NUMERICAL SIMULATION OF BUBBLE COALESCENCE USING A VOLUME OF FLUID (VOF) MODEL

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0. Abstract

This paper presents a Volume Tracking model developed with the specific objective of studying the time – dependent behavior of multiple, "large" gas bubbles rising in an initially quiescent liquid. The model, based on the Volume – Of – Fluid concept, employs an advanced interface tracking scheme known as Youngs' VOF to advance the gas – liquid interface through the Eulerian mesh. Additionally, the model solves the incompressible Navier – Stokes equations to obtain the flow field. Results obtained for four different cases will be discussed: the formation and rise of a skirted bubble and of a spherical cap bubble, the coalescence of two identical gas bubbles and the behavior of two gas bubbles emanating from two adjacent orifices. It could be concluded that the Volume Tracking model is able to track the motion of a gas – liquid interface, subject to appreciable changes in its topology, embedded in a flow field with significant vorticity.

1. Introduction

Gas – liquid bubble columns are employed throughout the biological, chemical and petrochemical industries in applications usually involving gas – liquid mass transfer and (exothermal) chemical reactions. This widespread application stems from the fact that bubble columns offer some distinct advantages over other multiphase reactors, among which its excellent heat transfer characteristics, its simple construction and its low operating costs should be mentioned (Shah *et al.*, 1982). However, despite their industrial relevance, many important hydrodynamic phenomena associated with the gas – liquid two – phase flow prevailing in bubble columns are still poorly understood. These phenomena include bubble formation, bubble coalescence and breakup and the transition between the various flow regimes observed in bubble columns.

Nowhere is this deficiency of fundamental knowledge regarding bubble column hydrodynamics more apparent than in the design and scale up of bubble columns operating in the heterogeneous or churn – turbulent regime. This regime, arguably the most important in industrial operation, is characterized by intermediate gas velocities, a fierce liquid circulation and the co – existence of "large" and "small" bubbles that differ considerably in shape (see for instance Grace, 1973, Grace *et al.*, 1976 and Deckwer and Schumpe, 1993). The larger bubbles observed in this regime are of particular importance because of their significant impact on gas – liquid contacting, and consequently on the overall performance of the bubble column as a chemical reactor. It is also in this regime that many of the aforementioned phenomena are of considerable importance and that traditional semi – empirical approaches often fail to provide adequate explanations for experimental observations.

To study the behavior of "large" gas bubbles rising in a liquid, in a more fundamental way, we have developed a Volume Tracking model based on the Volume – Of – Fluid (VOF) concept (Hirt and Nichols, 1981). This two – dimensional, finite difference Volume Tracking model resolves the time – dependent motion of the gas and liquid phases, and of the interface separating the two phases. Due to its advanced interface tracking scheme, referred to as Youngs' VOF (Youngs, 1982), the model is able to account for substantial changes in the topology of the gas – liquid interface induced by the relative liquid motion. This particular capability allows a detailed study of bubble formation, coalescence and breakup.

2. The Volume Tracking Model

The model presented in this paper consists of two intimately coupled parts: a part that tracks the gas – liquid interface through the Eulerian mesh and maintains an accurate and sharp representation of this interface, and a part that solves for the gas and liquid flow field. Both parts will subsequently be discussed in more detail.

2.1 Tracking the gas – liquid interface

The essential feature of the first part of the model is that it tracks the motion of the gas – liquid interface embedded in the overall motion of the flow field, while maintaining a compact interface thickness (one cell width). This requires a capability, on the part of the model, to uniquely identify the gas - liquid interface. The VOF concept achieves this by defining a fractional volume or 'color' function F (**x**, t) which specifies the fraction of a computational cell filled with liquid. More specific, a unit value of F indicates a computational cell completely filled with liquid, whereas a zero value of F indicates a cell containing only gas. Obviously, cells with intermediate F values contain a gas – liquid interface. The motion of this interface can now be tracked through the solution of the F transport equation given by:

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + (\mathbf{u} \cdot \nabla) F = 0 \qquad 1$$

The finite difference approximation of this equation relates the new time level value of F to its previous time level value and to the fluxes of F through the four cell faces. When calculating these convective fluxes special care must be taken to avoid computational smearing of the gas – liquid interface because this causes considerable inaccuracy in the interface representation. Several VOF algorithms have been developed that address this problem. Probably the most popular among these methods is the VOF algorithm originally developed by Hirt and Nichols (1981), also used to study gas bubbles rising in liquids by Tomiyama *et al.* (1993), Lin *et al.* (1996) and Delnoij *et al.* (1997). This algorithm uses an approximate interface reconstruction that forces the interface to align with one of the coordinate axes depending on the prevailing direction of the interface normal; meaning that according to the Hirt and Nichols VOF algorithm an interface can only be horizontal or vertical. For fluxes in a direction parallel to the reconstructed interface, upwind fluxes are used. Fluxes in a direction perpendicular to the reconstructed interface are estimated using a Donor – Acceptor method.

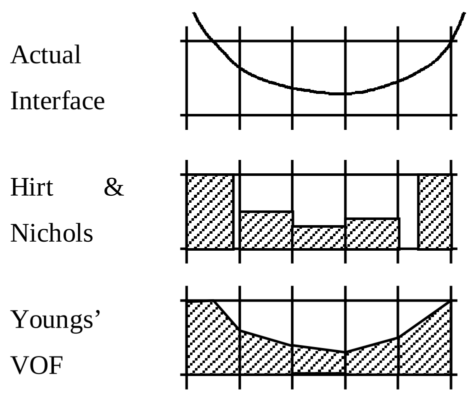

Figure 1. Hirt and Nichols' VOF interface reconstruction compared with Youngs' VOF method and actual interface.

However, the accuracy and capability of modern (so called piecewise linear) VOF algorithms greatly exceeds that of the older (piecewise constant) VOF algorithms such as the Hirt and Nichols VOF method (Kothe and Rider, 1995a and 1995b, Rider *et al.*, 1995, Rider and Kothe, 1995 and Rudman, 1997). A typical modern piecewise linear VOF method has been developed by Youngs (Youngs, 1982). Youngs' VOF method approximates the interface within a cell by a straight – line segment with a slope determined from the interface normal (see also Figure 1). This normal, in turn, is calculated from the gradient of the volume fraction using a nine point stencil. The line segment cuts the computational cell under consideration in such a way that the fractional fluid volume is equal to $F_{i,j}$. The resulting fluid polygon is then used to determine the fluxes through any cell face with an *outwards* directed velocity. The method described above is used in this study because of its superior accuracy and rigorous volume (mass) conservation, especially in flow fields with appreciable spatial and temporal variations.

2.2 Governing equations

The part of the Volume Tracking model that solves the gas and liquid phase flow fields employs the conservation equations for mass and momentum for an incompressible fluid:

$$\nabla \cdot \mathbf{u} = 0 \qquad 2$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla P + \nabla \cdot \mu\left((\nabla \mathbf{u}) + (\nabla \mathbf{u})^T\right) + \rho \mathbf{g} + \mathbf{F}_{SF} \qquad 3$$

Where the density and viscosity in equation (3) are defined as:

$$\rho = F(\mathbf{x}, t) \cdot \rho_l + (1 - F(\mathbf{x}, t)) \cdot \rho_g \qquad 4$$

$$\mu = F(\mathbf{x}, t) \cdot \mu_l + (1 - F(\mathbf{x}, t)) \cdot \mu_g \qquad 5$$

The model presented in this paper uses the Continuum Surface Force (CSF) model, originally developed by Brackbill *et al.* (1992), to describe interfacial surface tension. This CSF model replaces the interfacial force due to surface tension by a smoothly varying volumetric force ($\mathbf{F}_{SF}$) acting on all fluid elements in the interface transition region. The computer implementation of the CSF model, including wall adhesion, is similar to the approach followed by Kothe *et al.* in their RIPPLE code (Kothe *et al.*, 1991). The volumetric force due to surface tension is therefore represented as:

$$\mathbf{F}_{SF} = 2 \cdot F(\mathbf{x}, t) \cdot \sigma \cdot \kappa(\mathbf{x}, t) \cdot \tilde{\mathbf{n}}(\mathbf{x}, t) \qquad 6$$

In equation (6) F ($\mathbf{x}$, t) represents the fractional amount of liquid and κ represents the local surface curvature, which can be calculated using the average unit normal of the gas - liquid interface ($\tilde{\mathbf{n}}$ ($\mathbf{x}$, t)).

The volumetric force $\mathbf{F}_{SF}$ due to surface tension, as specified by equation (6), is located at (scalar) cell centers. This implies that the surface curvature κ and the average unit normal $\tilde{\mathbf{n}}$ must also be specified at cell centers. As the CSF model assumes that the normal vectors $\mathbf{n}$ are located at cell vertices, the required averaging (to calculate the cell centered normal $\tilde{\mathbf{n}}$) effectively yields a nine point stencil for $\tilde{\mathbf{n}}$. This rather large stencil leads to a better estimate of surface curvature (Kothe *et al.*, 1991) at the expense of reduced locality of the volumetric surface tension force (O ($2\delta x$)). Clearly, to enhance the accuracy of the CSF model, the Volume Tracking model has to maintain as compact and sharp an interface as possible (preferably O (δx)).

2.3 Numerical solution

The Volume Tracking algorithm outlined in the previous sections has been implemented in a computer code written in C, that solves the incompressible Navier - Stokes equations and tracks the motion of the gas - liquid interface in time. The system of linear equations arising from the finite difference approximation of the pressure – poisson equation, is solved using an Incomplete Choleski Conjugate Gradient method. A typical problem involving a single gas bubble rising during 1.0 s in a liquid, using a computational mesh of 100 x 150 cells and a time step of 1.0 x 10^{-4} s, requires 16 hours dedicated CPU time on a Silicon Graphics Indigo2 workstation. Approximately 50% of the CPU time used by the Volume Tracking code is required to solve the system of linear equations, whereas about 30% of the CPU time is used to track the interface.

3. Results and discussion

Key features of the Volume Tracking model outlined in the previous sections, are its capability to resolve the shape of a bubble under the prevailing flow conditions and physical properties of the liquid, and its capability to resolve the gas and liquid flow field associated with the rising bubble. In this section four typical results obtained with this model will be discussed. The first two case studies will explore the capability of the Volume Tracking model to accurately predict the formation and rise of a skirted bubble and of a spherical capped bubble. The third case study focuses on the co – axial rise, and eventual coalescence, of two gas bubbles emanating from the same orifice. Finally, the time – dependent behavior of two identical gas bubbles emanating from two adjacent orifices will be investigated.

3.1 The skirted bubble

Grace (1973) and Grace *et al.* (1976) presented a diagram that reflects the effect of fluid properties and equivalent bubble diameter on the shape and terminal rise velocity of an isolated bubble. According to their diagram, at Eö ≈ 4.0 x 10^2 and Mo = 1.0 x 10^2 a so – called skirted bubble should be obtained. Figure 2 shows the formation and rise of a single gas bubble emanating from a central orifice at Eö ≈ 4.0 x 10^2 and Mo = 1.0 x 10^2, as calculated with our Volume Tracking code. Figure 2 depicts the gas – liquid interface in precisely the same orientation as used by the Youngs' VOF algorithm to calculate the F fluxes; no smoothing has been applied. It can clearly be seen that a skirted bubble emerges, as is expected on basis of the aforementioned diagram. The bubble skirts are especially pronounced at t = 0.6 s, they stretch considerably as the bubble

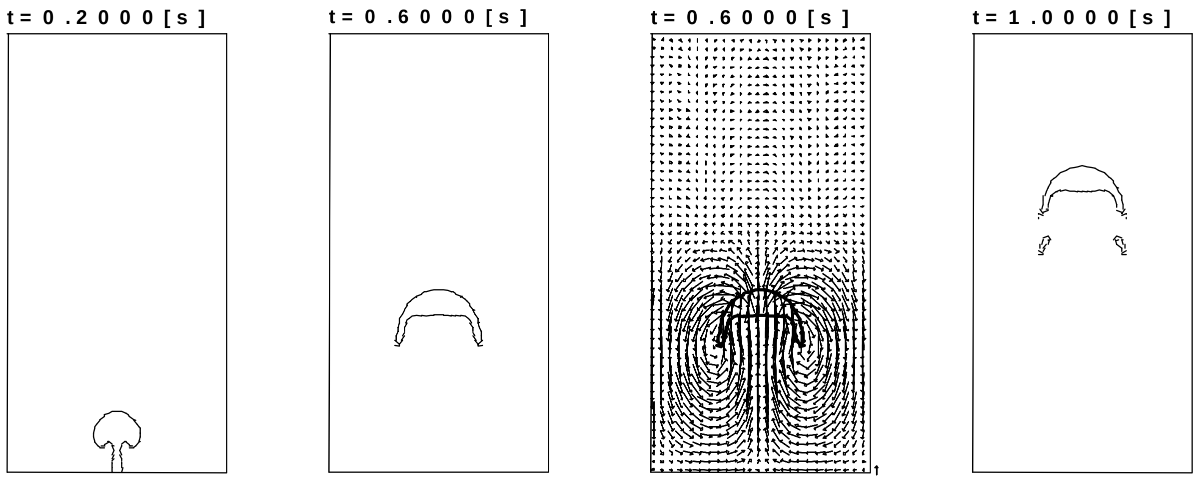

Figure 2 Bubble emanating from orifice at Eö ≈ 4.0 x 10^2 and Mo = 1.0 x 10^2. Results obtained with Youngs' VOF model. Height = 0.50 m, width = 0.25 m, NX = 50, NY = 100, DT = 1.0 x 10^{-5} s, liquid density = 1000 kg m^{-3}, gas density = 1.2 kg m^{-3}. The reference vector provided with the flow field corresponds to a velocity of 10 cm s^{-1}.

continues its ascent through the liquid and eventually break into smaller skirts and two small trailing bubbles (t = 1.0 s). Figure 2 also shows the gas – liquid flow pattern at t = 0.6 s, clearly revealing the structure of the wake trailing the skirted bubble. The skirts can be seen to extend into the eye of the vortices that make up the bubble wake.

3.2 The spherical cap bubble

At Eö ≈ 1.0×10^2 and Mo = 1.0×10^{-12}, the diagram presented by Grace (1973) and Grace *et al.* (1976) reports the existence of spherical capped bubbles. Figure 3 shows a sequence of snapshots depicting the instantaneous position of the gas – liquid interface of a gas bubble emanating from an orifice at (approximately) these Eö and Mo numbers. As can be seen from this Figure, a spherical cap bubble eventually emerges. The formation of this cap shaped bubble is worth discussing in more detail. At t = 0.06 s a bubble is formed that has sufficient buoyancy to start its ascent through the liquid. The liquid motion induced by this forming bubble causes severe necking (not shown). This neck, in turn, detaches from the primary bubble to form a second, elongated bubble (t = 0.12 s). This secondary bubble subsequently coalesces with the first bubble causing small pockets of liquid to be included in the bubble.

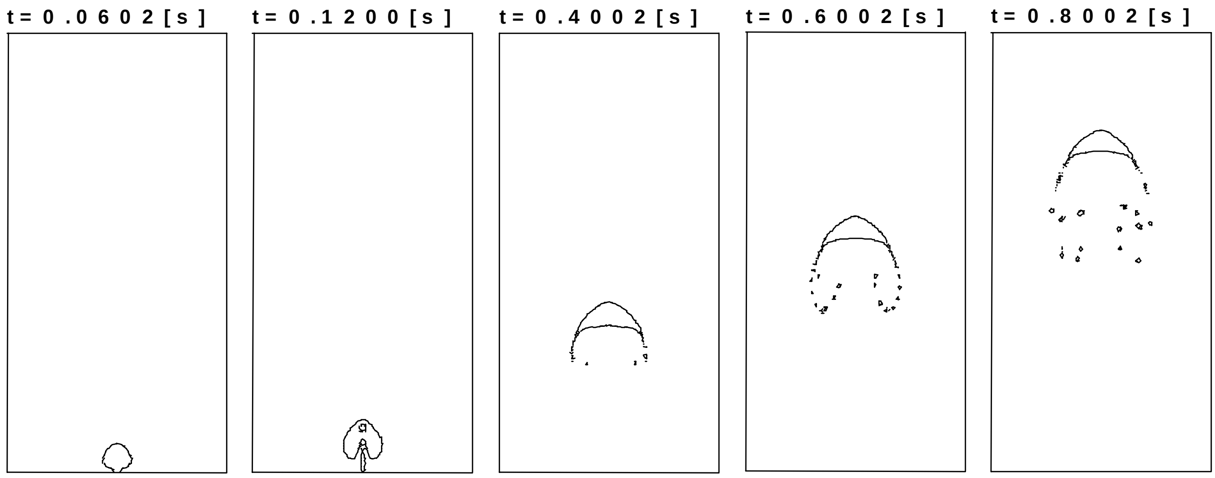

Figure 3 Bubble emanating from orifice at Eö ≈ 1.0×10^2 and Mo = 1.0×10^{-12}. Results obtained with Youngs' VOF model. Height = 0.20 m, width = 0.10 m, NX = 100, NY = 150, DT = 2.0×10^{-4} s, liquid density = 1000 kg m^{-3}, gas density = 1.0 kg m^{-3}.

At t = 0.6 s the distinctly spherical cap shaped bubble edges. These satellite bubbles, whose motion is also accumulate in the wake of the cap shaped bubble. This experiments, but (numerically) it might be exacerbated curvature, despite the considerable spatial resolution of Youngs' VOF method: the algorithm exhibits can be seen to shed small satellite bubbles from its rear tracked by the Volume Tracking code, tend to shedding of bubbles is frequently observed in by a locally (at the edges) under – resolved interface the Eulerian mesh. This reveals another aspect of numerical surface tension.

3.3 Co – axial coalescence of two gas bubbles

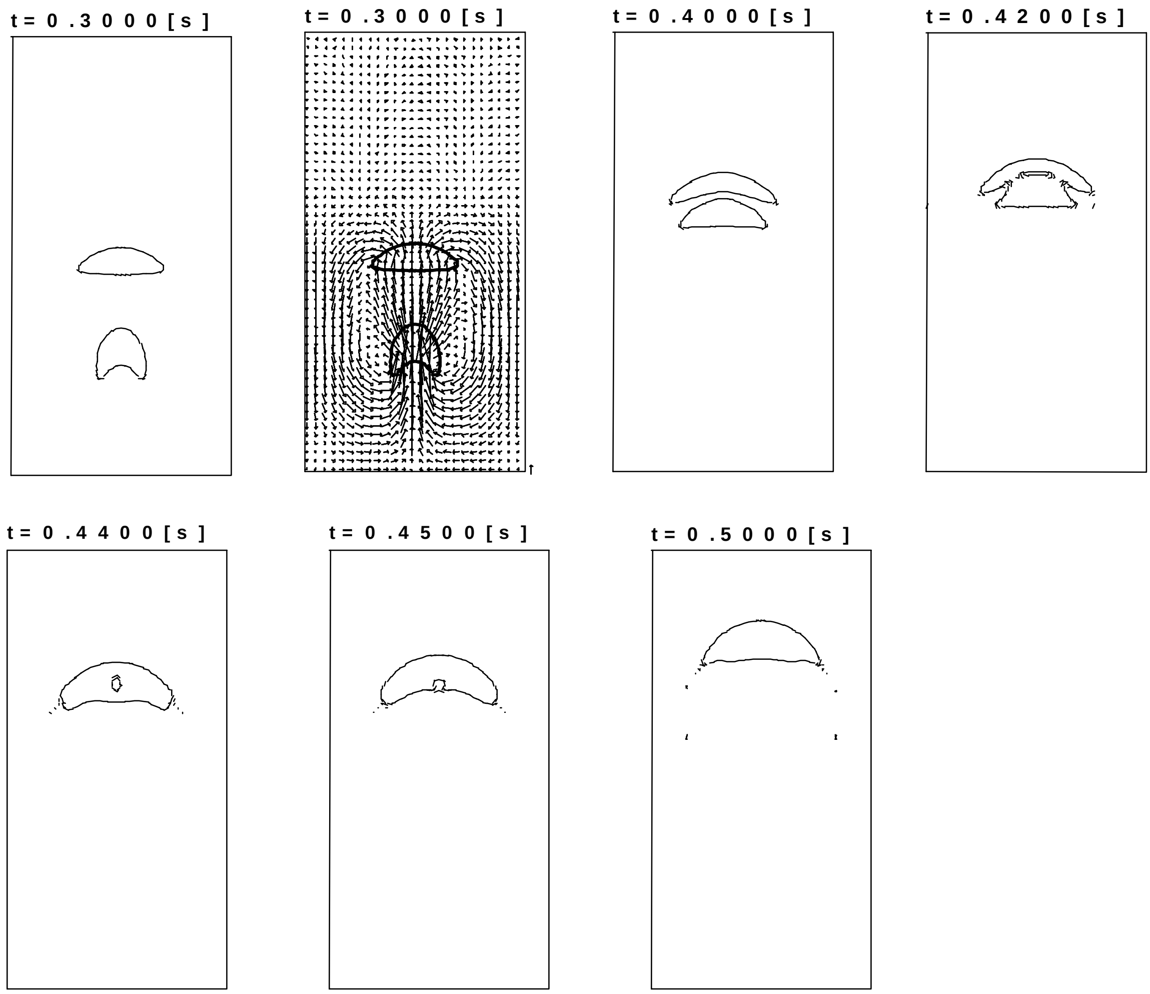

Figure 4 Co – axial coalescence of two bubbles emanating from the same orifice at Eö ≈ 16 and Mo = 2.0 x 10^{-4}. Results obtained with Youngs' VOF model. Height = 0.10m, width = 0.05 m, NX = 50, NY = 100, DT = 5.0 x 10^{-5} s, liquid density = 1000 kg m^{-3}, gas density = 1.2 kg m^{-3}. The reference vector corresponds to a velocity of 10 cm s^{-1}.

Brereton and Korotney (1991) presented experimental observations of the co – axial coalescence of two gas bubbles rising in an initially quiescent liquid. Using flash photography, the authors were able to analyze the coalescence process, and they were able to reveal the remarkable difference in shape between the leading and trailing bubble. The Volume Tracking model presented in this paper has also been used to study the co – axial coalescence of two identical gas bubbles at Eö ≈ 16 and Mo = 2.0 x 10^{-4}, conditions identical to those employed by Brereton and Korotney (1991). Snapshots depicting the instantaneous position of both the leading and the trailing bubble are shown in Figure 4. At t = 0.3 s the effect of the wake of the leading bubble on the shape of the trailing bubble can clearly be seen. The base of the trailing bubble is severely indented owing to the greater velocity of the liquid behind the trailing bubble compared to the velocity of the liquid preceding that bubble. At t = 0.40 s the base of the leading bubble deforms inward, due to interaction with the trailing bubble and the liquid immediately behind the leading bubble. Coalescence is imminent. At t = 0.42 s the inertia of the liquid behind the trailing bubble drives the coalescence of that bubble with the leading bubble. The gas – liquid interface of the coalesced bubble initially assumes a very complex shape, but eventually a spherical cap bubble emerges. It can also be seen that, during the coalescence of both bubbles, the coalesced bubble encapsulates a small drop of liquid that leaves the newly formed bubble through its base. These results agree remarkably well with the experimental observations reported by Brereton and Korotney, especially in view of the complexity of the coalescence process and the fundamental nature of our model.

3.4 Adjacent bubbles

In the previous section, we have studied the co – axial rise and eventual coalescence of two bubbles, as a fourth and final case we will study the formation and rise of two identical gas bubbles emanating from two adjacent orifices. It is interesting to see whether these bubbles will coalesce, as their co – axial counterparts did, or whether they will bounce. Figure 5 depicts the successive positions of both bubbles in a single frame; the associated flow field (one out of every two vectors is shown) of both phases at t = 0.18 s is also shown.

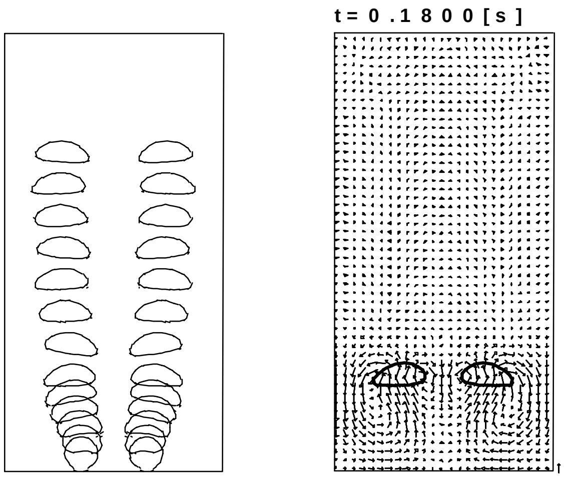

Figure 5 Two bubbles emanating from two adjacent orifices at Eö ≈ 4 and Mo = 2.0 x 10^{-4}. Both instantaneous bubble positions and the flow field at t = 0.18 s are shown. Results obtained with Youngs' VOF model. Heigth = 0.10 m, width = 0.05 m, NX = 50, NY = 100, DT = 5.0 x 10^{-5} s, liquid density = 1000 kg m^{-3}, gas density = 1.2 kg m^{-3}. The reference vector corresponds to a velocity of 10.0 cm s^{-1}.

It can be seen most clearly from Figure 5 that the two adjacent bubbles do not coalesce; instead the distance between the bubbles increases. In the early stages of their ascent, both bubbles exhibit a wobbling behavior that appears to diminish as the distance between the bubbles increases. The flow field depicted on the right hand side of Figure 5 clearly reveals the complex structure of the wake trailing the two bubbles. As can be inferred from this Figure, there is a considerable interaction between the wakes of both bubbles. Two vortex pairs make up the combined wake of the bubbles. Moreover, there appears to be a significant down flow of liquid in between the bubbles, preventing coalescence.

4. Conclusions

In this paper we have presented a Volume Tracking model developed with the specific objective of studying the behavior of multiple, "large" bubbles rising in an initially quiescent liquid. The model, based on the Volume – Of – Fluid (VOF) concept, solves the incompressible Navier – Stokes equations to obtain the gas and liquid flow fields. In addition, the model tracks the motion of the gas – liquid interface embedded in the overall motion of the flow field, and maintains a compact interface thickness through the use of an advanced interface tracking scheme known as Youngs' VOF (Youngs, 1982). Interface physics, surface tension in particular, have been incorporated in the model using the Continuum Surface Force (CSF) model.

Results obtained with this model for four different cases have been discussed: the formation and rise of a skirted bubble, and a spherical cap bubble, the co – axial rise and coalescence of two identical gas bubbles and the behavior of two gas bubbles emanating from adjacent orifices. From these results it can be concluded that the Volume Tracking code, in its present form, is able to accurately track the motion of a gas – liquid interface, subject to appreciable changes in its topology and embedded in a flow field with considerable vorticity. It is therefore that we believe that this Volume Tracking model offers a promising (perhaps not yet mature) tool for those involved in studying gas – liquid systems.

5. Notation

μ_l	Shear viscosity liquid [kg m^{-1} s^{-1}]
μ_g	Shear viscosity gas [kg m^{-1} s^{-1}]
δt	Time step [s]
δx	Grid size in x direction [m]
Eö	Dimensionless Eötvös number [-]
F	Fractional volume liquid [-]
$\mathbf{F}_{SF}$	Volumetric surface tension force [N]
$\mathbf{g}$	Acceleration due to gravity [m s^{-2}]
κ	Surface curvature [m]
Mo	Dimensionless Morton number [-]
$\mathbf{n}$	Normal to gas - liquid interface [-]
$\tilde{\mathbf{n}}$	Average unit normal to gas – liquid interface [-]
P	Pressure [N m^{-2}]
ρ_g	Density gas phase [kg m^{-3}]
ρ_l	Density liquid phase [kg m^{-3}]
σ	Surface tension coefficient [N m^{-1}]
t	Time [s]
τ_l	Stress tensor liquid [N m^{-2}]
$\mathbf{u}$	Velocity [m s^{-1}]
$\mathbf{x}$	X – coordinate [m]

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