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Numerical Simulation of a Single Air Bubble Rising in Water with Various Models of Surface Tension Force

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Abstract**—**Different numerical methods are employed and developed for simulating interfacial flows. A large range of applications belong to this group, e.g. two-phase flows of air bubbles in water or water drops in air. In such problems surface tension effects often play a dominant role. In this paper, various models of surface tension force for interfacial flows, the CSF, CSS, PCIL and SGIP models have been applied to simulate the motion of small air bubbles in water and the results were compared and reviewed. It has been pointed out that by using SGIP or PCIL models, we are able to simulate bubble rise and obtain results in close agreement with the experimental data.

Keywords**—**Volume-of-Fluid; Bubble Rising; SGIP model; CSS model; CSF model; PCIL model; interface; surface tension force.

I. Introduction

DIFFERENT numerical methods are employed and developed for simulating interfacial flows. The numerical methods can be divided into two groups depending on the type of grids used: moving grid or fixed grid. For the fixed-grid methods, the interface is moved through a fixed grid and its position is computed at each time step and in all partially filled cells. One important approach of fixed-grid methods, namely the volume-of-fluid, is among the most commonly used methods. The Volume-Of-Fluid method, tracks the volume of each fluid in all cells containing portions of the interface, rather than the interface itself. A volume fraction function F is defined as volume fraction of one the fluids in each cell. The VOF algorithm consists of the following three major part: 1) The interface reconstruction, which finds an explicit description of the interface in each multi-fluid cell based on void fractions; 2) The advection algorithm, which calculates the distribution of F at the next time step by solving an advection equation using the reconstructed interface and the underlying velocity field; 3) The surface tension model, which takes into account of surface tension effects at the interface. The VOF method solves a non-diffusive solution of the advection equation, by a geometrically based calculation technique of the void fraction fluxes at the cell faces based on the reconstructed interface. A significant improvement of the interface representation was achieved by Youngs [1] by introducing a piecewise-linear method. The PLIC method approximate the interface is by a straight line of arbitrary orientation in each cell. Its orientation is found the distribution of one of the fluids in the neighbor cell. Given the volume fraction of one of the two fluids in each computational cell and an estimate of the normal vector to the interface, a plane surface is constructed within the cell having the same normal and dividing the cell into two parts each of which contains the proper volume of one of the two fluids. This has several advantages: the fluxes of F with which the phase field F is updated, can be determined more accurately, and essentially free of numerical diffusion. Fluid properties can be calculated accurately. In contrast to the interface representation methods, the methods for introducing surface tension effects at the interface into the physical model remain a problem. Generally, the influence of surface tension is incorporated into the momentum equation following the continuum surface force (CSF) model of Brackbill et al. [2]. For doing so, the local curvature and the interface normal vector have to be calculated. This task is difficult, since the discontinuous void fraction function disallows the application of ordinary discretization schemes. An inconsistent calculation of the surface tension force can then result in the well-known phenomena of so-called "spurious currents" [11]. Usually problems with parasitic currents arise when flows with high density ratios are considered. Unfortunately, a large range of applications belong to this group, e.g. two-phase flows of air bubbles in water. In such problems surface tension effects often play a dominant role. The behavior of each algorithm under surface tension-dominant problems is discussed in the next section.

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II. Problem Formulation

We consider the three-dimensional, unsteady, laminar, incompressible Navier-Stokes equations without phase change. A volume-of-fluid (VOF) method along with a piecewise linear interface calculation (PLIC) is used to capture the fluid interfaces. It is assumed that the velocity field is continuous across the interface, but there is a pressure

jump at the interface due to the presence of the surface tension. The governing equations describing this problem are:

$$\frac{\partial u_i}{\partial x_i} = 0 , \tag{1}$$

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0 , \tag{2}$$

and

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \mathbf{F}_\mathbf{v}^{\mathbf{st}} . \vec{i} + \mu \frac{\partial^2 u_i}{\partial x_j^{\,2}} + \rho g_i . \tag{3}$$

where u_i's are the velocity components, and t and x_i are time and space coordinates respectively, F is the volume fraction of fluid, p is the pressure, $\mathbf{F}_\mathbf{v}^{\mathbf{st}}$ is the surface tension force per unit volume and ρ and μ are the average density and absolute viscosity in a cell, respectively, and they depend on the densities and viscosities of each fluid a the cell. That is:

$$\rho = \rho_2 + F(\rho_1 - \rho_2) \quad \text{and} \quad \mu = \mu_2 + F(\mu_1 - \mu_2) \tag{4}$$

Here we use pressure based numerical method, then the Poisson equation needs to be solved. The Poisson equation is obtained by taking the divergence of the momentum equation, Eq. (3), and then simplifying it by the continuity equation, Eq. (1). The resulting equation is:

$$\frac{\partial}{\partial x_i}\left(\frac{\partial p}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left[\frac{\partial}{\partial x_j}\left(\rho u_i u_j - 2\mu S_{ij} - \frac{\mathbf{F}_\mathbf{v}^{\mathbf{st}} . \vec{\mathbf{i}}}{\rho}\right)\right] . \tag{5}$$

III. Surface Tension Force

The complexity of simulation of interfacial flows is mainly due to the existence of surface tension force. The surface tension force is presented at the interface of two fluids when at least one of them is liquid. The surface tension force may be important in some interfacial flows. The surface tension force produces pressure jump across the interface. The boundary condition at the interface is stated as [4]:

$$(p_1 - p_2 + \sigma\kappa)n_i = (\tau_{1ik} - \tau_{2ik})n_k + \frac{\partial \sigma}{\partial x_i} \tag{6}$$

In this equation σ is surface tension coefficient, p_α is pressure, α denotes each of fluids and is defined as α=1,2, $\tau_{\alpha ik}$ is viscous tension tensor, n is unit vector perpendicular to the surface (toward fluid 2). If Eq. (6) is projected normal to the surface, the boundary condition for pressure is:

$$p_1 - p_2 + \sigma\kappa = 2\mu_1 n_k \left(\frac{\partial u_k}{\partial n}\right)_1 - 2\mu_2 n_k \left(\frac{\partial u_k}{\partial n}\right)_2 \tag{7}$$

From Eulerian point of view, surface tension force generates discontinuity in the pressure field. The discontinuity makes the numerical simulation of the interfacial flows difficult. There has been some efforts for implementing the effect of surface tension in Eulerian schemes. To eliminate the problem, the surface tension force is tuned into a volume force. One of attempts in this field, were done by Brackbill *et al.* [3]. This method, which is called CSF method, reformulates surface tension into an equivalent volume force F_v^{st} as follows:

$$\vec{\mathbf{F}}_\mathbf{v}^{\mathbf{st}} = \sigma\kappa\delta_s \mathbf{n} \tag{8}$$

This body force is added into the momentum equations and so the effect of surface tension is modeled. In this model it is necessary to calculate κ, n and δ_s. These variants are related to volume fraction function. By definition, they are calculated as follow [3]:

$$\mathbf{n} = \frac{\nabla \widetilde{F}}{\left|\nabla \widetilde{F}\right|} \quad , \quad \delta_s = \left|\nabla \widetilde{F}\right| \quad \text{and} \quad \kappa = -\nabla \cdot \tilde{\mathbf{n}} = -\nabla \cdot \frac{\nabla \widetilde{F}}{\left|\nabla \widetilde{F}\right|} \tag{9}$$

where the tilda denotes the filtered (smoothed) value. The strength of the spurious currents differs from one model to another. The amount of spurious velocity along with the accuracy of the pressure jump across the interface are use to evaluate the models. For CSF model, Eq. (8) is corrected to decrease the intensity of spurious currents by applying a density correction term [3, 5]:

$$\mathbf{F}_\mathbf{v}^{\mathbf{st}} = \sigma\kappa\boldsymbol{\delta}_\mathbf{s}\mathbf{n} = \sigma\kappa\mathbf{n}\left|\nabla \widetilde{F}\right| \frac{\rho(x)}{[\rho]} , \tag{10}$$

where *[ρ]* is the difference between the density of the heavier and the lighter fluids. The density correction term (the fraction in above Equation) is added to reduce the force in the region with lighter fluid in momentum equation. This dampens the acceleration of the lighter fluid in cells near the interface that contains large amounts of lighter fluid. Aleinov and Puckett [6] suggested another formulation of $\mathbf{F}^{\mathbf{st}}$. The surface force per unit volume is computed only within each surface cell and is placed at the center of the cell:

$$\mathbf{F}_{\mathbf{i,j,k}}^{\mathbf{st}} = \sigma\kappa_{i,j,k} \frac{A_{i,j,k}}{V_{i,j,k}} \mathbf{n}_{i,j,k} , \tag{11}$$

where $A_{i,j,k}$ is the surface area of the interface within the cell, $n_{i,j,k}$ is unit vector normal to the surface and ($V_{i,j,k}$) is the volume of the cell denoted by *i,j,k*. This force is then smoothed by convoluting it with a smoothing kernel, K:

$$\widetilde{\mathbf{F}}_{i,j,k}^{st} = K\mathbf{F}_{i,j,k}^{st} . \tag{12}$$

Another model was presented by Lafaurie *et al*. in 1999, and is called CSS model [7]. The CSS model, converts the surface tension force into stress form T, which is tangential to the interface. Then the capillary force is written as [7]:

$$\mathbf{F}_\mathbf{v}^{\mathbf{st}} = -\nabla . T = \sigma\nabla \cdot \left(\left|\nabla F\right|\mathbf{I} - \frac{\nabla F \otimes \nabla F}{\left|\nabla F\right|}\right) , \tag{13}$$

Meier *et al.* [8] modeled surface tension force based on VOF-PLIC method and calculated the surface tension force within each cell. In their model the surface tension force per unit area is determined in interfacial cells only and multiplied by interface area. But in the stagger grid numerical methods,

when the volume force is divided into the momentum cells and fluid accelerates as result of the surface tension. They used Eq. (11) to calculate the force at the center of each cell. Here we follow their notations which were given for two-dimensional case. They divided Eq. (11) by density to obtain the body force in the cell:

$$\mathbf{e}_{\mathbf{x,i,j}} = \frac{\sigma}{\rho_{i,j}} \kappa_{i,j} \frac{A_{i,j}}{V_{i,g}} \mathbf{n}_{\mathbf{i,j}} \tag{14}$$

Despite of their simplicity and being conservative, CSS and CSF models produce high spurious currents near the interface. For problems where the surface tension forces are dominant, the spurious currents can cause interface oscillations and deform or destroy the interface [9]. Meier's model was able to reduce spurious currents to some extent; however it still suffers by the generation of the spurious currents. PCIL model was presented by Shirani *et al.* [9] to reduce the amounts of these currents and produce more accurate pressure jump across the interface. This model is based on VOF-PLIC in which surface tension force is obtained by modified CSS and CSF models by introducing a dimensionless parameter H.

$$\mathbf{F}_{\mathbf{v}}^{\mathbf{st}} = H\sigma\kappa\mathbf{n}\frac{|\nabla\tilde{F}|}{[F]} \quad \text{and} \quad \mathbf{F}_{\mathbf{v}}^{\mathbf{st}} = H\sigma\nabla\cdot(|\nabla F|\mathbf{I} - \frac{\nabla F \otimes \nabla F}{|\nabla F|}) \tag{15}$$

Seifollahi and Shirani [10] presented a new model called SGIP for surface tension force based on VOF-PLIC and directly calculated the surface tension force at each interfacial cells. In this model, the surface tension force directly was calculated in each of the x- and y-momentum cells. In each of the momentum cells, the interface was assumed to be a straight line, see Fig. 1. The volumetric surface tension force acting on cell i+½,j at each staggered variable arrangement for two-dimensional case is as follows:

$$F_{vx,i+1/2,j}^{st} = \frac{\sigma\kappa_{i+1/2,j}\left(L_{x,i+1,j} - L_{x,i,j}\right)}{\Delta x\,\Delta y}. \tag{16}$$

The y-component of the surface tension may be obtained similarly. More details about obtaining the values of "L" components can be found in [10].

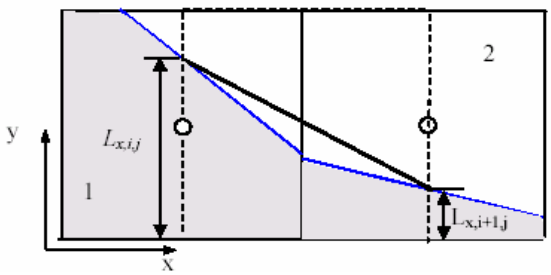

Fig 1 Interface in a x- momentum cell and interface function L_x

Ahmadi and Shirani [11] extended SGIP model for three-dimensional flows. Here, in each of the momentum cells, the interface is assumed to be a plane surface rather than a straight line, see Fig. 2 for the x-momentum cell. They replaced the two-dimensional interface lengths $L_{x,i,j}$ and $L_{x,i+1,j}$ with the three-dimensional interface surfaces $S_{x,i,j,k}$ and $S_{x,i+1,j,k}$. The volumetric surface tension force acting on cell $i+½,j,k$ at each staggered variable arrangement for three-dimensional case is as follows:

$$F_{vx,i+1/2,j,k}^{st} = \frac{\sigma\kappa_{i+1/2,j,k}\left(S_{x,i+1,j,k} - S_{x,i,j,k}\right)}{V_{i+1/2,j,k}}. \tag{17}$$

The y- and z- component of the surface tension may be obtained similarly. More details about obtaining the values of "S" components can be found in [11].

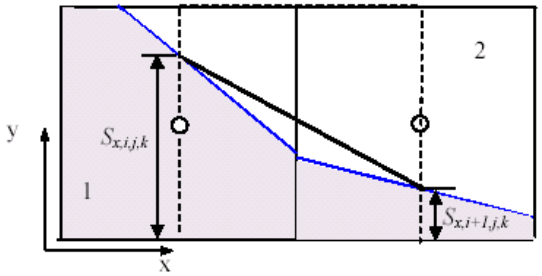

Fig. 2 Interface in a *x*- momentum cell and interface function S_x

IV. Numerical Method

A three-dimensional computer research code is modified and used to simulate the flow. The code is finite volume based and uses SIMPLEC algorithm along with QUICK method for convective terms. The code has the ability to solve laminar and turbulent, steady and unsteady flows. The code which was originally set up for solving single fluid flows was modified to solve interfacial flows. The VOF_PLIC method was used for interface tracking and the SGIP, CSF, CSS and PCIL models were implemented into the code.

V. Results

A small spherical air bubble starts to rise in water from stationary condition, influenced by buoyancy, surface tension and viscous effects. There has been a number of previous bubble simulations using VOF methods [8, 12-15], but only a few of them [8, 15] have been able to simulate very small bubbles of about 1 mm diameter and with such high density ratios. Clift et al. [16] realized that a moving bubble with diameter D=1.5 mm is spherical while for larger bubble with diameter D=3 mm, it is approximately ellipsoidal. We choose to simulate these two different bubbles as our dynamic test case. In order to reduce the spurious currents, some researchers use lower density ratios. Here, we used the actual densities of air and water. The bubble shapes are shown in Figs. 3 and 4 respectively. The parasitic velocities grow until they dramatically deform the bubble. The large bubble deformation happens i.e. at time 0.4 msec for smaller bubble, while for the larger bubble it takes around 3 msec for spurious currents to grow and cause significant bubble deformations. In fact, at these times, the magnitude of spurious velocities are so high that we need to decrease time step by orders of

magnitude to get converged solution. For both cases, we see that for CSF and CSS models, the bubble undergoes severe unphysical deformations. Similar unphysical bubble deformations are observed by Meier *et al.* [8] when CSF model is used.

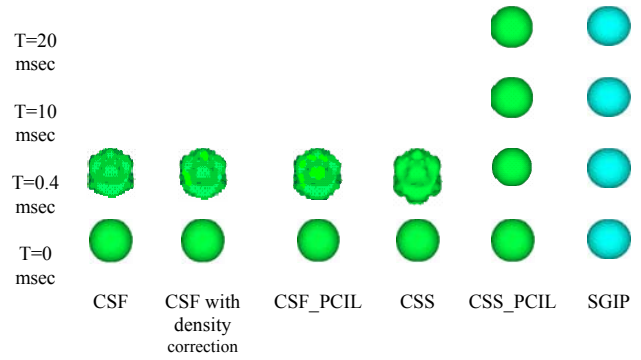

Fig. 3 Bubble shape with D=1.5 mm for different surface tension models at different times

Figs. 3 and 4 show that when using SGIP or CSS_PCIL models, the bubble maintains its shape and the spurious forces is reduced dramatically so that the bubble shapes are in accordance with experimental results. Comparing with Meier's results [15], for larger bubble we get similar results while for smaller bubble, our results are better since there is no unphysical deformation and bubble stays spherical as experiments suggest.

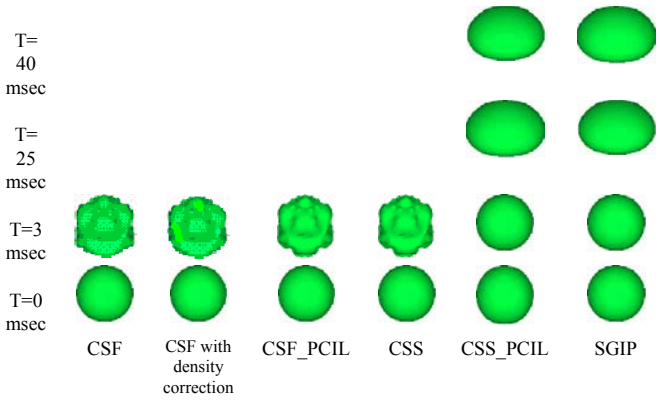

Fig. 4 Bubble shape with D=3 mm for different surface tension models at different times

Clift et al. [16] showed that the terminal rising velocity U_T for small air bubbles in pure water at room temperature can be determined using the following experimental correlation:

$$U_T = \sqrt{2.14\sigma/\rho d_e + 0.505 g d_e} \quad (18)$$

where d_e is the diameter of a sphere of equal volume. This correlation is also in accordance with the experimental results [17]. In addition to bubble shapes, the calculated bubble velocities for small and larger bubbles are compared to the experimental data in Figs. (5) and (6). Good agreement between numerical and experimental data [13, 15] is observed.

For the smaller bubble (D=1.5mm), since bubble stays spherical and there is less numerical error, the bubble rise velocity is much closer to that of experimental data than to the Meier's data [15].

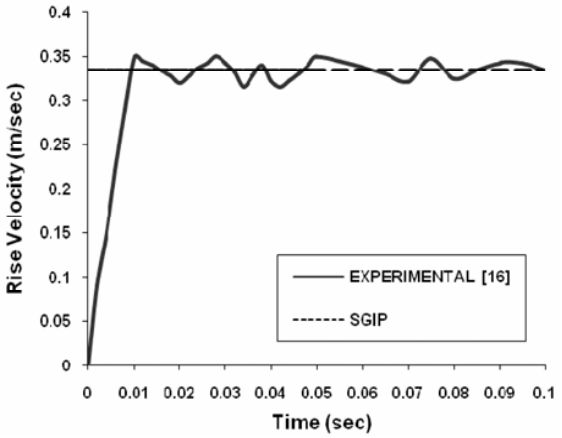

Fig. 5 Bubble velocity versus time for D=1.5 mm

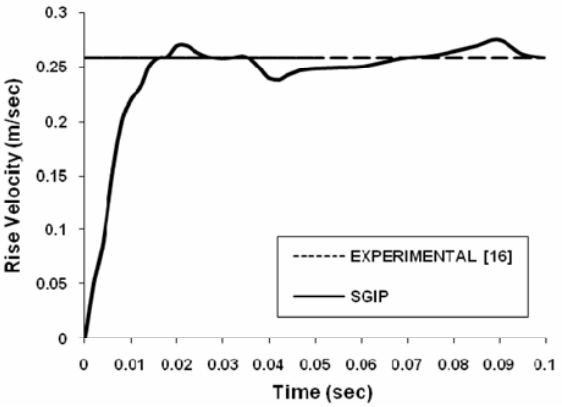

Fig. 6 Bubble velocity versus time for D=3 mm

VI. Conclusion

In this paper, six different surface tension models for interfacial flows were studied and compared for dynamic bubble rise case. It is shown that by using the CSF and CSS models, the magnitude of spurious currents is so high that it is not possible to simulate this type of surface tension dominated flows, while using SGIP or PCIL models, we are able to simulate bubble rise and obtain results in close agreement with the experimental data. For the case of smaller bubble, the bubble shape remains spherical and smooth as it is shown by experiments.

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