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Highlights

- We propose efficient, decoupled, and energy stable schemes for the hydrodynamics coupled a phase-field model.
- The proposed schemes are more accurate than other approaches and show better energy stability.
- We rigorously prove the unconditional energy stability of semi-implicit scheme and fully discrete scheme.
- Hydrodynamic behavior and energy changes during the bubble rising process are investigated in detail.

Efficient energy stable schemes for the hydrodynamics coupled phase-field model

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Abstract

In this paper, several efficient and energy stable semi-implicit schemes are presented for Cahn-Hilliard phase-field model of two-phase incompressible flows. A scalar auxiliary variable (SAV) approach is implemented to solve the Cahn-Hilliard equation while a splitting method based on pressure stabilization is used to solve Navier-Stokes equation. At each time step, the schemes involve solving only a sequence of linear elliptic equations and computations of phase-field variable, velocity and pressure are totally decoupled. A finite difference method on staggered grids is adopted to spatially discretize the proposed time marching schemes. We rigorously prove the unconditional energy stability for the semi-implicit schemes and fully discrete scheme. Numerical results in both two and three dimensions are obtained, which demonstrate accuracy and effectiveness of the proposed schemes. Using our numerical scheme, we compare the SAV, invariant energy quadratization (IEQ) and stabilization approaches. Bubble rising dynamics and coarsening dynamics are also investigated in detail. The results demonstrate that the SAV approach can be more accurate than the IEQ approach, and the stabilization approach is the least accurate among the three approaches. The energy stability of SAV approach appears better than other approaches at large time steps.

Keywords

Phase-field modelling; two-phase flows; Navier-Stokes equation; scalar auxiliary variable; energy stability

1. Introduction

Mixtures of two or more immiscible fluids components have always been attracting much attention due to its importance in many industrial applications, for instance, the CO₂ sequestration [1]. Numerous numerical methods have been used to understand the interfacial dynamics, including sharp interface methods [2], front tracking methods [3], lattice Boltzmann methods [4], and phase-field method considered in this study [5-8]. The phase-field model treats the interface as a thin and continuous layer, and a phase-field variable is introduced to distinguish two immiscible phases [9-11]. The phase-field model has been widely used in simulations of two-phase fluids. In this model, free energy functional dominates the interfacial dynamics of multiphase system, and it reads:

$$E_f(\phi) = \lambda \int_{\Omega} \left(\frac{1}{2} |\nabla \phi|^2 + F(\phi) \right) d\Omega, \quad (1.1)$$

where ϕ is the phase-field variable, and it is used to distinguish different fluids

$$\phi \begin{cases} 1 & \text{fluid 1,} \\ -1 & \text{fluid 2.} \end{cases}$$

At the interface of two fluids, ϕ varies continuously between -1 and 1. λ denotes the characteristic strength of phase mixing energy. The free energy E_f is also called the mixing energy of interface. The gradient term in (1.1) causes the interface to be diffused, and the second term, double well

potential $F(\phi) = (\phi^2 - 1)^2 / (4\varepsilon^2)$, expresses a preference to pure phases $\phi = \pm 1$. The competition between the two terms results in a diffuse interface at equilibrium. ε in $F(\phi)$ is a parameter that proportional to the interface thickness. Through the variational derivative of free energy E_f with respect to ϕ , we can obtain the chemical potential w

$$w_\phi := \frac{\delta E_f}{\delta \phi} = -\lambda \Delta \phi + \lambda F'(\phi). \quad (1.2)$$

The advective Cahn-Hilliard equation governs the evolution of ϕ

$$\phi_t + \nabla \cdot (\mathbf{u} \phi) - M \Delta w_\phi = 0, \quad (1.3)$$

where M is the mobility parameter.

The momentum equation for the hydrodynamics takes the usual form of Navier-Stokes equation [12, 13]

$$\begin{cases} \rho \mathbf{u}_t + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla \cdot \eta D(\mathbf{u}) + \nabla p + \phi \nabla w_\phi = 0, \\ \nabla \cdot \mathbf{u} = 0, \end{cases} \quad (1.4)$$

where $D(\mathbf{u}) = \nabla \mathbf{u} + \nabla \mathbf{u}^T$, $\mathbf{u}$ is the flow velocity field and p is the pressure. The Cahn-Hilliard equation and the Navier-Stokes equation is coupled through convection and stress terms. The total energy for the two-phase system is the sum of kinetic energy E_k and free energy E_f

$$E_{tot} = E_k + E_f = \int_{\Omega} \left(\frac{\rho}{2} |\mathbf{u}|^2 + \frac{\lambda}{2} |\nabla \phi|^2 + \lambda F(\phi) \right) d\Omega. \quad (1.5)$$

We can see that the phase-field model is completely derived from the energy-based variational formalism. The developed governing system is well-posed and satisfies a thermodynamically consistent energy dissipation law, which makes it possible to design efficient numerical methods. Several efficient numerical approaches have been proposed for the Cahn-Hilliard phase-field model, including convex splitting, stabilization, invariant energy quadratization (IEQ) and scalar auxiliary variable (SAV) approaches. The convex splitting approach [14-17] assumes that the double well potential $F(\phi)$ can be split as the difference of two convex functions (or the summation of one convex and one concave functions), namely $F(\phi) = F_c(\phi) - F_e(\phi)$ with $F_c(\phi) \geq 0$ and $F_e(\phi) \geq 0$. The first-order convex splitting scheme for the Cahn-Hilliard equation reads:

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} - M \Delta w_\phi^{n+1} = 0, \\ w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \lambda [F'_c(\phi^{n+1}) - F'_e(\phi^n)]. \end{cases} \quad (1.6)$$

The convection term is omitted in equation (1.6) to simplify the presentation. Although the convex splitting scheme is unconditionally stable and uniquely solvable, it still has some disadvantages. Firstly, this scheme usually involves a nonlinear coupled system, which is computational expensive to carry out numerical results. Secondly, the proof of unconditional energy stability for the nonlinear scheme is difficult. The stabilization approach [7, 12, 18] adds the term $\lambda(\phi^{n+1} - \phi^n) / \varepsilon^2$ artificially in the equation of chemical potential to balance the explicit nonlinear term $F'(\phi^n)$ so that the time step will not be severely constrained by the interface thickness

associated parameter. A first-order stabilization scheme for the Cahn-Hilliard equation reads:

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} - M \Delta w_\phi^{n+1} = 0, \\ w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda}{\varepsilon^2} (\phi^{n+1} - \phi^n) + \lambda F'(\phi^n). \end{cases} \quad (1.7)$$

The stabilization approach satisfies a discrete energy law and has been widely used due to its numerical efficiency and simplicity. Moreover, a totally decoupled, linear and unconditionally stable scheme for the Cahn-Hilliard phase-field model of two-phase incompressible flows has been constructed based on the stabilization approach [12]. However, this scheme requires the second derivative of the double well potential $F(\phi)$ to be bounded. Also, it is relatively difficult to construct an unconditionally stable second-order stabilization scheme. The IEQ approach [19-25] introduces an auxiliary variable q to transform $F(\phi)$ into an quadratic polynomial form (Obviously, $F(\phi)$ is positive and bounded from below in the whole domain). The auxiliary variable reads

$$q = \sqrt{F(\phi)}. \quad (1.8)$$

Then the free energy of system can be written as

$$E_f(\phi, q) = \lambda \int_{\Omega} \left(\frac{1}{2} |\nabla \phi|^2 + q^2 \right) d\Omega.$$

With the new free energy functional, we can obtain the following transformed Cahn-Hilliard equation [25],

$$\begin{cases} \phi_t - M \Delta w_\phi = 0, \\ w_\phi = -\lambda \Delta \phi + \frac{\lambda q}{\sqrt{F(\phi)}} F'(\phi), \\ q_t = \frac{F'(\phi)}{2\sqrt{F(\phi)}} \phi_t. \end{cases} \quad (1.9)$$

All nonlinear terms in the new system can be treated semi-explicitly, which in turn produces a set of linear elliptic equations. The first-order IEQ scheme can be written as

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} - M \Delta w_\phi^{n+1} = 0, \\ w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda q^{n+1}}{\sqrt{F(\phi^n)}} F'(\phi^n), \\ \frac{q^{n+1} - q^n}{\delta t} = \frac{F'(\phi^n)}{2\sqrt{F(\phi^n)}} \frac{\phi^{n+1} - \phi^n}{\delta t}. \end{cases} \quad (1.10)$$

If we substitute $F(\phi^n) = [(\phi^n)^2 - 1]^2 / (4\varepsilon^2)$ into (1.10), we can obtain

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} - M \Delta w_\phi^{n+1} = 0, \\ w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{2\lambda (\phi^n)^2}{\varepsilon^2} (\phi^{n+1} - \phi^n) + \lambda F'(\phi^n). \end{cases} \quad (1.11)$$

The stabilization term $2\lambda (\phi^n)^2 (\phi^{n+1} - \phi^n) / \varepsilon^2$ in (1.11) indicates that the IEQ approach can be viewed as a special stabilization approach when $F(\phi)$ is taken as the double well potential. The IEQ

approach has proven to be unconditionally stable and it can be easily extended to high-order schemes. But it also suffers from some shortcomings [25] such as: (1) It involves solving a linear fourth-order equation with variable coefficients for ϕ^{n+1} ; (2) It requires that the double well potential $F(\phi)$ is bounded from below, and this may not hold for some physically interesting models. To overcome these shortcomings, most recently, the SAV approach [25, 26] has been proposed. This approach almost shares the same idea with the IEQ approach. A scalar auxiliary variable r is introduced to transform the free energy functional into an equivalent form. Since the free energy $E_1(\phi)$ is bounded from below, we can define the following scalar variable r

$$r = \sqrt{E_1(\phi)}, \quad \text{where } E_1(\phi) = \int_{\Omega} F(\phi) d\Omega. \quad (1.12)$$

Then free energy of system is transformed into

$$E_f(\phi, r) = \int_{\Omega} \frac{\lambda}{2} |\nabla \phi|^2 d\Omega + \lambda r^2. \quad (1.13)$$

With the new free energy functional, we can obtain the transformed governing system

$$\begin{cases} \phi_t - M \Delta w_{\phi} = 0, \\ w_{\phi} = -\lambda \Delta \phi + \frac{\lambda r}{\sqrt{E_1(\phi)}} F'(\phi), \\ r_t = \frac{1}{\sqrt{E_1(\phi)}} \int_{\Omega} F'(\phi) \phi_t d\Omega. \end{cases} \quad (1.14)$$

By treating nonlinear terms in equation (1.14) semi-explicitly, we can get the first-order SAV scheme reads,

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} - M \Delta w_{\phi}^{n+1} = 0, \\ w_{\phi}^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda r^{n+1}}{\sqrt{E_1(\phi^n)}} F'(\phi^n), \\ \frac{r^{n+1} - r^n}{\delta t} = \frac{1}{2\sqrt{E_1(\phi^n)}} \int_{\Omega} F'(\phi^n) \frac{\phi^{n+1} - \phi^n}{\delta t} d\Omega. \end{cases} \quad (1.15)$$

Beside the unconditional energy stability, this scheme is extremely efficient and easy-to-implement. More precisely, the total cost at each step is essentially solving two linear fourth-order equations with constant coefficients [25].

From the numerical point of view, it is quite difficult to construct an efficient and energy stable scheme to solve the coupled Cahn-Hilliard and Navier-Stokes system [27, 28]. The main difficulties [9, 12] come from: (1) the small interfacial width in the Cahn-Hilliard equation that introduces stiffness into the governing system; (2) the nonlinear coupling between the phase-field variable and velocity through nonlinear convection and stresses; (3) the coupling between velocity and pressure through the incompressibility. Recently, several attempts [9, 10, 12, 29] have been made to develop efficient, decoupled and energy stable schemes for the Cahn-Hilliard phase-field models of two-phase incompressible flows. Shen et al. constructed two classes of totally decoupled, unconditionally stable schemes based on the stabilization and convex splitting approaches [12]. In particular, the scheme based on the stabilization approach involves solving only a sequence of linear and elliptic equations, which makes it extremely efficient and easy-to-implement. Yang and his collaborators constructed a series of first-order and second-order

schemes based the IEQ approach [19-21, 23, 24], which are efficient and satisfy discrete energy laws. The SAV approach is built upon the IEQ approach, and it enjoys all advantages of IEQ approach but overcoming most of its shortcomings [25, 26]. Therefore, it's necessary to develop numerical schemes, which are efficient, totally decoupled and satisfies the discrete energy law, for the hydrodynamics coupled phase-field model based on the SAV approach. However, to the best of the author's knowledge, no such work has ever been done before.

The rest of this paper is organized as follows. In section 2, we described a transformed Cahn-Hilliard and Navier-Stokes system. In section 3, we construct some efficient, decoupled and energy stable schemes for the hydrodynamics coupled phase-field model, and carry out the energy stability estimates for the proposed schemes. In section 4, we implement an efficient finite difference method on the staggered grids to spatially discretize the time marching schemes and prove the unconditional energy stability of the fully discrete scheme. Several 2D and 3D numerical examples are investigated in Section 5 and the paper is finally concluded in Section 6.

2. The governing equations

2.1. Case of matched density

In the case of matched density, we consider a transformed Cahn-Hilliard phase field model of two-phase incompressible flows. With the introduction of the scalar auxiliary variable in (1.8), the governing system can be written as

$$\phi_t + \nabla \cdot (\mathbf{u}\phi) - M \Delta w_\phi = 0, \quad (2.1a)$$

$$w_\phi = -\lambda \Delta \phi + \frac{\lambda r}{\sqrt{E_1(\phi)}} F'(\phi), \quad (2.1b)$$

$$r_t = -\frac{1}{2\sqrt{E_1(\phi)}} \int_{\Omega} F'(\phi) \phi_t d\Omega, \quad (2.1c)$$

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} - \eta \Delta \mathbf{u} + \nabla p + \phi \nabla w_\phi = 0, \quad (2.1d)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2.1e)$$

with periodic boundary conditions or

$$\mathbf{u} = 0, \quad \partial_n \phi = 0, \quad \partial_n w_\phi = 0, \quad \text{on } \Gamma.$$

Without loss of generality, we have set in the above $\rho=1$ and $\eta_1 = \eta_2 = \eta$. The purpose of this treatment is to simplify the presentation. By taking the inner product of (2.1a) with $-w_\phi$, (2.1b) with ϕ , (2.1c) with $-2\lambda r$, (2.1d) with $\mathbf{u}$, (2.1e) with p and adding these relations, we can find that the system satisfies the following energy law

$$\frac{d}{dt} E_{tot} = - \int_{\Omega} \left(\eta |\nabla \mathbf{u}|^2 + M |\nabla w_\phi|^2 \right) d\Omega \leq 0,$$

where

$$E_{tot} = \int_{\Omega} \left(\frac{1}{2} |\mathbf{u}|^2 + \frac{\lambda}{2} |\nabla \phi|^2 \right) d\Omega + \lambda r^2. \quad (2.2a)$$

2.2. Case of nonmatching density

For the case of nonmatching density, the governing system [12, 30] is shown as follows,

$$\phi_t + \nabla \cdot (\mathbf{u}\phi) - M \Delta w_\phi = 0, \quad (2.2a)$$

$$w_\phi = -\lambda \Delta \phi + \frac{\lambda r}{\sqrt{E_1(\phi)}} F'(\phi), \quad (2.2b)$$

$$r_t = \frac{1}{2\sqrt{E_1(\phi)}} \int_{\Omega} F'(\phi) \phi_t d\Omega, \quad (2.2c)$$

$$\rho(\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}) + \mathbf{J} \cdot \nabla \mathbf{u} - \nabla \cdot D(\mathbf{u}) + \nabla p + \phi \nabla w_\phi = 0, \quad (2.2d)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2.2e)$$

with periodic boundary conditions or

$$\mathbf{u} = 0, \quad \partial_n \phi = 0, \quad \partial_n w_\phi = 0, \quad \text{on } \Gamma.$$

where

$$\mathbf{J} = \frac{\rho_2 - \rho_1}{2} M \nabla w_\phi, \quad \rho = \frac{\rho_1 - \rho_2}{2} \phi + \frac{\rho_1 + \rho_2}{2}, \quad \eta = \frac{\eta_1 - \eta_2}{2} \phi + \frac{\eta_1 + \eta_2}{2}. \quad (2.2f)$$

We can easily derive the following conservation property from equations (2.2a), (2.2e) and (2.2f)

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) + \nabla \cdot \mathbf{J} = 0. \quad (2.3)$$

By taking the inner product of (2.2a) with $-w_\phi$, (2.2b) with ϕ_t , (2.2c) with $-2\lambda r$, (2.2d) with $\mathbf{u}$, of (2.1 e) with p and adding these relations, the following energy law can be obtained

$$\frac{d}{dt} E_{tot} = - \int_{\Omega} \left(\frac{\eta}{2} |D(\mathbf{u})|^2 + M |\nabla w_\phi|^2 \right) d\Omega \leq 0,$$

where

$$E_{tot} = \int_{\Omega} \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \frac{\lambda}{2} |\nabla \phi|^2 \right) d\Omega + \lambda r^2.$$

3. Linear, decoupled and energy stable numerical schemes

3.1. Case of matched density

We introduce a first-order stabilization term in the convective velocity [12, 31] and construct the following semi-implicit, totally decoupled numerical scheme for the governing system (2.1).

Given ϕ^n , $\mathbf{u}^n$ and p^n , the scheme calculates ϕ^{n+1} , $\tilde{\mathbf{u}}^{n+1}$, $\mathbf{u}^{n+1}$ and p^{n+1} for $n \geq 0$ in three steps. Step 1, we solve the transformed Cahn-Hilliard equation to update ϕ^{n+1} and r^{n+1} .

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} + \nabla \cdot (\mathbf{u}_*^n \phi^n) - M \Delta w_\phi^{n+1} = 0, \\ w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda r^{n+1}}{\sqrt{E_1(\phi^n)}} F'(\phi^n), \\ \frac{r^{n+1} - r^n}{\delta t} = \frac{1}{2\sqrt{E_1(\phi^n)}} \int_\Omega F'(\phi^n) \frac{(\phi^{n+1} - \phi^n)}{\delta t} d\Omega, \\ \partial_n \phi^{n+1} = 0, \quad \partial_n w_\phi^{n+1} = 0, \quad \text{on } \Gamma. \end{cases} \quad (3.1a)$$

$$\mathbf{u}_*^n = \mathbf{u}^n - \delta t \phi^n \nabla w_\phi^{n+1}. \quad (3.1b)$$

Step 2, Updating $\tilde{\mathbf{u}}^{n+1}$ by solving

$$\begin{cases} \frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^n}{\delta t} - \eta^n \Delta \tilde{\mathbf{u}}^{n+1} + \nabla p^n + (\tilde{\mathbf{u}}^n \cdot \nabla) \mathbf{u}^{n+1} + \phi^n \nabla w_\phi^{n+1} = 0, \\ \tilde{\mathbf{u}}^{n+1} = 0, \quad \text{on } \Gamma. \end{cases} \quad (3.1c)$$

Step 3, we update $\mathbf{u}^{n+1}$ and p^{n+1} by solving

$$\begin{cases} \mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1} + \delta t \nabla (p^{n+1} - p^n) = 0, \\ \nabla \cdot \mathbf{u}^{n+1} = 0, \\ \mathbf{u}^{n+1} \cdot \mathbf{n} = 0, \quad \text{on } \Gamma. \end{cases} \quad (3.1d)$$

Thanks to the second equation in (3.1d), we can rewrite the last term as follows,

$$\begin{cases} -\Delta (p^{n+1} - p^n) = -\frac{1}{\delta t} \nabla \cdot \tilde{\mathbf{u}}^{n+1}, \\ \partial_n (p^{n+1} - p^n)|_\Gamma = 0, \end{cases} \quad \mathbf{u}^{n+1} = \tilde{\mathbf{u}}^{n+1} - \delta t \nabla (p^{n+1} - p^n). \quad (3.2)$$

In the scheme (3.1), computations of the phase-field variable, the velocity and the pressure are totally decoupled, and each step consists of solving a linear elliptic equation, which indicates the scheme is uniquely solvable.

3.2. Case of nonmatching density

To deal with the case of nonmatching density, a cut-off function is defined

$$\hat{\phi}^{n+1} = \begin{cases} \phi^{n+1} & |\phi^{n+1}| \leq 1, \\ \text{sign}(\phi^{n+1}) & |\phi^{n+1}| > 1. \end{cases} \quad (3.3)$$

Similar to the previous case, we construct a semi-implicit and totally decoupled numerical scheme for the governing system (2.2). Given p^n , η^n , ϕ^n , $\mathbf{u}^n$, and p^n , the scheme calculates p^{n+1} , η^{n+1} , ϕ^{n+1} , $\mathbf{u}^{n+1}$ and p^{n+1} in three steps. Step 1, we solve the transformed Cahn-Hilliard equation to update ϕ^{n+1} and r^{n+1}

$$\begin{cases}
 \frac{\phi^{n+1} - \phi^n}{\delta t} + \nabla \cdot (\mathbf{u}_*^n \phi^n) - M \Delta w_\phi^{n+1} = 0, \\
 w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda r^{n+1}}{\sqrt{E_1(\phi^n)}} F'(\phi^n), \\
 \frac{r^{n+1} - r^n}{\delta t} = \frac{1}{2\sqrt{E_1(\phi^n)}} \int_{\Omega} F'(\phi^n) \frac{(\phi^{n+1} - \phi^n)}{\delta t} d\Omega, \\
 \partial_n \phi^{n+1} = 0, \quad \partial_n w_\phi^{n+1} = 0, \quad \text{on } \Gamma.
 \end{cases} \quad (3.4a)$$

$$\mathbf{u}_*^n = \mathbf{u}^n - \delta t \frac{\phi^n \nabla w_\phi^{n+1}}{\rho^n}. \quad (3.4b)$$

Step 2, updating $\mathbf{u}^{n+1}$, ρ^{n+1} and η^{n+1} by solving

$$\begin{cases}
 \rho^n \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\delta t} - \nabla \cdot \eta^n D(\mathbf{u}^{n+1}) + \nabla (2p^n - p^{n-1}) + \rho^n (\mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1} + \mathbf{J}^n \cdot \nabla \mathbf{u}^{n+1} \\
 + \phi^n \nabla w_\phi^{n+1} + \frac{1}{2} \frac{\rho^{n+1} - \rho^n}{\delta t} \mathbf{u}^{n+1} + \frac{1}{2} \nabla \cdot (\rho^n \mathbf{u}^n) \mathbf{u}^{n+1} + \frac{1}{2} (\nabla \cdot \mathbf{J}^n) \mathbf{u}^{n+1} = 0, \\
 \mathbf{u}^{n+1} = 0, \quad \text{on } \Gamma,
 \end{cases} \quad (3.4c)$$

where

$$\mathbf{J}^n = \frac{(\rho_2 - \rho_1)}{2} M \nabla w_\phi^n, \quad \rho^{n+1} = \frac{\rho_1 - \rho_2}{2} \hat{\phi}^{n+1} + \frac{\rho_1 + \rho_2}{2}, \quad \eta^{n+1} = \frac{\eta_1 - \eta_2}{2} \hat{\phi}^{n+1} + \frac{\eta_1 + \eta_2}{2}.$$

Step 3, we update p^{n+1} . To avoid solving an elliptic equation with a variable coefficient $1/\rho$, a pressure stabilization scheme is adapted to solve the pressure Poisson equation

$$\begin{cases}
 -\Delta(p^{n+1} - p^n) = -\frac{\chi}{\delta t} \nabla \cdot \mathbf{u}^{n+1}, \\
 \mathbf{n} \cdot \nabla p^{n+1} = 0, \quad \text{on } \Gamma.
 \end{cases} \quad (3.4d)$$

where $\chi = \frac{1}{2} \min(\rho_1, \rho_2)$.

The first-order stabilization term in (3.4b) is important for the unconditional stability of the proposed scheme, and we will give a clear demonstration in section 3.3. Combining (3.4a) and (3.4b), we have

$$\begin{cases}
 \phi^{n+1} - \delta t M \Delta w_\phi^{n+1} - \delta t^2 \nabla \cdot \left(\frac{(\phi^n)^2}{\rho^n} \nabla w_\phi^{n+1} \right) = \phi^n - \delta t \nabla \cdot (\mathbf{u}^n \phi^n), \\
 w_\phi^{n+1} = \lambda A \phi^{n+1} + \frac{\lambda}{2} (b^n, \phi^{n+1}) b^n + s^n, \\
 s^n = \lambda [r^n - (b^n, \phi^n)/2] b^n,
 \end{cases} \quad (3.5)$$

where

$$A \phi^{n+1} = -\Delta \phi^{n+1}, \quad b^n = F'(\phi^n) / \sqrt{E_1(\phi^n)},$$

and $(\cdot, \cdot)$ is the inner product in $L^2(\Omega)$. If we denote

$$A_p w_\phi^{n+1} = -\nabla \cdot \left(\frac{(\phi^n)^2}{\rho^n} \nabla w_\phi^{n+1} \right), \quad (3.6)$$

then equation (3.5) can be rewritten into

$$\begin{aligned} & \phi^{n+1} + \delta t M A \left[\lambda A \phi^{n+1} + \frac{\lambda}{2} (b^n, \phi^{n+1}) b^n + s^n \right] + \delta t^2 A_p \left[\lambda A \phi^{n+1} + \frac{\lambda}{2} (b^n, \phi^{n+1}) b^n + s^n \right] \\ & = \phi^n - \delta t \nabla \cdot (\mathbf{u}^n \phi^n). \end{aligned} \quad (3.7)$$

If we denote $A_w = I + \lambda M \delta t A^2 + \lambda \delta t^2 A_p A$ (where I is the identity matrix), then equation (3.7) can be written as

$$\begin{aligned} & A_w \phi^{n+1} + \frac{\lambda M \delta t}{2} (b^n, \phi^{n+1}) A b^n + \frac{\lambda \delta t^2}{2} (b^n, \phi^{n+1}) A_p b^n \\ & = \phi^n - \delta t \nabla \cdot (\mathbf{u}^n \phi^n) - M \delta t A s^n - \delta t^2 A_p s^n = S^n. \end{aligned} \quad (3.8)$$

Multiplying (3.8) with A_w^{-1} , and then taking the inner product with b^n , we have,

$$(b^n, \phi^{n+1}) + \frac{\lambda M \delta t}{2} (b^n, \phi^{n+1}) (b^n, A_w^{-1} A b^n) + \frac{\lambda \delta t^2}{2} (b^n, \phi^{n+1}) (b^n, A_w^{-1} A_p b^n) = (b^n, A_w^{-1} S^n). \quad (3.9)$$

The value of (b^n, ϕ^{n+1}) can be calculated from (3.9)

$$(b^n, \phi^{n+1}) = \frac{(b^n, A_w^{-1} S^n)}{1 + \alpha + \beta}, \quad (3.10)$$

where

$$\alpha = \frac{\lambda M \delta t}{2} (b^n, A_w^{-1} A b^n), \quad \beta = \frac{\lambda \delta t^2}{2} (b^n, A_w^{-1} A_p b^n).$$

Finally, we can obtain ϕ^{n+1} from (3.11)

$$\phi^{n+1} = A_w^{-1} S^n - \frac{\lambda M \delta t}{2} (b^n, \phi^{n+1}) A_w^{-1} A b^n - \frac{\lambda \delta t^2}{2} (b^n, \phi^{n+1}) A_w^{-1} A_p b^n. \quad (3.11)$$

At each time step, we need to solve three fourth-order equations with variable coefficients.

The transformed Cahn-Hilliard equation in (3.4a) can be solved very efficiently if the first-order stabilization term is removed from the convective velocity in (3.4b). Then, we can eliminate w^{n+1} and r^{n+1} to obtain

$$\begin{aligned} & (I + \lambda M \delta t A^2) \phi^{n+1} + \frac{\lambda M \delta t}{2} (b^n, \phi^{n+1}) A b^n \\ & = \phi^n - \lambda M \delta t \left[r^n - \frac{(b^n, \phi^n)}{2} \right] A b^n - \delta t \nabla \cdot (\mathbf{u}^n \phi^n) = S^n. \end{aligned} \quad (3.12)$$

ϕ^{n+1} can be obtained if the value of (b^n, ϕ^{n+1}) is determined. Multiplying (3.12) with $A_e^{-1} = (I + \lambda M \delta t A^2)^{-1}$, and then taking the inner product with b^n , we get

$$(b^n, \phi^{n+1}) + \frac{\lambda M \delta t}{2} (b^n, \phi^{n+1}) (b^n, A_e^{-1} A b^n) = (b^n, A_e^{-1} S^n). \quad (3.13)$$

The value of (b^n, ϕ^{n+1}) can be derived from (3.14)

$$(b^n, \phi^{n+1}) = \frac{(b^n, A_e^{-1} S^n)}{1 + \lambda M \delta t (b^n, A_e^{-1} A b^n)/2}. \quad (3.14)$$

Finally, the ϕ^{n+1} can be obtained by solving equation (3.15)

$$\phi^{n+1} = A_e^{-1} S^n - \frac{\lambda M \delta t}{2} (b^n, \phi^{n+1}) A_e^{-1} A b^n. \quad (3.15)$$

At each step, two fourth-order equations with constant coefficients are solved, demonstrating that the scheme (3.12) is extremely efficient and easy-to-implement. The scheme (3.12) is linear and decoupled, but not unconditionally energy stable. One can use the decoupled scheme (3.12) as a preconditioner for the unconditionally energy stable scheme (3.4), which can greatly improve the efficiency of scheme (3.4).

Remark 3.1. (1) Once we obtain ϕ^{n+1} , r^{n+1} can be calculated explicitly. Thus, the introduction of scalar auxiliary variable r does not involve extra computational cost; (2) Computations of the phase-field variable, the velocity and the pressure are totally decoupled; At each time step, the scheme (3.4) only needs to solve a sequence of elliptic equations; (3) The last three terms in equation (3.4c) is the first-order approximation of the term

$$\frac{1}{2} (\rho_t + \nabla \cdot (\rho \mathbf{u}) + \nabla \cdot \mathbf{J}) \mathbf{u} \quad (3.16)$$

at the time step $n+1$. This term vanishes in equation (2.2d) due to equation (2.3); (4) We can also replace (3.4c) with the following equation [32] to update $\mathbf{u}^{n+1}$

$$\begin{aligned} \rho^n \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\delta t} - \nabla \cdot \eta^n D(\mathbf{u}^{n+1}) + \nabla (2p^n - p^{n-1}) + (\rho^n \mathbf{u}^n) \cdot \nabla \mathbf{u}^{n+1} + \mathbf{J}^{n+1} \cdot \nabla \mathbf{u}^{n+1} \\ + \phi^n \nabla w_\phi^{n+1} + \frac{\rho_1 + \rho_2}{4} (\nabla \cdot \mathbf{u}^n) \mathbf{u}^{n+1} = 0. \end{aligned} \quad (3.17)$$

3.3. Energy stability analysis

Numerical schemes that do not respect energy dissipation laws may be “overloaded” with an excessive amount dissipation near singularities, which in turn lead to large numerical errors, particularly for long time integration. In this section, we will rigorously prove that the proposed schemes are unconditionally energy stable. We emphasize that the “unconditional” here only means the schemes have no constraints on the time step from the energy stability point of view. Large time step-sizes will definitely induce large errors in practice.

Theorem 3.1. Linear schemes (3.1) and (3.4) are unconditionally energy stable, and satisfy the following discrete energy law

$$\frac{E_{tot}^{n+1} - E_{tot}^n}{\delta t} = -\frac{1}{2} \left\| \sqrt{\eta^n} D(\mathbf{u}^{n+1}) \right\|^2 - M \left\| \nabla w_\phi^{n+1} \right\|^2 \leq 0, \quad (3.18)$$

where

$$\begin{cases} E_{tot}^n = \frac{1}{2} \left\| \sigma^n \mathbf{u}^n \right\|^2 + \frac{\delta t^2}{2\chi} \left\| \nabla p^n \right\|^2 + \frac{\lambda}{2} \left\| \nabla \phi^n \right\|^2 + \lambda \left| r^n \right|^2, \\ r^n = \sqrt{F(\phi^n)}, \sigma^n = \sqrt{\rho^n}, \end{cases} \quad (3.19)$$

here $\|\cdot\|$ denotes the L^2 -norm in Ω . E_{tot}^n is the total energy of the whole system at the time step n .

For the case of matched density, ρ and χ can be simply set to 1 in (3.19). The first term on the right side of equation (3.18) is the viscous dissipation, and the second term denotes the diffusion dissipation.

Proof. We only prove the unconditional energy stability for the case of nonmatching density, and the case of matched density can be similarly derived. Using integration by parts, we can easily derive

$$(\mathbf{u} \cdot \nabla \mathbf{v}, \mathbf{v}) + \frac{1}{2}((\nabla \cdot \mathbf{u}) \mathbf{v}, \mathbf{v}) = 0, \quad (3.20)$$

and

$$(\nabla \cdot \mathbf{u}, p) = -(\nabla p, \mathbf{u}). \quad (3.21)$$

with the identity (3.20), we have

$$\left((\rho^n \mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1} + \frac{1}{2} \nabla \cdot (\rho^n \mathbf{u}^n) \mathbf{u}^{n+1}, \mathbf{u}^{n+1} \right) = 0, \quad (3.22)$$

$$\left((\mathbf{J}^n \cdot \nabla) \mathbf{u}^{n+1} + \frac{1}{2} (\nabla \cdot \mathbf{J}^n) \mathbf{u}^{n+1}, \mathbf{u}^{n+1} \right) = 0. \quad (3.23)$$

According to the (3.4b), we have

$$\rho^n (\mathbf{u}^{n+1} - \mathbf{u}^n) + \delta t \phi^n \nabla w_\phi^{n+1} = \rho^n (\mathbf{u}^{n+1} - \mathbf{u}_*^n). \quad (3.24)$$

By taking the L^2 inner product of (3.4c) with $2\delta t \mathbf{u}^{n+1}$, using (3.21) -(3.24) and an identity of

$$(a - b, 2a) = \|a\|^2 - \|b\|^2 + \|a - b\|^2,$$

we can derive

$$\begin{aligned} & \|\sigma^n \mathbf{u}^{n+1}\|^2 - \|\sigma^n \mathbf{u}_*^n\|^2 + \|\sigma^n \mathbf{u}^{n+1} - \sigma^n \mathbf{u}_*^n\|^2 + \|\sigma^{n+1} \mathbf{u}^{n+1}\|^2 - \|\sigma^n \mathbf{u}^{n+1}\|^2 + \delta t \|\sqrt{\eta^n} D(\mathbf{u}^{n+1})\|^2 + \\ & + 2\delta t (p^{n+1} - 2p^n + p^{n-1}, \nabla \cdot \mathbf{u}^{n+1}) - 2\delta t (p^{n+1}, \nabla \cdot \mathbf{u}^{n+1}) = 0. \end{aligned} \quad (3.25)$$

By taking the L^2 inner product of (3.4d) with $2\delta t^2(p^{n+1} - 2p^n + p^{n-1})/\chi$ and with $-2\delta t^2 p^{n+1}/\chi$ separately, we obtain

$$\begin{aligned} & -\frac{\delta t^2}{\chi} \left(\|\nabla(p^{n+1} - p^n)\|^2 - \|\nabla(p^n - p^{n-1})\|^2 + \|\nabla(p^{n+1} - 2p^n + p^{n-1})\|^2 \right) \\ & = 2\delta t (p^{n+1} - 2p^n + p^{n-1}, \nabla \cdot \mathbf{u}^{n+1}), \end{aligned} \quad (3.26)$$

and

$$\frac{\delta t^2}{\chi} \left(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 + \|\nabla(p^{n+1} - p^n)\|^2 \right) = -2\delta t (p^{n+1}, \nabla \cdot \mathbf{u}^{n+1}). \quad (3.27)$$

By adding (3.26) and (3.27), we obtain

$$\begin{aligned} & 2\delta t (p^{n+1} - 2p^n + p^{n-1}, \nabla \cdot \mathbf{u}^{n+1}) - 2\delta t (p^{n+1}, \nabla \cdot \mathbf{u}^{n+1}) \\ & = \frac{\delta t^2}{\chi} \left(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 \right) + \frac{\delta t^2}{\chi} \|\nabla(p^n - p^{n-1})\|^2 \\ & - \frac{\delta t^2}{\chi} \|\nabla(p^{n+1} - 2p^n + p^{n-1})\|^2. \end{aligned} \quad (3.28)$$

Next, we take the difference of (3.4d) at step t^{n+1} and t^n , pair the resulting equation with $p^{n+1} - 2p^n + p^{n-1}$, then take integration by parts for both sides to derive

$$\frac{\delta t^2}{\chi} \|\nabla(p^{n+1} - 2p^n + p^{n-1})\|^2 \leq \chi \|\mathbf{u}^{n+1} - \mathbf{u}^n\|^2 \leq \frac{1}{2} \|\sigma^n(\mathbf{u}^{n+1} - \mathbf{u}^n)\|^2, \quad (3.29)$$

Combining (3.25), (3.28) and (3.29), we derive

$$\begin{aligned} & \|\sigma^{n+1}\mathbf{u}^{n+1}\|^2 - \|\sigma^n\mathbf{u}^n\|^2 + \|\sigma^n\mathbf{u}^{n+1} - \sigma^n\mathbf{u}^n\|^2 + \delta t \|\sqrt{\eta^n} D(\mathbf{u}^{n+1})\|^2 + \\ & + \frac{\delta t^2}{\chi} (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) + \frac{\delta t^2}{\chi} \|\nabla(p^n - p^{n-1})\|^2 \leq \frac{1}{2} \|\sigma^n(\mathbf{u}^{n+1} - \mathbf{u}^n)\|^2. \end{aligned} \quad (3.30)$$

To deal with the right side of equation (3.30), we rewrite (3.4b) as

$$\rho^n(\mathbf{u}^n - \mathbf{u}^n) = -\delta t \phi^n \nabla w_\phi^{n+1}, \quad (3.31)$$

By taking inner product of (3.31) with $2\mathbf{u}^n$, we have,

$$\|\sigma^n\mathbf{u}^n\|^2 - \|\sigma^n\mathbf{u}^n\|^2 + \|\sigma^n(\mathbf{u}^n - \mathbf{u}^n)\|^2 = -2\delta t (\phi^n \nabla w_\phi^{n+1}, \mathbf{u}^n), \quad (3.32)$$

On the other hand, according to the triangle inequality, we get

$$\|\sigma^n(\mathbf{u}^n - \mathbf{u}^n)\|^2 + \|\sigma^n(\mathbf{u}^{n+1} - \mathbf{u}^n)\|^2 \geq \frac{1}{2} \|\sigma^n(\mathbf{u}^{n+1} - \mathbf{u}^n)\|^2, \quad (3.33)$$

Then, by adding equations (3.30) and (3.32), and using the inequality (3.33), we have

$$\begin{aligned} & \|\sigma^{n+1}\mathbf{u}^{n+1}\|^2 - \|\sigma^n\mathbf{u}^n\|^2 + \delta t \|\sqrt{\eta^n} D(\mathbf{u}^{n+1})\|^2 \\ & + \frac{\delta t^2}{\chi} (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) + \frac{\delta t^2}{\chi} \|\nabla(p^n - p^{n-1})\|^2 \\ & \leq -2\delta t (\phi^n \nabla w_\phi^{n+1}, \mathbf{u}^n). \end{aligned} \quad (3.34)$$

By taking the inner product of the first equation in (3.4a) with $2\delta w_\phi^{n+1}$, we have

$$2(\phi^{n+1} - \phi^n, w_\phi^{n+1}) + 2\delta t (\nabla \cdot (\mathbf{u}^n \phi^n), w_\phi^{n+1}) + 2M\delta t \|\nabla w_\phi^{n+1}\|^2 = 0, \quad (3.35)$$

Taking the inner product of the second equation in (3.4a) with $-2(\phi^{n+1} - \phi^n)$, we obtain

$$-2(\phi^{n+1} - \phi^n, w_\phi^{n+1}) + \lambda (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \|\nabla \phi^{n+1} - \nabla \phi^n\|^2) + 2\lambda (r^{n+1} b^n, \phi^{n+1} - \phi^n) = 0, \quad (3.36)$$

Taking the inner product of the third equation in (3.4a) with $4\lambda r^{n+1}$, we get

$$2\lambda (|r^{n+1}|^2 - |r^n|^2 + |r^{n+1} - r^n|^2) - 2\lambda (r^{n+1} b^n, \phi^{n+1} - \phi^n) = 0, \quad (3.37)$$

Summing up equations (3.35), (3.36) and (3.37), we derive that

$$\begin{aligned} & \lambda (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \|\nabla \phi^{n+1} - \nabla \phi^n\|^2) + 2\lambda (|r^{n+1}|^2 - |r^n|^2 + |r^{n+1} - r^n|^2) \\ & + 2M\delta t \|\nabla w_\phi^{n+1}\|^2 = 2\delta t (\mathbf{u}^n, \phi^n \nabla w_\phi^{n+1}). \end{aligned} \quad (3.38)$$

Combining (3.34) and (3.38), and dropping off some positive terms, we arrive at

$$\begin{aligned} & \frac{1}{2} \|\sigma^{n+1}\mathbf{u}^{n+1}\|^2 - \frac{1}{2} \|\sigma^n\mathbf{u}^n\|^2 + \frac{\delta t^2}{2\chi} (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) \\ & + \frac{\lambda}{2} (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2) + \lambda (|r^{n+1}|^2 - |r^n|^2) \\ & = -\frac{1}{2} \delta t \|\sqrt{\eta^n} D(\mathbf{u}^{n+1})\|^2 - M\delta t \|\nabla w_\phi^{n+1}\|^2 \leq 0, \end{aligned} \quad (3.39)$$

which implies the desired result. $\square$

4. Fully discrete scheme and energy stability analysis

4.1 Fully discrete scheme

In this section, we will use an efficient finite difference method on staggered grids to spatially discretize the above time marching schemes [33-35], and carry out energy estimates for the proposed fully discrete schemes. The case of nonmatching density is taken as an example, and the case of matched density can be similarly derived. For a two-dimensional case, the computational domain is $\Omega = (0, L_x) \times (0, L_y)$, and cell centers are located on

$$x_i = \left(i - \frac{1}{2}\right)h_x, \quad i = 1, \dots, n_x, \quad y_j = \left(j - \frac{1}{2}\right)h_y, \quad j = 1, \dots, n_y,$$

where h_x and h_y are grid spacings in x and y directions, and n_x and n_y are the number of grids along the x and y coordinates respectively. To discretize the scheme (3.4), the following finite difference spaces are introduced. Ghost cells are also included in these spaces:

$$\begin{aligned} U_h &= (x_{i-1/2}, y_j) \Big| i = 1, \dots, n_x + 1; \quad j = 0, \dots, n_y + 1, \\ V_h &= (x_i, y_{j-1/2}) \Big| i = 0, \dots, n_x + 1; \quad j = 1, \dots, n_y + 1, \\ P_h &= (x_i, y_j) \Big| i = 0, \dots, n_x + 1; \quad j = 0, \dots, n_y + 1, \\ N_h &= (x_{i-1/2}, y_{j-1/2}) \Big| i = 1, \dots, n_x + 1; \quad j = 1, \dots, n_y + 1, \end{aligned}$$

where P_h is the cell-centered space, U_h and V_h are edge-centered spaces. ϕ , w , p , ρ , and η belong to P_h , u belongs to U_h and v belongs to V_h . We define some differential and averaged operators to complete the spatial discretization, including (a) edge-to-cell difference operators

$$d_x: U_h \rightarrow P_h \text{ \& } N_h \rightarrow V_h \text{ and } d_y: V_h \rightarrow P_h \text{ \& } N_h \rightarrow U_h;$$

(b) center-to-edge difference operators

$$D_x: P_h \rightarrow U_h \text{ \& } V_h \rightarrow N_h \text{ and } D_y: P_h \rightarrow V_h \text{ \& } U_h \rightarrow N_h;$$

(c) center-to-edge averaged operators

$$A_x: P_h \rightarrow U_h, U_h \rightarrow P_h \text{ \& } V_h \rightarrow N_h \text{ and } A_y: P_h \rightarrow V_h, V_h \rightarrow P_h \text{ \& } U_h \rightarrow N_h.$$

Figure 1 Finite difference spaces P_h , U_h , V_h and N_h

With these operators, we can fully discretize the governing system (3.4). Only the two-dimensional scheme is presented here, and the three-dimensional case is presented in the Appendix A.

$$\phi^{n+1} - \phi^n + \delta t \left[d_x \left(u_*^{n+1} A_x \phi^n \right) + d_y \left(v_*^{n+1} A_y \phi^n \right) \right] - \delta t M \left[d_x \left(D_x w_\phi^{n+1} \right) + d_y \left(D_y w_\phi^{n+1} \right) \right] = 0. \quad (4.1a)$$

$$w_\phi^{n+1} = -\lambda d_x (D_x \phi^{n+1}) - \lambda d_y (D_y \phi^{n+1}) + \lambda r^{n+1} b^n. \quad (4.1b)$$

$$r^{n+1} - r^n = \frac{h_x h_y}{2} \sum b^n (\phi^{n+1} - \phi^n), \quad (4.1c)$$

where $b^n = F'(\phi^n) / \sqrt{h_x h_y \sum F(\phi^n)}$.

$$A_x \rho^n (u_*^n - u^n) = -\delta t A_x \phi^n D_x w_\phi^{n+1}, \quad A_y \rho^n (v_*^n - v^n) = -\delta t A_y \phi^n D_y w_\phi^{n+1}. \quad (4.1d)$$

$$\begin{aligned} & A_x \rho^n (u^{n+1} - u^n) - \delta t \left[2D_x (\eta d_x u^{n+1}) + d_y (A_y (A_x \eta^n) D_y u^{n+1}) + d_y (A_y (A_x \eta^n) D_x v^{n+1}) \right] \\ & + \delta t D_x (2p^n - p^{n-1}) + \delta t A_x \rho^n \left[u^n D_x (A_x u^{n+1}) + A_x (A_y v^n) d_y (A_y u^{n+1}) \right] + \delta t A_x \phi^n D_x w_\phi^{n+1} \\ & + \delta t \left[J_x^n D_x (A_x u^{n+1}) + A_x (A_y J_y^n) d_y (A_y u^{n+1}) \right] + \frac{1}{2} u^{n+1} (A_x \rho^{n+1} - A_x \rho^n) \\ & + \frac{1}{2} \delta t \left[D_x (A_x J_x^n) + d_y (A_x J_y^n) \right] u^{n+1} + \frac{1}{2} \delta t A_x \rho^n \left[D_x (A_x u^n) + d_y (A_x v^n) \right] u^{n+1} = 0. \end{aligned} \quad (4.1e)$$

$$\begin{aligned} & A_y \rho^n (v^{n+1} - v^n) - \delta t \left(d_x (A_x (A_y \eta^n) D_y u^{n+1}) + d_x (A_x (A_y \eta^n) D_x v^{n+1}) + 2D_y (\eta^n d_y v^{n+1}) \right) \\ & + \delta t D_y (2p^n - p^{n-1}) + \delta t A_y \rho^n \left(A_x (A_y u^n) d_x (A_x v^{n+1}) + v^n D_y (A_y v^{n+1}) \right) + \delta t A_y \phi^n D_y w_\phi^{n+1} \\ & + \delta t \left(A_y (A_x J_x^n) d_x (A_x v^{n+1}) + J_y^n D_y (A_y v^{n+1}) \right) + \frac{1}{2} v^{n+1} (A_y \rho^{n+1} - A_y \rho^n) \\ & + \frac{1}{2} \delta t \left(d_x (A_y J_x^n) + D_y (A_y J_y^n) \right) v^{n+1} + \frac{1}{2} \delta t A_y \rho^n \left(d_x (A_y u^n) + D_y (A_y v^n) \right) v^{n+1} = 0. \end{aligned} \quad (4.1f)$$

$$d_x (D_x (p^{n+1} - p^n)) + d_y (D_y (p^{n+1} - p^n)) = \frac{\chi}{\delta t} (d_x u^{n+1} + d_y v^{n+1}), \quad (4.1g)$$

where

$$\begin{aligned} \rho^{n+1} &= \frac{\rho_1 - \rho_2}{2} \hat{\phi}^{n+1} + \frac{\rho_1 + \rho_2}{2}, \quad \eta^{n+1} = \frac{\eta_1 - \eta_2}{2} \hat{\phi}^{n+1} + \frac{\eta_1 + \eta_2}{2}, \\ J_x^n &= \frac{(\rho_2 - \rho_1)}{2} M D_x w_\phi^n, \quad J_y^n = \frac{(\rho_2 - \rho_1)}{2} M D_y w_\phi^n, \end{aligned}$$

here J_x belongs to U_h , J_y belongs to V_h . To fully discrete boundary conditions, an operator $\mathbf{D} = (D_x, D_y)$ is introduced to simplify the presentation.

$$\begin{cases} \mathbf{D} \phi^{n+1} \cdot \mathbf{n} = 0, \quad \mathbf{D} w_\phi^{n+1} \cdot \mathbf{n} = 0, & \text{on } \Gamma, \\ u^{n+1} = 0, \quad v^{n+1} = 0, & \text{on } \Gamma, \\ \mathbf{D} p^{n+1} \cdot \mathbf{n} = 0, & \text{on } \Gamma. \end{cases} \quad (4.1h)$$

In the fully discrete scheme (4.1), the central difference method is used to discretize advection terms in the Cahn-Hilliard and Navier-Stokes equations. We know that the central difference method is inaccurate and unstable at the large Péclet number, where the advection dominates flow. Hence, in all our simulations, advection terms are discretized by a composite high resolution scheme. More precisely, the fluxes at cell faces are evaluated with a MINMOD scheme, which is a combination of the central difference, first-order and second-order upwind schemes. The MINMOD scheme not only achieves the second-order accuracy, but also preserves the physical properties of convection. A preconditioner CG method (BiCGSATB) is used to solve the above fully discrete scheme. For variable-coefficient equations, matrices for the corresponding

constant-coefficient systems are used as preconditioners.

4.2 Energy stability analysis

In the component form, cell-centered functions (e.g., $\phi \in P_h$) can be identified via $\phi_{i,j} = \phi(x_i, y_j)$. Edge-centered functions in the U_h space (e.g., $f \in U_h$) can be identified via $f_{i+1/2,j} = f(x_{i+1/2}, y_j)$. Edge-centered functions in the V_h space (e.g., $g \in V_h$) can be identified via $g_{i+1/2,j} = g(x_{i+1/2}, y_j)$. To simplify the proof of energy stability of the proposed schemes, we define the following weighted inner products [34, 36]:

$$\langle \phi, \varphi \rangle_{P_h} = \sum_{i=1}^{nx} \sum_{j=1}^{ny} \phi_{i,j} \varphi_{i,j}, \quad \phi, \varphi \in P_h, \quad (4.2)$$

$$\langle f, g \rangle_{U_h} = \frac{1}{2} \sum_{i=1}^{nx} \sum_{j=1}^{ny} (f_{i+1/2,j} g_{i+1/2,j} + f_{i-1/2,j} g_{i-1/2,j}), \quad f, g \in U_h, \quad (4.3)$$

$$\langle f, g \rangle_{V_h} = \frac{1}{2} \sum_{i=1}^{nx} \sum_{j=1}^{ny} (f_{i,j+1/2} g_{i,j+1/2} + f_{i,j-1/2} g_{i,j-1/2}), \quad f, g \in V_h. \quad (4.4)$$

For any cell-centered function ϕ in the space P_h , we define

$$\|\phi\|_2 = \sqrt{h_x h_y \langle \phi, \phi \rangle_{P_h}}.$$

$$\|\nabla \phi\|_2 = \sqrt{h_x h_y \langle D_x \phi, D_x \phi \rangle_{U_h} + h_x h_y \langle D_y \phi, D_y \phi \rangle_{V_h}}.$$

For the edge-centered cell velocity $\mathbf{u}$, we define

$$\|\mathbf{u}\|_2 = \sqrt{h_x h_y \langle u, u \rangle_{U_h} + h_x h_y \langle v, v \rangle_{V_h}},$$

where u belongs to U_h , and v belongs to V_h . The following summation-by-parts formulae are important to prove the energy stability of the fully discrete scheme [34, 36].

Lemma 4.1. If $\phi \in P_h$ and $f \in U_h$, then

$$h_x h_y \langle D_x \phi, f \rangle_{U_h} = -h_x h_y \langle \phi, d_x f \rangle_{P_h} - h_y \sum_{j=1}^{ny} A_x \phi_{1/2,j} f_{1/2,j} + h_y \sum_{j=1}^{ny} A_x \phi_{nx+1/2,j} f_{nx+1/2,j}, \quad (4.5)$$

If $\phi \in P_h$ and $f \in V_h$, then

$$h_x h_y \langle D_y \phi, f \rangle_{V_h} = -h_x h_y \langle \phi, d_y f \rangle_{P_h} - h_x \sum_{i=1}^{nx} A_y \phi_{i,1/2} f_{i,1/2} + h_x \sum_{i=1}^{nx} A_y \phi_{i,ny+1/2} f_{i,ny+1/2}, \quad (4.6)$$

If $f \in N_h$, and $g \in U_h$, then

$$\begin{aligned} h_x h_y \langle d_y f, g \rangle_{U_h} &= -h_x h_y \langle f, D_y g \rangle_{N_h} - h_x \sum_{i=1}^{nx+1} A_y g_{i-1/2,1/2} f_{i-1/2,1/2} \\ &\quad + h_x \sum_{i=1}^{nx+1} A_y g_{i-1/2,ny+1/2} f_{i-1/2,ny+1/2}, \end{aligned} \quad (4.7)$$

If $f \in N_h$ and $g \in V_h$, then

$$\begin{aligned} h_x h_y \langle d_x f, g \rangle_{V_h} &= -h_x h_y \langle f, D_x g \rangle_{N_h} - h_y \sum_{j=1}^{ny+1} A_x g_{1/2,j-1/2} f_{1/2,j-1/2} \\ &\quad + h_y \sum_{j=1}^{ny+1} A_x g_{nx+1/2,j-1/2} f_{nx+1/2,j-1/2}. \end{aligned} \quad (4.8)$$

Theorem 4.1. The fully discrete scheme (4.1) is unconditionally energy stable and satisfies the

following discrete energy law

$$E_{tot}^{n+1} - E_{tot}^n \leq -\frac{\delta t}{2} \left\| \sqrt{\eta^n} D(\mathbf{u}^{n+1}) \right\|_2^2 - \delta t M \left\| \nabla w_\phi^{n+1} \right\|_2^2, \quad (4.9)$$

where

$$\begin{cases} E^n = \frac{1}{2} \left\| \sigma^n \mathbf{u}^n \right\|_2^2 + \frac{\lambda}{2} \left\| \nabla \phi^n \right\|_2^2 + \lambda |r^n|^2 + \frac{\delta t^2}{2\chi} \left\| \nabla p^n \right\|_2^2, \\ r^n = \sqrt{h_x h_y} \langle F(\phi^n), 1 \rangle_{P_h}. \end{cases} \quad (4.10)$$

Proof. According to the appendix in [8], we have

$$\begin{aligned} & \delta t \langle A_x \rho^n (u^n D_x (A_x u^{n+1}) + A_x (A_y v^n) d_y (A_y u^{n+1})), u^{n+1} \rangle_{U_h} \\ & + \delta t \langle A_y \rho^n (A_x (A_y u^n) d_x (A_x v^{n+1}) + v^n D_y (A_y v^{n+1})), v^{n+1} \rangle_{V_h} \\ & + \frac{1}{2} \delta t \langle A_x \rho^n (D_x (\rho^n A_x u^n) + d_y (A_x v^n)) u^{n+1}, u^{n+1} \rangle_{U_h} \\ & + \frac{1}{2} \delta t \langle A_y \rho^n (d_x (A_y u^n) + D_y (A_y v^n)) v^{n+1}, v^{n+1} \rangle_{V_h} = 0, \end{aligned}$$

and

$$\begin{aligned} & \delta t \langle (J_x^n D_x (A_x u^{n+1}) + A_x (A_y J_y^n) d_y (A_y u^{n+1})), u^{n+1} \rangle_{U_h} \\ & + \delta t \langle (A_y (A_x J_x^n) d_x (A_x v^{n+1}) + J_y^n D_y (A_y v^{n+1})), v^{n+1} \rangle_{V_h} \\ & + \frac{1}{2} \delta t \langle (D_x (A_x J_x^n) + d_y (A_x J_y^n)), u^{n+1} \rangle_{U_h} + \frac{1}{2} \delta t \langle (d_x (A_y J_x^n) + D_y (A_y J_y^n)), v^{n+1} \rangle_{V_h} = 0. \end{aligned}$$

According to the equation (4.1d), we have,

$$\begin{cases} A_x \rho^n (u^{n+1} - u^n) + \delta t A_x \phi^n D_x w_\phi^n = A_x \rho^n (u^{n+1} - u_*^n), \\ A_y \rho^n (v^{n+1} - v^n) + \delta t A_y \phi^n D_y w_\phi^n = A_y \rho^n (v^{n+1} - v_*^n). \end{cases} \quad (4.11)$$

Taking the discrete inner-product of (4.1e) and (4.1f) with $2u^{n+1}$ and $2v^{n+1}$ respectively, and using Lemma 4.1, Lemma 4.2 and (4.11), we can derive

$$\begin{aligned} & \langle \sigma_x^n u^{n+1}, \sigma_x^n u^{n+1} \rangle_{U_h} - \langle \sigma_x^n u_*^n, \sigma_x^n u_*^n \rangle_{U_h} + \langle \sigma_x^n (u^{n+1} - u_*^n), \sigma_x^n (u^{n+1} - u_*^n) \rangle_{U_h} \\ & + \langle \sigma_y^n v^{n+1}, \sigma_y^n v^{n+1} \rangle_{V_h} - \langle \sigma_y^n v_*^n, \sigma_y^n v_*^n \rangle_{V_h} + \langle \sigma_y^n (v^{n+1} - v_*^n), \sigma_y^n (v^{n+1} - v_*^n) \rangle_{V_h} \\ & + \langle \sigma_x^{n+1} u^{n+1}, \sigma_x^{n+1} u^{n+1} \rangle_{U_h} - \langle \sigma_x^n u^{n+1}, \sigma_x^n u^{n+1} \rangle_{U_h} + \langle \sigma_y^{n+1} v^{n+1}, \sigma_y^{n+1} v^{n+1} \rangle_{V_h} \\ & - \langle \sigma_y^n v^{n+1}, \sigma_y^n v^{n+1} \rangle_{V_h} + 2\delta t \langle p^{n+1} - 2p^n + p^{n-1}, d_x u^{n+1} \rangle_{P_h} - 2\delta t \langle p^{n+1}, d_x u^{n+1} \rangle_{P_h} \\ & + 2\delta t \langle p^{n+1} - 2p^n + p^{n-1}, d_y v^{n+1} \rangle_{P_h} - 2\delta t \langle p^{n+1}, d_y v^{n+1} \rangle_{P_h} \\ & + 2\delta t \langle \sqrt{\eta^n} d_x u^{n+1}, \sqrt{\eta^n} d_x u^{n+1} \rangle_{P_h} + 2\delta t \langle \sqrt{A_y (A_x \eta^n)} D_y u^{n+1}, \sqrt{A_y (A_x \eta^n)} D_y u^{n+1} \rangle_{N_h} \\ & + 2\delta t \langle \sqrt{A_x (A_y \eta^n)} D_x v^{n+1}, \sqrt{A_x (A_y \eta^n)} D_x v^{n+1} \rangle_{N_h} + 2\delta t \langle \sqrt{\eta^n} d_y v^{n+1}, \sqrt{\eta^n} d_y v^{n+1} \rangle_{P_h} = 0, \end{aligned} \quad (4.12)$$

where $\sigma_x^n = \sqrt{A_x \rho^n}$ and $\sigma_y^n = \sqrt{A_y \rho^n}$.

Taking the discrete inner-product of (4.1g) with $2\delta t^2(p^{n+1} - 2p^n + p^{n-1})/\chi$, we get

$$\begin{aligned}
 & \langle d_x(p^{n+1} - p^n), \frac{2\delta t^2}{\chi}(p^{n+1} - 2p^n + p^{n-1}) \rangle_{P_h} \\
 & + \langle d_y(p^{n+1} - p^n), \frac{2\delta t^2}{\chi}(p^{n+1} - 2p^n + p^{n-1}) \rangle_{P_h} \\
 & = -\delta t^2/\chi (\langle D_x(p^{n+1} - p^n), D_x(p^{n+1} - p^n) \rangle_{U_h} - \langle D_x(p^n - p^{n-1}), D_x(p^n - p^{n-1}) \rangle_{U_h} \\
 & \quad + \langle D_x(p^{n+1} - 2p^n + p^{n-1}), D_x(p^{n+1} - 2p^n + p^{n-1}) \rangle_{U_h}) \\
 & \quad - \delta t^2/\chi (\langle D_y(p^{n+1} - p^n), D_y(p^{n+1} - p^n) \rangle_{V_h} - \langle D_y(p^n - p^{n-1}), D_y(p^n - p^{n-1}) \rangle_{V_h} \\
 & \quad + \langle D_y(p^{n+1} - 2p^n + p^{n-1}), D_y(p^{n+1} - 2p^n + p^{n-1}) \rangle_{V_h}) \\
 & = 2\delta t \langle p^{n+1} - 2p^n + p^{n-1}, d_x u^{n+1} \rangle_{P_h} + 2\delta t \langle p^{n+1} - 2p^n + p^{n-1}, d_y v^{n+1} \rangle_{P_h}.
 \end{aligned} \tag{4.13}$$

Taking the discrete inner-product of (4.1g) with $-2\delta t^2 p^{n+1}/\chi$, we have

$$\begin{aligned}
 & \delta t^2/\chi (\langle D_x p^{n+1}, D_x p^{n+1} \rangle_{U_h} - \langle D_x p^n, D_x p^n \rangle_{U_h} + \langle D_x(p^{n+1} - p^n), D_x(p^{n+1} - p^n) \rangle_{U_h}) \\
 & + \delta t^2/\chi (\langle D_y p^{n+1}, D_y p^{n+1} \rangle_{V_h} - \langle D_y p^n, D_y p^n \rangle_{V_h} + \langle D_y(p^{n+1} - p^n), D_y(p^{n+1} - p^n) \rangle_{V_h}) \\
 & = -2\delta t \langle p^{n+1}, d_x u^{n+1} \rangle_{P_h} - 2\delta t \langle p^{n+1}, d_y v^{n+1} \rangle_{P_h},
 \end{aligned} \tag{4.14}$$

Now summing up equations (4.13) and (4.14), we obtain

$$\begin{aligned}
 & \delta t^2/\chi (\langle D_x(p^n - p^{n-1}), D_x(p^n - p^{n-1}) \rangle_{U_h} + \langle D_y(p^n - p^{n-1}), D_y(p^n - p^{n-1}) \rangle_{V_h}) \\
 & + \delta t^2/\chi (\langle D_x p^{n+1}, D_x p^{n+1} \rangle_{U_h} - \langle D_x p^n, D_x p^n \rangle_{U_h} + \langle D_y p^{n+1}, D_y p^{n+1} \rangle_{V_h} - \langle D_y p^n, D_y p^n \rangle_{V_h}) \\
 & = \delta t^2/\chi \langle D_x(p^{n+1} - 2p^n + p^{n-1}), D_x(p^{n+1} - 2p^n + p^{n-1}) \rangle_{U_h} \\
 & \quad + \delta t^2/\chi \langle D_y(p^{n+1} - 2p^n + p^{n-1}), D_y(p^{n+1} - 2p^n + p^{n-1}) \rangle_{V_h} \\
 & \quad + 2\delta t \langle p^{n+1} - 2p^n + p^{n-1}, d_x u^{n+1} \rangle_{P_h} + 2\delta t \langle p^{n+1} - 2p^n + p^{n-1}, d_y v^{n+1} \rangle_{P_h} \\
 & \quad - 2\delta t \langle p^{n+1}, d_x u^{n+1} \rangle_{P_h} - 2\delta t \langle p^{n+1}, d_y v^{n+1} \rangle_{P_h}.
 \end{aligned} \tag{4.15}$$

Next, we take the difference of (4.1g) at the time step t^{n+1} and t^n to derive

$$\begin{aligned}
 & \delta t^2/\chi \langle D_x(p^{n+1} - 2p^n + p^{n-1}), D_x(p^{n+1} - 2p^n + p^{n-1}) \rangle_{U_h} \\
 & + \delta t^2/\chi \langle D_y(p^{n+1} - 2p^n + p^{n-1}), D_y(p^{n+1} - 2p^n + p^{n-1}) \rangle_{V_h} \\
 & \leq \chi \langle u^{n+1} - u^n, u^{n+1} - u^n \rangle_{U_h} + \chi \langle v^{n+1} - v^n, v^{n+1} - v^n \rangle_{U_h} \\
 & \leq 1/2 \langle \sigma_x^n(u^{n+1} - u^n), \sigma_x^n(u^{n+1} - u^n) \rangle_{U_h} + \frac{1}{2} \langle \sigma_y^n(u^{n+1} - u^n), \sigma_y^n(u^{n+1} - u^n) \rangle_{V_h}.
 \end{aligned} \tag{4.16}$$

Combining the equations (4.12), (4.15) and (4.16), we get

$$\begin{aligned}
 & \langle \sigma_x^{n+1} u^{n+1}, \sigma_x^{n+1} u^{n+1} \rangle_{U_h} - \langle \sigma_x^n u^n, \sigma_x^n u^n \rangle_{U_h} + \langle \sigma_x^n(u^{n+1} - u^n), \sigma_x^n(u^{n+1} - u^n) \rangle_{U_h} \\
 & + \langle \sigma_y^{n+1} v^{n+1}, \sigma_y^{n+1} v^{n+1} \rangle_{V_h} - \langle \sigma_y^n v^n, \sigma_y^n v^n \rangle_{V_h} + \langle \sigma_y^n(v^{n+1} - v^n), \sigma_y^n(v^{n+1} - v^n) \rangle_{V_h} \\
 & + \delta t^2/\chi (\langle D_x p^{n+1}, D_x p^{n+1} \rangle_{U_h} - \langle D_x p^n, D_x p^n \rangle_{U_h} + \langle D_y p^{n+1}, D_y p^{n+1} \rangle_{V_h} - \langle D_y p^n, D_y p^n \rangle_{V_h}) \\
 & + \delta t^2/\chi (\langle D_x(p^n - p^{n-1}), D_x(p^n - p^{n-1}) \rangle_{U_h} + \langle D_y(p^n - p^{n-1}), D_y(p^n - p^{n-1}) \rangle_{V_h}) \\
 & + 2\delta t \langle \sqrt{\eta^n} d_x u^{n+1}, \sqrt{\eta^n} d_x u^{n+1} \rangle_{P_h} + 2\delta t \langle \sqrt{A_y(A_x \eta^n)} D_y u^{n+1}, \sqrt{A_y(A_x \eta^n)} D_y u^{n+1} \rangle_{N_h} \\
 & + 2\delta t \langle \sqrt{A_x(A_y \eta^n)} D_x v^{n+1}, \sqrt{A_x(A_y \eta^n)} D_x v^{n+1} \rangle_{N_h} + 2\delta t \langle \sqrt{\eta^n} d_y v^{n+1}, \sqrt{\eta^n} d_y v^{n+1} \rangle_{P_h} \\
 & \leq 1/2 \langle \sigma_x^n(u^{n+1} - u^n), \sigma_x^n(u^{n+1} - u^n) \rangle_{U_h} + \frac{1}{2} \langle \sigma_y^n(u^{n+1} - u^n), \sigma_y^n(u^{n+1} - u^n) \rangle_{V_h}.
 \end{aligned} \tag{4.17}$$

By taking discrete inner-product of (4.1d) with $2u_*^n$ and $2v_*^n$, respectively, we have

$$\begin{aligned}
 & \langle \sigma_x^n u_*^n, \sigma_x^n u_*^n \rangle_{U_h} - \langle \sigma_x^n u^n, \sigma_x^n u^n \rangle_{U_h} + \langle \sigma_x^n (u_*^n - u^n), \sigma_x^n (u_*^n - u^n) \rangle_{U_h} \\
 & + \langle \sigma_y^n v_*^n, \sigma_y^n v_*^n \rangle_{V_h} - \langle \sigma_y^n v^n, \sigma_y^n v^n \rangle_{V_h} + \langle \sigma_y^n (v_*^n - v^n), \sigma_y^n (v_*^n - v^n) \rangle_{V_h} \\
 & = -2\delta t \langle A_x \phi^n D_x w_\phi^{n+1}, u_*^n \rangle_{U_h} - 2\delta t \langle A_y \phi^n D_y w_\phi^{n+1}, v_*^n \rangle_{V_h},
 \end{aligned} \tag{4.18}$$

On the other hand, according to the triangle inequality, we can easily derive

$$\begin{aligned}
 & \langle \sigma_x^n (u_*^n - u^n), \sigma_x^n (u_*^n - u^n) \rangle_{U_h} + \langle \sigma_y^n (v_*^n - v^n), \sigma_y^n (v_*^n - v^n) \rangle_{V_h} \\
 & + \langle \sigma_x^n (u^{n+1} - u_*^n), \sigma_x^n (u^{n+1} - u_*^n) \rangle_{U_h} + \langle \sigma_y^n (v^{n+1} - v_*^n), \sigma_y^n (v^{n+1} - v_*^n) \rangle_{V_h} \\
 & \geq \frac{1}{2} \langle \sigma_x^n (u^{n+1} - u^n), \sigma_x^n (u^{n+1} - u^n) \rangle_{U_h} + \frac{1}{2} \langle \sigma_y^n (v^{n+1} - v^n), \sigma_y^n (v^{n+1} - v^n) \rangle_{V_h},
 \end{aligned} \tag{4.19}$$

By adding equations (4.17) and (4.18), and using the inequality (4.19), we get

$$\begin{aligned}
 & \langle \sigma_x^{n+1} u^{n+1}, \sigma_x^{n+1} u^{n+1} \rangle_{U_h} - \langle \sigma_x^n u^n, \sigma_x^n u^n \rangle_{U_h} + \langle \sigma_y^{n+1} v^{n+1}, \sigma_y^{n+1} v^{n+1} \rangle_{V_h} - \langle \sigma_y^n v^n, \sigma_y^n v^n \rangle_{V_h} \\
 & + \delta t^2 / \chi \left(\langle D_x p^{n+1}, D_x p^{n+1} \rangle_{U_h} - \langle D_x p^n, D_x p^n \rangle_{U_h} + \langle D_y p^{n+1}, D_y p^{n+1} \rangle_{V_h} - \langle D_y p^n, D_y p^n \rangle_{V_h} \right) \\
 & + \delta t^2 / \chi \left(\langle D_x (p^n - p^{n-1}), D_x (p^n - p^{n-1}) \rangle_{U_h} + \langle D_y (p^n - p^{n-1}), D_y (p^n - p^{n-1}) \rangle_{V_h} \right) \\
 & + 2\delta t \langle \sqrt{\eta^n} d_x u^{n+1}, \sqrt{\eta^n} d_x u^{n+1} \rangle_{P_h} + 2\delta t \langle \sqrt{A_y (A_x \eta^n)} D_y u^{n+1}, \sqrt{A_y (A_x \eta^n)} D_y u^{n+1} \rangle_{N_h} \\
 & + 2\delta t \langle \sqrt{A_x (A_y \eta^n)} D_x v^{n+1}, \sqrt{A_x (A_y \eta^n)} D_x v^{n+1} \rangle_{N_h} + 2\delta t \langle \sqrt{\eta^n} d_y v^{n+1}, \sqrt{\eta^n} d_y v^{n+1} \rangle_{P_h} \\
 & \leq -2\delta t \langle A_x \phi^n D_x w_\phi^{n+1}, u_*^n \rangle_{U_h} - 2\delta t \langle A_y \phi^n D_y w_\phi^{n+1}, v_*^n \rangle_{V_h}.
 \end{aligned} \tag{4.20}$$

Taking the discrete inner-product of (4.1a) with $2w_\phi^{n+1}$, we have

$$\begin{aligned}
 & 2\langle \phi^{n+1} - \phi^n, w_\phi^{n+1} \rangle_{P_h} - 2\delta t \langle A_x \phi^n u_*^n, D_x w_\phi^{n+1} \rangle_{U_h} - 2\delta t \langle A_y \phi^n v_*^n, D_y w_\phi^{n+1} \rangle_{V_h} \\
 & + 2M\delta t \langle D_x w_\phi^{n+1}, D_x w_\phi^{n+1} \rangle_{U_h} + 2M\delta t \langle D_y w_\phi^{n+1}, D_y w_\phi^{n+1} \rangle_{V_h} = 0.
 \end{aligned} \tag{4.21}$$

Taking the discrete inner-product of (4.1b) with $-2(\phi^{n+1} - \phi^n)$, we can derive

$$\begin{aligned}
 & -2\langle \phi^{n+1} - \phi^n, w_\phi^{n+1} \rangle_{P_h} + \lambda \left(\langle D_x \phi^{n+1}, D_x \phi^{n+1} \rangle_{U_h} - \langle D_x \phi^n, D_x \phi^n \rangle_{U_h} \right. \\
 & + \langle D_x (\phi^{n+1} - \phi^n), D_x (\phi^{n+1} - \phi^n) \rangle_{U_h} \left. + \lambda \left(\langle D_y \phi^{n+1}, D_y \phi^{n+1} \rangle_{V_h} - \langle D_y \phi^n, D_y \phi^n \rangle_{V_h} \right. \right. \\
 & \left. + \langle D_y (\phi^{n+1} - \phi^n), D_y (\phi^{n+1} - \phi^n) \rangle_{V_h} \right) + 2\lambda \langle r^{n+1} b^n, \phi^{n+1} - \phi^n \rangle_{P_h} = 0.
 \end{aligned} \tag{4.22}$$

Taking the discrete inner-product of (4.1c) with $4\lambda r^{n+1}$, we get

$$2\lambda / h_x h_y \left(|r^{n+1}|^2 - |r^n|^2 + |r^{n+1} - r^n|^2 \right) - 2\lambda \langle r^{n+1} b^n, \phi^{n+1} - \phi^n \rangle_{P_h} = 0. \tag{4.23}$$

Summing up equations (4.21), (4.22) and (4.23), we obtain

$$\begin{aligned}
 & \lambda \left(\langle D_x \phi^{n+1}, D_x \phi^{n+1} \rangle_{U_h} - \langle D_x \phi^n, D_x \phi^n \rangle_{U_h} + \langle D_x (\phi^{n+1} - \phi^n), D_x (\phi^{n+1} - \phi^n) \rangle_{U_h} \right) \\
 & + \lambda \left(\langle D_y \phi^{n+1}, D_y \phi^{n+1} \rangle_{V_h} - \langle D_y \phi^n, D_y \phi^n \rangle_{V_h} + \langle D_y (\phi^{n+1} - \phi^n), D_y (\phi^{n+1} - \phi^n) \rangle_{V_h} \right) \\
 & + 2\lambda / h_x h_y \left(|r^{n+1}|^2 - |r^n|^2 + |r^{n+1} - r^n|^2 \right) \\
 & + 2\delta t M \langle D_x w_\phi^{n+1}, D_x w_\phi^{n+1} \rangle_{U_h} + 2\delta t M \langle D_y w_\phi^{n+1}, D_y w_\phi^{n+1} \rangle_{V_h} \\
 & = 2\delta t \langle A_x \phi^n u_*^n, D_x w_\phi^{n+1} \rangle_{U_h} + 2\delta t \langle A_y \phi^n v_*^n, D_y w_\phi^{n+1} \rangle_{V_h}.
 \end{aligned} \tag{4.24}$$

Multiplying (4.20) and (4.24) with $h_x h_y / 2$, respectively, and summing up them together, we have

$$\begin{aligned} & \frac{1}{2} \|\sigma^{n+1} \mathbf{u}^{n+1}\|_2^2 - \frac{1}{2} \|\sigma^n \mathbf{u}^n\|_2^2 + \frac{\delta t^2}{2\chi} \left(\|\nabla p^{n+1}\|_2^2 - \|\nabla p^n\|_2^2 \right) + \frac{\lambda}{2} \left(\|\nabla \phi^{n+1}\|_2^2 - \|\nabla \phi^n\|_2^2 \right) \\ & + \lambda \left(|r^{n+1}|^2 - |r^n|^2 \right) = -M \delta t \|\nabla w_\phi^{n+1}\|_2^2 - \frac{\delta t}{2} \|\sqrt{\eta^n} D(\mathbf{u}^{n+1})\|_2^2 \leq 0, \end{aligned} \quad (4.25)$$

which implies the desired result. $\square$

5 Numerical Results

In this section, we conduct a series of numerical experiments to validate accuracy, efficiency and energy stability of the proposed schemes.

5.1. Bubble rising dynamics

5.1.1 Convergence and accuracy tests

To test the convergence and accuracy of the proposed numerical scheme, we simulate a lighter bubble rising process [37, 38] in a rectangular domain $\Omega = [0, 1] \times [0, 2]$. The initial profile of ϕ is set as

$$\phi(x, y) = -\tanh\left(\frac{1}{\sqrt{2}\varepsilon} \left(\sqrt{(x-x_0)^2 + (y-y_0)^2} - R\right)\right), \quad (5.1)$$

where (x_0, y_0) is the initial position of bubble center and R is the initial radius of bubble. If not explicit specified, the model parameters with default values are given below

$$\begin{aligned} \rho_1 &= 100, \quad \rho_2 = 1000, \quad \eta_1 = 1, \quad \eta_2 = 10, \quad M = 1 \times 10^{-5}, \quad \varepsilon = 0.01, \\ \lambda &= 0.26, \quad \gamma = 500, \quad x_0 = 0.5, \quad y_0 = 0.5, \quad R = 0.25. \end{aligned}$$

To test the convergence of time step-size δt , we used a spatial resolution $n_x = 250$ and $n_y = 500$ to reduce the error related to the spatial discretization. Because of the absence of the exact solution, the solution obtained with a small time step-size $\delta t = 2.5 \times 10^{-6}$ s selected as the reference solution. Various time step-sizes $\delta t = 4 \times 10^{-4}$, 2×10^{-4} , 1×10^{-4} and 5×10^{-5} are used to calculate the L^2 -norm error and convergence order for the phase-field variable ϕ , the velocity v and the pressure p at $t = 1$. It can be observed in Table 1 that the proposed numerical scheme can achieve the first-order accuracy in time.

Table 1. The L^2 norm error and convergence order for the phase-field variable ϕ , the velocity v and the pressure p at $t = 1$ with different temporal resolutions.

δt	Error(ϕ)	Order	Error(v)	Order	Error(p)	Order
4×10^{-4}	2.65×10^{-2}	-	8.23×10^{-2}	-	4.32×10^{-3}	-
2×10^{-4}	1.07×10^{-2}	1.31	2.97×10^{-3}	1.47	1.37×10^{-3}	1.66
1×10^{-4}	4.94×10^{-3}	1.12	1.15×10^{-3}	1.36	5.97×10^{-4}	1.19
5×10^{-5}	2.15×10^{-3}	1.18	4.65×10^{-4}	1.30	2.15×10^{-4}	1.47

We further perform the spatial convergence test with the ratio of n_x and n_y being 1:2. A series of $n_x = 100, 200, 300$ and 400 are selected and the solution at $n_x = 500$ is used as the exact solution. To decrease the error introduced by the time step-size, a small time step-size $\delta t = 0.1 h_{\min}$ is used in each simulation, where $h_{\min}$ is the minimum spatial step-size. The L^2 norm error for the phase-field variable, the velocity and the pressure at $t = 3$ is calculated. The system at $t = 3$ is close to a steady state, so the error related to the temporal discretization can be neglected. We can conclude from Figure 2 that the proposed scheme can achieve the desired accuracy in space.

Figure 2 The L^2 norm error for the phase-field variable ϕ , the velocity v and the pressure p at $t=3$ with different spatial resolutions

To quantitatively validate the proposed numerical scheme, two benchmark quantities: the center of mass and rising velocity are defined and measured during simulations[37, 38].

$$y_c = \int_{\phi \geq 0} y \rho d\Omega \bigg/ \int_{\phi \geq 0} \rho d\Omega, \quad V_c = \int_{\phi \geq 0} y d\Omega \bigg/ \int_{\phi \geq 0} 1 d\Omega \quad (5.2)$$

where y_c is the center of mass and V_c is the rising velocity. The spatial resolution for the validation simulation is $n_x=250$, $n_y=500$, and the time step-size is set as $\delta t = 0.1 h_{\min}$. We run each simulation until $t=3$. Figure 3 gives the shape of bubbles at $t=3$ with three different interface thicknesses and Figure 4 presents the evolutions of center of mass and mean rising velocity during the bubble rising process. Reference solutions obtained by a sharp interface method are also provided. Comparisons between simulated results and reference solutions indicate the accuracy of the proposed scheme.

Figure 3 Shape of bubbles (contour of $\phi=0$) at $t=3$ with three different interface thicknesses. $n_x=250$, $n_y=500$, $M=1$

$\times 10^{-5}$ and $\delta t = 1 \times 10^{-4}$.

Figure 4 Evolutions of center of mass and rising velocity of bubble with three different interface thicknesses. (a) center of mass; (b) rising velocity. $n_x=250$, $n_y=500$, $M=1 \times 10^{-5}$ and $\delta t=1 \times 10^{-4}$.

5.12 Comparisons of numerical schemes

Similar to the SAV approach, we can also construct decoupled, unconditionally energy stable schemes, based on the stabilization approach (cf. [15]) and IEQ approach (cf. Appendix B), for the hydrodynamics coupled phase-field model. In Figure 5, the bubble rising case is used to compare three approaches.

Figure 5 Shape of bubbles (contour of $\phi=0$) obtained by three different schemes. $n_x=250$, $n_y=500$, $M=1 \times 10^{-5}$, $\delta t=3 \times 10^{-4}$ and $\epsilon=0.01$

We can see obvious differences between results obtained by three schemes in Figure 5, especially when the rise velocity is large (at around $t = 1.5$). The differences almost disappear when the shape of bubble reach the steady state.

Figure 6 (a) Shape of bubbles (contour of $\phi=0$) at $t = 1.5$ and (b) mean rise velocities from $t = 0.35$ to 1.35 obtained by three different schemes. $n_x=250$, $n_y=500$, $M=1\times 10^{-5}$, $\delta t=3\times 10^{-4}$ and $\varepsilon=0.01$

Figure 6(a) is the partial enlargement of Figure 5(d), and Figure 6(b) gives the rising velocities obtained by three different approaches from $t = 0.35$ to 1.35 . It can be observed that the bubble contour obtained by the SAV approach has the largest deformation and rising velocity. To further compare the accuracy of the three approaches, we implement the IEQ and stabilization approaches with $\delta t=1\times 10^{-4}$ to simulate the bubble rising process, respectively, and the results are shown in Figure 7 and Figure 8.

Figure 7 (a) Shape of bubbles (contour of $\phi=0$) at $t = 1.5$ and (b) rising velocities from $t = 0.35$ to 1.35 obtained by the IEQ ($\delta t=1\times 10^{-4}$ and 3×10^{-4}) and SAV approaches ($\delta t=3\times 10^{-4}$). $n_x=250$, $n_y=500$, $M=1\times 10^{-5}$, and $\varepsilon=0.01$.

The results obtained by the IEQ approach with $\delta t=1\times 10^{-4}$ are consistent with those obtained by the SAV approach with $\delta t=3\times 10^{-4}$, as shown in Figure 7. This indicates that the SAV approach can be more accurate than the IEQ approach, possibly due to the fact that the SAV approach is directly related to the energy functional, not the energy density as in the IEQ approach. Similarly, it can also be concluded from Figure 8 that the SAV approach is more accurate than the stabilization approach. The introduction of stabilization term in the stabilization approach may result in the deviation from exact solutions. If the results obtained by the SAV approach with $\delta t=3\times 10^{-4}$ is used as the reference solutions, we can further derive that the IEQ approach is more

accurate than the stabilization approach form Figure 6.

Figure 8 (a) Shape of bubbles (contour of $\phi=0$) at $t = 1.5$ and (b) rising velocities from $t = 0.35$ to 1.35 obtained by the stabilization ($\delta t = 1 \times 10^{-4}$ and 3×10^{-4}) and SAV approaches ($\delta t = 3 \times 10^{-4}$). $n_x=250$, $n_y=500$, $M=1 \times 10^{-5}$, and $\varepsilon=0.01$.

5.13 Parameters analysis

The bubble rising process is affected by various parameters, such as the bubble size and viscosity ratio. A series of simulations are conducted to quantify the effect of these parameters.

(1) The effect of bubble size

Three different bubble sizes ($r=0.2$, 0.25 and 0.3) are selected to investigate the effect of bubble size, and each simulation runs until $t = 6$. Figure 9 gives the shape of bubbles at $t = 6$.

Figure 9 Shape of bubbles at $t=6$. (a) $r=0.2$; (b) $r=0.25$; (c) $r=0.3$.

Figure 10 Center of mass and rise velocity of bubbles. (a) center of mass; (b) rising velocity.

Figure 10(a) demonstrates that the smaller bubble rises faster. Mean rising velocity of the

small bubble ($r=0.2$) and the medium bubble ($r=0.25$) show similar trend in Figure 10(b). The velocity rises significantly at the initial stage and then drops slowly to a constant value, and the shape of bubble will temporarily reach a steady state when the rise velocity keeps constant. The rise velocity of bubble sees an obvious drop when it almost reaches the top wall. The shape of big bubble ($r=0.3$) varies with the rise velocity. At around $t=2$, the velocity decreases to a local minimum value and the deformation of bubble bottom almost reaches the maximum. Then, the deformation of bottom has been decreasing until the velocity rises to a crest (at around $t=3$). After that, the deformation increases with the decrease in rise velocity.

Figure 11. Evolutions of kinetic energy E_k and mixing energy of interface E_f .

Figure 11 shows evolutions of kinetic energy and mixing energy of interface. The kinetic energy and mixing energy of small bubble have been rising, which comes from part of the reduced gravity potential energy, until the bubble moves near the top wall. The small bubble is closer to the top wall than another two bubbles at $t = 6$ in Figure 9. The closer to the top wall, the greater the deformation of the bubble, which explains the obvious increment in mixing energy of small bubble at the later stage. The mixing energy of big bubble varies with the rising velocity. The large deformation of big bubble increases the interface length, and results in the increase of free energy. The kinetic energy shows the similar behavior with the rise velocity when bubble moves near the top wall.

(2) Viscosity ratio

We consider three different viscosity ratios ($\eta_1/\eta_2=1:10$, $1:1$ and $10:1$) in simulations, and run each simulation until $t=6$. Figure 12 gives the shape of bubbles at $t=6$.

Figure 12 Shape of bubbles at $t=6$. (a) $\eta_1/\eta_2=1:10$; (b) $\eta_1/\eta_2=1:1$; (c) $\eta_1/\eta_2=10:1$.

Figure 13 Center of mass and rising velocity of bubbles. (a) center of mass; (b) rising velocity.

It can be observed that the viscosity ratio has limited effect on the center of mass in Figure 13(a). The rising velocity of bubbles shows different behaviors under various viscosity ratios in Figure 13(b). Four important times are marked with red dotted lines on the velocity curve of the medium viscosity ratio ($\eta_1/\eta_2=1:1$), and the corresponding shape of bubbles are given. Two stages are divided by the four dotted lines, namely $t = 2.3 \sim 3$ and $t = 4.3 \sim 5.2$. The evolutions of bubble shape at the two stages are similar, and the deformation of bubble is determined by the rise velocity.

Figure 14 Evolutions of kinetic energy E_k and mixing energy of interface E_f .

Figure 14 gives the evolutions of kinetic energy and mixing energy of interface. The kinetic energies of small viscosity ratio ($\eta_1/\eta_2=1:10$) and medium viscosity ratio rise dramatically during the whole process.

5.14 3D bubble rising dynamics

We further extend the research of bubble rising dynamics to a three-dimensional domain $\Omega = [0, 1] \times [0, 1] \times [0, 2]$. The spatial resolution for the simulation is $n_x=90$, $n_y=90$ and $n_z=180$, and the time step is set as $\delta t = 0.001$. We run the simulation until $t = 3$. Figure 15 gives the 3D bubble rising dynamics. Obvious differences between 2D and 3D results can be observed in Figure 16.

Figure 15 3D bubble rising dynamics (contour of $\phi=0$). $n_x=90$, $n_y=90$, $n_z=180$, $M=1 \times 10^{-5}$, $t=1 \times 10^{-3}$ and $\varepsilon=0.013$.

Figure 16 Center of mass and rising velocity of bubbles. (a) center of mass; (b) rising velocity.

5.2. Coarsening Dynamics

To demonstrate the unconditional stability of the proposed numerical scheme, we start with a random phase-field variable in a two-dimensional domain $\Omega = [0, 1] \times [0, 1]$ to simulate the coarsening dynamics in the presence of flow. The parameters used in simulations are listed as follows,

$$\lambda = 0.01, \quad M = 1 \times 10^{-5}, \quad \varepsilon = 0.01, \quad \rho = 1, \quad \eta = 1, \quad n_x = 100, \quad n_y = 100, \quad \delta t = 1 \times 10^{-4}$$

Figure 17 Characteristic evolutions of phase-field variable at different times. (a) stabilization approach; (b) IEQ approach; (c) SAV approach

Figure 18 Evolutions of energy curves at different time step-sizes. (a) $\delta t = 1 \times 10^{-4}$; (b) $\delta t = 1 \times 10^{-3}$.

The results obtained by three approaches are shown in Figure 17 and Figure 18(a) with $\delta t = 1 \times 10^{-4}$, no visible difference is observed. With $\delta t = 1 \times 10^{-3}$, the original energy based on the SAV approach decreases faster than the other approaches, as shown in Figure 18(b).

Further, we extend the simulation to a 3D domain $\Omega = [0, 1] \times [0, 1] \times [0, 1]$, The parameters used in the simulation are listed as follows,

$$\lambda = 0.1, \quad M = 5 \times 10^{-5}, \quad \varepsilon = 0.012, \quad \rho = 1, \quad \eta = 1, \quad n_x = 100, \quad n_y = 100, \quad n_z = 100$$

Characteristic evolutions of phase-field variable at different times are presented in Figure 19. The energy decay cure of the whole system in Figure 20 demonstrates the unconditional energy stability of the proposed scheme.

Figure 19 Characteristic evolutions of phase-field variable (contour of $\phi=0$) at different times

Figure 20 Evolution of the total energy E_{tot} .

Conclusion remarks

In this work, we construct an efficient, totally decoupled and energy stable scheme for the Cahn-Hilliard phase field model of two-phase incompressible flows. A scalar auxiliary variable (SAV) approach is implemented to solve the Cahn-Hilliard equation while a splitting method based on pressure stabilization is used to solve the Navier-Stokes equation. At each step, the scheme involves solving only a sequence of linear elliptic differential equations and the computations of phase variable, velocity and pressure are totally decoupled. The finite difference spatial discretization on staggered grids is applied to verify efficiency and energy stability of the proposed scheme. We provide a rigorous proof of unconditional energy stability for semi-implicit scheme and fully discrete scheme. Using our numerical scheme, we compare the SAV, invariant

energy quadratization (IEQ) and stabilization approaches. Bubble rising dynamics and coarsening dynamics are also investigated in detail. The results demonstrate that the SAV approach can be more accurate than the IEQ approach, and the stabilization approach is the least accurate among the three approaches. The energy stability of SAV approach appears better than other approaches at large time steps.

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Appendix A

In this section, we provide a 3D fully discrete scheme for the time marching scheme (3.4). The computational domain is $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$, and cell centers are located on

$$x_i = \left(i - \frac{1}{2}\right)h_x, \quad i = 1, \dots, n_x, \quad y_j = \left(j - \frac{1}{2}\right)h_y, \quad j = 1, \dots, n_y, \quad z_k = \left(k - \frac{1}{2}\right)h_z.$$

Definitions of differential and averaged operators are similar to the 2D case. The 3D scheme is as follows

$$\begin{aligned} \phi^{n+1} - \phi^n + \delta t \left[d_x (u_*^{n+1} A_x \phi^n) + d_y (v_*^{n+1} A_y \phi^n) + d_z (w_*^{n+1} A_z \phi^n) \right] \\ - \delta t M \left[d_x (D_x w_\phi^{n+1}) + d_y (D_y w_\phi^{n+1}) + d_z (D_z w_\phi^{n+1}) \right] = 0. \end{aligned} \quad (A1)$$

$$w_\phi^{n+1} = -\lambda d_x (D_x \phi^{n+1}) - \lambda d_y (D_y \phi^{n+1}) - \lambda d_z (D_z \phi^{n+1}) + \lambda r^{n+1} b^n. \quad (A2)$$

$$r^{n+1} - r^n = \frac{h_x h_y h_z}{2} \sum b^n (\phi^{n+1} - \phi^n). \quad (A3)$$

where $b^n = F'(\phi^n) / \sqrt{h_x h_y h_z \sum F(\phi^n)}$.

$$\begin{cases} A_x \rho^n (u_*^n - u^n) = -\delta t A_x \phi^n D_x w_\phi^{n+1}, \\ A_y \rho^n (v_*^n - v^n) = -\delta t A_y \phi^n D_y w_\phi^{n+1}, \\ A_z \rho^n (w_*^n - w^n) = -\delta t A_z \phi^n D_z w_\phi^{n+1}. \end{cases} \quad (A4)$$

$$\begin{aligned}
 & A_x \rho^n (u^{n+1} - u^n) - 2\delta t D_x (\eta d_x u^{n+1}) - \delta t \left[d_y (A_y (A_x \eta^n) D_y u^{n+1}) + d_y (A_y (A_x \eta^n) D_x v^{n+1}) \right] \\
 & - \delta t \left[d_z (A_z (A_x \eta^n) D_z u^{n+1}) + d_z (A_z (A_x \eta^n) D_x w^{n+1}) \right] + \delta t D_x (2p^n - p^{n-1}) \\
 & + \delta t A_x \rho^n \left[u^n D_x (A_x u^{n+1}) + A_x (A_y v^n) d_y (A_y u^{n+1}) + A_x (A_z w^n) d_z (A_z u^{n+1}) \right] \\
 & + \delta t \left[J_x^n D_x (A_x u^{n+1}) + A_x (A_y J_y^n) d_y (A_y u^{n+1}) + A_x (A_z J_z^n) d_z (A_z u^{n+1}) \right] \\
 & + (A_x \rho^{n+1} - A_x \rho^n) u^{n+1} / 2 + \delta t \left[D_x (A_x J_x^n) + d_y (A_x J_y^n) + d_z (A_x J_z^n) \right] u^{n+1} / 2 \\
 & + \delta t A_x \rho^n \left[D_x (A_x u^n) + d_y (A_x v^n) + d_z (A_x w^n) \right] u^{n+1} / 2 + \delta t A_x \phi^n D_x w_\phi^{n+1} = 0.
 \end{aligned} \tag{A5}$$

$$\begin{aligned}
 & A_y \rho^n (v^{n+1} - v^n) - \delta t \left[d_x (A_x (A_y \eta^n) D_x v^{n+1}) + d_x (A_x (A_y \eta^n) D_y u^{n+1}) \right] - 2\delta t D_y (\eta^n d_y v^{n+1}) \\
 & - \delta t \left[d_z (A_z (A_y \eta^n) D_z v^{n+1}) + d_z (A_z (A_y \eta^n) D_y w^{n+1}) \right] + \delta t D_y (2p^n - p^{n-1}) \\
 & + \delta t A_y \rho^n \left[A_x (A_y u^n) d_x (A_x v^{n+1}) + v^n D_y (A_y v^{n+1}) + A_z (A_y w^n) d_z (A_z v^{n+1}) \right] \\
 & + \delta t \left[A_y (A_x J_x^n) d_x (A_x v^{n+1}) + J_y^n D_y (A_y v^{n+1}) + A_z (A_y J_z^n) d_z (A_z v^{n+1}) \right] \\
 & + v^{n+1} (A_y \rho^{n+1} - A_y \rho^n) / 2 + \delta t \left[d_x (A_y J_x^n) + D_y (A_y J_y^n) + d_z (A_y J_z^n) \right] v^{n+1} / 2 \\
 & + \delta t A_y \rho^n \left[d_x (A_y u^n) + D_y (A_y v^n) + d_z (A_y w^n) \right] v^{n+1} / 2 + \delta t A_y \phi^n D_y w_\phi^{n+1} = 0.
 \end{aligned} \tag{A6}$$

$$\begin{aligned}
 & A_z \rho^n (w^{n+1} - w^n) - \delta t \left[d_x (A_x (A_z \eta^n) D_x w^{n+1}) + d_x (A_x (A_z \eta^n) D_z u^{n+1}) \right] - 2\delta t D_z (\eta^n d_z w^{n+1}) \\
 & - \delta t \left[d_y (A_y (A_z \eta^n) D_y w^{n+1}) + d_y (A_y (A_z \eta^n) D_z v^{n+1}) \right] + \delta t D_z (2p^n - p^{n-1}) \\
 & + \delta t A_z \rho^n \left[A_x (A_z u^n) d_x (A_x w^{n+1}) + A_y (A_z v^n) d_y (A_y w^{n+1}) + w^n D_z (A_z w^{n+1}) \right] \\
 & + \delta t \left[A_z (A_x J_x^n) d_x (A_x w^{n+1}) + A_y (A_z J_y^n) d_y (A_y w^{n+1}) + J_z^n D_z (A_z w^{n+1}) \right] \\
 & + (A_z \rho^{n+1} - A_z \rho^n) w^{n+1} / 2 + \delta t \left[d_x (A_z J_x^n) + d_y (A_z J_y^n) + D_z (A_z J_z^n) \right] w^{n+1} / 2 \\
 & + \delta t A_z \rho^n \left[d_x (A_z u^n) + d_y (A_z v^n) + D_z (A_z w^n) \right] w^{n+1} / 2 + \delta t A_z \phi^n D_z w_\phi^{n+1} = 0.
 \end{aligned} \tag{A7}$$

$$\begin{aligned}
 & d_x \left[D_x (p^{n+1} - p^n) \right] + d_y \left[D_y (p^{n+1} - p^n) \right] + d_z \left[D_z (p^{n+1} - p^n) \right] \\
 & = \frac{\chi}{\delta t} (d_x u^{n+1} + d_y v^{n+1} + d_z w^{n+1}),
 \end{aligned} \tag{A8}$$

where

$$\begin{aligned}
 \rho^{n+1} &= \frac{\rho_1 - \rho_2}{2} \hat{\phi}^{n+1} + \frac{\rho_1 + \rho_2}{2}, \quad \eta^{n+1} = \frac{\eta_1 - \eta_2}{2} \hat{\phi}^{n+1} + \frac{\eta_1 + \eta_2}{2}, \\
 J_x^n &= \frac{(\rho_2 - \rho_1)}{2} MD_x w_\phi^n, \quad J_y^n = \frac{(\rho_2 - \rho_1)}{2} MD_y w_\phi^n, \quad J_z^n = \frac{(\rho_2 - \rho_1)}{2} MD_z w_\phi^n.
 \end{aligned}$$

To fully discrete boundary conditions, an operator $\mathbf{D} = (D_x, D_y, D_z)$ is introduced to simplify the presentation

$$\begin{cases} \mathbf{D} \phi^{n+1} \cdot \mathbf{n} = 0, \quad \mathbf{D} w_\phi^{n+1} \cdot \mathbf{n} = 0, & \text{on } \Gamma, \\ u^{n+1} = 0, v^{n+1} = 0, w_\phi^{n+1} = 0 & \text{on } \Gamma, \\ \mathbf{D} p^{n+1} \cdot \mathbf{n} = 0, & \text{on } \Gamma. \end{cases} \tag{A9}$$

Appendix B

Based on the IEQ approach, a semi-implicit, totally decoupled and energy stable scheme for

the governing system (2.2) is presented here. Given $\rho^n, \eta^n, \phi^n, \mathbf{u}^n$ and p^n , the scheme calculates $\rho^{n+1}, \eta^{n+1}, \phi^{n+1}, \mathbf{u}^{n+1}$ and p^{n+1} in three steps. Step 1, we solve the transformed Cahn-Hilliard equation to update ϕ^{n+1} ,

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} + \nabla \cdot (\mathbf{u}_*^n \phi^n) - M \Delta w_\phi^{n+1} = 0, \\ w_\phi^{n+1} = -\lambda \Delta \phi^{n+1} + \frac{\lambda q^{n+1}}{\sqrt{F(\phi^n)}} F'(\phi^n), \\ \frac{q^{n+1} - q^n}{\delta t} = \frac{F'(\phi^n)}{2\sqrt{F(\phi^n)}} \frac{(\phi^{n+1} - \phi^n)}{\delta t} \\ \partial_n \phi^{n+1} = 0, \quad \partial_n w_\phi^{n+1} = 0, \quad \text{on } \Gamma. \end{cases} \quad (\text{B1})$$

$$\mathbf{u}_*^n = \mathbf{u}^n - \delta t \frac{\phi^n \nabla w_\phi^{n+1}}{\rho^n}. \quad (\text{B2})$$

Step 2, $\mathbf{u}^{n+1}, \rho^{n+1}$ and η^{n+1} are updated.

$$\begin{cases} \rho^n \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\delta t} - \nabla \cdot \eta^n D(\mathbf{u}^{n+1}) + \nabla (2p^n - p^{n-1}) + \rho^n (\mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1} + \mathbf{J}^n \cdot \nabla \mathbf{u}^{n+1} + \\ \phi^n \nabla w_\phi^{n+1} + \frac{1}{2} \frac{\rho^{n+1} - \rho^n}{\delta t} \mathbf{u}^{n+1} + \frac{1}{2} \nabla \cdot (\rho^n \mathbf{u}^n) \mathbf{u}^{n+1} + \frac{1}{2} \nabla \cdot \mathbf{J}^n \mathbf{u}^{n+1} = 0, \\ \mathbf{u}^{n+1} = 0, \quad \text{on } \Gamma, \end{cases} \quad (\text{B3})$$

where

$$\mathbf{J}^n = \frac{(\rho_2 - \rho_1)}{2} M \nabla w_\phi^n, \quad \rho^{n+1} = \frac{\rho_1 - \rho_2}{2} \hat{\phi}^{n+1} + \frac{\rho_1 + \rho_2}{2}, \quad \eta^{n+1} = \frac{\eta_1 - \eta_2}{2} \hat{\phi}^{n+1} + \frac{\eta_1 + \eta_2}{2}.$$

Step 3, we update p^{n+1} . To avoid the elliptic equation with a variable coefficient $1/\rho$, the pressure-stabilized scheme is adapted to solve the pressure Poisson equation

$$\begin{cases} -\Delta(p^{n+1} - p^n) = -\frac{\chi}{\delta t} \nabla \cdot \mathbf{u}^{n+1}, \\ \mathbf{n} \cdot \nabla p^{n+1} = 0, \quad \text{on } \Gamma, \end{cases} \quad (\text{B4})$$

where $\chi = \frac{1}{2} \min(\rho_1, \rho_2)$.

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