Terminal shape and velocity of a rising bubble by phase-field-based incompressible Lattice Boltzmann model

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Abstract

This article describes the simulation of three-dimensional buoyancy-driven bubble rise using a phase-field-based incompressible Lattice Boltzmann model. The effect of the Cahn-Hilliard mobility parameter, which is the rate of diffusion relaxation from non-equilibrium toward equilibrium state of chemical potential, is evaluated in detail. In contrast with previous work that pursues a high density ratio of binary fluids in the hydrodynamic equation, we apply a large dynamic viscosity ratio, together with a matched density pair and a separate compensating gas phase buoyant force, and the numerical results fit previous experimental results well. Through analysis, it is noted that for cases with moderate Reynolds number, a large value of mobility keeps a relatively sharp interface, while smaller values of mobility would result in diffusive interfacial regions. Moreover, for cases with large Reynolds number, small bubbles at the tail tend to separate more easily when the value of mobility is larger. This article offers some potentially useful details for performing phase-field-based simulations.

Key words: bubble rise; Lattice Boltzmann method; phase-field model; Cahn-Hilliard mobility

1. Introduction

Multiphase flows are common phenomena and are of great significance in both scientific and engineering fields; bubble rising processes are typical flows of interest. Water resources-related problems include for example, methane and carbon dioxide ebullition in thawing high-latitude peat soils and bubble-based hazardous waste cleanup efforts at the U.S. Department of Energy's Hanford Site. There is also potential for liberation and release of gas bubbles into groundwater as a result of hydraulic fracturing. In different flow regimes, the shape and velocity of the rising bubble will be quite different [1,2], typically including oblate ellipsoidal, oblate ellipsoidal disk, oblate ellipsoidal cap, spherical cap, skirted, etc. A deeper understanding of the dynamic characteristic of a rising bubble can enable promising applications, e.g., bubble rise in porous media [3]. As a complement to experimental investigations that measure instantaneous bubble velocity and record changing bubble shape [1,2,4], numerical simulation methods may offer an alternative choice for developing such understanding [5–7].

For a numerical multiphase model, the key factor is to precisely track the interface and model the interfacial interaction, which can be achieved by solving a phase-tracking equation and modeling the interfacial tension force in the hydrodynamic equation. Typical methods to these problems include the volume of fluid (VOF) method [8], the level-set method (LSM) [9], phase-field-based models [10,11], etc.

Among these models, phase field theory is often adopted by researchers from scientific and engineering fields, and the most typical phase-tracking equation is the Cahn-Hilliard (CH) equation [12]. The CH equation is an equation of mathematical physics, describing spontaneously separated binary phases. Different from the temporal propagation and convection treatment in VOF and LSM, a diffusion term is also incorporated, where chemical potential and mobility are applied. Herein mobility is introduced as the rate of diffusion relaxation from non-equilibrium toward equilibrium state of chemical potential [13]. Although the phase field models have been solved and applied by many scholars, the physical meaning of mobility has not been fully understood, beyond its effect on the simulation results [13,14].

To solve the CH equation, conventional methods, including finite difference methods (FDM), finite

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volume methods (FVM), and finite element methods (FEM) [15], can be applied, each with advantages and drawbacks. In recent years, the Lattice Boltzmann method (LBM) has been developed to solve the CH equation and also the hydrodynamic equation [6,16–20]. It has drawn much attention due to its kinetic-based background, simple algorithm, and great performance in parallel computing. Single-relaxation time (SRT) and multi-relaxation time (MRT) schemes are two main branches of LBM, and the formulation of the MRT scheme is more general and stable. The difference lies in the choice of the relaxation times (described below), and if the elements of the matrix of the relaxation times in the MRT scheme are set to be the same, then it is reduced to the SRT scheme. In addition, other multiphase models based on LBM have been used for some time and include: the Rothman-Keller (color-gradient) model [21], the Shan-Chen (pseudopotential) model [22,23], the free-energy-based model [24], the He-Chen-Zhang model [25,26], etc.

Numerous investigations have been done to enhance understanding of the bubble rising process in the past. Clift *et al.* [1] and Bhaga *et al.* [2], respectively, conducted hydrodynamic experiments and measured the terminal shape, terminal velocity, and the wake behind the bubble. Hua *et al.* simulated the single-bubble and multi-bubble rising process using VOF [27] and LBM [28,29]. Huang *et al.* developed the axisymmetric model [30] based on the model of He *et al.* [25,26], and applied their model to simulate bubble rising processes. Ngachin *et al.* simulated the bubble rising process using a multicomponent Shan-Chen model based on their effective buoyancy method [31]. Amaya-Bower *et al.* used the CH equation and simulated bubble rising process under moderate Reynolds number [32]. In addition, similar numerical work is conducted for simulating falling droplet processes [33,34]. However, the above simulations share the same drawback of not being able to recover the correct incompressible continuity equation and operating in a compressible regime [30,35], which can make the results deviate from real situations in cases where the Reynolds number is high or cases where the deformation of bubbles/droplets is large. In problems involving bubble dynamics, another widely used approach is the boundary element method (BEM) [36–38], where the mesh is constructed over the modelled surface, thus greatly improving the computational efficiency. However, in the calculation, the viscosity and interfacial tension is usually ignored, which works in situations where the Reynolds number is extremely high.

The latest phase field model under the framework of LBM has been capable of correctly recovering the CH equation through the Chapman-Enskog analysis [17–19]. Moreover, the LB hydrodynamic equation has overcome the drawback of near-incompressible limit [17–19]. But in practice, the effect of mobility is often ignored, sometimes making the simulations deviate from real situations.

The aim of this work is to reveal the ability of the incompressible model to deal with the common bubble rising problem, and to present a direct investigation into the effect of the Cahn-Hilliard mobility. In our work, a flow regime with moderate Reynolds number is simulated to enable comparisons with previous experimental and numerical investigations. Gas bubbles can be considered relatively incompressible under certain conditions (for example, an ideal gas bubble rising through one meter of water will change its radius by only 3%); under other circumstances, an incompressible model like the one we use here would be most appropriate for lower-compressibility rising droplets, such as oil in water.

We outline this article as follows: in Sec. 2, we introduce the framework of the numerical model; in Sec. 3, we validate the model by conducting layered Poiseuille flow simulations; in Sec. 4, we perform bubble rising simulations and present our analysis; in Sec. 5, conclusions are drawn. The simulations are performed using an Intel Xeon CPU and an Nvidia K20m GPU, wherein the former acts as the control node and the latter executes almost all the calculation work.

2. Methodology

2.1. Phase tracking equation

By applying the phase-field theory, the interface can be captured using the order parameter, which is ϕ_l for the liquid phase, and ϕ_g for the gas phase, respectively. And the bulk free energy of an isothermal

liquid-gas system takes the double-well form [6]

$$E_f \approx \beta(\phi - \phi_l)^2(\phi - \phi_g)^2, \quad (1.)$$

where β is a parameter dependent on interfacial thickness and surface tension. The chemical potential can then be derived as

$$\mu(\phi) = \mu_0(\phi) - \kappa \nabla^2 \phi = 4\beta(\phi - \phi_l)(\phi - \phi_g)(\phi - \frac{\phi_l + \phi_g}{2}) - \kappa \nabla^2 \phi, \quad (2.)$$

where β and κ are related to surface tension, and the relationships are expressed as

$$\beta = \frac{12\sigma}{W(\phi_l - \phi_g)^4}, \quad (3.)$$

$$\kappa = \frac{3\sigma W}{2(\phi_l - \phi_g)^2}, \quad (4.)$$

where W is the interface width, and σ is surface tension.

By solving $\mu(\phi) = 0$, the analytical one-dimensional interfacial profile of the order parameter (along the z direction perpendicular to the interface) can be obtained:

$$\phi(z) = \frac{\phi_l + \phi_g}{2} + \frac{\phi_l - \phi_g}{2} \tanh\left(\frac{2z}{W}\right). \quad (5.)$$

In our simulations, Eq.5 is also used to initialize the values of order parameter along the normal direction of the interface.

Typically the diffusion-driven Cahn-Hilliard equation is used to track the interfaces of binary flow systems, and is formulated as

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = \nabla (M_\phi \nabla \mu), \quad (6.)$$

where M_ϕ is the mobility. To obtain a non-dimensional form of Eq. 6, we define the dimensionless variables as

$$\bar{x} = \frac{x}{x^*}, \bar{t} = \frac{t}{t^*}, \bar{u} = \frac{ut^*}{x^*}, \bar{\phi} = \frac{\phi}{\phi_l - \phi_g}. \quad (7.)$$

where x^* and t^* are the reference length and the reference time, respectively. Hence, Eq. 6 can be rewritten as

$$\partial_{\bar{t}} \bar{\phi} + \bar{\nabla} \cdot (\bar{\phi} \mathbf{u}) = \bar{\nabla} \left\{ \frac{1}{Pe} \bar{\nabla} \left[\frac{48}{Ch} (\bar{\phi} - \bar{\phi}_l)(\bar{\phi} - \bar{\phi}_l) \left(\bar{\phi} - \frac{\bar{\phi}_l + \bar{\phi}_g}{2} \right) - \frac{3Ch}{2} \bar{\nabla}^2 \bar{\phi} \right] \right\}. \quad (8.)$$

where $Pe = \frac{x^{*3}(\phi_l - \phi_g)^2}{M_\phi \sigma t^*}$ is the Péclet number, and $Ch = \frac{W}{x^*}$ is the Cahn number. These two parameters dominate the phase-tracking process.

Following the description of Liang *et al.* [17,18], the LB equation with MRT scheme for the CH equation has the following form

$$\mathbf{f}(\mathbf{x} + \mathbf{e}_i \delta t, t + \delta t) - \mathbf{f}(\mathbf{x}, t) = -(\mathbf{M}^{-1} \mathbf{\Lambda}^f \mathbf{M})[\mathbf{f}(\mathbf{x}, t) - \mathbf{f}^{eq}(\mathbf{x}, t)] + \left[\mathbf{M}^{-1} \left(\mathbf{I} - \frac{\mathbf{\Lambda}^f}{2} \right) \mathbf{M} \right] \mathbf{R}. \quad (9.)$$

where $\mathbf{M}$ is the transformation matrix from velocity space to moment space, and as described in [39]. With the three-dimension and fifteen-speed (D3Q15) scheme, the lattice vectors are

$$\mathbf{e} = c \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \end{bmatrix}, \quad (10.)$$

where $c = \delta x / \delta t$ is lattice speed, and $\delta x = 1lu$ and $\delta t = 1ts$ are lattice unit length and lattice time step, respectively. Herein lu and ts represent the lattice unit of length and time step [5], respectively, and in addition, mu is the lattice mass unit. The equilibrium function is

$$f_i^{eq} = \begin{cases} \eta\mu(w_i - 1) + \phi, & i = 0 \\ w_i\eta\mu + w_i \frac{\mathbf{e}_i \cdot \phi \mathbf{u}}{c_s^2}, & i \neq 0 \end{cases} \quad (11.)$$

where w_i are the weighing factors, and they are $w_0 = 2/9$, $w_{1-6} = 1/9$, and $w_{7-14} = 1/72$.

The parameter $c_s = 1/\sqrt{3} lu/ts$ is lattice sound speed. To recover the correct form of the CH equation, $\mathbf{R}$ in the source term is formulated as

$$R_i = \frac{w_i \mathbf{e}_i \cdot \partial_t(\phi \mathbf{u})}{c_s^2}. \quad (12.)$$

The order parameter is calculated as

$$\phi = \sum_i f_i. \quad (13.)$$

The MRT models used for both interface tracking (CH) and hydrodynamic equations employ a relaxation time matrix. The relaxation times $s_3^f = s_5^f = s_7^f = 1/\tau^f$ are required to ensure the derivation of the correct CH equation via the Chapman-Enskog expansion, and the remaining relaxation times mainly affect the numerical stability [40,41]. If every relaxation time is set to be $1/\tau^f$, then the scheme is reduced to the SRT scheme. The situation in dealing with the hydrodynamic equation is quite similar, where the relaxation times have to be set as $s_9^g = s_{10}^g = s_{11}^g = s_{12}^g = s_{13}^g = 1/\tau^g$ in order to recover the correct hydrodynamic equation. In fact, so far very few criteria concerning the choice of the free relaxation times have been introduced in the LBM community, especially for the D3Q15 scheme. Here our choices of relaxation times are based on the following considerations: first, keep relaxation times needed to recover the correct governing equations; second, in a simple way, choose uniform values of the remaining relaxation times to enhance numerical stability, and herein they are set to be 1.0 for simplicity.

By Chapman-Enskog expansion with an accuracy of $O(\delta t^2)$, mobility has the following form

$$M_\phi = \eta c_s^2 (\tau^f - 0.5) \delta t, \quad (14.)$$

where η is an independent constant introduced to permit the tuning of the mobility.

2.2. Hydrodynamic equation

The incompressible Navier-Stokes equations, including the continuity equation, are expressed as

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot [\rho \nu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \mathbf{F}_s + \mathbf{F}_B \end{cases} \quad (15.)$$

where $\mathbf{F}_s$ is the interfacial tension force, and $\mathbf{F}_B$ is the buoyant force. Different from some previous models that recover deviated NS equations, which commonly includes a compressible continuity equation and an artificial interfacial force in the hydrodynamic equation [25,26], we apply the latest model by Liang *et al.* [17,18], which is proven to be capable of correctly recovering the above NS equations to an accuracy of $O(\delta t^2 + \delta t Ma^2)$, where Ma denotes the Mach number. A similar model that recovers the incompressible NS equations can be found in the work of Zu *et al.* [19], which, by contrast, contains implicit calculation of pressure. Herein the LB equation with MRT scheme has the following for

$$\mathbf{g}(\mathbf{x} + \mathbf{e}_i \delta t, t + \delta t) - \mathbf{g}(\mathbf{x}, t) = -(\mathbf{M}^{-1} \Lambda^g \mathbf{M})[\mathbf{g}(\mathbf{x}, t) - \mathbf{g}^{eq}(\mathbf{x}, t)] + \left[\mathbf{M}^{-1} \left(\mathbf{I} - \frac{\Lambda^g}{2} \right) \mathbf{M} \right] \mathbf{S}. \quad (16.)$$

The equilibrium functions are

$$g_i^{eq} = \begin{cases} \frac{p}{c_s^2} (w_i - 1) + \rho s_i(\mathbf{u}), & i = 0 \\ \frac{p}{c_s^2} w_i + \rho s_i(\mathbf{u}), & i \neq 0 \end{cases} \quad (17.)$$

where $s_i(\mathbf{u})$ is calculated as

$$s_i(\mathbf{u}) = w_i \left(\frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2} \right). \quad (18.)$$

The source term $\mathbf{S}$ is formulated as

$$S_i = \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} \{s_i(\mathbf{u}) \cdot \nabla(\rho c_s^2) + [s_i(\mathbf{u}) + w_i] \cdot (\mathbf{F}_s + \mathbf{F}_B + \mathbf{F}_a)\}, \quad (19.)$$

where $\mathbf{F}_a$ is introduced to eliminate the artificial interfacial force. This compensating force is proposed by Li *et al.* [42] and is expressed as

$$\mathbf{F}_a = d_\phi \rho \cdot (M_\phi \nabla \mu) \mathbf{u}. \quad (20.)$$

To calculate the interfacial tension force, three forms are usually used. The first scheme [17] uses the chemical potential and the spatial derivative of the order parameter, by setting

$$\mathbf{F}_s^{(1)} = \mu \nabla \phi = -\kappa \nabla^2 \phi \nabla \phi + \mu_0 \nabla \phi. \quad (21.)$$

The second scheme [19] uses the derivative of chemical potential and the order parameter, i.e.

$$\mathbf{F}_s^{(2)} = -\phi \nabla \mu = \kappa \phi \nabla \nabla^2 \phi - \phi \nabla \mu_0. \quad (22.)$$

Note that the above schemes are developed from the original phase-field theory that usually ignores μ_0 or its first-order derivatives in the calculation of interfacial tension force [11]. In the work of Chao *et al.* [35] that applies the HCZ model, it is noted that a wiggle will appear over the interfacial region, which would cause an error in the direction of interfacial force. Thus another interfacial tension calculation scheme is recommended by Kim *et al.* [11,43] as

$$\mathbf{F}_s^{(3)} = -\kappa \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) |\nabla \phi| \nabla \phi. \quad (23.)$$

Since the third scheme contains the calculation of divergence, on the basis of Eq. 23, we have

$$\nabla^2 \phi = \nabla \cdot (\nabla \phi) = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} |\nabla \phi| \right) = |\nabla \phi| \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) + \frac{\nabla \phi}{|\nabla \phi|} \nabla \cdot (|\nabla \phi|), \text{ and} \quad (24.a)$$

$$\nabla \phi \frac{\nabla \phi}{|\nabla \phi|} \nabla \cdot (|\nabla \phi|) = |\nabla \phi| \nabla \cdot (|\nabla \phi|) = \frac{1}{2} \nabla \cdot (|\nabla \phi|^2). \quad (24b)$$

Hence, a new form can be derived as

$$\mathbf{F}_s = -\kappa \nabla^2 \phi \nabla \phi + \frac{\kappa}{2} \nabla \cdot (|\nabla \phi|^2). \quad (25.)$$

Eq. 25 is used in the remainder of the article to calculate interfacial tension force. The buoyant force is added only to the gas phase, as in the work of Ngachin *et al.* [31], and for each node, it is calculated as

$$\mathbf{F}_B = -\rho_l \mathbf{g} V_i, \quad (26.)$$

where $\mathbf{g}$ is gravitational acceleration, and V_i is the lattice volume. The buoyant force is actually $\mathbf{F}_B = -(\rho_l - \rho_g) \mathbf{g} V_i$, but it is quite reasonable to approximate it as $\mathbf{F}_B = -\rho_l \mathbf{g} V_i$ because ρ_g is often so small in comparison to ρ_l . In real bubble rising situations, the density ratio of the system is usually very high (water/air pair is around 800), and buoyancy can be approximated using Eq. 26 with little loss of accuracy. To compare with previous experimental work, Eq. 26, together with a high dynamic viscosity ratio, appears to be sufficient for simulating real situations, even though a matched density ratio is used in the hydrodynamic equation and the buoyant force is added separately as described below.

The macroscopic variables have the following explicit form

$$\mathbf{u} = \frac{\sum \mathbf{e}_i g_i + \frac{1}{2}(\mathbf{F}_s + \mathbf{F}_B)}{\rho - d_\phi \rho \cdot (M_\phi \nabla \mu)}, \text{ and} \quad (27.)$$

$$p = \frac{c_s^2}{1-w_0} \left[\sum_{i \neq 0} g_i + \frac{1}{2} \mathbf{u} \cdot \nabla \rho + \rho s_0(\mathbf{u}) \right]. \quad (28.)$$

Density has a linear relationship with the order parameter, calculated as

$$\rho = \rho_g + \frac{\phi - \phi_l}{\phi_l - \phi_g} (\rho_l - \rho_g). \quad (29.)$$

It is noted that by applying a matched density pair throughout the whole work, the density in the whole domain is set equal, i.e., $\rho = \rho_l = \rho_g$. As a result, the density gradient vanishes as zero. In addition, the buoyant force is added separately.

In addition, from the form of the equilibrium distribution and pressure, it can be noted that the velocity-based evolution as well as the calculation of macroscopic variables of the single-phase incompressible LBM model by Guo *et al.* [44] are inherited by this multiphase modeling work.

In order to ensure conservative stress across the binary interface and avoid the sharp-interface limit of phase-field models, we introduce a step form of dynamic viscosity, i.e.,

$$\mu_{vis} = \begin{cases} \mu_l, & \phi > 0.5(\phi_l + \phi_g) \\ \mu_g, & \phi < 0.5(\phi_l + \phi_g) \end{cases}. \quad (30.)$$

Similar to the phase-tracking equation, the diagonal matrix $\mathbf{A}^g = [s_0^g, s_1^g, s_2^g, \dots, s_{14}^g]^T$ contains the relaxation times, where $s_9^g = s_{10}^g = s_{11}^g = s_{12}^g = s_{13}^g = 1/\tau^g$.

The computational domain is partitioned into a uniform three-dimensional (3D) Cartesian grid (each node is $1 \times 1 \times 1 \text{ lu}^3$). The first and second order spatial derivatives are solved using an isotropic discretization scheme, involving the nearest-neighbor nodes [6,17,20], i.e.,

$$\nabla \chi(\mathbf{x}) = \frac{1}{c_s^2 \delta x} \sum w_i \mathbf{e}_i \chi(\mathbf{x} + \mathbf{e}_i \delta t), \quad (31.)$$

$$\nabla^2 \chi(\mathbf{x}) = \frac{2}{c_s^2 \delta x^2} \sum w_i [\chi(\mathbf{x} + \mathbf{e}_i \delta t) - \chi(\mathbf{x})], \quad (32.)$$

where χ can be any scalar variable appearing in the model. The temporal derivative in Eq.12 is calculated using the first-order Euler scheme, i.e.,

$$\partial_t \chi = \frac{\chi(t) - \chi(t - \delta t)}{\delta t}. \quad (33.)$$

3. Method validation by layered Poiseuille flow

For immiscible binary flow driven by a constant body force between two parallel plates, an analytical solution can be derived by applying the no-slip wall boundary condition, and the continuous velocity and shear stress condition in the interfacial region [6,19]. In our 3D simulation, the liquid phase flows in the region $0 < z \leq a$ and the gas phase flows in the region $-a \leq z < 0$. No-slip boundary condition is applied at $z = \pm a$. The driving force acts along the x direction, and periodic condition is applied along x and y directions.

The fluid flow is governed by the following equations:

$$\rho_l v_l \nabla^2 u_l = G, \rho_g v_g \nabla^2 u_g = G. \quad (34.)$$

The boundary conditions are

$$\begin{cases} u_l|_{y=0} = u_g|_{y=0} \\ \rho_l v_l (\partial_y u_l)|_{y=0} = \rho_g v_g (\partial_y u_g)|_{y=0} \\ u_l|_{y=a} = u_g|_{y=-a} = 0 \end{cases}. \quad (35.)$$

By solving Eq. 34 together with Eq. 35, the analytical velocity profiles of each region, which have parabolic forms, can be obtained. In addition, the analytical profile of the order parameter along the z direction follows the one-dimensional hyperbolic tangential form as given by Eq. 5.

First, three mesh resolutions are applied for the convergence study, i.e., $128 \times 32 \times 128$, $192 \times 48 \times 192$, and $256 \times 64 \times 256$. We set the density pair $\rho_l = \rho_g = 1 \text{ mu/lu}^3$, the dynamic viscosity

ratio $\mu_l/\mu_g = 58$, and $\mu_l = 0.1 \mu u/(lu \cdot ts)$ is also given. The constant driving force has a relationship with the central velocity [19], i.e., $u_c = Ga^2/(\mu_l + \mu_g)$, and we have $u_c = 0.001 lu/ts$. The mobility $M_\phi = 1$ is applied in all cases shown in this section. Relative errors of velocity, calculated through $Error_u = |1 - u_{simulated}/u_{analytical}| \times 100\%$, are shown in Fig. 1 for three mesh resolutions, where the maximum relative errors are 0.76%, 0.50%, and 0.37%, respectively, and even the coarsest mesh resolution is sufficient for most purposes.

Fig. 1. Mesh convergence study for layered Poiseuille flow: relative error of velocity along the z direction. Three mesh resolutions along x , y , and z directions are $128 \times 32 \times 128$, $192 \times 48 \times 192$, and $256 \times 64 \times 256$, respectively.

In order to present the performance of the step-formed dynamic viscosity scheme (denoted by Scheme I), we also compare the results with the continuous scheme proposed with a linear form as $\mu = \mu_g + \frac{\phi - \phi_l}{\phi_l - \phi_g}(\mu_l - \mu_g)$ (denoted as Scheme II). Results are shown in Fig. 2 and Fig. 3. It can be noted that both schemes show good results of the order parameter profile. With Scheme II, the velocity profile becomes continuous in the interfacial region, which deviates from the sharp analytical result. Meanwhile, by using Scheme I, the simulated velocity fits the analytical results well. Therefore, our step-formed dynamic viscosity shows better agreement with the analytical solution.

Fig. 2. Velocity profile along the z direction of layered Poiseuille flow, with mesh resolution of $128 \times 32 \times 128$.

Fig. 3. Order parameter profile along the z direction of layered Poiseuille flow, with mesh resolution of $128 \times 32 \times 128$.

4. Results and discussion

4.1. Computational setup

For the rising process of a single bubble, the dynamic behavior is dominated by buoyancy, interfacial tension and viscous stress. In addition to the Péclet number and the Cahn number defined in Sec 2.1, we apply the following non-dimensional parameters to characterize the flow regime and hydrodynamic properties, including the Eötvös number (Eo), the Morton number (Mo), and the Reynolds number (Re), defined as

$$Eo = \frac{g\rho_l d_0^2}{\sigma}, \quad (36.)$$

$$Mo = \frac{g\mu_l^4}{\rho_l \sigma^3}, \quad (37.)$$

$$Re = \frac{\rho_l V d_0}{\mu_l}, \quad (38.)$$

where g is the gravitational acceleration, ρ_l is the density of the liquid phase, d_0 is the initial diameter of the bubble, σ is surface tension, and V is the average velocity of the bubble.

It is noted that in some literature citations, the density difference, i.e., $\Delta\rho = \rho_l - \rho_g$, is applied in the definition of Eo and Mo. Herein the main objective is to be consistent with the experimental work of Clift *et al.* [1] and Bhaga *et al.* [2], and it is assumed that $\rho_l \gg \rho_g$ therein.

In addition, reference length $x^* = d_0$ and reference time $t^* = \sqrt{d_0/g}$ are chosen, and the definitions of the Péclet number and the Cahn number become

$$Pe = \frac{d_0^2 \sqrt{d_0 g} (\phi_l - \phi_g)^2}{M_\phi \sigma}, \quad (39.)$$

$$Ch = \frac{W}{d_0}. \quad (40.)$$

In the phase-field model, the density ratios of liquid/gas can be arbitrary, but numerical instability would occur if large density ratios are adopted. In our experience, the achievable density ratio is usually less than 10. In this article, we simulate using a matched density pair, i.e., $\rho_l/\rho_g = 1$ and incorporate buoyant force separately. Inspired by the fact that in the layered Poiseuille flow, both the shear stress and the streamwise velocity are continuous across the interface, and the dynamic viscosity ratio plays a critical role, we also apply a high dynamic viscosity, i.e., $\mu_l/\mu_g = 58$, in our simulations. Moreover, when a matched density pair is used in the simulations, the artificial interfacial force in Eq. 20 is eliminated.

In terms of boundary configuration, we apply periodic boundary conditions in the x and y horizontal

directions, and no-slip wall boundary condition in the z direction (direction of buoyant force). A no-flux boundary condition is also applied to the wall boundary, with ϕ and μ equaling the values of their neighboring fluid node, respectively.

Initially, the bubble is set to be of spherical shape, with a diffusive layer following the one-dimensional interface profile in Eq. 5. The initial diameter of the bubble is $d_0 = 50 lu$.

4.2. Terminal shape and velocity

Among the factors that dominate the terminal shape of the bubble, interfacial tension tends to promote the smallest surface area, i.e., circle in 2D and sphere in 3D; dynamic viscosity dominates the shear stress, thus determining the rate of approach to equilibrium and influencing drag force; buoyancy acts as the driving force and equals the value of drag force in the equilibrium state.

To validate our numerical results and make comparisons with experimental measurements, we follow the experimental studies of Clift *et al.* [1] and Bhaga *et al.* [2] with equal initial values of Eo and Mo . Herein we use three groups of simulation cases: Case A ($Eo=116$, $Mo=266$), Case B ($Eo=116$, $Mo=41.1$), and Case C ($Eo=116$, $Mo=5.51$). Different from Eo and Mo that measure interaction evolved in the momentum equation, the Péclet number considers the effect of mobility in the phase-tracking equation. In this section, we simulate situations with a constant mobility $M_\phi = 22.25$, thus the Péclet number is $Pe_0 = 44,194$. A constant interface, i.e., $W = 3 lu$ is also used, thus the Cahn number is $Ch = 0.06$. Table 1 lists the terminal Reynolds number simulated using different mesh resolutions in both the streamwise and spanwise directions, previous experimental results by Clift *et al.* [1], Bhaga *et al.* [2], and numerical results by Hua *et al.* [27], and Cheng *et al.* [29]. It is clear that the present results fit the experimental results quite well. Snapshots of terminal bubble shape in the 3D domain and comparisons with experimental results [2] are shown in Fig. 4.

Table 1 Comparisons of terminal Reynolds number and mesh convergence study

Case	Experimental		Numerical		Present study with different mesh resolutions					
	Clift <i>et al.</i>	Bhaga <i>et al.</i>	Hua <i>et al.</i>	Cheng <i>et al.</i>	160×160×352	192×192×320	192×192×352	192×192×384	224×224×352	256×256×352
A	3.48	3.57	3.62	3.62	3.404	3.464	3.465	3.465	3.479	3.482
B	6.81	7.16	7.00	7.20	6.702	6.823	6.825	6.825	6.857	6.861
C	13.0	13.3	13.2	13.7	12.71	12.95	12.96	12.96	13.03	13.04

From Table 1, firstly, in the flow direction, the mesh with $NZ = 352$ is sufficient for all three cases. In the horizontal direction, we note that the terminal Reynolds number is a bit influenced by the mesh resolution, however, good convergence is reached when the mesh resolution is $NX \times NY \times NZ = 192 \times 192 \times 352$, and compared to the results with finest mesh resolution, i.e., $NX \times NY \times NZ = 256 \times 256 \times 352$, the relative error is close to 0.5%. Through the convergence study, it is shown that the mesh resolution with $NX \times NY \times NZ = 192 \times 192 \times 352$ is sufficient and appropriate for simulating the cases. Moreover, the terminal velocities of Case A, Case B, and Case C are $0.00792 lu/ts$, $0.00978 lu/ts$, and $0.0112 lu/ts$, respectively, indicating that the incompressible limit $u_t \ll c_s$ is satisfied well.

Fig. 4. Time evolution of bubble shape and comparisons with experimental results (Case A: $Eo=116$, $Mo=266$; Case B: $Eo=116$, $Mo=41.1$; Case C: $Eo=116$, $Mo=5.51$). Experimental results are from Bhaga *et al.*

In each case, average velocity and centroid position are monitored every 100 lattice time steps ($0.04t^*$), and are calculated as

$$u_{average,z} = \frac{\sum \rho_i u_{i,z} s(\phi_i)}{\sum \rho_i s(\phi_i)}, \quad (41.)$$

$$Zc_{average,z} = \frac{\sum \rho_i Z_i s(\phi_i)}{\sum \rho_i s(\phi_i)}, \quad (42.)$$

where $s(\phi_i)$ is a switch function, i.e., $s(\phi_i) = 1$ when $\phi_i < (\phi_l + \phi_g)/2$, and indicates that the node is inside the bubble; or $s(\phi_i) = 0$ when $\phi_i > (\phi_l + \phi_g)/2$. The time evolution of the Reynolds number according to average bubble velocity, and the centroid position are shown in Fig. 5 and Fig. 6, respectively.

Fig. 5. Time evolution of Reynolds number at $Pe=44,194$ and $Ch=0.06$. Case A: $Eo=116$, $Mo=266$; Case B: $Eo=116$, $Mo=41.1$; Case C: $Eo=116$, $Mo=5.51$.

Fig. 6. Time evolution of bubble centroid position at $Pe=44,194$ and $Ch=0.06$. Case A: $Eo=116$, $Mo=266$; Case B: $Eo=116$, $Mo=41.1$; Case C: $Eo=116$, $Mo=5.51$.

In addition, drag force acting on the bubble is evaluated indirectly by measuring the momentum change during fixed intervals, i.e.

$$F_{drag,t} = F_B - \frac{1}{n\delta t} [\sum_{t+n\delta t/2} \rho_i u_{i,z} s(\phi_i) - \sum_{t-n\delta t/2} \rho_i u_{i,z} s(\phi_i)], \quad (43.)$$

where $n = 100$ is the statistical interval. Time evolution of calculated drag force is shown in Fig. 7. The final drag force of the bubble reaches its equilibrium value after approximately $3t^*$ time steps. Before that, it keeps changing as it rises and deforms towards the terminal shape. During that period of time, on one hand, smaller drag force will be acting on the bubble in cases where smaller viscosity is applied; on the other hand, with smaller drag force, the net force acting on the bubble will be larger, bringing a larger rate of deformation.

Fig. 7. Time evolution of drag force acting on the bubble at $Pe=44,194$. Case A: $Eo=116$, $Mo=266$; Case B: $Eo=116$, $Mo=41.1$; Case C: $Eo=116$, $Mo=5.51$.

4.3. Effect of mobility and interface width

Since it is still an open problem how to choose the value of mobility based on physical principles, it is important to explore the effect of mobility numerically before performing simulations. According to the CH equation and the definition of chemical potential, for a given flow regime, a relatively small value of mobility would result in a small rate of diffusion. In addition, based on the LB approach, the achievable value of mobility is often limited to a certain range, and numerical instability would occur beyond this range.

It has been reported recently that mobility has a close relationship with the interface width [14,45]. It is suggested that a value of mobility that is proportional to the square of the interface width is optimal for achieving thin interfaces. Since this conclusion is a general one, in specific problems, it is essential to identify an appropriate range of the mobility parameter.

Firstly, we conduct a rising bubble study to test the effect of interface width with a fixed value of mobility, and the results are shown in Fig. 8. The relative error in terminal Reynolds number compared with the case at $W = 3$ lu is less than 1.01%. Hence only minor influence of interface width on convergence to a constant Reynolds number is observed. Based on this study, we can conclude that interface width is not a major factor affecting the hydrodynamics of the rising bubble. At least at the interface width range of $W = 2 - 4$ lu, this justifies further consideration of the effect of mobility independent of the interface width.

Fig. 8. Terminal Reynolds number with different interface width. (Case A: $Eo=116$, $Mo=266$)

For the cases investigated, where the value of Reynolds number indicates a moderate flow regime, the effect of mobility on the bubble shape is minor when the shape is drawn simply with the surface where the order parameter equals to $(\phi_l + \phi_g)/2$. However, previous work has seldom presented the spatial distribution of the density or order parameter. To make comparisons, Fig. 9~11 show terminal bubble shapes (center cross section along y direction) with different values of Pe in Cases A, B, and C, each drawn by 11 equal-interval contours of order parameter ranging from -0.5 to 0.5.

Fig. 9. Terminal shape with different mobility. (Case A: $Eo=116$, $Mo=266$)

Fig. 10. Terminal shape with different mobility. (Case B: $Eo=116$, $Mo=41.1$)

Fig. 11. Terminal shape with different mobility. (Case C: $Eo=116$, $Mo=5.51$)

As the bubble rises, the shape deforms from its initial spherical shape and the lower part tends to shrink due to the wake, where the effect of mobility is significant. From Fig. 9~11, it can be noted that for relatively small values of mobility, the spatial distribution of the order parameter deviates from real situations where sharp interfaces exist. In order to obtain more detailed information on the influence of mobility on the interfaces, the minimum and maximum values of the order parameter in the whole domain are measured and are shown in Fig. 12 and Fig. 13, respectively.

Fig. 12. Minimum value of order parameter. Case A: $Eo=116$, $Mo=266$; Case B: $Eo=116$, $Mo=41.1$; Case C: $Eo=116$, $Mo=5.51$.

Fig. 13. Maximum value of order parameter. Case A: $Eo=116$, $Mo=266$; Case B: $Eo=116$, $Mo=41.1$; Case C: $Eo=116$, $Mo=5.51$.

Peak values of the order parameter exist near the interface. As the value of mobility decreases (higher Pe), the minimum value of order parameter decreases monotonically. And in cases where terminal velocity is larger, the minimum value of the order parameter will be decreased more. From the CH equation, it can be concluded that the above effect is caused by improper diffusion. In addition, the maximum value of the order parameter in the whole domain is only slightly influenced, and is close to the expected value in all cases. The above results also suggest that when conducting phase-field-based simulations, whether the value of mobility is appropriate can be checked through monitoring the maximum and minimum values of the order parameter.

Moreover, for cases with larger values of Mo , or small values of dynamic viscosity, when skirted tails or break-up appears, bifurcation induced by mobility is observed. For cases with large values of mobility, or small values of Péclet number, small bubbles appear to separate more easily in the simulations than in the experiments (see Fig. 14(b)). Meanwhile, it can be noted that the shape of the main part of the bubble is almost the same as the experimental results, and the position of the bubble is unaffected by the Péclet number, after $6t^*$ time steps. Although terminal shape can be captured after sufficient time steps, the effect of an improper value of mobility on the dynamic behavior is more complex.

Fig. 14. Terminal shape (a) with different mobility and (b) experimental results by Bhaga *et al.* at $Eo=116$ and $Mo=0.103$.

4.4. Effect of dynamic viscosity ratio

In order to assess the importance of the dynamic viscosity ratio, in this section we perform bubble rise simulations and apply a group of dynamic viscosity ratios at $Eo=116$ and $Mo=266$. Herein we keep all parameters fixed to the same values as those of Case A in Sec. 4.2, except for the dynamic viscosity of the gas phase and thereby the dynamic viscosity ratio. The time evolution of the Reynolds number is calculated to make comparisons, and the results are shown in Fig.15, where μ_r denotes the dynamic viscosity ratio of liquid to gas phases.

Fig. 15. Terminal Reynolds number with different dynamic viscosity ratio. (Case A: $Eo=116$, $Mo=266$, $Pe=44194$)

The results in Fig. 15 indicate that, for the modeled conditions (Case A), there is convergence of the Reynolds number to the experimental result ($Re=3.48$ listed in Table 1) for dynamic viscosity ratio greater than about 30. It is shown from Fig. 15 that at low dynamic viscosity ratios, more time steps are needed to reach the equilibrium state and the terminal velocity is smaller than experimental data. As a bubble rises at a moderate Reynolds number, the movement of the surrounding liquid phase owes much to the shear stress induced by the bubble, where the dynamic viscosity plays a significant role. In cases where large viscosity ratios are applied, the surrounding liquid phase is weakly influenced by the movement of the bubble.

Different from the intensively studied topic [6,20,29] to pursue a large density ratio in multiphase modeling, our simulations show that a correct treatment of dynamic viscosity across the interfacial region is also an important issue. A benefit of the current model is that it can achieve a very low viscosity in practical problems, both a high viscosity ratio and a relatively high Reynolds number can be achieved concurrently.

5. Conclusions

In this article, we present a numerical study of terminal shape and velocity of a rising bubble in various flow regimes, with an emphasis on the effect of the Cahn-Hilliard mobility. Based on the latest phase field model developed by Liang *et al.* [17], the incompressible multiphase flow of a rising bubble, including the phase-tracking and hydrodynamic equations, is fully evolved in a three-dimensional domain. Unlike previous numerical simulations, we apply a matched density pair, a high dynamic viscosity ratio, effective buoyancy, and a modified interfacial tension calculation scheme.

Using the LB model, the terminal shape and velocity of the rising bubble are in good agreement with previous experimental and numerical results. With constant Eo and Mo that dominate the dynamic process and various values of mobility, it is noted that large values of mobility maintain relatively sharp interfaces; while smaller values of mobility would result in non-physical diffusive interfacial regions. Moreover, for cases with large Reynolds number, small bubbles at the tail tend to separate more easily when the value of mobility is larger. Since the physical meaning of mobility is not yet fully understood, bifurcation induced by mobility should be noted and explored carefully.

In addition, simulations concerning the effect of dynamic viscosity show that a low dynamic viscosity would result in a considerably slower rate of evolution towards the equilibrium state, as well as deviated terminal velocity. A dynamic viscosity ratio that approaches the real system is recommended.

Overall, our work reveals good capability of the incompressible phase-field-based model, and offers useful tests concerning the effect of mobility.

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