CFD: a design and scale-up tool for multiphase reactors
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Chapter 6

Scaling up bubble columns using 2D simulations

Abstract
This paper develops a strategy for scaling up bubble column reactors operating in the churn-turbulent flow regime using Computational Fluid Dynamics (CFD). The bubble column is considered to be made up of three phases: (1) liquid, (2) "small" bubbles and (3) "large" bubbles and the Eulerian description is used for each of these phases. The three-phase description of bubble columns was implemented within the Eulerian framework of a commercial code CFX 4.2 of AEA Technology, Harwell, UK. Cylindrical axi-symmetry was assumed. Simulations for columns with diameters ranging from 1 to 6 m were carried out to emphasise the strong influence of scale on the hydrodynamics.

1. Introduction
Bubble column reactors operated in industry have several distinguishing features: (1) large column diameters are involved, ranging to 6 m, (2) high superficial gas velocities, in the 0.1 - 0.4 m/s range, are usually used, (3) the system pressure can range to 6 MPa and (4) the liquid phase often consists of a non-aqueous hydrocarbon mixture (Krishna et al., 1996). Laboratory studies on bubble column hydrodynamics are usually carried out with the air-water system, at ambient pressure conditions, in columns that are smaller than say 0.5 m in diameter (Deckwer, 1992). Even for the air-water system, available literature correlations give significantly different results. This is demonstrated by the predictions of the total gas holdup and the centre-line liquid velocity as a function of the superficial gas velocity and column diameter; see Figures 1 and 2. Only two correlations plotted in Fig. 1 anticipate that the gas holdup decreases with increasing column diameter. We see from Fig. 2 (b) that the predictions of the centre-line velocity for a bubble column of diameter 6 m diameter operating at \( U = 0.3 \) m/s varies between 0.9 and 4.5 m/s. This represents a variation of a factor of five and so there is a clear need for a reliable scale up strategy.

2. Eulerian simulations of large diameter bubble columns
Simulations were carried out for air-water and air-Tellus oil systems for column diameters ranging from 0.1 to 6 m, operating at two different superficial gas velocities, \( U = 0.16 \) and 0.30 m/s. Details of the column configurations and the grids used are specified in Table 1. Figure 4 shows the grid cell configuration. From the Reilly et al. (1994) correlation it was determined that the superficial gas velocity at the regime transition point for air-water \( U_{trans} = 0.034 \) m/s. For air-water operation at \( U < 0.034 \) m/s, homogeneous bubbly flow regime was taken to prevail. Therefore, only two phases, small bubbles and liquid are present. For churn-turbulent operation at \( U > 0.034 \) m/s, the complete three phase model was invoked. Following the model of Krishna and Ellenberger (1996) we assume that in the churn-turbulent flow regime the superficial gas velocity through the small bubble phase is \( U_{trans} = 0.034 \) m/s (see Fig. 3). The remainder of the gas \((U - U_{trans})\) was taken to rise up the column in the form of large bubbles. This implies that at the distributor the "large" bubbles constitute a fraction \((U - U_{trans}) / U\) of the total incoming volumetric flow, whereas the "small" bubble constitute a fraction \(U_{trans} / U\) of the total incoming flow. Strictly speaking, \(U_{trans}\) is a model parameter and its choice has a significant increasing effect on the small bubble holdup but its influence
on the centre-line velocity is negligible (Krishna et al., 1999b). The air-Tellus oil system was modelled as consisting of two phases: large bubbles and liquid, which corresponded closely with our experimental observations.

The major objective of the present paper is to develop a model for predicting the scale dependence of the hydrodynamics of bubble column reactors operating in the churn-turbulent regime. The model is identical to the one described in Chapter 5 and is pictured in Fig. 3.

**Fig. 1.** Comparison of literature correlations for the total gas holdup $\varepsilon$ for air-water system in column of 0.38 m diameter. (a) Variation of $\varepsilon$ with superficial gas velocity for a column of 0.38 m diameter. (b) Variation of $\varepsilon$ with column diameter for a superficial gas velocity of 0.3 m/s. The plotted correlations are: (1) Krishna and Ellenberger (1996); (2) Wilkinson et al. (1992); (3) Zehner (1989); (4) Akita and Yoshida (1973); (5) Bach and Pilhofer (1978); (6) Reilly et al. (1986); (7) Hikita et al. (1980); (8) Hughmark (1967).

**Fig. 2.** Comparison of literature correlations for the centre-line velocity $V_{L}(0)$ for air-water system. (a) Variation of $V_{L}(0)$ with superficial gas velocity for a column of 0.38 m diameter. (b) Variation of $V_{L}(0)$ with column diameter for a superficial gas velocity of 0.3 m/s. The plotted correlations are: (1) Ohki and Inoue (1970); (2) Ueyama and Miyauuchi (1979); (3) Joshi (1980); (4) Riquarts (1981); (5) Zehner (1986); (6) Nottenkämper et al. (1983); (7) Ulbrecht et al. (1985); (8) Kawase and Moo-Young (1989); (9) Bernemann (1989).
Fig. 3. Three-phase model for bubble columns operating in the churn-turbulent regime.

Table 1.
Column configurations, systems, operating conditions and grid details of CFD simulations. For operation at $U < U_{\text{trans}}$, homogeneous bubbly flow regime was taken to prevail. For operation at $U > U_{\text{trans}}$, the complete three phase model was invoked. The large bubble phase was injected over the central 32 of 75 grid cells. The small bubble phase was injected over the central 61 of 75 grid cells. The reported liquid velocity profiles are at the observation heights reported below. The reported values of the total gas holdup refer to the fractional gas volume below this observation height.

<table>
<thead>
<tr>
<th>Liquid Phase</th>
<th>Column Diameter $D_T$ [m]</th>
<th>Column height $h$ [m]</th>
<th>Initial Liquid height $h_L$ [m]</th>
<th>Observation Height $h_O$ [m]</th>
<th>Number of grid cells $N$ (radial) $\times$ (axial)</th>
<th>Superficial gas velocity, $U_{\text{gas}}$ [m/s]</th>
<th>$U_{\text{trans}}$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>1</td>
<td>7</td>
<td>4</td>
<td>4</td>
<td>$75 \times 150$</td>
<td>0.3</td>
<td>0.034</td>
</tr>
<tr>
<td>Water</td>
<td>1.5</td>
<td>8</td>
<td>4.8</td>
<td>4.8</td>
<td>$75 \times 410$</td>
<td>0.3</td>
<td>0.034</td>
</tr>
<tr>
<td>Water</td>
<td>2</td>
<td>13,12</td>
<td>10,7</td>
<td>9,7</td>
<td>$75 \times 250$</td>
<td>0.16, 0.3</td>
<td>0.034</td>
</tr>
<tr>
<td>Water</td>
<td>3</td>
<td>15</td>
<td>10</td>
<td>10</td>
<td>$75 \times 310$</td>
<td>0.3</td>
<td>0.034</td>
</tr>
<tr>
<td>Water</td>
<td>4</td>
<td>25</td>
<td>20</td>
<td>18</td>
<td>$75 \times 510$</td>
<td>0.16, 0.3</td>
<td>0.034</td>
</tr>
<tr>
<td>Water</td>
<td>6</td>
<td>35</td>
<td>25,20</td>
<td>18</td>
<td>$75 \times 710$</td>
<td>0.16, 0.3</td>
<td>0.034</td>
</tr>
<tr>
<td>Tellus oil</td>
<td>1.5</td>
<td>8</td>
<td>5.3</td>
<td>4.5</td>
<td>$75 \times 410$</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>Tellus oil</td>
<td>2</td>
<td>13</td>
<td>10</td>
<td>9</td>
<td>$75 \times 270$</td>
<td>0.16, 0.3</td>
<td>0</td>
</tr>
<tr>
<td>Tellus oil</td>
<td>2</td>
<td>13</td>
<td>10</td>
<td>9</td>
<td>$75 \times 780$ (finer grid)</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>Tellus oil</td>
<td>4</td>
<td>25</td>
<td>20</td>
<td>20</td>
<td>$75 \times 510$</td>
<td>0.16, 0.3</td>
<td>0</td>
</tr>
<tr>
<td>Tellus oil</td>
<td>6</td>
<td>35</td>
<td>20</td>
<td>20</td>
<td>$75 \times 710$</td>
<td>0.16, 0.3</td>
<td>0</td>
</tr>
</tbody>
</table>
A further assumption made is that the formation of the large bubbles takes place immediately at the distributor; this is essentially a simplification and the justification for this is that our experimental studies show that the "large" bubbles equilibrate within a distance of 0.1 m above the distributor (Ellenberger and Krishna, 1994). The diameter of the "small" bubbles was chosen to be 4 mm in all the simulations for the air-water system. The estimation of the drag coefficients for the small and large bubbles follows the same procedure as outlined in Chapter 5. The large bubbles were injected in the central core of the column because this is in conformity with visual observations. The small bubbles were distributed uniformly over the whole column with the exception of the wall region. The precise injection strategy was not found to influence the results provided the wall region was kept free of gas injection.

All simulations were carried out using cylindrical axi-symmetry. The time stepping strategy used in the transient simulations for attainment of steady state was typically: 20 steps at $5 \times 10^{-3}$ s, 20 steps at $1 \times 10^{-3}$ s, 460 steps at $5 \times 10^{-3}$ s, 3000 steps at $2 \times 10^{-2}$ s. Columns smaller than 2 m in diameter were carried out on a Silicon Graphics Power Indigo workstation with the R8000 processor. In all the runs, steady state was reached within 2500 time steps. Simulations of the columns larger than 2 m in diameter were carried out on a Power Challenge machine employing three R10000 processors in parallel.

Further details of the 2D simulations, including animations of column start-up dynamics are available on our web sites: http://ct-cr4.chem.uva.nl/euler2D and http://ct-cr4.chem.uva.nl/oil-water.
3. Simulation results

In all the simulations the column height to diameter ratio was kept to about five. For the 6 m diameter column the total column height was 35 m. Use of 10 mm grid cells, typically used in the simulations in Chapter 5, is not practical. Coarser grids were used as specified in Table 1. For columns larger than 2 m in diameter we use 50 mm grid cells in the vertical direction. For the 6 m column, for example, the total number of grid cells used was 75x710 = 53250 cells. Before proceeding to discuss the simulation results, we verify grid convergence. For this purpose the air-Tellus oil simulation in a 2 m diameter column operating at 0.16 m/s was run with two different grid configurations. In the coarse grid configuration a total of 270 cells were used along the column height. In the finer grid configuration a total of 780 cells were used along the column height. In both cases the number of grid cells in the radial direction was 75. The radial liquid velocity distributions with these two grid strategies are compared in Fig. 5. The results are indistinguishable. The gas holdup for these two grids agreed to within 2%.

The centre-line liquid velocity and cumulative gas holdup vary along the column height in the region close to the distributor; see Fig. 6. However for the high dispersion heights used the variations tend to even out. The reported $V_L(0)$ and $V_L(r)$ are at the observation heights specified in Table 1. The gas holdups are the cumulative values below the observation height specified.

The most dramatic expression of the scale effect is noticed when we compare the $V_L(r)$ as a function of the column diameter for a particular case, that of air-water operating at $U = 0.3$ m/s; see Fig. 7. The centre-line velocity for the 6 m diameter column $V_L(0) = 4.5$ m/s.

When comparing air-water and air-Tellus oil simulations at the same value of $U$, we note that the liquid velocity distribution $V_L(r)$ is virtually the same; see Fig. 8. A similar observation was reached earlier in Chapter 5 for a smaller diameter column.

For superficial gas velocities of 0.16 and 0.3 m/s, Eulerian simulations were carried out to study the influence of column diameter. The results for air-water and air-Tellus oil are shown in Figs 9 and 10. For air-water system the predictions of $V_L(0)$ agree remarkably well with that of Riquarts (1981)

$$V_L(0) = 0.21(gD_T)^{1/2}(U^3 / gV_L)^{1/8}$$

and demonstrate extremely strong scale dependence. The Riquarts correlation can also be used for the air-Tellus oil results provided we use the kinematic viscosity of water (!). The data for both systems are compared with the Riquarts (1981) correlation in Fig. 11.

Due to the strong liquid circulations with increasing column diameter, the bubbles will be accelerated. This acceleration effect causes a significant reduction in the large bubble holdup with increasing column diameter; see Figs 9 (a), (b) and 10 (a), (b). Also shown are the calculations of the large bubble holdup using the correlation of Krishna and Ellenberger (1996):

$$\epsilon_{b, large} = 0.268 \frac{1}{D_T^{0.18}} \frac{1}{(U-U_{trans})^{0.22}} (U-U_{trans})^{1/5}$$

where we have used $U_{trans} = 0$ for air-Tellus oil system. The decrease in the large bubble holdup with column diameter from the Eulerian simulations is stronger than anticipated by eq. (2).
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- **Fig. 5.** Test of grid convergence.

- **Fig. 6.** Variation of $V_L(0)$ and cumulative gas holdup with dispersion height.
Fig. 7. Scale effect on the radial distribution of liquid velocity.
Fig. 8. Comparison of air-water and air-Tellus oil simulations.
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Fig. 9. Influence of scale on the holdup of large bubbles and on the centre-line liquid velocity for air-water.

Fig. 10. Influence of scale on the holdup of large bubbles and on the centre-line liquid velocity for air-Tellus oil.
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Fig. 11. Comparison of Riquarts correlation (1) with Eulerian simulations for air-water and air-Tellus oil, details of which are given in Table 1. We take \( v_L = 10^{-6} \text{ m}^2/\text{s} \) for both water and Tellus oil, when applying eq. (1).

4. Conclusions

The following major conclusions can be drawn from the present work:

1) Eulerian simulations of the scale dependence of the centre-line \( V_L(0) \) shows that these velocities can approach values of about 4 – 5 m/s when the column diameter is increased to 6 m. The simulations further show that the liquid viscosity has practically no effect on \( V_L(0) \). On the basis of the Eulerian simulations we are able to recommend the use of the Riquarts correlation (eq. 1) provided we use the kinematic viscosity of water for all systems.

2) The strong increase in \( V_L(0) \) with scale has the effect of accelerating the gas bubbles leading to significant reduction in the gas holdup; this is underlined in the simulation results of Figs 9 and 10. The reduction in holdup is significantly stronger than that anticipated by the Krishna-Ellenberger (1996) correlation. Experimental data in the literature on gas holdup and \( V_L(0) \) in the churn-turbulent regime are restricted to columns smaller than 1 m in diameter. Therefore there is a need for experimental verification with larger column diameters in order to verify the strong scale dependence anticipated by the Eulerian simulations.