Direct numerical simulation of the drag force in bubble swarms

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Abstract

This paper studies the swarm effect on the drag force in bubbly flows. From literature it is well-known that for relatively small bubbles, the drag force increases with the bubble hold-up due to additional hindrance experienced by the bubbles caused by the modified flow field. Very large (spherical cap) bubbles on the other hand may rise cooperatively. The unique capabilities of a 3D Front Tracking model were used to investigate the influence of important parameters like the gas fraction, Reynolds number and the bubble size independently. It was found that the relative drag force increases for bubbles in the range of 2 to 5 mm when the gas fraction is increased up to 13%, while the bubbles become more spherical. Also the influence of the Reynolds number and the bubble aspect ratio on the increased drag force has been determined. It can be concluded that there is only a very weak effect over several decades of the Reynolds number, while there is a strong effect of the bubble aspect ratio. This also helps explaining why the increase in drag is smaller for larger bubbles: when the gas fraction is increased deformable bubbles become more spherical, thus reducing the drag force.

Introduction

Multiphase gas/liquid and gas/liquid/liquid flows are widely encountered, in natural phenomena as well as in (chemical) industry. The large scale of the industrial equipment contrasts sharply with the small scale of bubbles and droplets. Because of this difference in scales, it is virtually impossible to capture all the details of the flow field with the currently available computational resources in a single model. To overcome this problem a successful description of multi-phase flows therefore has to be based on a sound multi-level modelling approach (van Sint Annaland et al., 2003), which is schematically indicated in Fig. 1.

Figure 1: Schematic overview of a Multi-level modelling approach applied to gas-liquid flows.

Direct Numerical Simulations (DNS) are used at the smallest time and length scales to study the behaviour of one or a few gas bubbles or liquid droplets. Validated with dedicated experiments, these models can be used to derive closure equations for the momentum transfer (and analogously heat and mass transfer) between the dispersed phase and the continuous liquid, which can subsequently be used in higher level models. One step higher, the Euler-Lagrange or bubble tracking model can be used to study the interactions between large numbers of bubbles and their impact on the macroscopic flow structures. Each dispersed element in this model is treated as a discrete element and the forces acting on it are computed from closure equations. Because of this discrete approach a large number of bubbles ($\sim 10^5$) can be simulated with acceptable computation time. However, in industrial applications of multi-phase flows much more dispersed elements are encountered, which requires a continuum approach. Therefore, in the Euler-Euler models bubbles lose their discrete identity, which enables the simulation of very large systems and the study of large-scale heterogeneous structures in the flow.

Many different DNS models have been proposed and successfully used to simulate bubbly flows, each with their own strong and weak points (van Sint Annaland et al., 2006). By far the most popular model is Volume Of Fluid (VOF), which involves reconstruction of the interface using the spatial distribution of the phase fractions. The major advantage of this model is that the volume of the
dispersed elements can be well conserved, when a proper advection algorithm is used. However, there is also a significant downside: the interface is not explicitly tracked, but reconstructed from the phase fractions. This may cause problems associated with inaccuracies in the computation of the surface tension force, which is well known to cause artificial ‘parasitic’ currents at the interface. More specifically, using VOF it is at the moment very difficult to simulate small air bubbles (< 2 mm) in water, where a high density ratio and a high surface tension force are prevail simultaneously.

In this work a 3D Front Tracking (FT) model is used, following the work of Unverdi and Tryggvason (1992). The key feature of this model is that the interface is explicitly tracked by interconnected points, which form triangular markers (Fig. 2). In sharp contrast with VOF this makes it possible to describe the shape and location of the interface with a very high accuracy. As a consequence, the main advantage is that the accuracy of the surface tension force calculation is much higher and consequently there are significantly less parasitic currents. Another important advantage is that the explicit interface description does not automatically merge bubbles when they come very close, contrary to the VOF model, which is crucially important for the subject of this paper. However, this comes at a price: the volume of the dispersed phases is not intrinsically conserved and because of deformation, marker points have to be periodically added and removed (surface remeshing). For a detailed comparison of different DNS methods the interested reader is referred to Scardovelli and Zaleski (1999).

Figure 2: Low resolution example of the surface grid used in the 3D Front Tracking model, which clearly shows the points which make up the triangular markers on the bubble surface.

Over the years, many authors have demonstrated the difficulties of describing the behaviour of gas-liquid systems using the higher level models, because detailed knowledge about turbulence and the behaviour of bubbles or droplets in complex flow fields is lacking. As an example, even the behaviour of a single air bubble rising in quiescent water is not yet completely understood: not only well-defined physical properties like the density, viscosity and surface tension affect the behaviour of the bubbles, but also the presence of small amounts of surface active impurities (Grace et al., 1976). Not surprisingly, this leads to a large difference between existing relations for the drag force and numerical simulations (Dijkhuizen et al., 2005). This difference could be related to the presence of impurities, since the – inherently pure – numerical results compare well to experiments in ultrapure water (Duineveld, 1994; Veldhuis, 2007). Wu and Gharib (2002) and Tomiyama et al. (2002) independently pointed out that the initial shape of the bubble can affect its terminal rise velocity. Veldhuis (2007) even concluded that vibrations may have caused him to find a higher drag force, which indicates just how deceptively difficult the measurement of the terminal rise velocity of a single bubble actually is.

From literature it is known that the drag force coefficient derived for single bubbles in an infinite quiescent liquid is not valid for bubbles in bubble columns, as soon as there is a significant gas hold-up. Moreover, there are dozens of empirical correlations to describe the bubble rise velocity in a swarm of bubbles have been proposed in the literature, most of which have a formulation similar to the correlation of Richardson and Zaki (1954), who studied sedimentation of solid particles:

\[ \nu_{rel} = \nu_{\infty} (1 - \varepsilon_g)^n \]  

(1)

where \( n \) is referred to in literature as the “Richardson and Zaki” exponent and \( \varepsilon_g \) represents the gas fraction. Exactly how much the rise velocity of a bubble in a swarm changes is still very much an open question, where many variables are involved, especially for large deformed bubbles. Nevertheless, qualitatively most literature agrees.
on the mechanisms involved: for small bubbles and low gas fractions the presence of neighbouring bubbles hinders the fluid flow and consequently the drag force is increased (Ishii and Zuber, 1979). Also turbulence can cause an increase in drag as was found by Spelt and Biesheuvel (1997). Only for large deformed bubbles and high gas fractions a combination of the wake interaction, coalescence and bubble-induced turbulence may lower the drag coefficient (Simonnet et al., 2007). In their paper it was found that for air bubbles larger than 7 mm in water the drag force increases up to a gas fraction of 15%, after which it decreases sharply.

In sharp contrast, only very few articles have been published which deal with this subject using numerical simulations, even though the unique ability to control every parameter independently makes CFD ideally suited to study swarm effects in bubbly flows. For instance Krishna et al. (1999) studied the interaction between very large spherical cap bubbles using a 2D axisymmetric VOF model. They found an acceleration of three to six times compared to an isolated bubble. Sankaranarayanan et al. (2002) studied the bubble-bubble interaction by simulating a single bubble in a periodic box with an implicit version of the lattice-Boltzmann model. It was confirmed that for relatively small bubbles hindered rise occurs, while for highly distorted bubbles cooperative rise takes place.

The structure of this paper is as follows. First of all, a brief description of the numerical model is given, followed by a derivation of the drag coefficient for a swarm of bubbles. Then the simulation settings are given, after which the results obtained with the Front Tracking model are presented. Here, the effects of different parameters, such as the gas hold-up, bubble size and Reynolds number, on the drag coefficient are studied. Finally, this leads to the conclusions at the end of the paper.

Front tracking model

In the FT model a single Navier-Stokes equation (eq. 2) is solved together with the continuity equation (eq. 3) for all the phases at once. This so called one-field approximation is possible from a physical point of view, because the velocity field is continuous across phase boundaries (pure liquids). The surface tension force is included as a volumetric force \( F \) acting only in the vicinity of the interface.

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \rho g + \nabla \cdot \left( \mu \left( \nabla u + (\nabla u)^T \right) \right) + F \quad (2)
\]

\[
\nabla \cdot u = 0 \quad (3)
\]

The Navier-Stokes equations are discretised and solved on a staggered Cartesian mesh with a finite volume technique, using an explicit treatment of the convection and implicit treatment of the pressure gradient and viscous stresses. For the convection term a second order flux delimited Barton scheme (Centrella and Wilson, 1984) and for the diffusion term a standard second order finite difference scheme is used. To be able to simulate large density ratios, the Navier-Stokes equations are rewritten in their non-conservative form using the continuity equation (Van Sint Annaland et al., 2003):

\[
\rho \left( \frac{\partial u}{\partial t} + \nabla \cdot (uu) \right) = -\nabla p + \rho g + \nabla \cdot \left( \mu \left( \nabla u + (\nabla u)^T \right) \right) + F \quad (4)
\]

The discretised Navier-Stokes equations are solved in three steps. First of all a velocity estimate is calculated using all variables at the old time level. Secondly, an ICCG matrix solver is used to solve the system of discretised Navier-Stokes equations for each velocity direction separately, where the viscous stresses are treated implicitly in the direction for which the velocity is solved (Uhlmann, 2005). Implicit treatment of the viscous stresses is very important, especially for the cases with high viscosity, to avoid the requirement of small time steps because of numerical stability. Finally the velocity field is made divergence free using a standard pressure correction step.

Local fluid properties

In order to calculate the local physical properties in cells containing both gas and liquid, the phase fractions in each cell are required. Typically, for this purpose FT models following Unverdi and Tryggvason (1992) solve the Laplace equation near the interface:

\[
\nabla^2 F = \nabla \cdot G
\]

\[
G = \sum_m D(x - x_m) n_m \Delta s_m
\]

where \( n_m \) is the outwards pointing normal and \( \Delta s_m \) is the surface area of the triangular marker. First the gradient \( G \) is calculated from the interface markers, after which an ICCG method is used to solve this Poisson equation. However, the required discretisation of the gradient on the Eulerian grid effectively smears out the phase fraction. As a consequence, standard FT models cannot be considered as ‘sharp’ interface models, which may affect the calculation results when bubbles approach each other as happens in bubble swarms. To solve this, a simple geometric method was used to reconstruct the phase fractions directly from the surface triangulation, which yields the phase fraction in an Eulerian cell which is accurate down to the computer accuracy.

Now that the phase fractions have been computed, the local density can be obtained from linear weighing:

\[
\rho = F \rho_l + (1-F) \rho_g \quad (6)
\]

where \( F \) represents the liquid fraction. For the viscosity harmonic averaging is used (Prosperetti, 2001):

\[
\frac{\mu}{\mu_i} = F \frac{\mu}{\mu_i} + (1-F) \frac{\mu}{\mu_g} \quad (7)
\]

Surface tension force

Making direct use of the triangulation of the interface, the surface tension force acting on a triangular marker \( m \) is calculated by taking a contour integral along its edges (Fig. 4):

\[
\rho \left( \frac{\partial u}{\partial t} + \nabla \cdot (uu) \right) = -\nabla p + \rho g + \nabla \cdot \left( \mu \left( \nabla u + (\nabla u)^T \right) \right) + F \quad (4)
\]
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\[ F_{\sigma,n} = \frac{\sigma}{\Delta x \Delta y \Delta z} \sum_{m} t_{m,n} \times n_{m,n} \]  

(8)

where \( t_{m} \) is the counter clockwise unit tangent vector along the edges of marker \( m \).

**Figure 4:** Schematic illustration of the direct surface tension force calculation.

This method avoids the numerically inaccurate computation of the curvature and can be used for surfaces with a very high curvature with less numerical instability and better accuracy, provided that the remeshing procedure assures that the markers are of approximately the same size. The surface tension force is mapped onto the Eulerian grid using a summation over all the markers \( m \) and their edges \( l \):

\[ F_\sigma = \sum_m D(x-x_m) F_{\sigma,n} \]  

(9)

where \( t_{m,l} \) is the tangential vector and \( D \) is the distribution kernel, for which in this work density weighing (Deen et al., 2004) is used. Density weighing avoids mapping of the surface tension force to a cell with a low total mass, which can cause large distortions of the velocity field near the interface. Tryggvason et al. (2001) use a polynomial fit to obtain the normal and tangential vectors, but with our method the surface tension force is calculated directly from the discrete triangulation.

**Updating the interface**

Once the flow field has been computed on the Eulerian grid, each marker point of the interface triangulation is moved with the local flow field. After some time the surface grid will become deformed. Some markers will become too large or too stretched, while others become too small. To maintain an adequate resolution, points will have to be added at some places and removed at other places. In this work a similar approach as described by Unverdi and Tryggvason (1992) is followed.

**Drag force coefficient**

In order to provide closures for discrete elements models, where the bubbles or droplets are considered to be spherical, the drag coefficient will be based on a spherical equivalent diameter \( d \), thus effectively lumping the bubble shape into the drag force correlation. The drag force coefficient \( C_D \) for a single bubble can be computed from its steady terminal rise velocity \( v_t \) via a simple steady-state force balance in the z-direction:

\[ 0 = F_{x,z} + F_{z,c} = \frac{\pi}{6} d^3 (\rho_l - \rho_g) g \left( \frac{1}{2} C_D \frac{\pi}{4} d^2 \rho_l (v_t - u_z)^2 \right) \]  

(10)

By rewriting this force balance an expression for the drag force coefficient for a single bubble in an infinite liquid appears:

\[ C_{D,\infty} = \frac{4 \left( \rho_l - \rho_g \right) g d}{3 \rho_l (v_t - u_z)^2} \]  

(11)

For multiple bubbles in a swarm the situation is somewhat more complicated, since there will generally not be a well-defined steady state due to the random nature of the swarm, causing a continuous and lasting fluctuation of the bubble rise velocities. Since the goal of the obtained closures is to properly describe the momentum transfer between the different phases, the time-averaged drag coefficient is used. In addition, the decrease in buoyancy force due to the presence of the bubbles has been accounted for in the force balance for bubble \( I \) in a swarm of bubbles:

\[ 0 = \frac{\pi}{6} d^3 (\rho_l - \rho_g) g \left( \frac{1}{2} C_D \frac{\pi}{4} d^2 \rho_l \left( v_t - u_z \right)^2 \right) - \frac{N}{3} 4 \left( \rho_l - \rho_g \right) g d \left( 1 - \epsilon_i \right) \left( \rho_l - \rho_g \right) g d \left( v_t - u_z \right)^2 \]  

which finally gives a relation for the bubble-averaged drag coefficient:

\[ \langle C_D \rangle = \frac{\sum_{i=1}^{N} 4 \left( 1 - \epsilon_i \right) \left( \rho_l - \rho_g \right) g d \left( v_t - u_z \right)^2}{\sum_{i=1}^{N} 3 \rho_l \left( v_t - u_z \right)^2} \]  

(13)

**Simulation settings**

For the single bubble cases free-slip boundaries were used, with a relatively large domain (Fig. 5, left). The initial bubble diameter was equal to 20 Eulerian grid cells, which in the past has been proven sufficient for obtaining a grid-independent drag coefficient in many different physical systems.

**Table 1:** simulation settings and physical properties.

<table>
<thead>
<tr>
<th>Bubble size</th>
<th>2 mm</th>
<th>5 mm</th>
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<tbody>
<tr>
<td>Time step [s]</td>
<td>( 1.0 \times 10^{-4} )</td>
<td>( 1.0 \times 10^{-5} )</td>
</tr>
<tr>
<td>Grid size [m]</td>
<td>( 1.0 \times 10^{-4} )</td>
<td>( 2.5 \times 10^{-4} )</td>
</tr>
<tr>
<td>Simulation time [s]</td>
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<table>
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<tr>
<th>Physical system</th>
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<th>water</th>
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<tr>
<td>Gas density [kg·m(^{-3})]</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Gas viscosity [Pa·s]</td>
<td>( 1.8 \times 10^{-5} )</td>
<td>( 1.8 \times 10^{-5} )</td>
</tr>
<tr>
<td>Liquid density [kg·m(^{-3})]</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Liquid viscosity [Pa·s]</td>
<td>0.100</td>
<td>0.001</td>
</tr>
<tr>
<td>Surface tension [N·m(^{-1})]</td>
<td>0.073</td>
<td>0.073</td>
</tr>
</tbody>
</table>
Periodic boundaries were used to mimic large bubble swarms, using only a small number of bubbles (up to 8). Therefore a relatively small domain can be used, of which the size controls the gas fraction (0-15%). Note that in this way the resolution is always exactly the same in all simulations (Fig. 5, right). Additional simulation settings and the physical properties are listed in Table 1.

Figure 5: Initial bubble configuration (independent of selected bubble size). Left: free-slip boundaries were used to find the terminal rise velocity of a single bubble in an infinite initially quiescent liquid. Right: single bubble with periodic boundaries to mimic an infinite cubic array of bubbles (in this case 15% gas hold-up).

Results

First of all, the swarm effects will be investigated in a viscous liquid at low Reynolds numbers, where turbulence does not play a role. The influence of the bubble diameter, gas hold-up and the liquid viscosity on the drag force coefficient, bubble shape and flow profile is studied. Finally, the obtained knowledge about the swarm effects is used to study the industrially very important air-water system.

Viscous liquid (low Re)

First a viscous liquid (M=2.3·10⁻³) is used to investigate the influence of the bubble-bubble interactions at low Reynolds numbers, where turbulence does not play a role. Figure 6 shows the relative drag coefficient, i.e. compared to a single bubble in an infinite liquid, as a function of the gas fraction. It can be seen that for both 2 and 5 mm bubbles the drag force increases when the concentration of bubbles (gas fraction) is increased, thus the hindrance effect is dominant for these cases. This can be confirmed by investigating the flow profile around the bubbles (Fig. 7 and 8), which show a very small wake structure that is probably not sufficient for wake-acceleration of other bubbles. Only for the random array of bubbles any significant asymmetry occurs, which however does not affect the average drag coefficient. For the larger (slightly deformed) bubble the drag increases less, which might be caused by either the higher Reynolds number or the deformability. Both the simulations using a periodic box containing a single bubble, as well as the simulations using eight randomly positioned bubbles in a periodic box give very similar results. Note that there is a considerable deviation in the average drag of the individual bubbles, as indicated by the “error” bars in Fig. 6.

Figure 6: Relative drag coefficient versus the gas fraction for 2 mm (∆) and 5 mm bubbles (○) in a viscous liquid. Single bubble in a periodic box (open symbols) and random swarm of eight bubbles in a periodic box (closed symbols). The standard deviation for the random bubbles is shown as error bars.

First of all the influence of the gas fraction on the bubble shape is studied by plotting the aspect ratio E of the bubble (defined as height/width) in Fig. 9. For the small spherical bubbles the shape is only slightly affected by the presence of other bubbles in its vicinity, while for the larger bubbles there is a significant effect. It can be concluded that when the gas fraction is increased the bubble shape becomes more spherical, which is consistent with a dominant hindrance effect. More importantly, it is demonstrated that in the random configuration of eight bubbles there is more shape deformation, because the bubbles have more freedom to expand in the horizontal plane compared to a cubic array. Also it can be seen that there is a significant deviation in the shape of the random bubbles, as indicated by the “error” bars.

Secondly, the influence of the Reynolds number and bubble shape on the relative drag coefficient are investigated by varying the liquid viscosity (0.05-0.4 Pa·s) for a constant gas fraction of 13%. First of all, the effect of the Reynolds number is studied for a 2 mm bubble, because of the more or less constant spherical shape. It can be discerned from Fig. 10 that there is hardly any effect of the Reynolds number, even though it spans several decades. On the other hand, the effect of the bubble shape can be studied using the larger deformable 5 mm bubble (Fig. 11). It can be concluded that there is a much stronger effect: a small deformation already increases the relative drag force considerably. This effect also explains why the relative drag force increase as a function of the gas hold-up is less for larger bubbles: deformable bubbles have the capability to become more spherical which partly counteracts the increase in drag force and therefore do not have the same drag increase as smaller spherical bubbles.
Figure 7: Flow profile around 2 mm bubble in a viscous liquid. From top to bottom: single bubble in an infinite liquid, single periodic bubble (cubic array) and a random swarm of eight bubbles.

Figure 8: Flow profile around 5 mm bubble in a viscous liquid. From top to bottom: single bubble in an infinite liquid, single periodic bubble (cubic array) and a random swarm of eight bubbles.
Finally, the swarm effect on the drag force has been studied for higher Reynolds numbers, studying gas bubbles rising in water. As expected, it was found that the flow is much more dynamic, also because the larger bubbles tend to oscillate. Fig. 12 shows that for both 2 and 5 mm bubbles – similar to the viscous case – the drag coefficient increases with the gas fraction. This means that even with the very low viscosity of water, there is no net acceleration of the bubbles up to a diameter of 5 mm, which is in accordance with the experimental results by Simonnet et al. (2007). Also the aspect ratio of the bubbles increases with the gas fraction in a similar way as was observed for the viscous case (Fig. 13). Finally, the velocity profile around the bubbles is shown in Fig. 14. It can be seen that the influence of the bubble wakes is much more pronounced and there is a very dynamic bubble motion.
Conclusions

In this paper the influence of swarm effects on the drag force in bubbly flows is studied at both low and high Reynolds numbers. It was found that the relative drag force increases for bubbles in the range 2 to 5 mm when the gas fraction is increased up to 13%, and the bubbles become more spherical. Secondly, the influence of the Reynolds number and the bubble aspect ratio on this drag increase has been investigated. It can be concluded that there is only a very weak effect of the Reynolds number and a strong effect of the aspect ratio. This also helps to explain why the relative increase in the relative drag force is smaller for large bubbles: when the gas fraction increases the bubbles become more spherical, thus decreasing the drag force.

Acknowledgement

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Nomenclature

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<thead>
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<th>Symbol</th>
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<tbody>
<tr>
<td>C</td>
<td>coefficient</td>
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<tr>
<td>d</td>
<td>equivalent bubble diameter (m)</td>
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<td>D</td>
<td>distribution function</td>
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<td>F</td>
<td>liquid fraction</td>
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<td>F</td>
<td>force density (Nm⁻³)</td>
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<td>G</td>
<td>phase fraction gradient</td>
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<td>g</td>
<td>gravity constant (ms⁻²)</td>
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<tr>
<td>M</td>
<td>Morton number</td>
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<tr>
<td>n</td>
<td>surface normal vector</td>
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<tr>
<td>N</td>
<td>number of bubbles</td>
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<tr>
<td>p</td>
<td>pressure (Nm⁻²)</td>
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<td>Reynolds number</td>
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<td>s</td>
<td>surface (m²)</td>
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<td>t</td>
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<tr>
<td>t</td>
<td>tangential vector (m)</td>
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<tr>
<td>u</td>
<td>velocity field (ms⁻¹)</td>
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<tr>
<td>v</td>
<td>bubble velocity (ms⁻¹)</td>
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Greek symbols

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<tr>
<td>ε</td>
<td>hold-up</td>
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<tr>
<td>µ</td>
<td>dynamic viscosity (Pas)</td>
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<tr>
<td>ρ</td>
<td>density (kgm⁻³)</td>
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<tr>
<td>σ</td>
<td>surface tension coefficient (Nm⁻¹)</td>
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Subscripts

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<thead>
<tr>
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<tr>
<td>D</td>
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<td>g</td>
<td>gas</td>
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<td>liquid</td>
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