Numerical simulation for multi-phase fluids considering different densities with continuous finite element method

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Abstract. In this paper, we compute a phase field model of Cahn-Hilliard type for multi-component mixture fluids considering surface tension and buoyancy effects. We discretize Navier-Stokes and Cahn-Hilliard coupled equations with a continuous finite element scheme in space and the finite difference in time. Also, we apply a penalty formulation to the continuity equation which may increase the stability in solving the continuity condition and momentum equation. The dynamic of a rising lighter drop due to different densities between other two immiscible fluids is studied as the numerical example with a relatively coarse grid. Numerical results show that this model can be solved with a relative simple scheme and coarse grid which leads to the higher efficiency.

1. Introduction

Multiphase flows play an increasingly important role in many scientific and bio-medical engineering applications, such as, gas bubble trapped in water \cite{1}, oil-water mixtures \cite{2}, nanofluids \cite{3, 4}, biological fluids and cells in blood \cite{5}. Multiphase fluid motions have been extensively studied both theoretically and experimentally, yet still remain an active interdisciplinary research field. Interface tracking and interface capturing are two main viewpoint for simulating the interface structure of multiphase fluids and lots of work on the numerical simulation of the interface have been done with different methods like, front tracking \cite{6, 7} and immersed boundary \cite{8, 9} which belong to interface tracking and also the method with the interface capturing such as level set method \cite{10, 11}, volume of fluid \cite{12, 13} and phase field method \cite{14, 15}.

There are two kinds of theoretical models named sharp interface model and phase field model due to different treatment for the interface which are widely used for multi-phase fluids with clear interface. Sharp interface model uses the single phase fluid model to simulate each phase apart. It treats the interface as the boundary which makes the jump of boundary conditions exists at the interface due to the different property parameters of different phase. As boundary conditions at interface not continuous any more, it increases the difficulty in the computing of the system. Many people investigate multi-phase fluids numerically with sharp interface model as this model is closer to the reality \cite{8, 14}, even though they have to deal with the jump condition.

Phase-field model \cite{16} has become one of the major tools to deal with many dynamical processes in biological morphology, which can be traced back to Cahn et al. \cite{17, 18}. For the multiphase fluid...
systems, Lin et al. [19, 20] developed the model and its advantage is the well-posed nonlinear partial differential equations can satisfy thermodynamics-consistent energy dissipation laws. In [21], a mass-conserved diffuse interface method is proposed for simulating incompressible flows of binary fluids with large density ratio. Aland [22] presented time integration for diffuse interface models for two-phase flow. Chen and Shen [23] introduced a fully adaptive energy stable scheme for Navier-Stokes-Cahn-Hilliard system. Recently, Kim [24] proposed a generalized continuous surface tension force formulation for the phase-field model with any number of fluids. In [25], Kim introduced phase-field models for multi-component fluid flows. But, it could not eliminate spurious phases at binary interfaces. In [26], Lee and Kim extended their previous works and proposed a new diffuse interface model for the mixture of N incompressible immiscible fluids. They employed a new chemical potential that can eliminate spurious phases at binary interfaces. Various numerical methods are used to solve the phase field model, such as the lattice Boltzmann [27, 28], adaptive moving mesh methods [23, 29, 30], finite element methods [31, 32, 33], Euler methods [34, 35].

In this paper, we use the phase field model proposed by Lee and Kim [26] to compute the multiphase fluids with the continuous finite element method. In Section 2, we introduce the phase-field model for multi-component immiscible fluids. In Section 3, we present the weak form and the fully discretized Navier-Stokes-Cahn-Hilliard system. We perform the numerical experiment of rising lighter drop in three-component fluids in Section 4. Section 5 is the conclusion.

2. Multi-phase model, weak form and fully discretized form

The model for the multi-component immiscible fluids proposed by Lee and Kim [26] is composed of Navier Stokes equations and Cahn-Hilliard models as follows:

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \left( \eta \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) + SF(c) + \rho g \]

(1)

\[ \nabla \cdot \mathbf{u} = 0 \]

(2)

\[ \frac{\partial c_i}{\partial t} + \nabla \cdot (c_i \mathbf{u}) = \nabla \cdot [M(c) \nabla \mu_i] \]

(3)

\[ \mu_i = f(c_i) - \epsilon^2 \Delta c_i + \beta_i, \quad i=1,2,L,N \]

(4)

Here \( c = (c_1, \ldots, c_N) \) is a vector-valued phase parameter and each \( c_i \) is the concentration of each component in the mixture satisfying \( \sum_{i=1}^{N} c_i = 1, 0 \leq c_i \leq 1 \). \( \mathbf{u} = (u_1, u_2) \) represents the velocity of the mixture and \( p \) is the hydrostatic pressure. \( M, \epsilon, \eta, \rho, \mu \) denote phenomenological mobility, interface thickness, fluid viscosity, density and chemical potential, respectively. \( \rho \) and \( \eta \) due to the different densities and multi-component have the expression of \( \rho = \sum_{i=1}^{N} \rho_i c_i \) and \( \eta = \sum_{i=1}^{N} \eta_i c_i \). where \( \rho_i \) and \( \eta_i \) are the \( \text{th} \) fluid density and viscosity, respectively. The acceleration of gravity is \( g = (0, -g) \). In addition, we have

\[ f(c_i) = c_i (c_i - 0.5)(c_i - 1), \beta_i = -\frac{\epsilon^2}{N} \sum_{j=1}^{N} f(c_j) SF(c) = \sum_{j=1}^{N} \frac{0.5 \sigma}{c_i} \left( sf(c_j) + sf(c_j) \delta(c_i, c_j) \right) \]

(5)

which is the surface tension force and \( sf(c_j) = -6 \sqrt{2} \epsilon \nabla \cdot (\nabla c_j / |\nabla c_j|) |\nabla c_j| \nabla c_i \). \( \sigma_j \) is the physical surface tension coefficient between two components and \( \delta(c_i, c_j) = 5c_i c_j \). The boundary condition \( c_i \)
and $\mu_i$ is $\delta_{c_i} c_i = 0, \delta_{a_i} \mu_i = 0$. However, the boundary condition of $\mathbf{u}$ for top and bottom is $\mathbf{u} = \mathbf{0}$ and the periodic boundary condition for left and right. The dimensionless physical quantities are introduced as

$$
\mathbf{x}' = \frac{x}{L_c}, \mathbf{u}' = \frac{\mathbf{u}}{U_c}, \rho' = \frac{\rho}{\rho_c}, \rho' = \frac{\rho}{\rho_c}, \eta' = \frac{\eta}{\eta_c}, \mathbf{g}' = \frac{\mathbf{g}}{g}, \mathbf{M}' = \frac{\mathbf{M}}{M_c}, \mu' = \frac{\mu}{\mu_c}.
$$

(6)

Applying equation (6) to equation (1)-(4) and without loss of generality letting $\mathbf{u} = \mathbf{u}', \rho = \rho', \rho = \rho', \eta = \eta', \mathbf{g} = \mathbf{g}', \mathbf{M} = \mathbf{M}', \mu = \mu'$, the whole system becomes

$$
\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla p + \frac{1}{Re} \nabla \cdot \left(\eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T)\right) + \mathbf{SF}(c) + \frac{\rho}{Fr^2} \mathbf{g},
$$

(7)

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

(8)

$$
\frac{\partial \mathbf{c}}{\partial t} + \nabla \cdot (\mathbf{c} \mathbf{u}) = \frac{1}{Pe} \nabla \cdot [\mathbf{M}(c) \nabla \mu_i],
$$

(9)

$$
\mu_i = f(c_i) - c_i^2 \Delta c_i + \beta_i, \quad i = 1, 2, L, N
$$

(10)

where

$$
\mathbf{SF}(c) = \sum_{i=1}^{N} \sum_{j=1}^{i} 0.5 \sigma_j \left( \mathbf{sf}(c_i) + \mathbf{sf}(c_j) \right) \frac{\delta(c_j, c_j)}{W_{ij}}, \quad \mathbf{g} = (0, -1).
$$

(11)

$$
Re = \frac{\mu_c U L_c}{\eta_c}, \quad We = \frac{\rho_c L_c^2}{\mu_c}, \quad Fr = \frac{U}{\sqrt{gL}}, \quad Pe = \frac{UL_c}{M_c \mu_c}.
$$

(12)

Please see more details in [19, 35] for the finite element space and we define that $T = [\mathcal{V}_c]$, the weak form reads: Find $\mathbf{u} \in W^{1,3}, p \in L_0^2, c_i, \mu_i \in W^{1,3}$ such that:

$$
\int_{\Omega} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u}\right) \cdot \mathbf{v} + \nabla p : \mathbf{v} + \frac{\eta}{Re} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : \nabla \mathbf{v} + \sum_{i=1}^{N} \sum_{j=1}^{i} 15 \sqrt{2} \left( \frac{\nabla c_i}{T_i} \otimes (T c_i \nabla c_i) + \frac{\nabla c_i}{T_j} \otimes (T_j \nabla c_j) \right) \cdot \nabla (c_i c_j) \cdot \mathbf{v} + \frac{\rho}{Fr^2} \mathbf{g} : \mathbf{v} \right) dx
$$

(13)

$$
\int_{\Omega} \mathbf{v} \cdot \nabla q dx = 0, \quad \forall q \in W^{1,3}(\Omega)
$$

(14)

$$
\int_{\Omega} \left(\frac{\partial \mathbf{c}}{\partial t} s_i + \nabla \cdot (\mathbf{c} \mathbf{u}) s_i + \frac{\mathbf{M}}{Pe} \nu_{\mu_i} \cdot \nabla s_i \right) dx = 0, \quad \forall s_i \in W^{1,3}(\Omega)
$$

(15)

$$
\int_{\Omega} \mu_i m_i - f(c_i) m_i - c_i^2 (\nabla c_i, \nabla m_i) - \beta_i m_i dx = 0, \quad \forall m_i \in W^{1,3}(\Omega)
$$

(16)

We make $\mathbf{W} = W^{1,3}(\Omega) \times L_0^2(\Omega) \times W^{1,3}(\Omega) \times W^{1,3}(\Omega)$, $\mathbf{W}^h = \mathbf{U}^h \times P^h \times \mathbf{H}^h \times \mathbf{H}^h \subset \mathbf{W}$ as a finite dimensional subspace of $\mathbf{W}$ given by a continuous finite element discretization. We let $\Delta t > 0$ denote the time step size and $(\mathbf{u}^n, p^n, c^n, \mu^n) \in \mathbf{W}^h$ is an approximation of $\mathbf{u}(t^*) = \mathbf{u}(n \Delta t), \quad p(t^*) = p(n \Delta t), \quad c(t^*) = c(n \Delta t), \quad \mu(t^*) = \mu(n \Delta t)$. Here we need to rewrite the continuity condition equation (14) as
\[ \nabla \cdot \mathbf{u} + \delta p = 0 \] with \( \delta = 10^{-6} \) and the chemical potential \( \mu = \omega + \alpha c, \alpha = 0.5 \). And \( (\mathbf{u}_{\text{ret}}, p_{\text{ret}}, c_{\text{ret}}, \mu_{\text{ret}}) \) is the approximation at time \( t^{n+1} = (n+1) \Delta t \) and the discretized formulas are as follows:

\[
\int_{\Omega} \left( \rho_{\text{ret}}^{n+1} \left( \mathbf{u}_{\text{ret}}^{n+1} + (\mathbf{u}_h^* \cdot \nabla) \mathbf{u}_h^* \right) \cdot \mathbf{v} + \nabla p_{\text{ret}}^{n+1} \cdot \mathbf{v} + \frac{\eta}{Re} \left( \nabla \mathbf{u}_{\text{ret}}^{n+1} + \left( \nabla \mathbf{u}_{\text{ret}}^{n+1} \right)^T \right) : \nabla \mathbf{v} + \int_{\Gamma_d} \sum_{t=1}^{\Delta t} \frac{15 \sqrt{e}}{We_g} \left( - \frac{\nabla c_{\text{ret}}^{n+1}}{T_{ij}^e} \otimes (T_{ij}^{n+1} \nabla c_{\text{ret}}^{n+1} \iota) \right) \cdot \left( \nabla (c_{\text{ret}}^{n+1} \mathbf{c}_{\text{ret}}^{n+1}) \mathbf{v} \right) + \frac{(T_{ij}^{n+1})^2}{2} + \left( T_{ij}^{n+1} \right)^2 \left( \nabla (c_{\text{ret}}^{n+1} \mathbf{c}_{\text{ret}}^{n+1}) \mathbf{v} \right) \) \right) + \int_{\Omega} g \cdot \mathbf{v} + \int_{\Gamma_d} \sum_{t=1}^{\Delta t} \frac{15 \sqrt{e}}{We_g} \left( \mathbf{n} \left( c_{\text{ret}}^{n+1} \mathbf{c}_{\text{ret}}^{n+1} \right) \mathbf{v} \right) ds = 0 \]

where \( \mathbf{u}_{\text{ret}}^* = (\mathbf{u}_{\text{ret}}^{n+1} - \mathbf{u}_h^* )/\Delta t \), \( c_{\text{ret}}^* = (c_{\text{ret}}^{n+1} - c_{\text{ret}}^0 )/\Delta t \), \( T_{ij}^{n+1} = \left| \nabla c_{\text{ret}}^{n+1} \right| , f (c_{\text{ret}}^0) = c_{\text{ret}}^0 (c_{\text{ret}}^0 - 0.5) (c_{\text{ret}}^0 - 0.5) \).

3. Numerical result and discussion

In the computation of the system, we use \( P_2 \) (piecewise quadratic) continuous finite element to compute \( \mathbf{u}, c, \rho \) and \( p \) under the FreeFem++ platform [36].

In this section, we simulate the buoyancy-driven evolution of a rising bubble with equation (17)-(20). A lighter bubble is set in a two phase fluids distributed at the top and bottom of the pipe and the bubble rises from the bottom of this two phase media to the top of the computing domain. The density ratio is 1:4:3 ( \( \rho_1 = 1, \rho_2 = 4, \rho_3 = 3, c_1 \) means the lighter bubble set in phase 2 in the initial time, \( c_3 \) represents the bottom fluid and \( c_3 \) denotes the top fluid) the same as the numerical example in [1] and other parameters are set as \( Re = 30, Fr = 1, Pe = 0.01/\varepsilon, \varepsilon = 0.01, M = 0.0001 \), \( We_{12} = 30, We_{13} = 20, We_{c3} = 15 \). The initial value of phase parameter \( c_1 \) is

\[
c_1 (x, y) = \begin{cases} 0.5 & \frac{1}{2} \left( 1 + \tanh \left( \frac{r - \left( (x - 2)^2 + (y - 1)^2 \right)^{1/2}}{2 \sqrt{2} \varepsilon} \right) \right) \end{cases}, \quad c_2 (x, y, 0) = 1 - \begin{cases} 1 & \frac{1}{2} \left( 1 + \tanh \left( \frac{y - 1.6}{2 \sqrt{2} \varepsilon} \right) \right) - c_1 (x, y, 0) \end{cases} (21) \]

\[
c_1 (x, y, 0) = 1 - c_1 (x, y, 0) - c_2 (x, y, 0) \] (22)

The computing domain is \( \Omega = [0.4] \times [0.4] \times [0, 32] \times [0, 32] \) and 32 x 32 relatively coarse grid is used to compute this system. \( r \) is the radius of the lighter bubble ( \( c_1 \) ) and we make the comparison between \( r = 0.3 \) and \( r = 0.2 \).

Figure 1 shows the interface structure of the rising bubble ( \( c_1 = 0.5 \) ) with different radii at different time ( \( t = 0, 2.15, 9.85, 11.1, 11.5, 12.4 \) ). We can see that both cases give the similar behavior before \( t = 2.15 \) as the bubble rises gradually with the buoyancy effect and also contributes to the change of the interface of \( c_1 = 0.5 \) and \( c_3 \). The bubble with \( r = 0.3 \) rises faster than the other one but
they still stay in phase 2. When $t = 9.85$, some parts of the bubble have crossed the interface and filtered into phase 3 in both cases. And the bubble with $r = 0.3$ crosses the interface between other two phases and filters into the phase 3 completely with some parts of phase 2 at $t = 11.1$ which well agreed with the result in [1].

**Figure 1.** The evolution of the bubble and the horizontal interface. (Top) $r = 0.3$; (Bottom) $r = 0.2$.

We may consider that the bubble with $r = 0.2$ would not cross the horizontal interface completely as the horizontal interface returns to the original position compared between $t = 11.5$ and $t = 12.45$. But the result in figure 2 shows that the bubble crosses the interface and filters into another phase completely at $t = 20.85$, but this process is not smooth. According to the numerical simulation in
figure 1 and figure 2, we may conclude that a bigger bubble can move into the other fluid more easily and smoothly. We also give the evolution of the velocity in this system in figure 3.

Figure 3. The velocity of the system at the time matched with figure 1.

4. Conclusions
In this paper, we numerical investigate the evolution of the interface structure in multiphase fluid considering the surface tension and buoyancy effect with the continuous finite element method. We treat the continuity condition with a penalty method to enhance the stability of pressure. The buoyancy driven bubble is simulated as a numerical example to examine the accuracy and efficiency of the continuous finite element method. Different sizes of the lighter bubble would have influence on the numerical solutions and the rising process of the bigger bubble would be more smoothly.

Acknowledgements
Yongyue Jiang is partially supported by Beijing Postdoctoral Research Foundation.

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