in a 0.051 m diameter column. To enable such a prediction we resort to Eulerian simulations of the slurry reactor hydrodynamics.

3. Development of Eulerian simulation model

We consider the catalyst particles to be uniformly distributed in the liquid phase and we consider the slurry phase to be a pseudo-liquid phase. For either gas or liquid phase the volume-averaged mass and momentum conservation equations in the Eulerian framework are given by

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

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

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

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

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

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 and Eigenberger [7]. The added mass and lift force contributions were both ignored in the present analysis. We propose the following relation for estimation of the square bracketed term in Eq. (3) containing the drag coefficient C_D:

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

where V_{b0} is the rise velocity of the bubble swarm at low superficial gas velocities. In the simulations, the value of ρ_L was chosen to coincide with the experimentally determined value of the density of the slurry, i.e. 881 kg/m^3. From the gas holdup data we can estimate the average bubble swarm velocity $V_b = U/\varepsilon$ and determine V_{b0} by extrapolation of the data at low values of U; see Fig. 2. For 16 wt.% slurry, the value of V_{b0} is estimated as 0.235 m s^{-1}; this is denoted by the large filled circle in Fig. 2. 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. Increased liquid circulations cause the bubble swarm velocity V_b to increase with increasing U. Our approach for the estimation of C_D from V_{b0} is valid when the bubble size does not increase significantly with increasing U; this is a good approximation for non-coalescing systems, but will not generally hold for air–water. It is important to note that we do not need to know the bubble

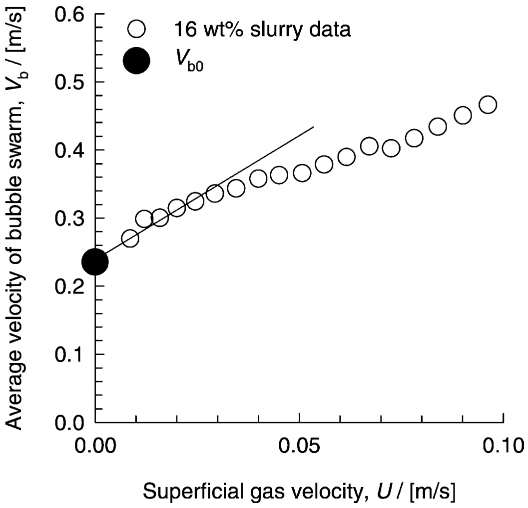


Fig. 2. Average bubble swarm velocity for air–ethanol containing 16 wt.% catalyst. The large filled black circle denotes the extrapolated value of V_{b0}.

diameter d_b in order to calculate the momentum exchange $\mathbf{M}_{L,G}$.

For the continuous, liquid (i.e. slurry) phase, the turbulent contribution to the stress tensor is evaluated by means of 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

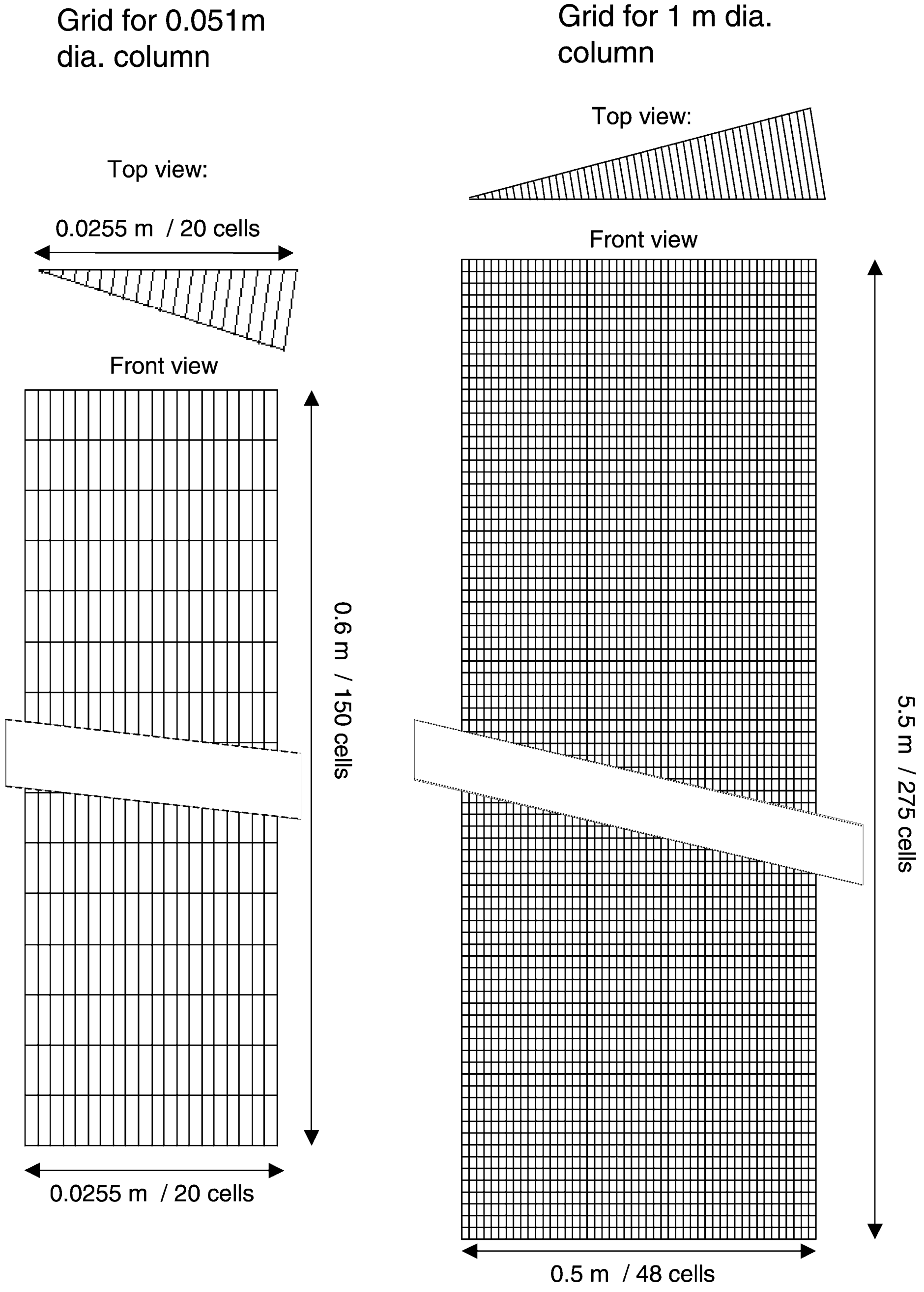


Fig. 3. Grid used in the 2D cylindrical axi-symmetric Eulerian simulations for 0.051 and 1 m diameter columns.

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 non-staggered and all variables are evaluated at the cell centres. An improved version of the Rhie–Chow algorithm [17] is used to calculate the velocity at the cell faces. The pressure–velocity coupling is obtained using the SIMPLEC algorithm [18]. 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 0.051 and 1 m, with superficial gas velocities U ranging up to 0.10 m s^{-1}. The total column height used in the simulations in the 0.051 m diameter column is 0.6 m. For height to diameter ratios higher than 5, the simulation results do not change and therefore we choose a column height of 0.6 m, rather than the 1 m used in the experiments; this results in saving of computation time. For the 1 m diameter column, the total column height is taken to be 5.5 m. The grids used for the simulations are uniform in both directions; see Fig. 3. The total number of cells for the 0.051 m diameter column is 3000. The total number of cells for the 1 m diameter column is 13,200.

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 0.051 m diameter column and 36 out of 48 cells in the 1 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 time stepping strategy used in all 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 the remaining steps until steady state at 1×10^{-2} s.

The simulations were carried out on Silicon Graphics Power Indigo workstations with 75 MHz R8000 processors, a Silicon Graphics O2 workstation with a 150 MHz R10000 processor, a Silicon Graphics Power Challenge with 6 200 MHz R10000 processors and a Windows NT pc with a single Pentium Celeron processor running at 500 MHz. For the smaller diameter column, each simulation was completed within a day. Each of the 1 m diameter column simulation took several days to complete.

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

4. Simulation results and comparison with experiments

The Eulerian simulations for the total gas holdup ε are compared with the experimental data in Fig. 4. The agreement is very good. Clearly, the CFD simulations are able to describe the variation of gas holdup with increasing superficial gas velocity U in the 0.051 m diameter column using only V_{b0} as the experimentally determined input parameter. In order to understand the variation of ε with U, we examine the radial distribution of the liquid and gas (bubble) velocities, respectively, $V_L(r)$ and $V_b(r)$ in Fig. 5(a) and (b) for the 0.051 m diameter column. We see from Fig. 5(a)

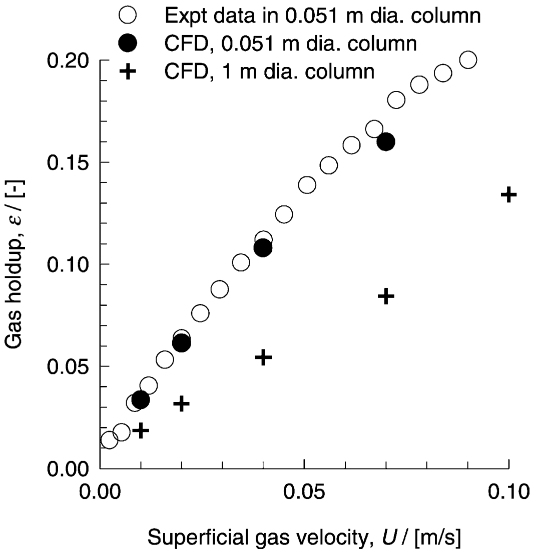
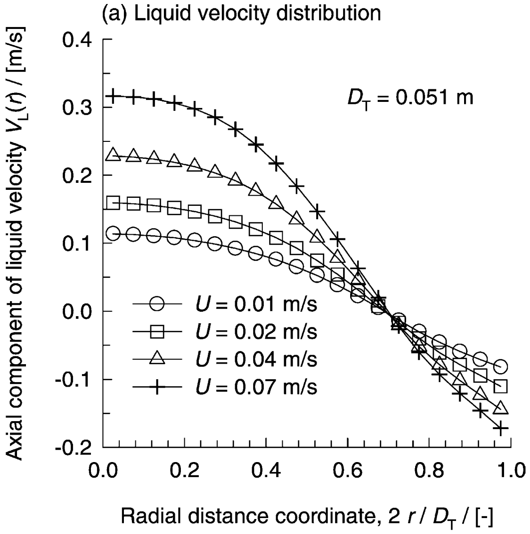


Fig. 4. Gas holdup vs. superficial gas velocities for 0.051 and 1 m diameter columns. Comparison of simulations with experiments, and scale effect shown by simulations.


(a) Liquid velocity distribution

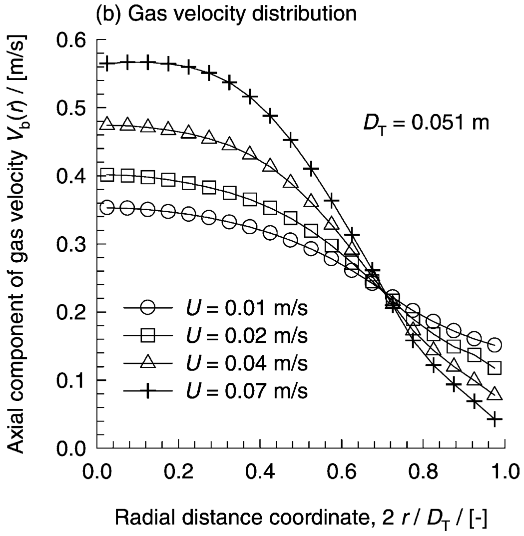
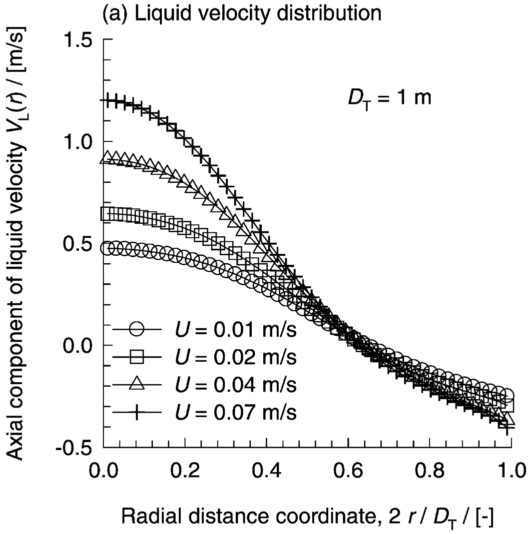

(b) Gas velocity distribution

Fig. 5. Radial distribution of (a) liquid velocity $V_L(r)$ and (b) gas velocity $V_b(r)$ for varying superficial gas velocities U in 0.051 m diameter column.


(a) Liquid velocity distribution

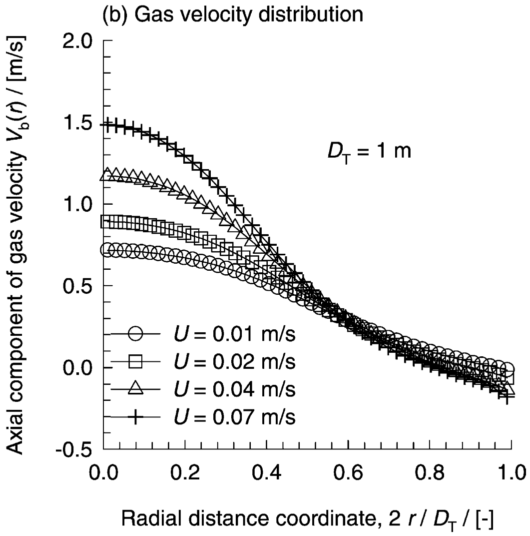

(b) Gas velocity distribution

Fig. 6. Radial distribution of (a) liquid velocity $V_L(r)$ and (b) gas velocity $V_b(r)$ for varying superficial gas velocities U in 1 m diameter column.

that the liquid circulation velocities increase strongly with increasing superficial gas velocity U. As a result of the increased liquid circulations, the bubbles tend to rise faster in the central core, as is evidenced in the simulation results $V_b(r)$ in Fig. 5(b).

The simulated values of the gas holdup in the 1 m diameter column are significantly lower than for the 0.051 m diameter column; see Fig. 4. This result can be rationalised when we consider the radial distribution of the liquid and gas (bubble) velocities, respectively, $V_L(r)$ and $V_b(r)$ for the 1 m diameter column; see Fig. 6(a) and (b). The circulation velocities are significantly higher than the corresponding values for the 0.051 m diameter column. This is further emphasised in Fig. 7 in which the axial component of the liquid velocity $V_L(0)$ is compared for the two column diameters as a function of the superficial gas velocity.

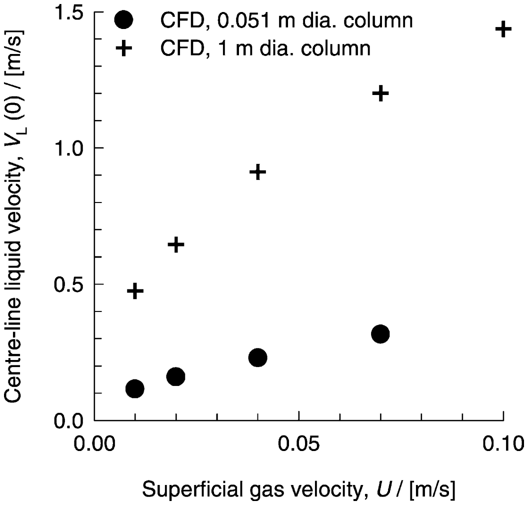


Fig. 7. Influence of column diameter on the axial component of liquid velocity in the centre of column $V_L(0)$.

5. Conclusions

In this paper, we have put forward a scale-up strategy for bubble column slurry reactors with concentrated slurries, using CFD as a pivotal tool. In such columns, the bubble dispersion consists almost exclusively of 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 ethanol with 16 wt.% Co catalyst a value $V_{b0} = 0.235\,\mathrm{m\,s^{-1}}$ is obtained; see Fig. 2. This value of V_{b0} is used to estimate the drag coefficient C_D (or actually $(3/4)(C_D/d_b)\rho_L$) 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 the 0.051 m diameter column. Simulations for a 1 m diameter column show the extremely strong scale dependence, which tends to reduce the gas holdup significantly.

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