A COMPARATIVE STUDY OF LATTICE BOLTZMANN AND VOLUME OF FLUID METHOD FOR TWO-DIMENSIONAL MULTIPHASE FLOWS

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The volume of fluid (VOF) model of FLUENT and the lattice Boltzmann method (LBM) are used to simulate two-phase flows. Both methods are validated for static and dynamic bubble test cases and then compared to experimental results. The VOF method does not reduce the spurious currents of the static droplet test and does not satisfy the Laplace law for small droplets at the acceptable level, as compared with the LBM. For single bubble flows, simulations are executed for various Eotvos numbers, Morton numbers and Reynolds numbers, and the results of both methods agree well with the experiments in the case of low Eotvos numbers. For high Eotvos numbers, the VOF results deviated from the experiments. For multiple bubbles, the bubble flow characteristics are related by the wake of the leading bubble. The coaxial and oblique coalescence of the bubbles are simulated successfully and the subsequent results are presented. In conclusion, the LBM performs better than the VOF method.

KEYWORDS : Volume of Fluid, Two-phase Flow, Spurious Current, Laplace Law, Rising Bubble, Lattice Boltzmann, Bubble Coalescence

1. INTRODUCTION

Two-phase flow has many industrial and academic applications. Condensation and boiling phenomena are especially important for the design of the core, the steam generator, and the condensation heat exchanger of nuclear reactors [1]. Studies of two-phase flow have been carried out mainly by theoretical analysis and experiment, but there have been few studies about numerical analysis [1, 2]. This lack is due to the difficulties of numerical analysis for two-phase flow. The interface and topology change of each phase should be calculated and heat and mass transfer must be considered in the case of the boiling process [2].

Many methods to predict the interface of each phase have been proposed in the past. These can generally be classified into an interface capturing method and an interface tracking method. The typical methods to track the interface are the marker and cell (MAC) and the front tracking method (FTM) [2, 3]. For the interface tracking method, the interface is estimated by the virtual particles to trace the trajectory of the flow using the Lagrangian grids. The traditional methods of the interface capturing

method are the volume of fluid (VOF) and level set (LS) methods, which introduce an order parameter [4, 5]. The convection or diffusion of the order parameter is used to capture the interface.

The interface tracking method is relatively accurate at conserving the interface, but it is complex and does not predict the interface well. On the other hand, the interface capturing method is fairly good at predicting the interface, but it does not conserve the interface well. For the interface capturing schemes, a geometry reconstruction and a re-initialization scheme are needed. Recently, the commercial code FLUENT has implemented a modified HRIC and CICSAM scheme with the VOF options, which together make a simple and efficient method for calculating interface problems [6].

The traditional CFD is based on the Navier-Stokes equations, but the lattice Boltzmann method (LBM) is based on a kinetic Boltzmann equation. The LBM has been proposed by many researchers since the 1980s [7, 8]. The Boltzmann equation for the simulation of the motion of molecules results in the incompressible Navier-Stokes equations with the Chapman-Enskog expansion under the assumption of 2nd order approximation. For the Boltzmann

equation, the distribution function at any location is defined as a dependent variable, instead of as the velocity and the pressure. By integrating the distribution function, macroscopic variables such as density and velocity can be obtained.

Two-phase models for the LBM, which are color gradient, potential method, and free energy method, have recently been proposed [8, 9]. The two-phase model based on free energy [9] was used in the present study. For the free energy based model, the chemical potential as a thermodynamic variable is introduced in the Cahn-Hilliard equation [8, 10] to capture the interface. Surface tension on the interface of each phase can be easily obtained using the gradient of the chemical potential. For more information, refer to references [8, 9].

Single or multiple bubble rising flows have been studied in the past years by numerical analysis and experiments [9-18]. Bhaga and Weber [11] performed extensive experiments about single bubble rising in liquids and reported a flow regime map that was correlated with dimensionless variables like Eotvos, Morton, and Reynolds numbers. Hou and Lou [12] have executed numerical analysis for single bubble flows and obtained results consistent with the aforementioned experiments [11]. For multiple bubbles, Brereton and Korotney [13] have reported the characteristics of the coalescence of two rising bubbles at different positions through visual experiments. Numerical simulations of coaxial and oblique coalescence have been carried out by several researchers [14-17]. Although many numerical calculations have been done, the results for identical flow conditions were not consistent owing to the numerical schemes and initial assumptions, including boundary conditions. Also, there have been few comparative studies about any two methods, such as the VOF method and the LBM [14]. We are now developing an in-house LBM code to simulate nucleate pool boiling flows. During the process of this, a quantitative comparison about similar problems for the two methods is needed to validate our code, whereas the performance of the two methods is known from previous studies.

In this study, the accuracy and the performance of the VOF method and the LBM were compared through several tests. For validation purposes, a disk under shear flow and a static droplet in a stationary flow were simulated. It was shown that the two methods satisfy the Laplace law through the static droplet test. The final shape and the terminal velocity of the single rising bubble in the two methods were compared with experimental results [11]. In addition, the characteristics of multiple rising bubble flows, positioned inline or obliquely, were studied.

2. MATHEMATICAL MODELS AND NUMERICAL ANALYSIS METHODS

2.1 Governing Equations for the VOF Method

Governing equations for incompressible multiphase

flow [6] are as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (1)$$

$$\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \mu \nabla^2 \vec{u} + \vec{F}_b \quad (2)$$

$$\frac{\partial F}{\partial t} + \nabla \cdot (F \vec{u}) = 0 \quad (3)$$

, where F is the volume fraction. Each mixture property is defined as

$$\rho = F\rho_A + (1-F)\rho_B, \quad \mu = F\mu_A + (1-F)\mu_B \quad (4)$$

, where ρ_A and ρ_B are the density of the fluid A and B, respectively, and μ_A and μ_B are the dynamic viscosity of the fluid A and B.

2.2 Analysis Method for the VOF Method [6]

In order to solve the above governing equations, PISO, a pressure velocity coupling algorithm, was adopted. PISO, which introduced neighbor and skewness corrections to the SIMPLE algorithm, is known as for efficiently treating the skewness of computational grids and transient calculations. The VOF calculations are basically transient and, therefore, PISO is appropriate.

The convection schemes used for the momentum equations were 2nd order Upwind, QUICK, and 3rd order MUSCL. The sensitivity tests of these schemes were performed but showed almost no difference among their results. In the following calculations, a second order Upwind scheme was mainly used.

For the interface capturing options, Geo-Reconstruct, QUICK, modified High Resolution Interface Capturing (HRIC) and Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM) were used. Geo-Reconstruct is related to the geometry reconstruction. QUICK, modified HRIC and CICSAM are the convection schemes for the VOF equation (Eq. 3). Upwind schemes are generally unstable for interface capturing because of their numerical diffusion. Central differencing schemes are unbounded and often give unphysical results. The modified HRIC and CICSAM schemes are composite schemes that consist of a non-linear blend of upwind and downwind differencing by which the above deficiencies are overcome.

Unsteady formulation was the 1st order, and, as a transient control, the Non-Iterative Time Advancement (NITA) was selected. In the iterative time advancement scheme, all the equations are solved iteratively for each time-step until the convergence criteria are met. However, the NITA scheme needs no outer iteration per time-step, which is required in the iterative time advancement scheme. Thus, the NITA scheme significantly speeds up transient calculations.

2.3 Lattice Boltzmann Method

In this section, the lattice Boltzmann method, based on the free energy concept, is briefly described. More details can be found in Zheng *et al.* [9].

Prior to describing the lattice Boltzmann equations, the macroscopic governing equations to solve are as follows:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{u}) = 0 \quad (5)$$

$$\frac{\partial (n\vec{u})}{\partial t} + \nabla \cdot (n\vec{u}\vec{u}) = -\nabla P + \mu \nabla^2 \vec{u} + \vec{F}_b \quad (6)$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \vec{u}) = \theta_M \nabla^2 \mu_\phi \quad (7)$$

, where μ_ϕ is the chemical potential, θ_M is mobility, P is a pressure tensor, and $\vec{F}_b$ is the volumetric force. Also, n and ϕ are defined as

$$n = \frac{\rho_A + \rho_B}{2}, \phi = \frac{\rho_A - \rho_B}{2} \quad (8)$$

, where n is the total density and ϕ is an order parameter that represents each phase.

An interface capturing scheme was modeled using the Cahn-Hilliard equation shown in Eq. (7), which has been introduced by many researchers [8, 10, 18] who have obtained the successful prediction of the interface.

It is converted to the lattice Boltzmann equation, as follows:

$$g_i(\vec{x} + \vec{e}_i \delta t, t + \delta t) = g_i(\vec{x}, t) + \Omega_i + (1 - q)[g_i(\vec{x} + \vec{e}_i \delta t, t) - g_i(\vec{x}, t)] \quad (9)$$

$$\Omega_i = \frac{g_i^{(eq)}(\vec{x}, t) - g_i(\vec{x}, t)}{\tau_\phi}$$

, where g_i is the particle distribution function, τ_ϕ is a single relaxation time, $\vec{e}_i$ is the lattice velocity, and $q(=\frac{1}{1+\tau_\phi})$ means the constant related to the partial streaming. The order parameter is obtained from

$$\phi = \sum_i g_i \quad (10)$$

In this study, the D2Q5 model (D2 means 2-dimensional and Q5 means the number of the lattice) to solve Eq. (9) was used. The lattice velocities for the D2Q5 model (Fig. 1) are as follows:

$$\vec{e}_0 = c(0,0)^T, \vec{e}_{1,3} = c(\pm 1,0)^T, \vec{e}_{2,4} = c(0,\pm 1)^T \quad (11)$$

, where $c (= \delta x / \delta t = \delta y / \delta t)$ is the magnitude of the lattice velocity. In LBM, the value of the lattice velocity equals unity because the grid spacing and the time step are generally defined as unity ($\delta x = \delta y = \delta t = 1$).

The equilibrium distribution function is expressed as:

$$g_0^{(eq)} = \phi - 2\Gamma\mu_\phi + (\phi\vec{e}_i \cdot \vec{u})/2q \quad (12)$$

$$g_{1,2,3,4}^{(eq)} = 0.5\Gamma\mu_\phi + (\phi\vec{e}_i \cdot \vec{u})/2q$$

, where Γ is used to control the mobility [19].

In Eq. (6), the gradient of the pressure tensor is the important term related to the surface tension of the multiphase flows. Again, it is expressed as a potential term [8, 10]

$$\vec{F}_{st} = -\nabla P = -\nabla p_i - \phi \nabla \mu_\phi \quad (13)$$

, where $p_i (= nc_s^2 = \frac{1}{3}c_s^2)$, c_s is the speed of sound) means the equation of state for an ideal gas. The chemical potential

is obtained from a free energy density functional. The free energy functional in a closed system is expressed as:

$$F = \int \mathfrak{S} dV = \int dV [\psi(\phi) + \frac{\kappa}{2}(\nabla \phi)^2 + nc_s^2 \ln(n)] \quad (14)$$

, where V is a control volume, κ is a coefficient related to the surface tension and the interface thickness, and ψ is the volume free energy density. In addition, ψ can be expressed in the double-well form as:

$$\psi(\phi) = A(\phi^2 - \phi^{*2})^2 \quad (15)$$

and

$$\phi^* = \frac{\rho_H - \rho_L}{2}$$

, where ρ_H and ρ_L mean the liquid and the vapor density, respectively. A is a variable that controls the interaction of the two phase energy. The order parameter maintains $-\phi^*$ and ϕ^* in the equilibrium state, which results in the minimum free energy.

The chemical potential is defined as

$$\mu_\phi = \frac{\partial \mathfrak{S}}{\partial \phi} - \nabla \cdot \frac{\partial \mathfrak{S}}{\partial \nabla \phi} = 4A(\phi^3 - \phi^{*2}\phi)^2 - \kappa \nabla^2 \phi \quad (16)$$

The pressure tensor and the pressure can be derived as follows:

$$P_{\alpha\beta} = \phi \mu_\phi - \mathfrak{S} = p \delta_{\alpha\beta} + \kappa \nabla_\alpha \phi \nabla_\beta \phi$$

$$p = A(3\phi^4 - 2\phi^{*2}\phi^2 - \phi^{*4}) - \kappa \phi \nabla^2 \phi - \frac{\kappa(\nabla \phi)^2}{2} + nc_s^2 \quad (17)$$

The profile with the normal direction of the interface is

$$\phi = \phi^* \tanh\left(\frac{2\xi}{W}\right) \quad (18)$$

, where ξ is the coordinate perpendicular to the interface and W is the thickness of the interface, which is measured from the interface zero level. The surface tension coefficient and the interface thickness are expressed in terms of κ, A, ϕ^* .

$$\sigma = \frac{4\sqrt{2\kappa A}}{3} \phi^{*3}, W = \frac{\sqrt{2\kappa/A}}{\phi^*} \quad (19)$$

The lattice Boltzmann equations of Eqs. (5) and (6) can be described as

$$f_i(\vec{x} + \vec{e}_i \delta t, t + \delta t) = f_i(\vec{x}, t) + \Omega_i \quad (20)$$

$$\Omega_i = \frac{f_i^{(eq)}(\vec{x}, t) - f_i(\vec{x}, t)}{\tau_n} + A_i(-\phi \nabla \mu_\phi + \vec{F}_b) \delta t$$

with

$$A_i = (1 - \frac{1}{2\tau_n}) \frac{w_i}{c_s^2} \left[(\vec{e}_i \cdot \vec{u}) + \frac{(\vec{e}_i \cdot \vec{u})}{c_s^2} \vec{e}_i \right]$$

, where $\vec{F}_b (= 2\phi^* \vec{g})$ means the gravitational terms and τ_n is a single relaxation time associated with the viscosity, $\nu (= c_s^2 (\tau_n - 0.5) \delta t)$ [14, 20].

The equilibrium distribution functions satisfy the following conservation equations

$$n = \sum_i f_i^{(eq)} \quad (21)$$

$$\vec{u} = \left[\sum_i f_i^{(eq)} \vec{e}_i + \frac{1}{2}(-\phi \nabla \mu_\phi + \vec{F}_b) \right] / n \quad (22)$$

The equilibrium distribution functions to satisfy Eqs. (21)-(22) are as follows:

$$f_i^{(eq)} = w_i n [1 + 3\vec{e}_i \cdot \vec{u} - \frac{3}{2} \vec{u} \cdot \vec{u} + \frac{9}{2} (\vec{e}_i \cdot \vec{u})^2] \quad (23)$$

, where

$$w_0 = \frac{4}{9}, w_{i=1,2,3,4} = \frac{1}{9}, w_{i=5,6,7,8} = \frac{1}{36}$$

In this study, the D2Q9 model (D2 means 2-dimensional and Q9 means the number of lattice) to solve Eq. (20) was used. The lattice velocities for the D2Q9 model (Fig. 1) are as follows:

$$\begin{aligned} \vec{e}_0 &= c(0,0)^T, \vec{e}_{1,3} = c(\pm 1,0)^T, \vec{e}_{2,4} = c(0,\pm 1)^T, \\ \vec{e}_{5,7} &= c(\pm 1,\pm 1)^T, \vec{e}_{6,8} = c(\mp 1,\pm 1)^T \end{aligned} \quad (24)$$

In the lattice Boltzmann method, boundary conditions are another important issue. Since they are not a major subject in this study, a bounce-back rule [7, 8], which is simple and efficient is applied for the wall as a no-slip boundary condition. Also, a periodic boundary condition, which has no issue, is used.

2.4 Comparison of Concepts for the VOF Method and Two Phase LBM

Two approaches of the VOF method based on the Navier-Stokes equation and the free-energy model based on the lattice Boltzmann equation are briefly described in this section.

In the VOF method, a volume fraction F is represented as one of the phases depending on the volume fraction values. Hence, F is zero or unity in a control volume (cell) containing a pure fluid (liquid or gas) and has a value of $0 < F < 1$ in a cell containing an interface. To solve an evolution equation for the volume fraction, the volume of fluid method consists of two major parts: the interface reconstruction schemes, such as a donor-acceptor scheme

and a geometric reconstruction (piecewise-linear) scheme, and the non-diffusive schemes of the convection equation for the volume fraction such as QUICK, modified HRIC and CICSAM schemes. Generally, the surface tension model based on the continuum surface force (CSF) model of Brackbill *et al.* [25] is incorporated into the momentum equation.

In the two phase LBM, the interface is defined by an order parameter ϕ , which varies smoothly across the interface (diffuse interface). It is similar to the level set function ϕ , which is initialized as a signed distance function from the interface, i.e., positive on one side, negative on the other side, and zero at the interface. The order parameter in the LBM has a value of $-\phi^* < \phi < \phi^*$ ($\phi^* = \frac{\rho_H - \rho_L}{2}$, density difference), and the interface is represented by the zero level of ϕ . In contrast to the VOF method, the free energy LBM captures the interface by solving a convection-diffusion equation that is called the Cahn-Hilliard equation, which involves the chemical potential. It does not severely suffer numerical diffusion, as the VOF method does, because of the diffusion term in the Cahn-Hilliard equation. The surface tension is modeled as a source term associated with the order parameter and gradient of the chemical potential. The potential form of the surface tension related term is implemented in the lattice Boltzmann equation for momentum.

3. RESULTS AND DISCUSSION

3.1 A disk under Shear Flow

The transitional and rotational movements of a rigid body, and a disk under shear flow have been proposed for benchmark tests of the interface capturing performance [19, 21]. Unlike other tests, the disk under shear flow undergoes a deformation of its interface because of the

Fig. 1. Lattice Systems for the LBM

imposing velocity field. Thus, the interface capturing methods of the VOF method and LBM could be clearly evaluated in regard to the deformation of the interface.

The computational domain has 200×200 grids. A circular disk with a radius of 40 is located (100, 60) in the computational domain. In this section, the parameters are set at $\kappa = 0.002$, $\Gamma = 0.4$, $A = 0.001$ and $\tau_\phi = 0.7$. The order parameter is set at ϕ^* inside the disk and $-\phi^*$ elsewhere ($\phi^* = 1$). Periodic boundary conditions are applied at all directions.

The velocity fields are

$$u = u_0 \pi \cos X \sin Y \quad (25)$$

$$v = -u_0 \pi \sin X \cos Y \quad (26)$$

, where $u_0 = 0.01$, $X = \pi (\frac{i}{iEnd} - 0.5)$, $Y = \pi (\frac{j}{jEnd} - 0.5)$, $iEnd = jEnd = 200$ [19].

At first, it was rotated by 2 cycles in the counter-clockwise direction, and then backward in the clockwise direction. Finally, it returned to the initial condition in the case of an ideal case. However, a perfect restoration of the initial configuration is difficult to obtain even when higher order convection schemes in the VOF method are used. In Fig. 2, the previous results of the VOF method and the present results of the LBM are presented.

Hirt-Nichols VOF [4], which is known as a donor-acceptor scheme, and Youngs VOF [21], as a Georeconstruct scheme in FLUENT, show many jetsam and

sawteeth at the interface, as is shown in Fig. 2 (a), (b). However, for the present LBM, the disk returns to its initial configuration after 2 rotation cycles without jetsam, as shown in Fig. 2 (c). Also, a little deformation is found in the final shape, but it is not more severe than the deformation found in the results for the VOF method. As is mentioned in sections 2.2 and 2.3, the interface capturing schemes in the VOF method have been known to suffer numerical diffusion, which is inherited from the pure convection equation of the volume fraction (Eq. (3)). However, the interface capturing schemes in the LBM have been modeled with a convection-diffusion equation (Eq. (7)), which can greatly reduce the numerical diffusion. The test results show that the LBM is superior to the VOF method for interface capturing performance.

3.2 Static Droplet in a Quiescent Fluid

The static droplet ($g = 0$) in a quiescent fluid does not actually exist in the gravitational field. However, it is proposed in order to validate the numerical scheme as an ideal case [22-24]. In this section, the parameters for the LBM are set at $\tau_n = 1.0$ and $\tau_\phi = 0.7$, unless otherwise noted. The order parameter is set at ϕ^* inside the droplet and at $-\phi^*$ elsewhere. Periodic boundary conditions are applied at all directions. For the VOF method, the volume fraction (F) is set at unity inside the droplet and at zero elsewhere. The other parameters are set equivalent to the LBM.

The existing two-phase flow models, such as the level set or the VOF method, cause spurious currents around the

Fig. 2. Shear Flows Computed by Various Methods (Top : Forward 2 Revolutions, Bottom : Backward 2 Revolutions) (a) VOF of Hirt-Nichols [21], (b) VOF of Youngs [21], (c) LBM (Present) [From Rudman (1997)-Copyright © John Wiley and Sons 1997-Used with Permission.]

bubbles or droplets. This is mainly due to the differencing error of the surface tension gradient that appears in the momentum equation [23, 24]. This is especially the case with the model proposed by Brackbill *et al.* [6, 25], which is used in the VOF method, in which the spurious currents occur severely. The spurious currents can lessen the convergence and accuracy of the numerical results. Efforts to reduce these spurious currents have been performed in the past, but it was not possible to obtain satisfactory results. Recently, Shin *et al.* [26] proposed a surface tension model to suppress the spurious currents by nearly two orders of magnitude using the level contour reconstruction method, which improves the front tracking method [2]. A method proposed by Popinet [27], which combined an adaptive grid, VOF representation, balanced-force continuum-surface-force surface tension formulation [22] and height-function curvature estimation, is shown to recover exact equilibrium between the surface tension and the pressure gradient in the case of a stationary droplet. However, the above successful methods relative to the present LBM are

complex to implement and difficult to extend to three-dimensional cases.

Figure 3 shows the VOF results of 4 interface capturing options in FLUENT. In all cases, spurious currents occurred and could not be reduced further. As shown in Fig. 4, the Geo-reconstruct scheme shows the greatest magnitude of spurious currents among all schemes, but the currents of the QUICK and modified HRIC Schemes are smaller than any others. The modified HRIC scheme has been used in many previous tests and is known to be robust [6]. Therefore, it is used in the following calculations.

In Fig. 5, the results of the LBM and VOF method are compared. The VOF method utilized the modified HRIC scheme. When the LBM was used, the spurious currents were magnified 10^7 times. In LBM, the surface tension is represented as a potential term and then discretized by higher-order isotropic approximation. These differencing errors are smaller than those of the conventional finite difference method [23, 24].

The Laplace law states that the internal pressure of a

Fig. 3. Velocity Fields of the VOF Options in FLUENT ($\times 5$ Times Magnification, Density Ratio=10, $R=0.25$, $\sigma=0.002187$, 50×50 Grids)

bubble or droplet is greater than the external pressure because of the curvature of the interface caused by the surface tension [18].

$$\Delta p = \frac{\sigma}{R} : \text{2-dimensional case} \quad (27)$$

To verify whether this law is valid or not, the pressure difference between the inside and outside of the droplet was calculated by varying the droplet radii. The grid size for the computational domain is fixed as 100×100 , or 200×200 . Figure 6 shows that the linear relationship of the slope and the results of the VOF method and LBM with coarse grids (100×100 grids) for the large droplets ($1/R$ is small) are consistent with Laplace's law. However, the VOF results (100×100 grids) for the small droplets ($1/R$ is large) have differences of up to 20% from the analytical solution. It seems that the grids of the droplets with small radius are lacking to resolve the curvature of

the interface because the grid size for the computational domain is fixed. Therefore, calculated results with the refined grids (VOF, 200×200 grids) were found to follow the analytical solution, shown in Fig. 6. However, in the case of utilizing the LBM, no significant difference ($< 1\%$) could be detected between the analytical solution and the numerical calculation, even though the coarse grids (LBM, 100×100 grids) were used for the small droplets. According to Shin *et al.* [26], accurate estimation of the interface curvature for small droplets required the fine grids in the model by Brackbill *et al.* [6, 25]. In contrast to the VOF method, the present LBM does not require the calculation of the interface curvature, which is replaced by differencing the potential form of Eq. (13). To reduce

Fig. 4. Effect of the Interface Capturing Schemes in FLUENT

Fig. 6. Comparison of the Present Results with the Laplace Law (Density Ratio=1000, $\sigma=0.01$, Solid Line : Analytical, Symbol : Numerical)

(a) VOF modified HRIC (x5 times)

(b) LBM (x10⁷ times)

Fig. 5. Comparison of the Velocity Fields (Density Ratio=10, $\sigma=0.002187$, 50×50 Grids)

the differencing error, accurate prediction of the interface and the small spurious currents, which are verified from the above tests, are prerequisites, in addition to the higher-order isotropic approximation [24]. Therefore, the LBM can perform better than the VOF method for the static bubble test.

3.3 Rising Bubble Flows in a Gravitational Field

In the following calculations, a density ratio of 1000 and viscosity ratio of 1000, which values are similar to those of substances such as water and air, were applied in the VOF method and the LBM. For the LBM, because the mobility acts as the diffusion coefficient of the Cahn-Hilliard equation (Eq. 7), too large a value (>1000) can cause numerical diffusion; too small a value (<100) can cause numerical instability. Also, the discretization error decreases with the thickness of the interface. And, the calculated results changed little for the values larger than $W = 5$ [9]. Therefore, $\Gamma = 400$ and $W = 5$ were used, and the other parameters were

$$\sigma = 2, \tau_\theta = 0.7, \tau_n = 0.8$$

3.3.1 Single Rising Bubble Flow

In this section, we discuss the results of our simulation about single rising bubble flows. To minimize the effect of the walls, a computational domain must be selected through sensitivity tests (mainly horizontal direction). Figure 7 displays the final shapes of the bubble at the same time, and there are slight differences among the shapes in the sizes wider than the horizontal direction of $8d$ (d is the initial bubble diameter).

Also, grid sensitivity tests for the bubbles were performed. The number of grids of the bubble diameter was changed from 20 to 40, and then to 60. The 40 grids of the

bubble are reasonable, as can be seen in Fig. 7. Unless otherwise noted, the LBM calculations were carried out by 40 grids of the bubble diameter and $8d \times 12d$ of the computational domain. The VOF calculations were similarly done by $8d \times 12d$ (320×480 grids) of the computational domain.

The terminal shapes and final velocities of a rising bubble have been obtained by numerical analysis and experiments in the past [9, 11, 12, 14, 15]. The types of bubbles are dependent on variables such as Eotvos (Eu), Morton (M), and Reynolds (Re) number.

$$Eu = \frac{g(\rho_H - \rho_L)d^2}{\sigma}, \quad M = \frac{g(\rho_H - \rho_L)\mu_H^4}{\rho_H^2\sigma^3}, \quad Re = \frac{\rho_H V_T d}{\mu_H} \quad (28)$$

, where g is the gravitational acceleration, d is the bubble diameter, σ is the surface tension coefficient, μ is the dynamic viscosity, and V_T is the terminal velocity. When the buoyancy and the drag force of the bubble are in balance, the velocity is constant; this is called the terminal velocity of the bubble. The Eu number, a dimensionless variable, is the ratio of gravity and surface tension; it is also related to the bubble size. The Morton number is related to the properties of viscosity and surface tension and represents the dynamic behavior of the rising bubbles. The Reynolds number is a dimensionless variable associated with the terminal velocity of the bubbles.

Bhaga and Weber [11] obtained the final shapes and the terminal velocities of a rising bubble by extensive experiments and presented the flow regime map shown in Fig. 8. Bubble shapes are classified in Fig. 8 as follows: spherical (S), oblate ellipsoid (OE), oblate ellipsoidal (OED), oblate ellipsoidal cap (OEC), spherical cap with closed, steady wake (SCC), spherical cap with open, unsteady wake (SCO), skirted with smooth, steady skirt (SKS), and skirted with wavy, unsteady skirt (SKW). Figure 8 also shows the relationship between Re and Eu numbers with lines of constant M number. In general, the

Fig. 7. Effect of the Domain Sizes (Left) and the Bubble Grid Sizes (Right); $d_1=20$, $d_2=40$, $d_3=60$ (Test Case C in Table 1)

greater the surface tension (Eo is small) and viscosity (M is large) the steadier the bubble form and, thus, the less likely it is that the bubble will experience significant deformation. Bubbles in this region, i.e., in the bottom left part of the flow regime map, will maintain spherical shapes during rising. Smaller values for surface tension (Eo is large) and viscosity (M is small) lead to more significant deformation and unsteady behavior in the rising bubble. At high Eo and intermediate M number, the rising bubble has an ellipsoidal or spherical cap shape, as can be seen in the right part of the flow regime map. With further lowering of M number, the rise velocity of the bubble (Re) is larger and, subsequently, the bubble shape becomes skirted because of the enhanced inertia forces. Increasing Eo number with constant M number results in the increase of the rise velocity (Re). This trend can be clearly seen in Fig. 8.

The numerical simulations were carried out by varying

the parameters such as Eo and M number, and then the final shapes and the terminal velocities of the bubble were obtained from the numerical simulations. The test cases are listed in Table 1, which also presents the terminal Re numbers secured by the two methods for various Eo , M numbers.

The final shapes of the bubble for the present simulations are presented in the right part of Fig. 8. In Fig. 8, the locations of the simulation cases are marked on the flow regime map. These cases are ranged from ellipsoidal to skirted shapes. The test case A ($Eo = 5$ and $M = 0.012$) is located on the border of the spherical and oblate ellipsoidal regime in Fig. 8, and, thus, its shape is expected to be an ellipsoidal one. Consequently, oblate ellipsoidal shapes are observed as shown in Fig. 8, and those of both methods are nearly the same. The shape of the bubble, which was initially assumed to be a circle, is well maintained in case A because of the large surface tension, i.e. small Eo . In

Fig. 8. The Flow Regime Map of Experiments by Bhaga and Weber [11]; VOF and LBM Numerical Results (Right) [From Bhaga and Weber (1981)-Copyright © Cambridge University Press 1981-Used with Permission.]

Table 1. Comparison of Numerical Results with Experiments

Test case	Eo (M)	Re_{exp} [11]	Re_{cal} (VOF)	Error_VOF* (%)	Re_{cal} (LBM)	Error_LBM* (%)
A	5 (0.012)	5.5	5.8	6.8	6.2	12.7
B	16 (0.038)	13.4	9.3	30.6	12.2	9.0
C	40 (0.096)	20.0	14.0	30.0	16.0	20.0
D	240 (0.574)	52.1	33.2	36.3	41.0	21.3

*error = $| (exp. value - numerical value) / exp. value | \times 100$

case B (intermediate Eo), the shape of the bubble can be expected to be OEC from the flow regime map. Both results (case B) have oblate ellipsoidal cap shapes and are relatively consistent with the flow regime map. However, the difference between the both methods begins to show. The LBM shows a deeper indentation or dimple in the bottom surface of the bubble than does the VOF method. From the photographs in experiments by Bhaga and Weber [11], bubbles in the regime of OEC have an indentation or dimple in their bottom surface. Therefore, the prediction of the LBM is reasonable for the case B. Considering the parameters in case C ($Eo = 40$ and $M = 0.096$), the OEC type is still expected to be the shape of the bubble and the size of the dimple region is also expected to be large because of the increased rise velocity of the bubble. The LBM for case C predicts the bubble shape to be OEC type with a wide dimple region and symmetrical geometry. However, the VOF calculations result in the skirt type and symmetry breaking structure shown in Fig. 8 (case C). With further increase of the Eo number, the dimple region grows larger and the rim of the bubble becomes thinner. Finally, the bubble shape appears to be skirted, as shown in Fig. 8 (case D). For case D ($Eo = 240$ and $M = 0.574$) of the VOF method, the SKS type occurred for the final shape of the bubble, as expected. However, the edges of the skirt are irregularly torn away from the interface of the bubble tip. According to Bhaga and Weber [11], these unstable behaviors of bubbles are observed at the values of $Eo = 641$ and $M = 43.1$, which values correspond to the middle right region of the flow regime map. It is expected that these unsteady motions of skirts will not occur for case D. The LBM result for case D shows a smooth steady skirt with symmetry, as can be seen in Fig. 8. This deviation is due to the limited performance of the interface prediction of the VOF method in the case of the large deformation as is shown in section 3.1.

The terminal velocities (Re number) of both methods and experiments [11] are compared in Table 1. When the Eo number is small, the rise velocity can be obtained analytically with good accuracy assuming spherical shape although there is little deformation of the rising bubble. As the Eo number increases, the bubbles undergo their deformation. Therefore, the simple assumption of spherical shape is not valid for large Eo number. In case A, the results of both methods are in quantitative agreement with the experiments [11], as shown in Table 1. This is due to the small deformation of the bubble, which has a nearly spherical shape (see Fig. 8) and stable flow fields [28]. However, the deviation between the numerical results and the experiments can be seen when the Eo number increases (case C, D). This is due to both the initial condition difference between the numerical analysis and the experiments, and the 3-dimensional effect. For the numerical analysis, the initial condition of the bubble shape is ideally assumed to be a perfect circle, which is a simple initial condition to apply. However, in experiments

with limited test sections, it is difficult to maintain circular shape as an initial experimental condition, especially in the case of large Eo numbers; the data are different case by case. For comparison purposes, the above assumption is reasonable, although deviation between the numerical results and the experiments occurs. In both cases, for small Eo numbers (case A, B), there are small deviations relative to the cases for large Eo numbers (case C, D), owing to the small deformation and small rise velocity (Re). Nevertheless, the LBM always has consistent results and better performance than the VOF method.

Figure 9 presents the interfacial contours of the VOF method and the LBM at different times for test case B in Table 1 in order to provide a better comparison of bubble shapes. Initially, the circular bubble with a distance of $1d$ from the bubble center to the bottom wall is positioned at rest. In the first stage, the bubble rises fast because of the buoyancy force. At that time, the bubble starts to deform, flattening the bottom surface. Then, the drag force of the bubble increases with time. Finally, when the buoyancy and the drag force are in equilibrium, the bubble rises at a steady rate and with a steady shape. As mentioned above, this constant speed is called the terminal velocity and this steady form is called the final shape. Overall, the results of the LBM are similar to those of the VOF method except for the final position and the degree of deformation.

Figure 10 shows the relative velocity fields and interfaces of each phase for the VOF method and the LBM in case B. The relative velocity means the one measured in a moving coordinate frame. A closed wake, which was also observed in experiments by Bhaga and Weber [11], can be seen at the bottom of the rising bubble. In addition, circulation inside the bubble is produced as can be seen in Fig. 10. Both methods did a good job of predicting the internal circulation of the bubble, the wake behind the bubble, and the elliptical shape, as was expected.

It is clear that as the Eo number increases, the bubble shapes change from spherical to oblate ellipsoidal, and then to skirt-like. High Eo number is interpreted to be a low surface tension of liquid-gas interface or large sized bubble. Low M number, which is interpreted to be a low viscosity of the surrounding liquid, results in a high rise velocity of bubble. Generally, for high Eo and low M numbers, bubble rises fast, tends to deform, and then the wake behind the bubble is enlarged. Also, there are symmetry shapes except for the case of high Eo (> 640) and low M numbers ($< 4 \times 10^{-3}$) [11]. The bubble shapes in the numerical results are found to match well with those in the flow regime map in Fig. 8. However, the LBM is better than the VOF method for predicting the bubble shapes, symmetry structure and the terminal velocity.

3.3.2 Multiple Rising Bubble Flows

In this section, we discuss the results of our simulation about multiple rising bubble flows at $Eo = 16$ and $M = 2$

Fig. 9. Transient Interfacial Profiles for Test case B in Table 1; VOF (Left), LBM (Right)

Fig. 10. Relative Velocity Fields and Interface Contours for Test Case B in Table1; VOF (Left), LBM (Right)

$\times 10^{-4}$. The other parameters are the same as those of the single bubble cases, including the computational domain. The effects of the initial bubble position on the flow field and the shape evolution of the trailing bubble are studied.

No-slip boundary conditions were imposed at the surrounding walls. Two bubbles, which have the same diameter of $d = 40$, were initially positioned either inline or staggered, as shown in Figs. 11 and 14, at $t=0$ [13, 15, 17]. In Fig. 11, the two bubbles are separated by a distance of $1.5d$ from their centers. For the inline cases, the calculated results and those from the experiments [13] are presented in Fig. 11 (VOF), Fig. 12 (experiment), and Fig. 13 (LBM).

The bubbles rise because of buoyancy after they are released at $t = 0$. From the flow regime map (Fig. 8), the OEC or OED type, which is similar to those in case B in section 3.3.1, is expected for the leading bubble. As can be seen in Figs. 11-13, the leading bubble rises with the shape of an ellipsoid, but the trailing bubble is different from the leading one. As discussed in the previous section, a closed wake occurs behind the leading bubble and then the trailing bubble enters its wake region. As compared with the data in Fig. 9, the leading bubble resembles the shape of single rising bubble. As time increases, the leading bubble becomes an oblate ellipsoidal cap while the

Fig. 11. Coaxial Coalescence of the Two Bubbles at Different Times ($Eo = 16$, $M = 2 \times 10^{-4}$); VOF Results

Fig. 12. Coaxial Coalescence of the Two Bubbles at Different Times by Brereton and Korotney [13] ($Eo = 16$, $M = 2 \times 10^{-4}$); Experimental Results [From Brereton and Korotney (1991)-Copyright © ASME 1991-Used with Permission.]

Fig. 13. Coaxial Coalescence of the Two Bubbles at Different Times ($Eo = 16$, $M = 2 \times 10^{-4}$); VOF Results

trailing bubble is elongated. The trailing bubble within the wake experiences a lower drag than that of the leading bubble. Thus, the trailing bubble, under the influence of the wake, catches up with the leading bubble. Finally, the two bubbles coalesce into the one large bubble shown in Fig. 11. For the inline cases, the movement of bubbles is symmetrical about the center line. Thus, the bubbles move rectilinearly because of the balance of the net lateral forces acting on the bubbles. This process is observed in the experiment performed by Brereton and Korotney [13]. Comparing Fig. 11 with Fig. 12, it can be said that the numerical results of the VOF methods are similar to the experimental results. It should also be noted that the initial conditions of the VOF method (Fig. 11) and the experiment (Fig. 12) are different and it is difficult to match their conditions, as was discussed in the previous section. Actually, the bubbles can be seen in Fig. 12, have dimples in their bottom surfaces, but, when viewed from the side, the indentation or dimples of the bubbles cannot be seen. Figure 13 shows the coalescence process of two bubbles simulated by the LBM. When viewed from the side, the process is similar to that of the VOF method, shown in Fig. 11. However, the internal process is different. Just before the bubbles collide ($t=0.0638$ in Fig. 13), a liquid film is captured between two bubbles and is then squeezed to the outside and finally ruptured. These processes can

be clearly seen in Fig. 13.

For the staggered case, the oblique coalescence of two bubbles is studied. Figures 14, 15, 16 show the results of VOF, experiment [13], and LBM, respectively. In Fig. 14, two bubbles are separated by a distance of $1.5d$ of their centers in the vertical direction. Unlike the inline case, the lower bubble is positioned to the right at a distance of $0.8d$. Although the process is similar to the coaxial process, the shape of the trailing bubble is different. The trailing bubble goes through a large asymmetrical deformation when it approaches the leading bubble, unlike the coaxial case. The asymmetrical structure of the trailing bubble can be seen in Figs. 14-16. The wake occurs behind the leading bubble, which is similar to the case of the coaxial flow. The velocity fields of the wake affecting the trailing bubble are not symmetrical about the center axis because of the staggered position of the bubbles. The net lateral forces acting on the trailing bubble are unbalanced, and then the lower bubble is deformed into a "tongue" shape. The experimental results of Brereton and Korotney [13] support this simulation result, when comparing Fig. 14 with Fig. 15. In addition, the effect of the asymmetrical horizontal velocity in the wake region on the trailing bubble was noted by [15].

Generally, the results of both numerical methods for two bubble coalescence are in good agreement with the

Fig. 14. Oblique Coalescence of the Two Bubbles at Different Times ($Eo = 16$, $M = 2 \times 10^{-4}$); VOF Results

Fig. 15. Oblique Coalescence of the Two Bubbles at Different Times by Brereton and Korotney [13] ($Eo = 16$, $M = 2 \times 10^{-4}$); Experimental Results [From Brereton and Korotney (1991)-Copyright © ASME 1991-Used with Permission.]

Fig. 16. Oblique Coalescence of the Two Bubbles at Different Times ($Eo = 16$, $M = 2 \times 10^{-4}$); LBM Results

experiment [13]. However, the LBM has better smoothness of interface than does the VOF method. However, no decisive conclusion was drawn from the above results because of the lack of experimental results for the internal observation of the bubbles just after collision. The process of the above coalescence is characterized as a 3 step phenomenon, as follows: (1) the collision between bubbles (2) the squeezing of the liquid film, and (3) the emission or destruction of the liquid film [16]. This phenomenon is difficult to simulate because of the topological change. The interface tracking method, which transforms the grid along the interface, is especially difficult to solve; however, the interface capturing methods such as the VOF method and the LBM can be done successfully [16, 17].

4. CONCLUSION

The volume of fluid (VOF) and the lattice Boltzmann method (LBM) were used to simulate the two-phase flows. The disk under shear flow and the static droplet flow were simulated for the validation tests. From the tests, the QUICK and modified HRIC schemes of the interface capturing methods in FLUENT were shown to perform

better than the Geo-Reconstruct and the CICSAM. However, the VOF method performed worse than the LBM in terms of spurious currents and satisfying of the Laplace law.

In the case of the single rising bubble flows, the final shape and the terminal velocity of the bubble are dependent on the Eotvos (Eo) and Morton (M) numbers. For larger surface tensions (Eo number is small), the results of both methods were in good agreements with the experiments by Bhaga and Weber [11]. For smaller surface tensions (Eo number is large), the deviations between numerical results and experiments occur at the terminal velocity, but those deviations of LBM are less than the VOF method. For multiple bubbles, the coalescence and dynamics of bubbles are affected by the wake pattern of the leading bubble. The coaxial and oblique coalescence of two rising bubbles was simulated successfully with the VOF method and the LBM.

Considering the above results, the LBM performs better than the VOF method in the case of the interface capturing, spurious currents, and rising bubble flows. The contact angle with the wall, bubble necking, and phase change including heat and mass transfer, which are important for the nucleate boiling, will be investigated in the future.

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