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Chapter 3  

Rise of spherical cap bubbles and in-line bubble pair interaction

Abstract
The rise velocity of a single spherical cap bubble in an infinitely large liquid medium is given by the classical Davies-Taylor (1950) relation \( V_b^0 = 0.71 \sqrt{g d_b} \). In order to account for wall-effects, Collins (1967) introduced a scale factor SF that is a function of the ratio of the bubble diameter \( d_b \) to the column diameter \( D_c \): \( V_b^0 = 0.71 \sqrt{g d_b} (SF) \). We carried out Volume-of-Fluid (VOF) simulations to confirm the validity of the Davies-Taylor-Collins relations for a variety of liquid properties.

We also studied in-line interaction between two spherical cap bubbles. The trailing bubble gets sucked into the wake of the leading bubble and gets accelerated. The rise velocity of the trailing bubble can be expressed as \( V_h = 0.71 \sqrt{g d_b} (SF) (AF) \). The acceleration factor \( AF \) accounts for the increase in the rise velocity of a bubble because of its interaction with the wake of a bubble preceding it. It is found that the acceleration factor \( AF \) increases linearly as the vertical distance of separation between the two bubbles decreases. Increasing liquid viscosity reduces this wake acceleration effect. Volume-of-Fluid simulations of in-line interactions of spherical cap bubbles show excellent agreement with experiments carried out by Urseanu (2000).

On the basis of the insights gained in this work we develop a relation for the large bubble swarm velocity which could be used in Eulerian simulations of bubble columns operating in the churn-turbulent flow regime.

1. Introduction
For estimation of the gas holdup in bubble columns operating in the churn-turbulent flow regime we need to predict the rise velocity of a swarm of large spherical cap gas bubbles in liquids. There are two empirical correlations for estimating the rise velocity of swarms of large bubbles. The first one due to Wilkinson et al. (1992) is

\[
\frac{V_h \mu_L}{\sigma} = 2.25 \left( \frac{\sigma^3 \rho_L}{g \mu_L^4} \right)^{0.273} \left( \frac{\rho_L}{\rho_\infty} \right)^{0.053} + 2.4 \left( \frac{U - U_{\text{trans}}}{\mu_L} \right)^{0.757} \left( \frac{\sigma^3 \rho_L}{g \mu_L^4} \right)^{0.077} \left( \frac{\rho_L}{\rho_\infty} \right)^{0.077}
\]

(1)

where \( U_{\text{trans}} \) is the superficial gas velocity at the point of transition from homogeneous to heterogeneous flow regime. The superficial gas velocity through the large bubble phase is \((U - U_{\text{trans}})\). It is important to note that the Wilkinson correlation does not anticipate that the large bubble rise velocity is column diameter dependent. In a more recent paper, Krishna and Ellenberger (1996) used an extensive set of experimental data obtained in columns of 0.1, 0.174, 0.19, 0.38 and 0.63 m in diameter and with liquids of varying physical properties. They found that the large bubble rise velocity is virtually independent of the properties of the liquid phase but increases significantly with increasing column diameter. They developed the correlation:

\[
V_h \equiv (U - U_{\text{trans}}) / \epsilon_b = D_f^{0.18} (U - U_{\text{trans}})^{0.42} / 0.268
\]

(2)
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Krishna and Ellenberger recommend the use of the Reilly et al. (1994) correlation for the estimation of $U_{\text{trans}}$. An important disadvantage of the Krishna-Ellenberger correlation (2) is that extrapolation to commercial scale reactors is fraught with danger because of the power-law dependence of the large bubble rise velocity on the column diameter. Krishna et al. (1996) suggest the use of eq. (2) up to diameters of 1 m and assert, using analogy with gas-solid fluid beds, that the column diameter dependence ceases after this point. A further point of criticism of both correlations (1) and (2) above is that these cannot be incorporated into more fundamentally based bubble column reactor models using Computational Fluid Dynamics (CFD). Such CFD models, within the Eulerian framework require information on the large bubble sizes and on the interface momentum exchange, or drag, coefficients. (see e.g. Jakobsen et al., 1997).


The objective in this chapter is to use Volume-of-Fluid (VOF) simulation techniques to study the rise of single spherical cap bubbles in liquids and their interactions. Furthermore, on the basis of this insight we develop a relationship for the large bubble swarm velocity. Experimental data of Urseanu (2000) are used for validation of the VOF simulations.

2. Rise velocity of single spherical cap bubbles

When the criterion $E_o > 40$, single gas bubbles assume a spherical cap shape (see Clift et al., 1978). In order to describe the rise velocity of these bubbles we introduce a scale factor correction into the Davies-Taylor (1950) relation

$$V_{b_0} = 0.71 \sqrt{gd_b} \text{(SF)}$$

(3)

where the superscript 0 is used to emphasise that the rise velocity refers to that of a single, isolated, bubble. Collins (1967) has derived the following empirical relations for the scale factor:

$$SF = 1 \quad \text{for } \frac{d_b}{D_t} < 0.125$$

$$SF = 1.13 \exp(- \frac{d_b}{D_t}) \quad \text{for } 0.125 < \frac{d_b}{D_t} < 0.6$$

$$SF = 0.496 \sqrt{D_t/d_b} \quad \text{for } \frac{d_b}{D_t} > 0.6$$

(4)

The measured experimental data of Urseanu (2000) conform exceedingly well with the calculations using eqs (3) and (4); see Figs 1 (a) and (b) for water and Tellus oil respectively. The strong influence of scale on the bubble rise velocity is demonstrated graphically in Fig. 2 which shows retraced video images recording the rise of a 34 mm bubble in columns of 0.051 and 0.1 m diameter filled with water. It is to be noted that the bubble appears to be flatter in the 0.1 m diameter column.
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**Fig. 1.** Scale effects for rise of single gas bubbles in cylindrical columns.  
(a) comparison of data for air-water with the Davies-Taylor-Collins model, eqs (3)-(4).  
(b) comparison of data for air-Tellus oil with eqs (3)-(4).  
(c) Comparison of VOF simulations with eqs (3)-(4).

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**Fig. 2.** Comparison of the rise trajectories of a 34 mm diameter bubble rising in water in columns of 0.051 and 0.1 m diameter. Experimentally obtained video images have been retraced. Measurements of Urseanu (2000).
3. Volume-of-Fluid simulations

To understand the scale effects on rise of spherical cap bubbles we undertook Volume-of-Fluid (VOF) simulations. The VOF model (Delnoij et al. 1997b, Hirt and Nichols 1981, Tomiyama et al. 1993a/1993b) resolves the transient motion of the gas and liquid phases using the Navier-Stokes equations, and accounts for the topology changes of the gas-liquid interface induced by the relative motion between the dispersed gas bubble and the surrounding liquid. The finite-difference VOF model uses a donor-acceptor algorithm, originally developed by Hirt and Nichols (1981), to obtain, and maintain, an accurate and sharp representation of the gas-liquid interface. The VOF method defines a fractional volume or "colour" function $c(x,t)$ that indicates the fraction of the computational cell filled with liquid. The colour function varies between 0, if the cell is completely occupied by gas, and 1, if the cell consists only of the liquid phase. The location of the bubble interface is tracked in time by solving a balance equation for this function:

$$\frac{\partial c(x,t)}{\partial t} + \nabla \cdot (uc(x,t)) = 0 \quad (5)$$

The liquid and gas velocities are assumed to equilibrate over a very small distance and essentially $u_t = u$ for $\alpha = L, G$ at the bubble interface. The mass and momentum conservation equations can be considered to be homogenous:

$$\nabla \cdot (\rho u) = 0 \quad (6)$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p - \nabla \cdot \tau + \rho g + F_{sf} \quad (7)$$

where $p$ is the pressure, $\tau$ is the viscous stress tensor, $g$ is the gravitational acceleration. The density and viscosity used in eqs (6) and (7) are calculated from:

$$\rho = \varepsilon_L \rho_L + \varepsilon_G \rho_G$$

$$\mu = \varepsilon_L \mu_L + \varepsilon_G \mu_G \quad (8)$$

where $\varepsilon_\alpha$ denotes the volume fraction of the phase $\alpha = L, G$. The continuum surface force model, originally proposed by Brackbill et al. (1992), is used to model the force due to surface tension acting on the gas-liquid interface. In this model the surface tension is modelled as a body force $F_{sf}$ that is non-zero only at the bubble interface and is given by the gradient of the colour function:

$$F_{sf} = \sigma \vartheta(x) \nabla c(x,t) \quad (9)$$

where $\vartheta(x)$ is the local mean curvature of the bubble interface:

$$\vartheta(x,t) = -\nabla \cdot \left( \frac{n}{|n|} \right) \quad (10)$$

where $n$ is the vector normal to the bubble interface:

$$n = \nabla c(x,t) \quad (11)$$

The set of equations (5) – (11) were solved using the commercial flow solver CFX 4.1c of AEA Technology, Harwell, UK. 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 (1983) algorithm is used to calculate the velocity at the
cell faces. The pressure-velocity coupling is obtained using the SIMPLER algorithm (Van Doormal and Raithby, 1984).

Table 1 lists the VOF simulations performed for single bubbles rising in a cylindrical column filled with liquid, which was taken to be water, paraffin oil or ethylene glycol. Since spherical cap bubbles rise vertically in a straight line, axis-symmetry was assumed in these simulations. A uniform grid of 1 mm size in both \( r \) and \( z \) directions was used. The column was modelled as an open system, so the pressure in the gas space above the initial liquid column is equal to the ambient pressure (101.325 kPa). For the convective terms in the equations hybrid differencing was used. Upwind differencing was used for the time integration. The time step used in the simulations were usually 0.0004 s or smaller. To counteract excessive smearing of the liquid-gas interface by numerical diffusion, a surface sharpening routine was invoked. This routine identifies gas and liquid on the “wrong” side of the interface, and moves it back to the correct side, while conserving volume of the respective phases. In order to avoid “dissolution” of the bubble due to surface sharpening we found it necessary to ensure that each bubble area encompassed a few hundred cells; a grid cell size of 1 mm satisfied this requirement and in all the simulations there was less than 10% volume (or area) change during the simulation. Simulations carried out with a 2 mm grid size did not meet with the above requirement while simulations with a finer grid size than 1 mm did not yield significantly different results.

**Table 1.**

Results of axi-symmetric VOF simulations in cylindrical coordinates. In all cases the grid size chosen was \( \Delta r, \Delta z = 1 \) mm. The systems were either air-water (\( \rho_L = 998; \mu_L = 0.001; \sigma = 0.072 \)), air-paraffin oil (\( \rho_L = 795; \mu_L = 0.0023; \sigma = 0.028 \)) or air-ethylene glycol (\( \rho_L = 1109; \mu_L = 0.0199; \sigma = 0.0477 \)).

<table>
<thead>
<tr>
<th>Bubble diameter, ( d_b / [\text{m}] )</th>
<th>Column diameter, ( D_c / [\text{m}] )</th>
<th>System</th>
<th>Time step, ( \Delta t / [\text{s}] )</th>
<th>Rise velocity, ( V_r / [\text{m s}^{-1}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.021</td>
<td>0.1</td>
<td>air-water</td>
<td>0.0004</td>
<td>0.289</td>
</tr>
<tr>
<td>0.021</td>
<td>0.051</td>
<td>air-water</td>
<td>0.0004</td>
<td>0.244</td>
</tr>
<tr>
<td>0.029</td>
<td>0.051</td>
<td>air-water</td>
<td>0.0004</td>
<td>0.248</td>
</tr>
<tr>
<td>0.027</td>
<td>0.051</td>
<td>air-paraffin oil</td>
<td>0.0003</td>
<td>0.249</td>
</tr>
<tr>
<td>0.039</td>
<td>0.051</td>
<td>air-ethylene glycol</td>
<td>0.0003</td>
<td>0.25</td>
</tr>
</tbody>
</table>

All simulations were carried out using the parallel version of CFX 4.1c running on Silicon Graphics Power Challenge machine with six R8000 processors. To give an indication of the required CPU time, the axi-symmetric simulation of the rise of a 27 mm bubble for 0.83 s in a 0.051 m diameter cylindrical column of 0.5 m height, filled with paraffin oil, involving 13000 grid cells took 4 days. Snapshots at various time steps for this simulation are shown in Fig. 3. As initial condition a spherical bubble, was placed near the bottom of the column. To ensure convergence in the initial period when the bubble “adjusts” itself to its surrounding and begins its ascent, the following time stepping strategy was used: 50 steps at \( 5 \times 10^{-5} \) s, 50 steps at \( 2.5 \times 10^{-5} \) s, 50 steps at \( 5 \times 10^{-5} \) s and 3000 steps at \( 3 \times 10^{-4} \) s. For each time step about 40 iterations were typically required to obtain convergence of the governing equations. The grid size and time steps used in our work are significantly finer than those used by other workers using VOF simulations (e.g. Delnoij et al., 1997b). This would tend to compensate for the fact that the Hirt-Nichols Donor-Acceptor algorithm used in the CFX implementation of the VOF algorithm is considered to be rather "crude" compared to the more sophisticated algorithms.
available currently (Delnoij et al., 1997b). It can be noted from Fig. 3 that small fragments of the bubble are torn off in the initial stages and these fragments “dissolve” away due to application of the surface sharpening procedure and also due to numerical diffusion. The bubble diameters reported in Table 1 were determined from the volume of the remaining bubble, which typically attains its terminal velocity after about 0.15 s from the start of the simulation. The bubble rise velocity was determined by a linear regression of the z-coordinates of the nose of the bubble during steady-rise.

![Figure 3](image1.png)

**Fig. 3.** Snapshots obtained with axi-symmetric cylindrical VOF simulations of rise of a 27 mm diameter bubble in a column of 0.051 m diameter. The system is air-paraffin oil.

![Figure 4](image2.png)

**Fig. 4.** VOF simulations of the rise trajectories of a 21 mm diameter bubble in 0.051 and 0.1 m diameter columns. The insets show the liquid phase velocity profiles surrounding the bubble.
Figure 4 compares the z-coordinates of the nose of 21 mm bubbles rising in columns of 0.1 and 0.051 m diameters filled with water; this figure shows that the bubble rises faster in the wider column. The reason for this is the restraining effect of the walls. The insets to Fig. 4 show the liquid phase velocity profiles for these two simulations. We notice that the 21 mm bubble assumes a flatter shape in the 0.1 m wide column and is less influenced by the wall than the same bubble placed in a 0.051 m wide column. This is in accordance with the video images obtained experimentally; see Fig. 2. Put another way, the drag between the bubble and the liquid is higher in the column of smaller width due to the higher downward liquid velocity in the vicinity of the bubble.

The five axi-symmetric cylindrical simulations for air-water, air-paraffin oil and air-ethylene glycol are in excellent agreement with the Davies-Taylor-Collins relations (3, 4); see Fig. 1 (c). Since the simulations were carried out with widely varying density, surface tension and viscosity values, we also conclude the general validity of eqs (3, 4) provided the condition of $E_o > 40$ is met.

4. In-line interactions of bubble pairs

Typical rise trajectories are shown in Fig. 5 for the in-line interactions of two 31-mm diameter bubbles in water. It is clear that the acceleration effect increases as the trailing bubble approaches the leading bubble.

![Fig. 5. Retraced video images of in-line interactions of 31 mm diameter bubbles rising in a 0.051 m diameter column filled with water. Experiments of Urseanu (2000).](http://ct-cr4.chem.uva.nl/axissym)

The VOF simulation of this experiment is shown in Fig. 6. The reason that the shape of the bubbles in the VOF simulations appears to be hollower than in the experiment is due to the fact that in the video recordings only the outer periphery of the bubbles can be visualised. The contours of the bubbles in Fig. 6, however, are drawn for a slice in the r-z plane. The liquid phase velocity profiles at 0.07 s before coalescence of the bubbles are indicated in the inset in Fig. 6. A comparison of the measured trajectories for both leading and trailing bubbles with VOF simulations shows very good agreement; see Fig. 7 (a). A similar good agreement between VOF simulations and experiment is obtained for the rise trajectories of two 31 mm bubbles rising in aqueous 86 wt% glycerol solution with a viscosity of 0.1 Pa s; see Fig. 7 (b). Animations of the VOF simulations performed to study in-line interactions of bubbles in various liquids can be viewed on our web site (http://ct-cr4.chem.uva.nl/axissym).
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Fig. 6. VOF simulations, using cylindrical axi-symmetry, of the experiment shown in Fig. 5. The inset shows the liquid phase velocity profiles for the situation corresponding to 0.07 s before coalescence. Animations of this VOF simulation can be viewed on our web site (http://ct-cr4.chem.uva.nl/axissym).

Fig. 7. Comparison between experiment and VOF simulations of the rise trajectories of the leading and trailing bubbles in a 0.051 m diameter column filled with (a) water and (b) 86 wt% glycerol solution. Animations of these VOF simulations can be viewed on our web site (http://ct-cr4.chem.uva.nl/axissym).
5. The acceleration factor

The slope of the rise trajectory at any instant of time yields the rise velocity. We define an acceleration factor, $AF$, for the trailing bubble as the ratio of the actual velocity to the velocity it would have were the same bubble uninfluenced by other bubbles; this latter velocity can be obtained from eqs (3) and (4). In Fig. 8 the experimentally observed acceleration factor (which corresponds to that from VOF simulations) for the trailing bubble is plotted against its distance of separation, $\Delta z$, from the leading bubble. The acceleration factor $AF$ is seen to increase as $\Delta z$ decreases in a more or less linear fashion. For a given separation distance, the value of $AF$ decreases with increasing liquid viscosity. For example when $\Delta z = 0.05$ m, the value of $AF$ for water ($\mu_L = 0.001$) is 3, for Tellus oil ($\mu_L = 0.075$), $AF = 2.5$ and for 86 wt% glycerol ($\mu_L = 0.147$), $AF = 2$. The wake interaction effects are weaker in highly viscous liquids. The wake interaction effects in low viscosity liquids (say with $\mu_L < 0.003$ Pa s) can be expected to be of comparable magnitude.

![Image](Figura 8.png)

**Fig. 8.** The acceleration factor for the trailing bubble as function of its distance of separation from the preceding bubble. The measurements with Tellus oil were made in a 0.1 m diameter column and those with water and 86 wt% aqueous glycerol solution were made in a 0.051 m diameter column.

6. Rise velocity of large bubble swarms

For steady-state mode of operation in the churn-turbulent regime, every large bubble is a “trailing” bubble. The large bubble swarm velocity can therefore be expected to be much higher than that of a single, isolated, bubble, $V_b^0$. From the foregoing section we should expect the acceleration factor to increase linearly with decreasing distance of separation of the bubbles. With increasing values of $(U - U_{trans})$ we should expect the average distance of separation between the large bubbles to decrease. We therefore assert that

$$V_b = V_b^0 (AF)$$

$$AF = \alpha + \beta(U - U_{trans})$$

(12)
where $V_b^0$ is given by eqs (3) and (4). The experimental data on $V_b$ as a function of $(U - U_{trans})$ we collected earlier (Krishna and Ellenberger 1996, De Swart 1996), comprising of more than 1000 measured points with liquids of relatively low viscosity (less than 0.0029 Pa s) were used to obtain the following expressions for the average large bubble diameter and the acceleration factor, $AF$:

$$d_b = 0.069(U - U_{trans})^{0.376}$$
$$AF = 2.73 + 4.505(U - U_{trans})$$  \hspace{1cm} (13)$$

In obtaining the fits, only experimental data with $(U - U_{trans})$ values exceeding 0.05 m/s were used. This truncation was necessary in order to ensure that the large bubble sizes met with the Eö > 40 criterion required of the Davies-Taylor-Collins relations (3) and (4). The four fit parameters in eq. (13) were determined by the multiple regression solver routine of Microsoft Excel 97 in which the mean square deviation between experiments and model equations were minimised. The correlation (13) is only valid when the Eö > 40 criterion is met for the predicted bubble sizes. The fitted bubble size correlation agrees remarkably well with the measured data on average large bubble diameters carried out earlier in our group (De Swart 1996, De Swart et al. 1996) for the systems air-water and air-paraffin oil in a 2D rectangular column of 0.3 m width; see Fig. 9. There are no other reported large bubble size correlations available in the literature. In Fig. 10 (a) we compare the experimental values of the acceleration factor $AF$ (calculated with the fitted bubble size expression) against the correlation line given by eq. (13).

![Graph showing correlation for average bubble size of large bubble swarm as function of superficial gas velocity through large bubble population. The experimental data is from De Swart (1996) measured with systems air-water and air-paraffin oil in a 2D rectangular column of 0.3 m width at different heights $h$ above the distributor.]

**Fig. 9.** Correlation for the average bubble size of large bubble swarm as function of the superficial gas velocity through the large bubble population. The experimental data is from De Swart (1996) measured with the systems air-water and air-paraffin oil in a 2D rectangular column of 0.3 m width at different heights $h$ above the distributor.
From the measurements made by Urseanu (2000) in her study with the system air-Tellus oil ($\mu_L = 0.075$), the corresponding fits for the bubble size and acceleration factors are:

\[
\begin{align*}
    d_b &= 0.069(U - U_{\text{trans}})^{0.376} \\
    AF &= 2.25 + 4.09(U - U_{\text{trans}})
\end{align*}
\]  

(14)

As expected the $AF$ for the high viscosity Tellus oil is lower by about 20% than for low viscosity liquids such as water and paraffin oil; see Fig. 10 (b).

The results of the present chapter can be easily incorporated into CFD models of bubble columns by using the drag coefficient defined by

\[
    C_D = \frac{4}{3} \frac{\rho_L - \rho_G}{\rho_L} g d_b \frac{1}{V_{h}^2}
\]

(15)

for the large bubble population. The drag coefficient thus calculated represents an averaged value over the range of bubble sizes actually encountered in practice. The acid test of the validity of the developed drag relation would be to carry out Eulerian simulations of bubble columns in the churn-turbulent regime. Eulerian simulations of bubble columns using eq. (15) for the drag coefficient for the large bubbles are presented in Chapters 5, 6 and 7.

**Fig. 10.** The acceleration factor for large bubble velocity swarm in (a) low viscosity liquids (water, paraffin oil, tetradecane) and (b) high viscosity liquids (Tellus oil).
7. Conclusions

1. For rise of single spherical cap bubbles (meeting with the criterion $E_0 > 40$) in cylindrical columns, the Davies-Taylor-Collins relations (3) and (4) are found to be of excellent accuracy. VOF simulations, using axi-symmetric cylindrical coordinate geometry, are in excellent agreement with experiments and represent a powerful tool for \textit{a priori} prediction of scale effects on single bubble rise for gas-liquid systems with widely varying properties.

2. VOF simulations of in-line bubble pair interactions are in excellent agreement with experiment.

3. The acceleration factor $AF$ depends on the liquid viscosity; higher viscosities lead to lower wake acceleration effects.

4. The empirically fitted relations (13) and (14) allow estimation of the large bubble size and acceleration factor in liquids of low and high viscosity respectively. These relations are used in Eulerian simulations of bubble columns in Chapters 5, 6 and 7.