Research News

Simulating the Rise Characteristics of Gas Bubbles in Liquids Using CFD

By *R. Krishna* and *J. M. van Baten**

With the advent of modern tools of computational fluid dynamics (CFD), it is now possible to obtain detailed information on the bubble shape, morphology and rise characteristics from knowledge of system properties and geometry. In this paper we try to give a flavor of the power of CFD tools and summarize recent advances.

1 Introduction

The gentle rise of bubbles in a glass of beer or champagne is a familiar sight in our daily life. Bubbly dispersions are also encountered in many branches of engineering and technology. Aeration typically supplies the gas needed for a chemical reaction in a liquid, or the oxygen demanded by organisms in bioengineering. Aeration of fluids is used in rectification, absorption, wastewater treatment, and biotechnological processes. In all such processes, a component is required to be transferred from the gas bubbles to the surrounding liquid. In the ozone treatment of water, for example, ozone is dispersed as gas bubbles in water. The ozone dissolves in water and reacts chemically with organic pollutants. The chemical reaction is fast and the overall process is limited by the efficiency of transfer of ozone from the gas bubbles to the liquid phase. Edible oils require to be partially hydrogenated in order to modify their melting behavior and their taste stability. Industrially, the hydrogenation is usually carried out in a bubble column reactor in which fine catalyst particles are dispersed in the liquid phase into which hydrogen is dispersed in the form of gas bubbles.

In all the above-mentioned process applications, it is important in practice to estimate the contact time between the gas bubbles and the liquid. The contact time is dictated by the bubble rise velocity V_b and the trajectory followed. The rise characteristics of a bubble are strongly dependent on the bubble size (diameter d_b) and system properties (phase viscosity, μ; phase density, ρ ; interfacial tension, σ). A generalized graphical representation [1,2] of the rise velocity V_b is possible in terms of the Eötvös number ($Eö = g(\rho_L - \rho_G) d_b^2/\sigma$, Morton number ($M = g\mu_L^4(\rho_L - \rho_G)/\rho_L^2\sigma^3$) and Reynolds number ($Re = \rho_L d_b V_b/\mu_L$); see Fig. 1. The chart such as presented in Fig. 1 has been developed on the basis of vast amounts of experimental data and theoretical analysis [1,2]. A variety of bubble shapes are possible, e.g., spherical, ellipsoidal, spherical cap, etc. For the air-water system ($M = 2.63 \times 10^{-11}$; $\log(M) = -10.6$) we note that increasing the bubble size from say 4 mm (corresponding to Eö = 2.2) to 20 mm (Eö = 54.4) the regime changes from "wobbling" to "spherical cap".

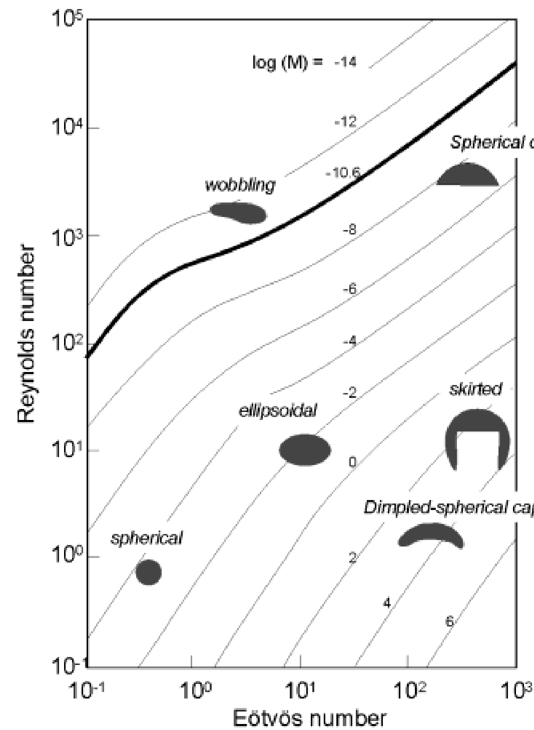

Figure 1. Shape regimes for bubble rising in a column of liquid. The thick line drawn in this figure, log(M) = –10.6, corresponds to the properties of an air-water system, with Morton number $M = 2.63 \times 10^{-11}$.

It was Leonardo da Vinci, who, about five centuries ago, summarized his observations on the motion of air bubbles in the "wobbling" regime in the following manner. "*The air that submerged itself with the water which percussed upon the other water, returns to the air, penetrating the water in sinuous movement, changing its substance into a great number of forms. And this happens because "the light thing cannot remain under the heavy"; rather it is continuously pressed by the part of the liquid which rests upon it; and because the water that stands there perpendicular is more powerful than the other in its decent, this water is always driven away by the part of the water*

[*] R. Krishna (author to whom correspondence should be addressed), J. M. van Baten, Department of Chemical Engineering, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands; e-mail: krishna@its.chem.uva.nl

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that forms its coverings, and so moves more continually sideways where it is less heavy and in consequence offers less resistance, according to the 5th [proposition] of the 2nd [Book]; and because this "has to make its movement by the shortest way", it never spreads itself out from its path except to the extent to which it avoids the water which covers it above." Leonardo da Vinci was clearly describing the meandering motion of bubbles in the 3–6 mm size range in water.

With the advent of modern tools of computational fluid dynamics (CFD), it is now possible to obtain detailed information on the bubble shape, morphology and rise characteristics. In this paper we try to give a flavour of the power of CFD tools and summarize recent advances. Specifically we use the volume-of-fluid (VOF) technique developed by Hirt and Nichols [3] to describe the bubble rise in liquids.

2 VOF Methodology

The VOF model [3–9] 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 gas and liquid phases share the same velocity field. Hence, a single velocity field is solved that is valid for both phases. A single scalar variable C, also called the color function, keeps track of whether a volume element is filled with gas or liquid, or a combination thereof; see Fig. 2. If the value of C is zero (white in the picture), the content of the volume at that location is liquid, and if the value of C is unity (dark gray in the picture), the content of the volume at that location is gas. The color function C, therefore, defines the local mixture density and viscosity at that location. Values of C between one and zero represent a mixture of gas and liquid. This usually occurs at the gas-liquid interface. The color variable C obeys the usual continuity relations of mass and momentum for a conserved quantity.

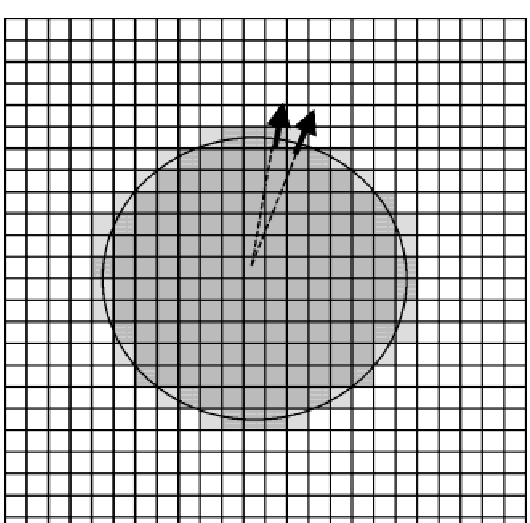

Figure 2. Pictorial representation of the VOF technique.

For proper resolution of the gas-liquid interface a few hundred grid cells need to be used for each bubble. Furthermore, grid size and time step should be fine enough to capture fluctuations in local velocities. Since gas-liquid interfaces usually have a very limited thickness, a scheme has to be incorporated that prevents smearing out the gas-liquid interface over a thickness of several grid cells. This is achieved by identifying the gas-liquid interface by means of using a cut-off value (say 0.5) for the color function. After the interface location is determined, gas and liquid on the wrong side of the interface are placed back on the right side of the interface, while conserving the mass balance, i.e., gas and liquid are exchanged from the wrong side to the right side of the gas-liquid interface.

Finally, surface tension effects need to be included in the model. The thick black arrows in the picture show the directions of the gradient of the color function. The curvature of the bubble interface between these arrows is defined by the angle between the vectors. This curvature has a magnitude and a direction; these are used to calculate surface tension forces at the locations with gradients of the color function. The resulting surface tension force is added to the CFD model as a body force in the Navier-Stokes equation, acting on whatever phase is present at that location.

3 VOF Simulation Results

Simulations were carried out to determine the rise characteristics of bubbles varying in size between 4 and 20 mm in a rectangular column using a uniform 2-D Cartesian co-ordinate grid. A uniform grid was used. The front of the 2-D rectangular grid is formed by the x-z plane. No account is taken of the variation along the depth of the system, and the simulations are truly two-dimensional. At the two walls, the no-slip boundary condition is imposed. The column is 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). The time step used in the simulations were usually 0.0003 s or smaller. For simulations of bubble sizes smaller than 12 mm, we found that the rich dynamic features could be captured only by allowing at least 800 grid cells per bubble cross section. This constraint resulted in grid sizes as small as 0.125 mm for the smallest bubble size we could simulate with adequate accuracy. All simulations were carried out using the parallel version of CFX 4.1c running on a Silicon Graphics Power Challenge machine with six R8000 processors. To give an indication of the required CPU time, the simulation of the rise of a 7 mm diameter bubble for 0.75 s in a column of 0.025 m width and 0.09 m height, involving 144000 grid cells, required about two weeks.

Initially, a circular shaped bubble is placed near the bottom of the column filled with liquid and the simulations are started. As illustration, the time trajectories of a 20 mm circular bubble placed in a column of 0.04 m width and 0.09 m height are shown in Fig. 3. The bubble first adjusts itself to a circular cap shape and, in doing so, there is a breakage of bubbles at the edges. The circular shape form is attained after about 0.1 s from the start of the simulations. For bubbles smaller than 20 mm, no bubble breakage was observed and the time trajectories are shown in Fig. 4. The 4 and 5 mm bubbles show meandering trajectories. The 7 mm bubble oscillates from side to side when moving up the column. The 8 and 9 mm bubbles behave like jellyfish. The 12 mm bubble flaps its "wings" like a bird. The 20 mm bubble has a vertical trajectory. These rich dynamic features can be viewed by looking at the animations on our web site http://ct-cr4.chem.uva.nl/single_bubble. From Fig. 4 we see that as the bubble size increases the amplitude of these excursions in the x-directions decrease.

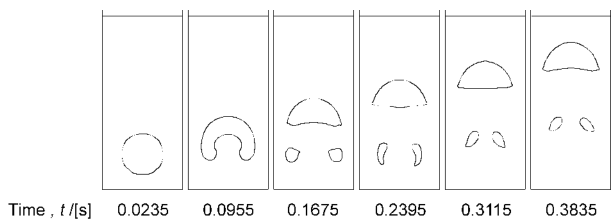

Figure 3. Rise of a 20 mm air bubble in a column of 0.04 m width and 0.09 m height. Animations of this VOF simulations can be viewed on our web site http://ct-cr4.chem.uva.nl/single_bubble.

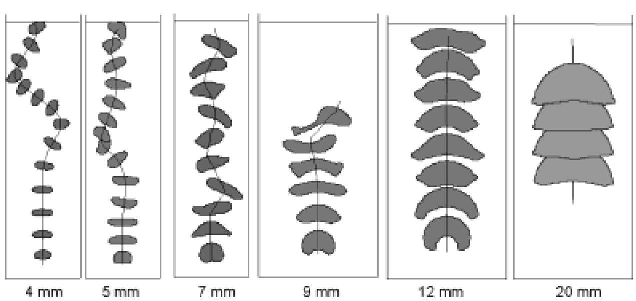

Figure 4. Snapshots obtained with 2-D VOF simulations of the rise trajectories of bubbles in the 4–12 mm size range. Animations of all these VOF simulations can be viewed on our web site http://ct-cr4.chem.uva.nl/single_bubble.

The jellyfish- and bird-like motions of the bubbles are intriguing and in order to verify these we tracked the rise characteristics of air bubbles in a 2-D rectangular column of water [10]. The bubble trajectories were recorded on video at 25 frames per second. The retraced video images for bubbles of 9.7, 12.3, 13.7 and 15.5 mm in size are shown in Fig. 5. Although there is no one-to-one correspondence with the VOF simulation results seen in Fig. 3 we see several qualitatively similar dynamic features. The 9.7 mm bubble meanders from side to side. The 12.3 mm bubble exhibits jellyfish-like characteristics. Close observation of the edges of the 13.7 mm bubble confirms the vertical oscillation of the edges of the bubbles, analogous to the flapping of the wings of a bird. When the bubble size increases to 15.5 mm, these vertical oscillations of the edges vanish and the bubble moves more or less in a vertical line.

VOF simulations also help us understand the influence of column width on the rise velocity of circular cap bubbles in 2-D rectangular columns. Fig. 6 compares the z-coordinates of the

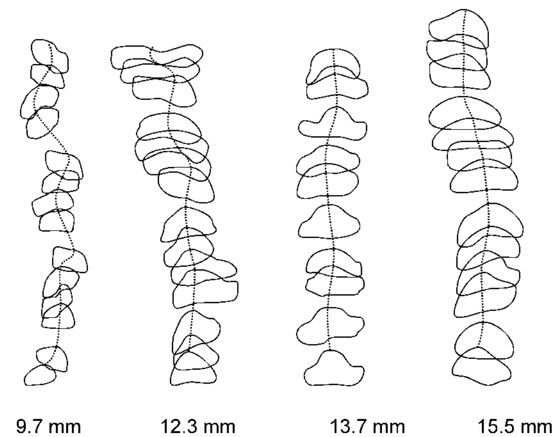

Figure 5. Retraced video recordings of the rise characteristics of 9.7, 12.3, 13.7 and 15.5 mm bubbles observed in a 2-D rectangular column.

nose of 33 mm bubbles rising in 2-D rectangular columns of 0.1 and 0.051 m widths; this figure shows that the bubble rises faster in the wider column. The reason for this is the restraining effect of the walls. Also shown in the inset to Fig. 6 are the liquid velocity profiles for these two simulations. We notice that the 33 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 [6]. 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 wall effect is a function of the ratio of the bubble diameter to the column width, d_b/D_T. The Froude number, $V_b/(g\ d_b)^{1/2}$ obtained from experiments, carried out both with liquids and powders, match very well with those obtained from VOF simulations [7] (see Fig. 7).

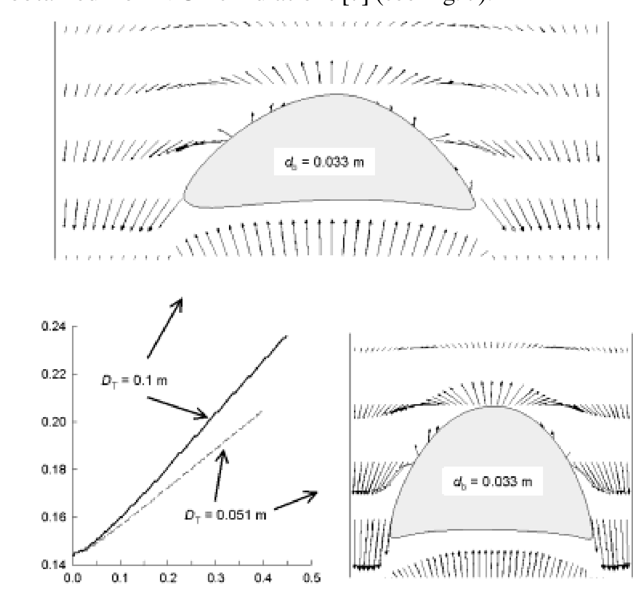

Figure 6. The rise trajectories of 33 mm diameter bubbles in water determined from VOF simulations. Liquid phase velocity profiles surrounding a 33 m diameter bubble rising in columns of 0.051 and 0.1 m width are also shown. Animations of all these VOF simulations can be viewed on our web site http://ct-cr4.chem.uva.nl/cartesian.

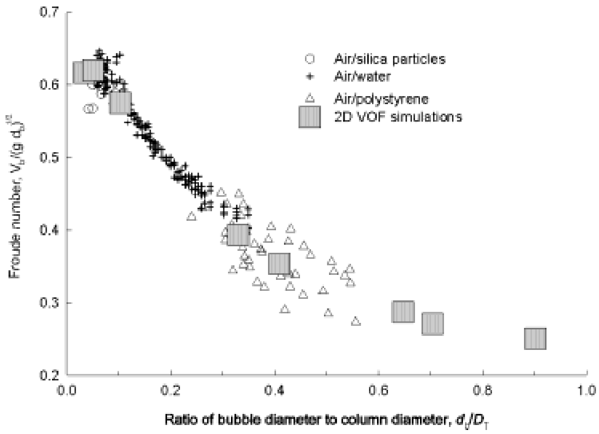

Figure 7. Rise velocities determined from VOF simulations for air-water system are compared with the experimental data for the rise of circular cap bubbles in a 2-D rectangular column of 0.3 m width filled with water and powders.

4 Conclusions

We have demonstrated that the volume-of-fluid (VOF) simulation technique is a powerful tool for studying the rise characteristics of air bubbles in a 2-D rectangular column of water. Bubbles in the 4–20 mm size range reveal rich dynamic features. When the bubble size increases from 4 mm to 20 mm, there is a gradual decrease in the lateral movement. There are also several qualitative changes in the bubble morphology and rise characteristics. In particular the jellyfish-like behavior of 7–9 mm bubbles and the vertical oscillations of the edges of bubbles in the region of 12 mm are noteworthy. These features were confirmed experimentally using video-imaging techniques. VOF simulations help us understand the influence of column diameter on the rise velocity of spherical cap bubble.

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