Numerical simulation of bubble formation by breaking waves in turbulent two-phase Couette flow

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1. Motivation and objectives

Turbulent bubbly flows are often encountered in nature and in industries: petroleum, biochemical, power generation, and ship industries. In naval applications, for example, it is important to understand the mechanisms of surface wave breaking and bubble generation resulting from the interaction between turbulent boundary-layer (TBL) and free surface. The bubble size generated by the wave breaking is typically from the order of microns to centimeters. Moreover, the micron-sized bubbles reside for a long time beneath the free surface because of their slow buoyant force. However, it is very challenging to model such a phenomenon because of its complex and broad-band characteristics.

Two-phase flows are generally classified into three regimes according to the shape of the interface: separated flows, dispersed flows, and mixed flows. In dispersed flows, one phase is assumed to be dilute and the dispersed dilute phase is often treated in a Lagrangian way. The particles, droplets or bubbles, are assumed as point particles because the particle size is very small as compared to the macroscopic scale. The individual particles are tracked by solving Newton’s second law considering the forces acting on the particles. The flow inside the particles does not need to be solved and the interaction between flow and particles is taken into account by adding source terms in the Navier-Stokes equations. Many numerical models have been proposed and validated for turbulent bubbly flows in dilute phase (Riley & Patterson 1974; Squires & Eaton 1990; Elghobashi & Truesdell 1992). However, the disadvantage is that it is inaccurate for the dense regime where the interaction between particles is significant.

In the case of separated two-phase flows, no empirical model or hypothesis can be assumed for the shape of the each phase. In order to capture the physical process occurring at the interface, the phase interface should be resolved and tracked in the numerical simulation. Among several phase-tracking methods based on the Eulerian approach, the marker particle method (Tryggvason et al. 2001), the volume-of-fluid (VoF) method (Gueyffier et al. 1999) and the level set method (Sussman et al. 1994) are popular schemes. Each tracking method has its advantages and disadvantages. The marker particle method can conserve the volume of each phase with high accuracy but it is too complex to model topological changes of the interface, especially in three-dimensional cases. Although the level-set method can handle topology changes automatically, its main drawback is that volume conservation is not inherently guaranteed. The VoF method shows good volume conservation, but requires a specific advection scheme for the transport equation of VoF scalar, thereby affecting the accuracy of the scheme and volume conservation. Moreover, calculating geometric quantities such as surface normal and curvature remains problematic.

The research and development described in this paper arise from the need for modeling
a realistic turbulent bubbly flow in a mixed flow regime. Our objective is to perform turbulent bubbly flows in a mixed flow regime using a high-fidelity computational tool and to predict turbulent bubbly flow behavior with greater accuracy and reliability. However, a number of challenges must be overcome for numerical simulations. First of all, mass conservation should be guaranteed because even a small numerical diffusion error in each phase mass is critical to the small-size bubbles. Thus, 100% mass conservation is necessary to maintain small bubbles in the mixed two-phase flow where the separated and dispersed phase coexist. In addition to the mass conservation, one must also ensure solver robustness at realistic density ratios. In the area of high-performance computing, achieving speed and scalability is complicated by the highly dynamic workload associated with the moving interface, as well as the variable coefficient unstructured Poisson system that must be solved in each time step.

In the present study, we use a novel geometric unstructured VoF method recently developed at Cascade Technologies, Inc. The VoF-based scheme is fully conservative and un-split, allowing exact mass conservation and robust handling of high-density ratios. Before applying to bubbly flows, the method is tested on several canonical problems: Zalesak's disk, sphere in a deformation field, stationary column in equilibrium, and damped surface waves. These tests demonstrated stability and the accuracy of the present VoF method.

The numerical method is then applied to a realistic turbulent bubbly flow in a Couette flow with moving sidewalls. Two-phase turbulent boundary layers (TBL) in a Couette-type setting have been simulated, capturing the unsteady evolution of complex phase interface as well as bubbles beneath the free surface. Computations were carried out for water and air properties with the Reynolds number of 12,000 and Weber numbers of 200 based on the water properties. The primary objective of these calculations is to show the capability of the newly developed VoF method.

2. Canonical test cases

The following subsections present canonical test problems to verify the accuracy of the present numerical method.

2.1. Solid body rotation of Zalesak’s disk

To test the capability of the present method to adequately transport a body with sharp corners, the rigid body rotation of Zalesak’s disk in a solid body velocity field is simulated. The initial shape of a notched circle is centered at (0.5, 0.75) in a 1 × 1 domain box with a radius 0.15, a width of 0.05, and a slot length of 0.25. The velocity field is given by

\[
\begin{align*}
    u(x, y, t) &= 0.5 - y \\
    v(x, y, t) &= x - 0.5.
\end{align*}
\]

Time integration is performed until one revolution is reached. Figure 1 shows the shape of Zalesak’s disk after one full rotation for different grid sizes. The notched disk is distorted in the coarse grid, however, the shape approaches to the exact solution by refining the grid.

2.2. Sphere in a deformation field

As a test for a three-dimensional case, the evolution of a sphere in a deformation field is simulated. A sphere of radius 0.15 is placed at (0.35,0.35,0.35) in a unit box. The velocity field is set to
Figure 1. The interface shape of Zalesak’s disk after one rotation with the exact solution (dashed line). CFL=0.5: (a) 50 × 50 mesh; (b) 100 × 100 mesh; (c) 200 × 200 mesh; (d) 400 × 400 mesh.

Figure 2. Time evolution of the iso-surface of VoF = 0.5 in a deformation field with 256³ grids: (a) t = 0; (b) t = T/8; (c) t = T/4; (d) t = 3T/8; (e) t = T/2.

Figure 3. The iso-surface of VoF = 0.5 at t = T/2 for different grid resolutions: (a) 64³; (b) 128³; (c) 256³.

\[
\begin{align*}
    u(x, y, z, t) &= 2 \cos(\pi t/T) \sin^2(\pi x) \sin(2\pi y) \sin(2\pi z), \\
v(x, y, z, t) &= -\cos(\pi t/T) \sin(2\pi x) \sin^2(\pi y) \sin(2\pi z), \\
w(x, y, z, y) &= -\cos(\pi t/T) \sin(2\pi x) \sin(2\pi y) \sin^2(\pi z),
\end{align*}
\]  

where, T = 3. Figure 2 shows the time evolution of the iso-surface of VoF = 0.5 with 256³ grids. The sphere is stretched in time and the thin structure is found at t = T/2. The iso-surfaces of VoF = 0.5 at t = T/2 for different grid resolutions are depicted for comparison in Fig. 3. With the coarse grid of 64³, the thin structure is almost gone and a few large droplets are observed instead. In the case of a fine grid of 256³, the thin structure maintains its shape and the under-resolved region is replaced with fine scale
droplets and ligaments. Note that the total volume of each phase is conserved regardless of the grid size.

2.3. Stationary column in equilibrium

A stationary column in equilibrium is considered in order to test the spurious current induced by curvature errors. The diameter of the column is $D = 4$, which is placed at the center of an $8 \times 8$ domain. The surface tension coefficient is $\sigma = 1$ and the densities inside and outside the column are $\rho_1 = 1000$ and $\rho_2 = 1$, respectively. The Laplace numbers, $La = \sigma \rho_1 D/\mu_1$, used in the simulations are 40000 and $\infty$ to study the viscous effect.

Owing to errors in curvature evaluation, non-zero spurious currents are produced for the equilibrium column as explained in Francois et al. (2006). The long-time behavior of the spurious velocities has been studied in order to check whether the errors are accumulated and result in large erroneous spurious velocities. Figure 4(a) shows the temporal evolution of the kinetic energy of the inviscid column ($La = \infty$) in the whole computational domain for different grid resolutions. It shows oscillations of kinetic energy are not growing in time and decreasing with grid resolution. Figure 4(b) illustrates the evolution of kinetic energy for $La = 40,000$. The kinetic energy with viscosity shows rapid decay in time and tends toward zero where numerical balance is reached between surface tension and pressure. The results demonstrate that the balanced-force implementation with the present VoF method is accurate enough to obtain an equilibrium solution in the case of a stationary column.

2.4. Damped surface waves

In order to verify the accuracy of the surface tension term with the viscous term, a small perturbed surface wave between two immiscible fluids without gravity are solved and compared with the initial value theory of Prosperetti (1981). The cosine wave with wavelength $\lambda = 2\pi$ and amplitude $A_0 = 0.01\lambda$ is placed in a $[0, 2\pi] \times [0, 2\pi]$ domain as

$$G(x, t = 0) = y - \pi + A_0 \cos(x),$$  \hfill (2.3)
Figure 5 shows the temporal evolution of the non-dimensional disturbance amplitude $A$ under grid refinement. Figure 6 shows the rms amplitude error $E_{rms}$ for $0 < t < 20$.

2.5. Rising bubble

To illustrate the stability and mass-conserving nature of the scheme, Figure 7 illustrates six different frames from a numerical simulation of a rising bubble inside a rectangular enclosure. A computational domain of [-0.1m, 0.1m] x [-0.1m, 0.2m] is considered, which is initially filled with water with density 1000kg/m$^3$ where the free surface is located at $y = 0.15$m. A circular air bubble of radius 1/30m is centered at the origin with density 1.364kg/m$^3$. The viscosities of air and water are set to $1.8 \times 10^{-5}$kg/m/s and $1.0 \times 10^{-3}$kg/m/s, respectively. The effect of surface tension is included with the coefficient $\sigma = 0.07$N/m.

Even after the first bursting of the main bubble, small bubbles remain entrained in the fluid, floating slowly to the surface. While we do not claim that this sort of numerical experiment properly captures every scale of bubble breakup for this type of problem, it nevertheless illustrates the potential benefit of a fully conservative un-split scheme for resolving and tracking small-scale bubbles.
Figure 7. Visualizations from a numerical simulation of a rising bubble inside the rectangular water box: (a) $t=0.28s$; (b) $t=0.46s$; (c) $t=0.64s$; (d) $t=1.17s$; (e) $t=1.88s$; (f) $t=3.06s$. 
3. Numerical simulation of turbulent two-phase Couette flow

3.1. Numerical configuration

The flow configuration and domain size are described in Fig. 8. The initial shape of the interface is a flat surface in an $xy$ plane at the midpoint of the $z$-axis. Two sidewalls are moving in the opposite direction with speed of $U = 1.2\text{m/s}$, respectively. The no-slip conditions are used for the moving sidewalls and the top and bottom walls are $w = 0$, $\frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = 0$. (3.1)

The flow is assumed to be statistically homogeneous in the $x$-direction where periodic boundary conditions are used. The computational domain size is set to $h = 0.01\text{m}$. Initially, the half bottom of the domain is filled with water with a density of $1000\text{kg/m}^3$ where the free surface is located at the center, $z = 0.0\text{m}$. The upper part is air with a density of $1.2\text{kg/m}^3$. The viscosities of air and water are set to $1.8 \times 10^{-5}\text{kg/m/s}$ and $1.0 \times 10^{-3}\text{kg/m/s}$, respectively. The effect of surface tension is included with the coefficient $\sigma = 0.07\text{N/m}$ and the Weber number based on the water and $h$ is $We_h = 200$. Here, gravity is $9.81\text{m/s}^2$ acting in the $-z$ direction.

3.2. Grid resolution requirement

In order to correctly capture the physical process occurring at the interface, every meaningful scale of the interface should be resolved, as well as the scale of turbulent flow. The Reynolds number in water, based on $h$, is about $12,000$, which corresponds to $Re_\tau \approx 600$ in the case of a single water turbulent Couette flow. The grid resolution near the wall is then determined based on the viscous length scale assuming a single-phase turbulent flow. In the case of the two-phase flow, the smallest length scale of the phase interface should be considered in addition to Kolmogorov length scale for fully resolved numerical simulations. In the present study, we choose the Hinze scale (Hinze 1955) as the smallest interfacial scale, where the interfacial energy is balanced by the turbulent kinetic energy of eddies. Thus, the turbulent fragmentation ceases at the scale smaller than the Hinze scale where the surface tension is large enough to prevent breaking up. The ratio of these forces can be represented by the bubble Weber number as
\[ We = \frac{\rho_l u^2 d}{\sigma}, \quad (3.2) \]

where \( \rho_l \) is the liquid density, \( u \) is the turbulent velocity, \( \sigma \) is the surface tension coefficient, and \( d \) is the bubble diameter. The critical Weber number, \( We_c \), can be defined by the condition for bubble fragmentation when exceeding a critical value, \( We_c \). The recent experiments reported that \( We_c \) is \( 3 \sim 4.7 \) (Lewis & Davidson 1982; Martinez-Bazan et al. 1999). This condition limits the grid size in the domain where the phase interface exists. In the present computation, the grid size is chosen such that the Weber number based on the grid size is less than \( We_\Delta = 3.4 \) to satisfy the condition. The grid resolution based on the viscous length scale is then \( \Delta x^+ = 8, \Delta y_{\text{min}}^+ = 0.1, \Delta y_{\text{max}}^+ = 8, \) and \( \Delta z^+ = 8 \).

3.3. Results

The simulation has been performed at least 50 flow-through times to obtain a statistically converged number of bubbles. Figure 9 shows a snapshot of the iso-surface of \( \text{VoF} = 0.5 \) for different points of view to illustrate the free surface and bubbles. On the free surface, the oblique wave structure is observed and the phase interface is oscillating, leading to breakup of the phase interface. The air cavities are found underneath the free surface, which was trapped between the breaking free surface waves. This air cavity is subsequently fragmented into air bubbles in the water. The mean volume fraction of air shown in Fig. 10(a) is averaged in time and the periodic direction (x) and measured at three different planes in the gravitational direction. Note that the volume fraction is 0 in the water phase and 1 in the air phase. The averaged volume fraction of air is increased as the height is increased in z. The volume fraction is observed to be small near the sidewall compared to the center region. The Sauter mean diameter (SMD) of the bubble is also measured at the same locations and shown in Fig. 10(b). The large-size of bubbles are concentrated away from the sidewall, while the small-size bubbles are concentrated near the sidewall.

4. Conclusion

A novel unstructured VoF method, developed at Cascade Technologies, Inc, is tested for canonical verification cases to assess the accuracy and performance of the method. The VoF-based scheme is geometric and un-split and exactly conserves the mass. As a demonstration of the conservative capability, turbulent two-phase Couette flow with moving sidewalls was simulated in the periodic boundary conditions. Computation was performed for water and air with the Reynolds number of 12,000 and Weber numbers of 200 based on the water properties. The grid resolution is determined to correctly resolve the turbulent flow and bubble size larger than the Hinze scale.

The simulation successfully predicts the breaking surface wave and resulting air cavities and tracks even small bubbles near the sidewall without losing them. With this conservative benefit of our method, the statistical data on the mean volume fraction and bubble size distribution can be obtained. It is observed from the bubble statistics that large bubbles are concentrated away from the wall whereas small bubbles are concentrated near the side walls. In the future, the numerical result will be compared with the experimental data, which is currently conducted by James Duncan at the University of Maryland.
Figure 9. Snapshots of the iso-surface of $V_oF = 0.5$ of the turbulent two-phase Couette flow for different points of view: (a) front view; (b) top view; (c) side view.

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Figure 10. Statistics of the volume fraction and bubble size averaged in time and x direction for different heights, ---, z/h = -0.3; - - - - - - - , z/h = -0.6; - - - - - - , z/h = -1.2: (a) mean volume fraction of air; (b) Sauter mean diameter of bubble.

REFERENCES


