Direct numerical simulation of single gas bubbles in pure and contaminated liquids

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Disperse gas bubbles play an important role in many industrial applications. Knowing the rising velocity, the interfacial area, or the critical size for break–up or coalescence in different systems can be crucial for the process design. Hence, knowing the fundamental behaviour of a single bubble appears mandatory for the examination of bubble swarms and for the Euler–Lagrange or Euler–Euler modelling of disperse systems. In the present work a level–set–based volume–tracking method is implemented into the CFD–code OpenFOAM to follow the free interface of a single bubble. The volume–tracking method is coupled with a transport model for surfactants on the interface, including adsorption and desorption processes. The dependency of surface tension on the local surfactant concentration on the interface is modelled by a non–linear (Langmuir) equation of state. Marangoni forces, resulting from surface tension gradients, are included. The rise of a single air bubble (i) in pure water and (ii) in the presence of surfactants of different strengths is simulated. The results show good agreement with available correlations from literature.

1 Model

To describe an incompressible two–phase flow in the context of a volume–tracking method, the immersed–boundary formulation of the Navier–Stokes equation is used. In its non–dimensional form, including gravity and surface tension, it has the form

\[ \rho(\phi) \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla p + \frac{\mu(\phi)}{Re} \Delta \vec{u} + \frac{\rho(\phi)}{Fr} \vec{y} - \frac{\delta(\phi)}{We} \left( \nabla \sigma(c_s) + \vec{n} \kappa \sigma(c_s) \right). \]

(1)

The dimensionless groups are the Reynolds number \( Re = \frac{u_0 d_0 \rho_{\text{ref}}}{\mu_{\text{ref}}} \), the Froude number \( Fr = \frac{u_0^2}{g d_0} \), and the Weber number \( We = \frac{u_0 d_0 \rho_{\text{ref}}}{\sigma} \). The phase distribution is obtained from the colour function \( \phi \). In this work a modified level–set method, proposed by Olsson et al. [1], is used for the colour function. It is defined as \( \phi = 1 \) in phase 1, \( \phi = 0 \) in phase 2, and \( 0 < \phi < 1 \) on the interface. The colour function is transported within the flow field according to eq. (2). Due to numerical diffusion the shape and distribution of \( \phi \) is distorted during the simulation. To resolve this problem, a compression step according to eq. (3) is solved to steady–state after each time step.

\[ \frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0, \]

(2)

\[ \frac{\partial \phi}{\partial \tau} + \nabla \cdot \phi (1 - \phi) \vec{n} = \epsilon \Delta \phi. \]

(3)

The compression step is set up such that in areas where \( 0 < \phi < 1 \) the colour function is advected normal to the interface. This is opposed by a small amount of diffusion, with the diffusion coefficient \( \epsilon \) being proportional to the grid size. This results in a smooth transition from \( \phi = 0 \) to \( \phi = 1 \) and in a constant thickness of the transition zone.

Surface active impurities, so–called surfactants, in any of the phases can adsorb on the interface. They are convected along the interface and desorb on the downstream side of the bubble. The influence of surfactant diffusion appears to be negligible, given Peclet numbers in the order of \( Pe \sim 10^6 \). The resulting transport equation (4) for the surfactant concentration \( c \) is given in non–dimensional form.

\[ \frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \delta k_a (1 - c) - k_d c, \]

(4)

\[ \frac{\partial c}{\partial \tau} + (2 \phi - 1) \vec{n} \cdot \nabla c = \epsilon (\vec{n} \otimes \vec{n}) \Delta c. \]

(5)

Here \( k_a \) and \( k_d \) are the (non–dimensional) adsorption and desorption rates, respectively. Again, a compression step is necessary to compensate numerical diffusion. It is similar to the compression step above (see eq. (3)), but the convection term acts
from both sides of the interface. It is governed by eq. (5).
Surface tension depends on the local (integrated) concentration $c_s$ of a surfactant. The (Langmuir) equation of state
\[ \sigma(c_s) = 1 + E \ln (1 - c_s) \] (6)
reflects this dependency. The parameter $E$ characterizes the strength of the surfactant. If concentration is constant, surface tension contributes to normal stress only. In contrast, a varying surfactant concentration leads to surface tension gradients and, therefore, to tangential stresses, so–called Marangoni stresses, along the interface (see last term in eq. (1)).

2 Results

Numerical simulations have been performed for a pure system without surfactant and for systems with surfactants of different strength. Three predictions have been chosen for comparison: one for ideal spherical bubbles [2], one for ideal spherical particles [3], and one for ideal non–spherical bubbles [4]. The numerical results are shown in figure 1 together with the predictions from literature. The simulated terminal velocities for bubbles in pure water closely follow the prediction for ideal bubbles. Small bubbles match that for spherical bubbles, larger bubbles that for non–spherical bubbles. If a weak surfactant is present, small bubbles with an equivalent diameter $d_{eq} < 1 \text{ mm}$ are slowed down, while bigger bubbles remain unaffected. As the surfactant strength increases, this effect gets stronger and even bigger bubbles are slowed down. Eventually, the bubble rise velocity reaches a minimum, which is identical to the prediction for solid particles. Consequently, it can be concluded that the contamination of the interface of a free rising gas bubble may be responsible for bubbles behaving like solid particles. In other words, only in pure systems a bubble can behave like an ideal bubble.

3 Summary and outlook

A modified level–set method is implemented and used to simulate the rise of gas bubbles in liquids. The model is extended to include effects of contaminations on the interface; for this purpose a method for transporting a scalar on the interface is applied. Simulation results are compared to available correlations in literature. The agreement is very good for both pure and contaminated systems. It is shown that Marangoni forces, resulting from contamination of the interface, are a possible candidate to explain the rise of small bubbles, in agreement with that of solid particles. Future investigation will concentrate on characterizing different types of contaminations and their effect on the bubble behaviour. Further experimental validation of the simulation results is in progress both at the Ruhr-Universit ät Bochum and the Technische Universität Dortmund.

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References