NUMERICAL APPROXIMATIONS FOR ALLEN-CAHN TYPE PHASE FIELD MODEL OF TWO-PHASE INCOMPRESSIBLE FLUIDS WITH MOVING CONTACT LINES

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ABSTRACT. In this paper, we present some efficient numerical schemes to solve a two-phase hydrodynamics coupled phase field model with moving contact line boundary conditions. The model is a nonlinear coupling system, which consists the Navier-Stokes equations with the general Navier Boundary conditions or degenerated Navier Boundary conditions, and the Allen-Cahn type phase field equations with dynamical contact line boundary condition or static contact line boundary condition. The proposed schemes are linear and unconditionally energy stable. The energy stability of the proposed schemes are proved rigorously. Ample numerical tests are performed to show the accuracy and efficiency thereafter.

1. Introduction

Phase field (or diffuse interface) methods have been used widely and successfully to simulate a variety of interfacial phenomena, and have become one of the major tools to study the interfacial dynamics in many science and engineering fields (cf. [3, 5, 6, 8, 9, 12, 13, 15, 16, 26] and the references therein). The starting point of the phase-field approach is that the interface between multiple material components is viewed as a transition layer, where the two components are assumed to mix to a certain degree. Hence, the dynamics of the interface can be determined by the competition between the kinetic energy and the “elastic” mixing energy. Based on the variational formalism, the derived phase field model usually follows the thermodynamically consistent (or called energy stable) energy dissipation law, making it possible to carry out mathematical analysis, to develop efficient numerical schemes, and further to obtain reliable numerical simulations.

In typical phase field models, there are mainly two categories of system equations: the Allen-Cahn equation (Bray [2]) and the Cahn-Hilliard equation (Cahn and Hilliard, [4]) based on choices of diffusion rates. From the numerical point of view, the Allen-Cahn equation is a second-order equation, which is easier to solve numerically but does not conserve the
volume fraction, while the Cahn-Hilliard equation is a fourth-order equation which conserves the volume fraction but is relatively harder to solve numerically. Since the PDE system of either of phase field models usually follows the energy law, people are particularly interested in developing efficient numerical schemes that can satisfy a thermo-consistent energy law in the discrete level. Moreover, it is specifically desirable to develop some “easy-to-implement” (linear or decoupled) schemes in order to avoid expensive computational cost spent on the iterations needed by the nonlinear schemes.

In [18–22], the authors developed an efficient phase field model to simulate the so called “moving contact line” (MCL) problem, where the fluid-fluid interface may touch the solid wall. For such situation, the simple no-slip boundary conditions implying that the position of the contact line does not move, are not applicable since there may exist quite a few molecules near the surface that they “bounce along” down the surface. Thus the phase field model derived in [18–22] consists of Navier-Stokes equations with the general Navier boundary condition (GNBC), and the equations for the phase field variable with the so-called dynamical contact line boundary condition (DCLBC). Due to the considerations of volume conservation, the dynamics of the phase field variable is governed by the fourth order Cahn-Hilliard equations. We recall that a nonlinear, energy stable numerical scheme was proposed in [10], where the convective term was treated semi-implicitly, and the double well potential was handled by the convex splitting approach. Thus such scheme anyhow requires solving a coupled nonlinear system which usually is not convenient for the computations and its solvability is not easy to be proved.

Therefore, in this paper, we aim to develop some efficient numerical schemes to solve the phase field model with MCLs. To avoid the difficulties to solve the fourth order Cahn-Hilliard equation, we adopt the second order Allen-Cahn equation by assuming that the relaxation of the phase variable is governed by the $L^2$ gradient flow. To overcome non-conservation of the volume fraction, an extra term is added in the free energy to penalize the volume, which is one of the common practices in the framework of phase field models [9,27]. We develop two numerical schemes, one for the static contact line boundary condition (SCLBC) and the other for the DCLBC. Both schemes are linear and unconditionally energy stable. Moreover, the computations of the phase variable are completely decoupled from that of the velocity in the scheme for the SCLBC. Ample numerical examples are implemented to show the accuracy and efficiency thereafter.

The rest of the paper is organized as follows. In section 2, we present the phase-field model of moving contact line condition and show the energy dissipation law for the system. In section 3, we propose two energy stable schemes and prove their energy stabilities. In section 4, we present some numerical simulations to illustrate the efficiency and accuracy of the proposed numerical schemes. Some concluding remarks are given in section 5.
2. The PDE system and its energy law

In the pioneering work of Wang and Qian et al. (cf. [18–22]), the flow coupled phase field model consists the Navier-Stokes (NS) equations with the GNBC (cf. (2.4)) for the momentum equation, and the Cahn-Hilliard equations (CH) with the DCLBC (cf. (2.8)) for the phase field variable. Thus the non-dimensional version of the system reads as follows.

Incompressible Navier-Stokes equations for hydrodynamics:
\[
\begin{align*}
    \mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} &= \nu \Delta \mathbf{u} - \nabla p + \lambda \mu \nabla \phi, \\
    \nabla \cdot \mathbf{u} &= 0, \\
    \mathbf{u} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega, \\
    l(\phi)(\mathbf{u}_\tau - \mathbf{u}_w) + \nu \partial_n \mathbf{u}_\tau - \lambda L(\phi) \nabla_\tau \phi &= 0, \quad \text{on } \partial \Omega.
\end{align*}
\]

Cahn-Hilliard type phase field equations:
\[
\begin{align*}
    \phi_t + \nabla \cdot (\mathbf{u} \phi) &= M \Delta \mu, \\
    \mu &= -\varepsilon \Delta \phi + f(\phi), \\
    \partial_n \mu &= 0, \quad \text{on } \partial \Omega, \\
    \phi_t + \mathbf{u}_\tau \cdot \nabla_\tau \phi &= -\gamma L(\phi), \quad \text{on } \partial \Omega.
\end{align*}
\]

Now we give the detailed description for all the variables. \( \mathbf{u} \) is the fluid velocity, \( p \) is the pressure, \( \phi \) is the phase field variable, \( \mu \) is the chemical potential, the function \( L(\phi) \) is given by
\[
L(\phi) = \varepsilon \partial_n \phi + g'(\phi),
\]
where \( g(\phi) \) is the boundary interfacial energy, \( l(\phi) \geq 0 \) is a given coefficient function meaning the ratio of the thickness of interface and characteristic length. The function \( f(\phi) = F'(\phi) \) with \( F(\phi) \) being the Ginzburg-Landau double well potential. More precisely, \( F(\phi) \) and \( g(\phi) \) are defined as
\[
F(\phi) = \frac{1}{4\varepsilon}(\phi^2 - 1)^2, \quad g(\phi) = -\frac{\sqrt{2}}{3} \cos \theta_s \sin(\frac{\pi}{2} \phi),
\]
where \( \theta_s \) is the static contact angle, \( \nu \) is the viscosity coefficient, \( \lambda \) denotes the strength of the capillary force comparing to the Newtonian fluid stress, \( M \) is the mobility coefficient, \( \gamma \) is a boundary relaxation coefficient, \( \varepsilon \) denotes the interface thickness. \( \nabla \) denotes the gradient operator, \( \mathbf{n} \) is the outward normal direction on boundary \( \partial \Omega \), \( \tau \) is the boundary tangential direction, and vector operator \( \nabla_\tau = \nabla - (\mathbf{n} \cdot \nabla) \mathbf{n} \) is the gradient along tangential direction, \( \mathbf{u}_w \) is the boundary wall velocity, \( \mathbf{u}_\tau \) is the boundary fluid velocity in tangential direction. From (2.3), we have \( \mathbf{u} = \mathbf{u}_\tau \) on boundary \( \partial \Omega \).

When \( \gamma \to +\infty \), the DCLBC (2.8) reduces to the (SCLBC),
\[
L(\phi) = 0, \quad \text{on } \partial \Omega,
\]
and the GNBC (2.4) reduces to the NBC,
\begin{equation}
(l(\phi)(u_r - u_w) + \nu \partial_n u_r = 0, \quad \text{on } \partial \Omega.
\end{equation}

The above system provides quite a few challenges for the numerical algorithms development. To design numerical scheme that can satisfy the discrete energy dissipation law, naturally, one must overcome the following difficulties: (i) the fourth order Cahn-Hilliard equation with complicated boundary conditions; (ii) the coupling of the velocity and pressure through the incompressible condition; (iii) the stiffness in the phase equation associated with the interfacial width; (iv) the nonlinear couplings between the velocity and the phase variable in the stresses and convections; and (v) the nonlinear couplings between the velocity and the phase variable on the boundary conditions.

In this paper, to avoid the difficulty to solve the fourth order Cahn-Hilliard equation with complicated boundary conditions, we assume the relaxation of the interface follows the $L^2$ gradient flow. Namely, the fourth order Cahn-Hilliard equation is replaced by the second order Allen-Cahn equation. Thus the phase field equation is given as follows.

\begin{align}
\phi_t + \mathbf{u} \cdot \nabla \phi &= -M \mu, \\
\mu &= -\varepsilon \Delta \phi + f(\phi), \\
\phi_t + \mathbf{u}_r \cdot \nabla \phi &= -\gamma L(\phi), \quad \text{on } \partial \Omega.
\end{align}

It is well known that the Allen-Cahn equation does not conserve the volume. Inspired by the Allen-Cahn type phase field vesicle model in [9, 27], we add a penalty term in the phase field equation, to enforce this conservation property. Thus the modified Allen-Cahn (AC) equation reads as follows.

\begin{align}
\phi_t + \mathbf{u} \cdot \nabla \phi &= -M \mu, \\
\mu &= -\varepsilon \Delta \phi + f(\phi) + \Lambda (\phi - \alpha), \\
\phi_t + \mathbf{u}_r \cdot \nabla \phi &= -\gamma L(\phi), \quad \text{on } \partial \Omega,
\end{align}

where $\alpha = \int_{\Omega} \phi(t = 0) dx$ is the initial volume and $\Lambda$ is the positive penalty parameter.

We now derive the energy dissipation law for PDEs system (2.1)-(2.4) and (2.16)-(2.18). Here and after, for any function $f, g \in L^2(\Omega)$, we use $(f, g)$ to denote $\int_{\Omega} fg dx$, $(f, g)_{\partial \Omega}$ to denote $\int_{\partial \Omega} fg ds$, and $\|f\|^2 = (f, f)$ and $\|f\|^2_{\partial \Omega} = (f, f)_{\partial \Omega}$.

**Theorem 2.1.** The NS-AC-GNBC-DCLBC system ((2.1)-(2.4), (2.16)-(2.18)) is a dissipative system satisfying the following energy dissipation law,
\begin{equation}
\frac{d}{dt} E = -\nu \|\nabla \mathbf{u}\|^2 - \lambda M \|\mu\|^2 - \lambda \gamma \|L(\phi)\|^2_{\partial \Omega} - \|l(\phi)_{\frac{1}{2}} \mathbf{u}_s \|^2_{\partial \Omega} - (l(\phi)_{\frac{1}{2}} \mathbf{u}_s, \mathbf{u}_w)_{\partial \Omega},
\end{equation}
where $\mathbf{u}_s = \mathbf{u}_r - \mathbf{u}_w$ is the velocity slip on boundary $\partial \Omega$, and
\begin{equation}
E = \frac{\|\mathbf{u}\|^2}{2} + \lambda \left( \varepsilon \frac{\|\nabla \phi\|^2}{2} + (F(\phi), 1) + \frac{\Lambda}{2} \|\phi - \alpha\|^2 \right) + \lambda (g(\phi), 1)_{\partial \Omega}.
\end{equation}
Proof. By taking the inner product of (2.1) with \( u \), using the incompressible condition (2.2) and the zero flux boundary condition (2.3), we have

\[
\frac{1}{2} \frac{d}{dt} \|u\|^2 = \nu (\partial_n u, u_{\partial \Omega}) - \nu \|\nabla u\|^2 + \lambda (\nabla \phi, u).
\]

By taking the inner product of (2.16) with \( \lambda \mu \), we get

\[
\lambda (\phi_t, \mu) + \lambda (u \cdot \nabla \phi, \mu) = -\lambda M \|\mu\|^2.
\]

By taking the inner product of (2.17) with \( \lambda \phi_t \), we have

\[
\lambda (\mu, \phi_t) = -\lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega} + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\nabla \phi\|^2 + \lambda \varepsilon \frac{d}{dt} (F(\phi), 1) + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\phi - \alpha\|^2.
\]

Summing up equations (2.20)-(2.22), we obtain

\[
\frac{1}{2} \frac{d}{dt} \|u\|^2 + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\nabla \phi\|^2 + \lambda \varepsilon \frac{d}{dt} (F(\phi), 1) + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\phi - \alpha\|^2
\]

\[
= -\nu \|\nabla u\|^2 - \lambda M \|\mu\|^2 + \nu (\partial_n u, u_{\partial \Omega}) + \lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega}.
\]

Then, by using (2.8), (2.9) and boundary condition (2.4), we have

\[
u (\partial_n u, u_{\Omega}) = \nu (\partial_n u_r, u_r)_{\partial \Omega} = (\lambda L(\phi) \nabla r \phi - l(\phi)(u_r - u_w), u_r)_{\partial \Omega}
\]

\[
(2.24)
\]

and

\[
\lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega} = \lambda (\phi_t - g'(\phi), \phi_t)_{\partial \Omega}
\]

\[
= \lambda (\phi_t, \phi_t)_{\partial \Omega} - \lambda (g'(\phi), \phi_t)_{\partial \Omega}
\]

\[
= \lambda (\phi_t, \nabla r \phi - \gamma L(\phi))_{\partial \Omega} - \lambda \frac{d}{dt} (g(\phi), 1)_{\partial \Omega}
\]

\[
= -\lambda (\phi_t, \nabla r \phi, u_r)_{\partial \Omega} - \lambda \gamma \|L(\phi)\|^2_{\partial \Omega} - \lambda \frac{d}{dt} (g(\phi), 1)_{\partial \Omega}.
\]

Summing up (2.23), (2.24) and (2.25), we obtain the energy desired energy estimate (2.19). \( \square \)

Even though the above PDE energy law is straightforward, the nonlinear terms in \( \mu \) involves the second order derivatives, and it is not convenient to use them as test functions in numerical approximations, making it difficult to prove the discrete energy dissipation law. To overcome this difficulty, we have to reformulate the momentum equation (2.1) in an alternative form which is convenient for numerical approximation, we let \( \dot{\phi} = \phi_t + u \cdot \nabla \phi \), and notice that \( \mu = \frac{1}{-M} \dot{\phi} \), then the momentum equaiton (2.1) can be rewritten as the following equivalent form,

\[
(2.26)
\]

This equivalent form (2.26)-(2.2)-(2.3)-(2.4) and (2.16)-(2.18) still admits the similar energy law. To this end, by taking the \( L^2 \) inner product of (2.26) with \( u \), of (2.16) with \( \frac{\lambda}{-M} \dot{\phi} \), and of
(2.17) with $-\lambda \phi_t$, we derive

\[
\frac{1}{2} \frac{d}{dt} \|u\|^2 = \nu (\partial_n u, u)_{\partial \Omega} - \nu \|\nabla u\|^2 - \frac{\lambda}{M} (\phi \nabla \phi, u). 
\]

(2.27)

\[
\frac{\lambda}{M} \|\dot{\phi}\|^2 - \frac{\lambda}{M} (\phi, u \cdot \nabla \phi) = -\lambda (\mu, \phi_t).
\]

(2.28)

\[
-\lambda (\mu, \phi_t) = \lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega} - \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\nabla \phi\|^2 - \frac{\lambda}{M} \frac{d}{dt} (F(\phi), 1) - \frac{1}{2} \lambda \Lambda \frac{d}{dt} \|\phi - \alpha\|^2.
\]

Taking the summation of the above equalities, we have

\[
\frac{1}{2} \frac{d}{dt} \|u\|^2 + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\nabla \phi\|^2 + \frac{\lambda}{M} \frac{d}{dt} (F(\phi), 1) + \frac{1}{2} \lambda \Lambda \frac{d}{dt} \|\phi - \alpha\|^2 = -\nu \|\nabla u\|^2 - \frac{\lambda}{M} \|\dot{\phi}\|^2 + \nu (\partial_n u, u)_{\partial \Omega} + \lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega}.
\]

Using (2.24) and (2.25), we have the energy dissipation law.

\[
\frac{d}{dt} E = -\nu \|\nabla u\|^2 - \frac{\lambda}{M} \|\dot{\phi}\|^2 - \lambda \gamma \|L(\phi)\|_{\partial \Omega}^2 - \|l(\phi) \frac{1}{2} u_s\|_{\partial \Omega}^2 - (l(\phi) u_s, u_w)_{\partial \Omega}.
\]

3. Energy Stable Numerical Schemes

We aim to develop easy-to-implement energy stable schemes where the word “easy” means linear or decoupling. To this end, we assume that $F(\phi)$ satisfies the conditions as follows.

- There exists a constant $L$ such that

\[
(3.1) \quad \max_{|\phi| \in \mathbb{R}} |F''(\phi)| \leq L.
\]

We note that this condition is not satisfied by the usual Ginzburg-Landau double-well potential $F(\phi) = \frac{1}{4\varepsilon} (\phi^2 - 1)^2$. However, since it is well-known that the Allen-Cahn equation satisfies the maximum principle, we can truncate $F(\phi)$ to quadratic growth outside of an interval $[-M_1, M_1]$ without affecting the solution if the maximum norm of the initial condition $\phi_0$ is bounded by $M_1$. Therefore, it has been a common practice [7, 11, 23]) to consider the Allen-Cahn equation with a truncated double-well potential $\hat{F}(\phi)$. Without loss of generality, we introduce the following $\hat{F}(\phi)$ to replace $F(\phi)$:

\[
(3.2) \quad \hat{F}(\phi) = \frac{1}{4\varepsilon} \begin{cases} 
2(\phi + 1)^2, & \text{if } \phi < -1, \\
(\phi^2 - 1)^2, & \text{if } -1 \leq \phi \leq 1, \\
2(\phi - 1)^2, & \text{if } \phi > 1.
\end{cases}
\]

We drop the $\cdot$ in symbols for convenience. Correspondingly, we define $f(\phi) = F'(\phi)$ and two lipschitz constants

\[
(3.3) \quad L_1 := \max_{\phi \in \mathbb{R}} |f'(\phi)| = \frac{2}{\varepsilon}, \quad L_2 := \max_{\phi \in \mathbb{R}} |g''(\phi)| = \frac{\sqrt{2} \pi^2}{12} |\cos \theta_s|.
\]
3.1. **Linear, Decoupled schemes (LD).** We first focus on the NS-AC-NBC-SCLBC system where the boundary conditions are relatively simpler. We emphasize that there is no coupling between the velocity and phase field variable on the boundary, that makes it possible to develop the following decoupled, linear scheme. For convenience, we relist the governing system as follows.

The hydrodynamics equations:

\begin{align}
\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \frac{\lambda}{M} \dot{\phi} \nabla \phi &= 0, \quad (3.4) \\
\nabla \cdot \mathbf{u} &= 0, \quad (3.5) \\
\mathbf{u} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega, \quad (3.6) \\
l(\phi)(\mathbf{u}_\tau - \mathbf{u}_w) + \nu \partial_n \mathbf{u}_\tau &= 0, \quad \text{on } \partial \Omega. \quad (3.7)
\end{align}

The Allen-Cahn type phase field equations:

\begin{align}
\phi_t + (\mathbf{u} \cdot \nabla) \phi &= M(\varepsilon \Delta \phi - f(\phi) - \Lambda(\phi - \alpha)), \quad (3.8) \\
L(\phi) &= 0, \quad \text{on } \partial \Omega. \quad (3.9)
\end{align}

Let \( \delta t > 0 \) be a time discretization step and suppose \( \mathbf{u}^n, \phi^n \) and \( p^n \) are given, where the superscript \( n \) on variables denotes approximations of corresponding variables at time \( n\delta t \). Assuming \( S_1, S_2 \) are two positive stabilizing coefficients to be determined, the first-order time discretization scheme to solve NS-AC-NBC-SCLBC system (3.4)-(3.9) reads as follows.

**Step 1:** We first solve for \( \phi^{n+1} \) from

\begin{align}
\frac{\phi^{n+1} - \phi^n}{\delta t} + (\mathbf{u}_n^* \cdot \nabla) \phi^n &= M(\varepsilon \Delta \phi^{n+1} - f(\phi^n) - S_1(\phi^{n+1} - \phi^n) - \Lambda(\phi^{n+1} - \alpha)), \quad (3.10) \\
\tilde{L}^{n+1} &= 0, \quad \text{on } \partial \Omega, \quad (3.11)
\end{align}

where

\begin{align}
\mathbf{u}_n^* &= \mathbf{u}^n - \frac{\lambda}{M} \delta t \dot{\phi}^{n+1} \nabla \phi^n, \quad (3.12) \\
\dot{\phi}^{n+1} &= \frac{\phi^{n+1} - \phi^n}{\delta t} + (\mathbf{u}_n^* \cdot \nabla) \phi^n. \quad (3.13) \\
\tilde{L}^{n+1} &= \varepsilon \partial_n \phi^{n+1} + g'(\phi^n) + S_2(\phi^{n+1} - \phi^n). \quad (3.14)
\end{align}

**Step 2:** We solve \( \tilde{\mathbf{u}}^{n+1} \) from

\begin{align}
\frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}_k}{\delta t} + (\mathbf{u}^n \cdot \nabla) \tilde{\mathbf{u}}^{n+1} - \nu \Delta \tilde{\mathbf{u}}^{n+1} + \nabla p^n &= 0, \quad (3.15) \\
\tilde{\mathbf{u}}^{n+1} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega, \quad (3.16) \\
\nu \partial_n \mathbf{u}_s^{n+1} + l(\phi^n) \tilde{\mathbf{u}}_s^{n+1} &= 0, \quad \text{on } \partial \Omega. \quad (3.17)
\end{align}
**Step 3:** We update $u^{n+1}$ and $p^{n+1}$ from

\begin{align}
\frac{u^{n+1} - \tilde{u}^{n+1}}{\delta t} + \nabla (p^{n+1} - p^n) &= 0, \\
\nabla \cdot u^{n+1} &= 0, \\
 (3.19) \\
\n u^{n+1} \cdot n &= 0, \quad \text{on} \quad \partial \Omega.
\end{align}

(3.18)

**Remark 3.1.** We recall that $f(\phi)$ takes the form $\frac{1}{\varepsilon} \phi (\phi^2 - 1)$, so the explicit treatment of this term usually leads to a severe restriction on the time step $\delta t$ when $\varepsilon \ll 1$. It is common practice to add a “stabilizing” term to improve the stability [14, 23–25].

**Remark 3.2.** Inspired by [1, 17, 24, 25], we introduce the explicit convective velocity $u^\star_n$ in (3.10) by combining the term $u^n$ with surface tension term $\dot{\phi} \nabla \phi$. This term helps us to decouple the computations of $\phi$ from the velocity. From (3.13), we obtain

\begin{equation}
(3.21)
\end{equation}

where $B = (I + \frac{\delta t}{M/\Lambda} \nabla \phi_n \nabla \phi_n)$. It is easy to get the det $(I + c \nabla \phi \nabla \phi) = 1 + c \nabla \phi \cdot \nabla \phi$, thus $B$ is invertible.

We have the energy stability as follows.

**Theorem 3.1.** Assuming $u_w = 0$, and $S_1 \geq (L_1 - \Lambda)/2$ and $S_2 \geq L_2/2$, the scheme (3.10)-(3.20) is energy stable in the sense that

\begin{equation}
E_{\text{tot}}^{n+1} + \frac{\delta t^2}{2} \| \nabla p^{n+1} \|^2 + \delta t \left( \nu \| \nabla \tilde{u}^{n+1} \|^2 + \frac{\lambda}{M} \| \dot{\phi}^{n+1} \|^2 + \| l^{1/2} (\phi^n) \tilde{u}^{n+1} \|^2 \right) \\
\leq E_{\text{tot}}^n + \frac{\delta t^2}{2} \| \nabla p^n \|^2, \quad n = 0, 1, 2, \cdots,
\end{equation}

(3.22)

where

\begin{equation}
(3.23)
E_{\text{tot}}^n = \frac{1}{2} \| u^n \|^2 + \lambda \left( \frac{\nu \| \nabla \phi^n \|^2}{2} + (F(\phi^n), 1) + \frac{\Lambda}{2} \| \phi^n - \alpha \|^2 \right) + \lambda (g(\phi^n), 1) \partial \Omega.
\end{equation}

(3.22)

**Proof.** By taking inner product of (3.10) with $\frac{\lambda}{M} \dot{\phi}^{n+1} - \dot{\phi}^n$, and notice the identity

\begin{equation}
(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2,
\end{equation}

(3.24)

we have

\begin{equation}
\frac{\lambda}{M} \| \dot{\phi}^{n+1} \|^2 - \frac{\lambda}{M} (u^n \cdot \nabla \phi^n, \dot{\phi}^{n+1}) - \lambda \varepsilon (\Delta \dot{\phi}^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t}) \\
+ \lambda (f(\phi^n), \frac{\phi^{n+1} - \phi^n}{\delta t}) + \frac{\lambda S_1}{\delta t} \| \phi^{n+1} - \phi^n \|^2 \\
+ \frac{\lambda \Lambda}{2 \delta t} \left( \| \phi^{n+1} - \alpha \|^2 - \| \phi^n - \alpha \|^2 + \| \phi^{n+1} - \phi^n \|^2 \right) = 0,
\end{equation}

(3.25)
and  
\[-\lambda \varepsilon (\Delta \phi^{n+1}, \phi^{n+1} - \phi^n) = \frac{\lambda \varepsilon}{2\delta t} (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \|\nabla (\phi^{n+1} - \phi^n)\|^2) \]

\[+ \lambda (\partial_n \phi^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t})_{\partial \Omega}. \quad (3.26)\]

For the boundary integral terms in (3.26), by using (3.11) and (3.14), we have  
\[-\lambda \varepsilon (\partial_n \phi^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t})_{\partial \Omega} = \lambda (g'(\phi^n) + S_2(\phi^{n+1} - \phi^n), \frac{\phi^{n+1} - \phi^n}{\delta t})_{\partial \Omega}. \quad (3.27)\]

To handle the nonlinear term associated with $f$ in (3.25) and the term associated with $g$ in (3.27), we need the following identities  
\[f(\phi^n)(\phi^{n+1} - \phi^n) = F(\phi^{n+1}) - F(\phi^n) - \frac{f'(\eta)}{2}(\phi^{n+1} - \phi^n)^2, \quad (3.28)\]
\[g'(\phi^n)(\phi^{n+1} - \phi^n) = g(\phi^{n+1}) - g(\phi^n) - \frac{g''(\zeta)}{2}(\phi^{n+1} - \phi^n)^2. \quad (3.29)\]

Combining equations (3.25), (3.26), (3.27), (3.28) and (3.29), we get  
\[\frac{\lambda \varepsilon}{2\delta t} (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \|\nabla (\phi^{n+1} - \phi^n)\|^2) \]
\[+ \frac{\lambda}{\delta t} \left( (F(\phi^{n+1}) - F(\phi^n), 1) + (S_1 + \frac{\Lambda}{2} - \frac{f'(\eta)}{2}, (\phi^{n+1} - \phi^n)^2) \right) \]
\[+ \frac{\lambda}{\delta t} \left( (g(\phi^{n+1}) - g(\phi^n), 1)_{\partial \Omega} + (S_2 - \frac{g''(\zeta)}{2}, (\phi^{n+1} - \phi^n)^2)_{\partial \Omega} \right) \]
\[+ \frac{\lambda \Lambda}{2\delta t} (\|\phi^{n+1} - \alpha\|^2 - \|\phi^n - \alpha\|^2) - \frac{\lambda}{M} (\hat{u}_n^* \cdot \nabla \phi^n, \dot{\phi}^{n+1}) \]
\[= -\frac{\lambda}{M} \|\dot{\phi}^{n+1}\|^2. \quad (3.30)\]

By taking the $L^2$ inner product of equation (3.13) with $u_n^*/\delta t$, we obtain  
\[\frac{1}{2\delta t} (\|u_n^*\|^2 - \|u^n\|^2 + \|u_n^* - u^n\|^2) = -\frac{\lambda}{M} (\dot{\phi}^{n+1} \nabla \phi^n, u_n^*). \quad (3.31)\]

By taking the inner product of equation (3.15) with $\dot{u}^{n+1}$, and notice $\nabla \cdot u^n = 0, u^n \cdot n_{\partial \Omega} = 0$, we have  
\[(u^n \cdot \nabla)\dot{u}^{n+1}, \dot{u}^{n+1}) = 0, \quad (3.32)\]
and  
\[\frac{1}{2\delta t} (\|\dot{u}^{n+1}\|^2 - \|u_n^*\|^2 + \|\dot{u}^{n+1} - u_n^*\|^2) \]
\[= -\nu \|\nabla \dot{u}^{n+1}\|^2 + \nu (\partial_n \dot{u}^{n+1}, \dot{u}^{n+1})_{\partial \Omega} - (\nabla p^n, \dot{u}^{n+1}). \quad (3.33)\]
For the boundary term in the above equation, using equation (3.17) and noticing that \( \tilde{u}_{n+1} - \tilde{u}_{w}^{n+1} = \tilde{u}_{s}^{n+1} \) and \( u_{w}^{n+1} = 0 \), we have

\[
\nu(\partial_{n} \tilde{u}_{n+1}, \tilde{u}_{n+1})_{\partial\Omega} = -||l^{1/2}(\phi^n)\tilde{u}_{s}^{n+1}||_{\partial\Omega}^2.
\]

By taking inner product of (3.18) with \( u_{n+1} \), using (3.19) and (3.20), we have

\[
\frac{1}{2\delta t}(\|u_{n+1}\|^2 - \|\tilde{u}_{n+1}\|^2) = 0.
\]

We can also obtain the following equation directly from the equation (3.18),

\[
\frac{1}{2\delta t}(\|\nabla p_{n+1} - \nabla p_{n}\|^2 = \frac{1}{2\delta t}\|\tilde{u}_{n+1} - u_{n+1}\|^2.
\]

In addition, by taking inner product of (3.18) with \( \delta t \nabla p_{n} \), using incompressible condition (3.19) and boundary condition (3.20), we can get

\[
\frac{\delta t}{2}(\|\nabla p_{n+1}\|^2 - \|\nabla p_{n}\|^2 - \|\nabla p_{n+1} - \nabla p_{n}\|^2) = (\tilde{u}_{n+1}, \nabla p_{n}).
\]

By taking the summation of equations (3.30), (3.31), (3.33)–(3.37), we derive

\[
\frac{1}{\delta t}(E_{tot}^{n+1} - E_{tot}^{n}) + \frac{\delta t}{2}(\|\nabla p_{n+1}\|^2 - \|\nabla p_{n}\|^2) + \frac{\lambda \varepsilon}{2\delta t}\|\nabla (\phi^{n+1} - \phi^n)\|^2 = \\
- \left( \nu\|\nabla \tilde{u}_{n+1}\|^2 + \frac{\lambda}{M}\|\tilde{u}_{s}^{n+1}\|^2 + ||l^{1/2}(\phi^n)\tilde{u}_{s}^{n+1}||_{\partial\Omega}^2 \right) \]

\[
- \frac{1}{2\delta t}(\|u_{s} - u_{n}\|^2 + \|\tilde{u}_{n+1} - u_{s}^{n}\|^2) \]

\[
- \frac{\lambda}{\delta t} \left( S_1 + \frac{\Lambda}{2} - \frac{f'(\xi)}{2}, (\phi^{n+1} - \phi^n)^2 \right) + \left( S_2 - \frac{g''(\zeta)}{2}, (\phi^{n+1} - \phi^n)^2\right)_{\partial\Omega}.
\]

Thus, assuming \( S_1 \geq (L_1 - \Lambda)/2 \) and \( S_2 \geq L_2/2 \) and dropping some unnecessary positive terms, we get the desired energy estimate (3.22). \( \square \)

3.2. Linear, Coupled Scheme (LC). For the GNBC-DCLBC, the velocity and phase field variable are both coupled together on the boundary conditions. Such couplings make it be a very challenging issue to construct any decoupled schemes for GNBC-DCLBC. Thus the best scheme we can develop is the following linear coupled scheme, to solve the NS-AC-GNBC-DCLBC system.

For convenience, we relist the governing equations as follows.

The hydrodynamics equations:

\[
u \tau + (u \cdot \nabla) u - \nu \Delta u + \nabla p + \frac{\lambda}{M} \nabla \phi = 0,
\]

\[
\nabla \cdot u = 0,
\]

\[
u \tau \cdot n = 0, \quad \text{on} \quad \partial \Omega,
\]

\[
\nabla \cdot \phi - u \cdot n = 0, \quad \text{on} \quad \partial \Omega.
\]
The Allen-Cahn type phase field equations:

\[ \phi_t + (u \cdot \nabla)\phi = M(\varepsilon \Delta \phi - f(\phi) - \Lambda(\phi - \alpha)), \]
\[ \phi_t + (u \cdot \nabla)\phi = -\gamma L(\phi), \quad \text{on} \quad \partial \Omega, \]

Assuming \( S_1, S_2 \) are two positive stabilizing coefficients to be determined, the first-order time discretization scheme to solve PDE system (3.39)-(3.44) reads as follows.

**Step 1:** We first solve for \( \tilde{u}^{n+1}, \phi^{n+1} \) from

\[ \frac{\tilde{u}^{n+1} - u^n}{\delta t} + (u^n \cdot \nabla)\tilde{u}^{n+1} + \nabla p^n + \frac{\lambda}{M} \dot{\phi}^{n+1} \nabla \phi^n = 0, \]
\[ \frac{\dot{\phi}^{n+1} - \phi^n}{\delta t} + (\tilde{u}^{n+1} \cdot \nabla)\phi^{n+1} = M(\varepsilon \Delta \phi^{n+1} - f(\phi^n) - S_1(\phi^{n+1} - \phi^n) - \Lambda(\phi^{n+1} - \alpha)), \]

with the boundary conditions

\[ \tilde{u}^{n+1} \cdot n = 0, \quad \text{on} \quad \partial \Omega, \]
\[ \nu \partial_n \tilde{u}_{\phi}^{n+1} + f(\phi^n)\tilde{u}_{\phi}^{n+1} - \lambda \tilde{L}^{n+1} \nabla \phi^n = 0, \quad \text{on} \quad \partial \Omega, \]
\[ \frac{\dot{\phi}^{n+1} - \phi^n}{\delta t} + (\tilde{u}^{n+1} \cdot \nabla)\phi^{n+1} = -\gamma \tilde{L}^{n+1}, \quad \text{on} \quad \partial \Omega, \]

where

\[ \dot{\phi}^{n+1} = \frac{\phi^{n+1} - \phi^n}{\delta t} + (\tilde{u}^{n+1} \cdot \nabla)\phi^n, \]
\[ \tilde{L}^{n+1} = \varepsilon \partial_n \phi^{n+1} + g'(\phi^n) + S_2(\phi^{n+1} - \phi^n). \]

**Step 2:** We update \( u^{n+1} \) and \( p^{n+1} \) from

\[ \frac{u^{n+1} - \tilde{u}^{n+1}}{\delta t} + \nabla (p^{n+1} - p^n) = 0, \]
\[ \nabla \cdot u^{n+1} = 0, \]
\[ u^{n+1} \cdot n = 0, \quad \text{on} \quad \partial \Omega. \]

We now present the energy stability proof is as follows.

**Theorem 3.2.** Assuming \( u_w = 0 \), and \( S_1 \geq (L_1 - \Lambda)/2 \) and \( S_2 \geq L_2/2 \), the scheme (3.45)-(3.54) is energy stable in the sense that

\[ E_{tot}^{n+1} + \frac{\delta t^2}{2} ||\nabla p^{n+1}||^2 + \delta t \left( \nu ||\nabla \tilde{u}^{n+1}||^2 + \frac{\lambda}{M} ||\dot{\phi}^{n+1}||^2 + ||1/2(\phi^n)\tilde{u}_{\phi}^{n+1}||_{\partial \Omega}^2 + \gamma \lambda ||\tilde{L}^{n+1}||_{\partial \Omega}^2 \right) \]
\[ \leq E_{tot}^{n} + \frac{\delta t^2}{2} ||\nabla p^n||^2. \quad n = 0, 1, 2, \cdots , \]

where \( E_{tot} \) is defined in (3.23).
Proof. By taking inner product of (3.46) with \( \frac{\lambda}{M} \phi^{n+1} - \phi^n \), we have
\[
\frac{\lambda}{M} \|\dot{\phi}^{n+1}\|^2 - \frac{\lambda}{M} (\dot{u}^{n+1} \cdot \nabla \phi^n, \dot{\phi}^{n+1}) + \frac{\lambda \varepsilon}{2\delta t} (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \|\nabla (\phi^{n+1} - \phi^n)\|^2)
\]
(3.56)
\[
- \lambda \varepsilon (\partial_n \phi^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t})_{\partial \Omega} + \lambda (f(\phi^n), \frac{\phi^{n+1} - \phi^n}{\delta t}) + \frac{\lambda S_1}{\delta t} \|\phi^{n+1} - \phi^n\|^2
\]
\[
+ \frac{\lambda A}{2\delta t} (\|\phi^{n+1} - \alpha\|^2 - \|\phi^n - \alpha\|^2 + \|\phi^{n+1} - \phi^n\|^2) = 0.
\]
For the boundary integral terms above, using (3.51), we have
\[
- \lambda \varepsilon (\partial_n \phi^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t})_{\partial \Omega}
\]
(3.57)
\[
= \lambda (-\bar{L}^{n+1} + g'(\phi^n) + S_2 (\phi^{n+1} - \phi^n), \frac{\phi^{n+1} - \phi^n}{\delta t})_{\partial \Omega}.
\]
and
\[
\lambda (\bar{L}^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t}) = -\gamma \lambda \|\bar{L}^{n+1}\|_{\partial \Omega} - \lambda (\bar{L}^{n+1}, (\tilde{u}^{n+1} - \nabla) \phi^{n+1}).
\]
Combining equations (3.56), (3.57), (3.28) and (3.29), we get
\[
\frac{\lambda \varepsilon}{2\delta t} (\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \|\nabla (\phi^{n+1} - \phi^n)\|^2)
\]
\[
+ \frac{\lambda}{\delta t} (F(\phi^{n+1}) - F(\phi^n), 1) + \frac{\lambda}{\delta t} \left( S_1 + \frac{\lambda}{2} - \frac{f'(\eta)}{2}, (\phi^{n+1} - \phi^n)^2 \right)
\]
(3.59)
\[
+ \frac{\lambda}{\delta t} \left( g(\phi^{n+1}) - g(\phi^n), 1 \right)_{\partial \Omega} + \frac{\lambda}{\delta t} \left( S_2 - \frac{g''(\zeta)}{2}, (\phi^{n+1} - \phi^n)^2 \right)_{\partial \Omega}
\]
\[
+ \frac{\lambda A}{2\delta t} \left( \|\phi^{n+1} - \alpha\|^2 - \|\phi^n - \alpha\|^2 \right) - \frac{\lambda}{M} (\tilde{u}^{n+1} \cdot \nabla \phi^n, \frac{\phi^{n+1} - \phi^n}{\delta t})
\]
\[
= -\gamma \lambda \|\bar{L}^{n+1}\|^2_{\partial \Omega} - \lambda (\bar{L}^{n+1}, (\tilde{u}^{n+1} - \nabla) \phi^{n+1}) - \frac{\lambda}{M} \|\dot{\phi}^{n+1}\|^2.
\]
By taking the inner product of equation (3.45), we obtain
\[
\frac{1}{2\delta t} (\|\tilde{u}^{n+1}\|^2 - \|u^n\|^2 + \|\tilde{u}^{n+1} - u^n\|^2)
\]
(3.60)
\[
= -\nu \|\nabla u^{n+1}\|^2 + \nu (\partial_n u^{n+1}, u^{n+1})_{\partial \Omega} - (\nabla p^n, \tilde{u}^{n+1}).
\]
For the boundary term in the above equation, using equation (3.48), we have
\[
\nu (\partial_n \tilde{u}^{n+1}, u^{n+1})_{\partial \Omega} = -\|u^{1/2}(\phi^n)\|_{\partial \Omega}^2 + \lambda (\bar{L}^{n+1} \nabla \phi^n, \tilde{u}^{n+1})_{\partial \Omega}.
\]
Exactly as Theorem 3.1, for (3.52), we derive
\[
\frac{1}{2\delta t} (\|u^{n+1}\|^2 - \|\tilde{u}^{n+1}\|^2 + \|u^{n+1} - \tilde{u}^{n+1}\|^2) = 0,
\]
(3.62)
\[
\frac{\delta t}{2} \|\nabla p^{n+1} - \nabla p^n\|^2 = \frac{1}{2\delta t} \|\tilde{u}^{n+1} - u^{n+1}\|^2,
\]
(3.63)
and
\begin{equation}
\frac{\delta t}{2} (\| \nabla p^{n+1} \|^2 - \| \nabla p^n \|^2 - \| \nabla p^{n+1} - \nabla p^n \|^2) = (\tilde{u}^{n+1}, \nabla p^n).
\end{equation}

By taking the summation of equations (3.59)-(3.64), we derive
\begin{equation}
\frac{1}{\delta t} (E_{tot}^{n+1} - E_{tot}^n) + \frac{\delta t}{2} (\| \nabla p^{n+1} \|^2 - \| \nabla p^n \|^2) + \frac{\lambda \varepsilon}{2 \delta t} \| \nabla (\phi^{n+1} - \phi^n) \|^2 =
\end{equation}
\begin{align*}
& - \left( \nu \| \tilde{u}^{n+1} \|^2 + \frac{\lambda}{M} \| \phi^{n+1} \|^2 + \| l^{1/2} (\phi^n) \tilde{u}_s^{n+1} \|^2_{\partial \Omega} - \gamma \lambda \| \tilde{L}^{n+1} \|^2_{\partial \Omega} \right) \\
& - \frac{1}{2 \delta t} (\| \tilde{u}^{n+1} - u^{n+1} \|^2 + \| \tilde{u}^{n+1} - u^n \|^2) \\
& - \frac{\lambda}{\delta t} \left( (S_1 + \Lambda - \frac{f'(\xi)}{2}, (\phi^{n+1} - \phi^n)^2) + (S_2 - \frac{g''(\zeta)}{2}, (\phi^{n+1} - \phi^n)^2)_{\partial \Omega} \right).
\end{align*}

Thus, assuming $S_1 \geq (L_1 - \Lambda)/2$ and $S_2 \geq L_2/2$ and dropping some unnecessary postive terms, we get the desired energy estimate (3.55).

\[\square\]

4. Numerical Simulations

In this section, we present some 2D numerical simulations to validate our proposed schemes. For simplicity, we assume the system in $x$ direction is periodic, and only the top and bottom boundaries take the GNBC (or NBC) and DCLBC (or SCLBC). For the spatial operators in the scheme, we use second-order central finite difference methods to discretize them over an uniform spatial grid, where the velocity fields are discretized on the center of mesh surface, and pressure $p$, phase variables $\phi$ are discretized on cell center.

4.1. Shear flow. We consider the flow between two parallel plates which move in opposite directions at a constant speed. We fix the domain size to be $L_y = 0.4, L_x = 2$, and use $201 \times 101$ grid points to discretize the space. The other parameters are given as follows.
\begin{equation}
\lambda = \frac{1}{3}, \nu = \frac{1}{36}, M = 0.0125, \gamma = 100, \varepsilon = 0.01, l(\phi) = 1/1.14, \Lambda = \frac{10}{M}.
\end{equation}
The initial velocity field takes the profile of Couette flow, and the initial value of $\phi$ is given as follows.
\begin{equation}
\phi_0(x, y) = \tanh \left( \frac{1}{\sqrt{2\varepsilon}} \left( \frac{L_x}{4} - \left| x - \frac{L_x}{2} \right| \right) \right).
\end{equation}

Figure 5.1 (a) shows the interface contour of $\phi_0$.

We present two numerical results for a classical benchmark numerical simulation from [10, 25]. In simulation I, $u_w = \pm 0.7, \theta_s = 64^\circ$, where $u_w$ is the speed of top and bottom plates, $\theta_s$ is the static contact angle; $\pm$ sign means the values on top boundary and bottom boundary have different signs (directions). In simulation II, $u_w = \pm 0.2$ and $\theta_s = \pm 77.6^\circ$. In spite of the fact that our numerical schemes are stable for any time step, we still have to choose some
reasonable small time step in order to get the desired accuracy. In the two simulations, the time step is $\delta t = 0.001$.

The interface contours of $\phi$ at the steady state ($t = 5$) are presented in Figure 5.1 (b)-(c) using both of the LC scheme and LD scheme. These results are consistent to the numerical results in [10, 25]. We notice that the LD scheme for NBC-SCLBC actually gives almost identical results as the LC scheme for GNBC-DCLBC.

We test the accuracy for both of the two schemes for the parameters of simulation I. We take $\delta t = 1.25e - 5$ as the exact solution, and compare numerical $L^2$ error of phase function $\phi$ and the Euclidian norm of the velocity $u$ at $T = 0.5$, for various time step. We show the temporal convergence rate of the LD scheme and LC scheme in Table (4.1) and Table (4.2) respectively. We note that both schemes are at least first order in time.

4.2. Dewetting and Spreading of a drop. We simulate the dynamics of a drop initially resided on a surface. For various contact angles, the drop will perform different dynamics of dewetting or spreading. We set two contact angles and perform the simulations using both of the LD and LC schemes. We fix the domain size to be $[-1, 1] \times [-0.5, 0.5]$, and set the other

<table>
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<th>$\delta t$</th>
<th>$\text{Err } u$</th>
<th>order</th>
<th>$\text{Err } \phi$</th>
<th>order</th>
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</table>

Table 4.1. Numerical errors for velocity $u$ and $\phi$ at $t = 0.5$ for different time steps using the LD scheme.

<table>
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<tr>
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<th>$\text{Err } u$</th>
<th>order</th>
<th>$\text{Err } \phi$</th>
<th>order</th>
</tr>
</thead>
<tbody>
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</tr>
</tbody>
</table>

Table 4.2. Numerical errors for velocity $u$ and $\phi$ at $t = 0.5$ for different time steps using the LC scheme.
parameters as follows.

\begin{equation}
\lambda = 1, \nu = \frac{1}{12}, M = 0.0125, \gamma = 100, \varepsilon = 0.01, l(\phi) = 1/0.19.
\end{equation}

We take $201 \times 101$ grid points for $x$ and $y$ direction respectively.

In Figure 5.2 and Figure 5.3, we plot the contour of the drop interface using the LD scheme for NBC-SCLBC system for $\theta_s = 30^\circ$ and $\theta_s = 150^\circ$, respectively. We notice that for the acute contact angle, the drop performs the dewetting process, and for the obtuse contact angle, the drop tends to spread over the solid surface. The detailed results using the LC scheme are omitted because they are essentially the same as the results of the LD scheme. For comparisons, we plot the two contour lines of the steady state ($t = 5$) using LD scheme and LC scheme for these two contact angles in Figure. 5.4 and Figure 5.5, respectively.

5. Concluding Remarks

In this paper, for the hydrodynamics coupled, Allen-Cahn type phase-field model that incorporates the moving contact line boundary problems, we construct two efficient, linear numerical schemes. The first scheme is decoupled for the simple version of the boundary conditions (NBC-SCLBC), where one only needs to solve a series of decoupled elliptic equations. The other is linear coupled for the more complicated version of the boundary conditions (GNBC-DCLBC). Both schemes are energy stable and the unconditional energy stability are rigorously proved. Ample numerical simulations are presented to verify the accuracy and efficiency of the proposed model and numerical schemes.

Acknowledgments

The work of X. Yang is partially supported by NSF DMS-1200487, NSF DMS-1418898, AFOSR FA9550-12-1-0178, NSFC-11471372, and NSFC-11571385. X. Yang thank the hospitality of Hong Kong University of Science and Technology during his winter visit. The work of H. Zhang is partially supported by NSFC grant No. 11471046, 11571045 and the Ministry of Education Program for New Century Excellent Talents Project NCET-12-0053.
(a) The initial profile of the phase field $\phi_0$.

(b) Simulation I: The steady state of $\phi$ for $\theta_s = 64^\circ$.

(c) Simulation II: The steady state of $\phi$ for $\theta_s = 77.6^\circ$.

**Figure 5.1.** The contours of the interfaces of phase variable $\phi$. (a) The initial configuration of $\phi$ given by (4.2); (b) Contour of $\phi$ at $t = 5$ with contact angle $\theta_s = 64^\circ$ and $u_w = \pm 0.7$; (c) Contour of $\phi$ at $t = 5$ with contact angle $\theta_s = 77.6^\circ$ and $u_w = \pm 0.2$. The results are generated by both of the LD and LC scheme with $200 \times 100$ grid points and $\delta t = 0.001$. 
Figure 5.2. The snapshots of the interface contour of the phase variable \( \phi \) using the LD scheme for the system of NBC-SCLBC at \( t = 0, 1, 1.5, 2, 2.5, 3.5, 4, 5 \). The contact angle is \( \theta_s = 30^\circ \).
Figure 5.3. The interface contour of the phase variable $\phi$ using the LD scheme for the system of GNBC-DCLBC. The contact angle is $\theta_s = 150^\circ$. 
Figure 5.4. The comparison of the interface contour of the steady state using the LD scheme for NBC-SCLBC, and LC scheme for GNBC-DCLBC with $\theta_s = 30^\circ$.

Figure 5.5. The comparison of the interface contour of the steady state using the LD scheme for NBC-SCLBC, and LC scheme for GNBC-DCLBC with $\theta_s = 150^\circ$.

REFERENCES


