Numerical approximations and error analysis of the Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions

Xuelian Bao; Hui Zhang

Abstract We consider numerical approximations and error analysis for the Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions (P. Knopf et. al., arXiv, 2020). Based on the stabilized linearly implicit approach, a first-order in time, linear and energy stable scheme for solving this model is proposed. The corresponding semi-discretized-in-time error estimates for the scheme are also derived. Numerical experiments, including the comparison with the former work, the convergence results for the relaxation parameter \( K \to 0 \) and \( K \to \infty \) and the accuracy tests with respect to the time step size, are performed to validate the accuracy of the proposed scheme and the error analysis.

1 Introduction

The Cahn-Hilliard equation, first introduced in [2], was originally utilized to describe the phase separation and de-mixing processes of binary mixtures. The standard Cahn-Hilliard equation can be written as follows:

\[
\begin{align*}
\phi_t &= \Delta \mu, \quad \text{in } \Omega \times (0,T), \\
\mu &= -\varepsilon \Delta \phi + \frac{1}{\varepsilon} F'(\phi), \quad \text{in } \Omega \times (0,T),
\end{align*}
\]

where the parameter \( \varepsilon > 0 \), \( \Omega \subseteq \mathbb{R}^d \) (\( d = 2, 3 \)) denotes a bounded domain whose boundary \( \Gamma = \partial \Omega \) with the unit outer vector field \( n \). The function \( \phi \) denotes the difference of two local relative concentrations, in order to describe the binary alloys. The regions with \( \phi = \pm 1 \) in the domain \( \Omega \) correspond to the pure phases of the materials, which are separated by a interfacial region whose thickness is proportional to \( \varepsilon \).

In the Cahn-Hilliard equation, \( \mu \) denotes the chemical potential in \( \Omega \), which can be expressed as the Fréchet derivative of the bulk free energy:

\[
E^{\text{bulk}}(\phi) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} F(\phi) \, dx,
\]

where \( F \) denotes the potential in \( \Omega \). The classical choice of \( F \) is the smooth double-well potential

\[
F(x) = \frac{1}{4}(x^2 - 1)^2, \quad x \in \mathbb{R},
\]
which has a double-well structure with two minima at -1 and 1 and a local unstable maximum at 0.

Since the time-evolution of $\phi$ is confined in a bounded domain, suitable boundary conditions are needed. The classical choice is the homogeneous Neumann conditions:

\begin{align}
\partial_n \mu &= 0, \quad \text{on } \Gamma \times (0, T), \\
\partial_n \phi &= 0, \quad \text{on } \Gamma \times (0, T),
\end{align}

where $\partial_n$ represents the outward normal derivative on $\Gamma$. Obviously, the mass conservation law holds in the bulk (i.e., in $\Omega$) with the no-flux boundary condition (1.4):

\begin{align}
\int_\Omega \phi(t) \, dx &= \int_\Omega \phi(0) \, dx, \quad t \in [0, T].
\end{align}

In addition, the time evolution of the bulk free energy $E^{\text{bulk}}$ (Eq. (1.2)) is decreasing with the boundary conditions (1.4) and (1.5), namely,

\begin{align}
\frac{d}{dt} E^{\text{bulk}}(\phi(t)) + \int_\Omega |\nabla \mu|^2 \, dx = 0, \quad t \in (0, T).
\end{align}

When some particular applications (for instance, the hydrodynamic applications such as contact line problems) are taken into consideration, it’s necessary to describe the short-range interactions between the mixture and the solid wall. However, the standard homogeneous Neumann conditions neglects the effects of the boundary to the bulk dynamics. Thus, several dynamic boundary conditions have been proposed and analysed in recent years, see for instance, [22, 27, 10, 12, 5, 6, 21, 17, 19, 18]. These dynamic boundary conditions are based on the system with added surface free energy [7, 8, 16]. The total free energy can be written as

\begin{align}
E^{\text{total}}(\phi) &= E^{\text{bulk}}(\phi) + E^{\text{surf}}(\phi), \\
E^{\text{surf}}(\phi) &= \int_\Gamma \frac{\delta}{2} |\nabla_\Gamma \phi|^2 + \frac{1}{\delta} G(\phi) \, dS,
\end{align}

where $\nabla_\Gamma$ represents the tangential or surface gradient operator on $\Gamma$, $G$ is the surface potential, $\delta$ denotes the thickness of the interfacial region on $\Gamma$ and the parameter $\kappa$ is related to the surface diffusion. When $\kappa = 0$, it corresponds to the moving contact line problem [25].

In the present work, we summarize three Cahn-Hilliard models with dynamic boundary conditions in detail. All the dynamic boundary conditions of the three models have a Cahn-Hilliard type structure. And they can be interpreted as an $H^{-1}$-gradient flow of the total free energy.

The first Cahn-Hilliard model with dynamic boundary conditions was proposed by G.R. Goldstein, A. Miranville, and G. Schimperna [12]:

\begin{align}
\begin{cases}
\phi_t = \Delta \mu, & \text{in } \Omega \times (0, T), \\
\mu = -\epsilon \Delta \phi + \frac{1}{\epsilon} F'(\phi), & \text{in } \Omega \times (0, T), \\
\phi|_\Gamma = \psi, & \text{on } \Gamma \times (0, T), \\
\psi_t = \Delta_\Gamma \mu - \partial_n \mu, & \text{on } \Gamma \times (0, T), \\
\mu = -\delta \epsilon \Delta_\Gamma \psi + \frac{1}{\delta} G'(\psi) + \epsilon \partial_n \phi & \text{on } \Gamma \times (0, T).
\end{cases}
\end{align}
In the present work, we denote the model as the GMS model for convenience. Here, $\Delta_{\Gamma}$ denotes the Laplace-Beltrami operator on $\Gamma$. Note that this model describes the chemical reactions occurring on the boundary and the chemical potentials in the bulk and on the boundary are the same. Moreover, the dynamic boundary conditions ensure the conservation of the total mass (namely, the sum of the bulk and boundary mass):

\[
(1.11) \quad \int_{\Omega} \phi(t)dx + \int_{\Gamma} \psi(t)dS = \int_{\Omega} \phi(0)dx + \int_{\Gamma} \psi(0)dS, \quad \text{for all} \ t \in [0, T],
\]

and the energy dissipation law:

\[
(1.12) \quad \frac{d}{dt} E_{\text{total}}(\phi, \psi) = -\|\nabla \mu\|^2_{\Omega} - \|\nabla_{\Gamma} \mu\|^2_{\Gamma} \leq 0.
\]

The second Cahn-Hilliard model with dynamic boundary conditions was proposed by C. Liu and H. Wu [19]:

\[
(1.13) \begin{cases}
\phi_t = \Delta \mu, & \text{in } \Omega \times (0, T), \\
\mu = -\varepsilon \Delta \phi + \frac{1}{\varepsilon} F'(\phi), & \text{in } \Omega \times (0, T), \\
\partial_{n\mu} = 0, & \text{on } \Gamma \times (0, T), \\
\phi|_{\Gamma} = \psi, & \text{on } \Gamma \times (0, T), \\
\psi_t = \Delta_{\Gamma} \mu_{\Gamma}, & \text{on } \Gamma \times (0, T), \\
\mu_{\Gamma} = -\delta \kappa \Delta_{\Gamma} \psi + \frac{1}{\delta} G'(\psi) + \varepsilon \partial_n \phi, & \text{on } \Gamma \times (0, T).
\end{cases}
\]

We denote it as the Liu-Wu model for short. Here, $\mu_{\Gamma}$ denotes the chemical potential on the boundary. The model assumes that there is no mass exchange between the bulk and the boundary, namely, $\partial_{n\mu} = 0$. Different from the GMS model ($\mu = \mu_{\Gamma}$), the chemical potential $\mu$ and $\mu_{\Gamma}$ are not directly coupled. Similarly, we can obtain the following mass conservation law:

\[
(1.14) \quad \int_{\Omega} \phi(t)dx = \int_{\Omega} \phi(0)dx \quad \text{and} \quad \int_{\Gamma} \psi(t)dS = \int_{\Gamma} \psi(0)dS, \quad t \in [0, T],
\]

indicating that the Liu-Wu model satisfies the mass conservation law in the bulk and on the boundary respectively. Moreover, the energy dissipation law [1.12] also holds for the Liu-Wu model. The readers can find the well-posedness results for the Liu-Wu model and the GMS model in [19] and [12] respectively.

Recently, Knopf [18] proposed a new model, which can be interpreted as an interpolation between the Liu-Wu model and the GMS model. It reads as follows,

\[
(1.15) \begin{cases}
\phi_t = \Delta \mu, & \text{in } \Omega \times (0, T), \\
\mu = -\varepsilon \Delta \phi + \frac{1}{\varepsilon} F'(\phi), & \text{in } \Omega \times (0, T), \\
K\partial_{n\mu} = \mu_{\Gamma} - \mu, & \text{on } \Gamma \times (0, T), \\
\phi|_{\Gamma} = \psi, & \text{on } \Gamma \times (0, T), \\
\psi_t = \Delta_{\Gamma} \mu_{\Gamma} - \partial_{n\mu}, & \text{on } \Gamma \times (0, T), \\
\mu_{\Gamma} = -\delta \kappa \Delta_{\Gamma} \psi + \frac{1}{\delta} G'(\psi) + \varepsilon \partial_n \phi, & \text{on } \Gamma \times (0, T).
\end{cases}
\]
In the present work, we use the authors’ initials and refer it to be the KLLM model for convenience. Here, $\mu$ and $\mu_\Gamma$ represent the chemical potentials in $\Omega$ and on $\Gamma$, respectively. Notice that $\mu$ and $\mu_\Gamma$ are coupled by the Robin type boundary condition $K\partial_n\mu = \mu_\Gamma - \mu$, where the positive parameter $K$ is the relaxation parameter. The constant $1/K$ can be interpreted as the reaction rate, since the reactions between the materials are described by (1.15). The well-posedness of the system (1.15) and convergence to the Liu-Wu model (as $K \to \infty$) and the GMS model (as $K \to 0$) in both the weak and the strong sense have been investigated by Knopf [18].

The numerical approximations of the Cahn-Hilliard equation and its variants have already been well investigated. There exists extensive efficient techniques for the time discretization, such as the stabilized linearly implicit approach [14], the convex splitting approach [23, 13], the invariant energy quadratization (IEQ) method [28, 29] and the scalar auxiliary variable (SAV) method [24]. Recently, there have been numerical approximations for the Cahn-Hilliard equation with dynamic boundary conditions, see for instance, [3, 4, 15, 9, 26]. Specifically, for the Liu-Wu model, the finite element scheme has been proposed in [26, 11], where the straightforward discretization based on piecewise linear finite element functions was utilized to simulate the model, and the corresponding nonlinear system was solved by Newton’s method. A recent contribution on the numerical analysis can be found in [20]. For the KLLM model, we refer the readers to [18] for the finite element numerical approximations and numerical analysis. However, the backward implicit Euler method was used for time discretization in the above finite element schemes, where one needs to solve nonlinear systems at each time step. Recently, based on the stabilized linearly implicit approach, a linear and energy stable numerical scheme has been proposed for the Liu-Wu model [1] and the corresponding semi-discrete-in-time error estimates are carried out.

Inspired by the numerical scheme in [1], a first-order in time, linear and energy stable scheme for solving the KLLM model is proposed in the present work. The scheme allows us to simulate the KLLM model as well as the two limit models – the Liu-Wu model and the GMS model. Note that the scheme is highly efficient since one only needs to solve a linear equation at each time step. Numerical simulations are performed in the two-dimensional space to validate the accuracy and stability of the scheme by comparing with the former work. We also investigate the error estimates in semi-discrete-in-time for the scheme. To the best of the authors’ knowledge, the proposed scheme is the first linear numerical scheme to solve the KLLM model and it is the first work to give the corresponding semi-discrete-in-time error estimates.

The rest of the paper is organized as follows. We first present some notions and notation appearing in this article in Section 2. In Section 3, the stabilized scheme for the KLLM model and the energy stability are derived. The error estimates are constructed in Section 4. In Section 5, we present the numerical examples and illustrate the convergence results for $K \to 0$ and $K \to \infty$. The accuracy tests are also displayed in this section. Finally, the conclusion is presented in Section 6.

2 Preliminaries

Before giving the stabilized scheme and the corresponding error analysis, we make some definitions in this section. The norm and inner product of $L^2(\Omega)$ and $L^2(\Gamma)$ are denoted by $\|\cdot\|_\Omega$, $(\cdot, \cdot)_\Omega$ and $\|\cdot\|_\Gamma$, $(\cdot, \cdot)_\Gamma$ respectively. The usual norm in $H^k(\Omega)$ and $H^k(\Gamma)$ are denoted by $\|\cdot\|_{H^k(\Omega)}$ and $\|\cdot\|_{H^k(\Gamma)}$ respectively.
We consider a finite time interval \([0, T]\) and a domain \(\Omega \subset \mathbb{R}^d\) \((d = 2, 3)\), which is a bounded domain with sufficient smooth boundary \(\Gamma = \partial \Omega\) and \(\mathbf{n} = \mathbf{n}(x)\) is the unit outer normal vector on \(\Gamma\).

Let \(\tau\) be the time step size. For a sequence of functions \(f^0, f^1, \ldots, f^N\) in some Hilbert space \(E\), we denote the sequence by \(\{f^n\}\) and define the following discrete norm for \(\{f^n\}\):

\[
\|f^n\|_{l^n(E)} = \max_{0 \leq n \leq N}(\|f^n\|_E).
\]

We denote by \(C\) a generic constant that is independent of \(\tau\) but possibly depends on the parameters and solutions, and use \(f \lesssim g\) to say that there is a generic constant \(C\) such that \(f \leq Cg\).

### 3 The Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions and its numerical scheme

In this section, we first summarize the mass conservation and the energy dissipation law of the KLLM model. Then we propose the stabilized linear numerical scheme and prove the discrete energy dissipation law.

Since \(\phi\) is the phase-field order parameter in the bulk, denote its trace \(\phi|_\Gamma \doteq \psi\) as the order parameter on the boundary. In the bulk \(\Omega\), assume that \(\phi\) is a locally conserved quantity that satisfies the continuity equation

\[
\phi_t + \nabla \cdot (\phi \mathbf{u}) = 0, \quad (x, t) \in \Omega \times (0, T),
\]

where \(\mathbf{u}\) is the microscopic effective velocity.

We assume that there exists mass exchange between the bulk \(\Omega\) and the boundary \(\Gamma\), which is denoted by the flux \(J = \phi \mathbf{u}\). Assume that the mass flux is directly driven by differences between the chemical potentials in the sense that

\[
K(J \cdot \mathbf{n}) = K(\phi \mathbf{u} \cdot \mathbf{n}) = \mu - \mu_\Gamma, \quad (x, t) \in \Gamma \times (0, T),
\]

where \(K\) is a positive parameter describing the extent of mass exchange. Eq. (3.2) is the boundary condition of \(\mathbf{u}\).

Assume that the boundary dynamics is characterized by a local mass conservation law analogous to (3.1), such that

\[
\psi_t + \nabla_\Gamma \cdot (\psi \mathbf{v}) - J \cdot \mathbf{n} = 0, \quad (x, t) \in \Gamma \times (0, T),
\]

where \(\mathbf{v}\) denotes the microscopic effective tangential velocity field on the boundary \(\Gamma\). Assume that \(\Gamma\) is a closed manifold, thus, there is no need to impose any boundary condition on \(\mathbf{v}\).

The mass is conserved in the sense that

\[
\int_\Omega \phi(t) d\mathbf{x} + \int_\Gamma \psi(t) d\mathbf{S} = \int_\Omega \phi(0) d\mathbf{x} + \int_\Gamma \psi(0) d\mathbf{S}, \quad \forall t \in [0, T].
\]

To this end, integrating (3.1) over \(\Omega\), we have

\[
\frac{d}{dt} \int_\Omega \phi(\cdot, t) d\mathbf{x} + \int_\Gamma \phi \mathbf{u} \cdot \mathbf{n} d\mathbf{S} = 0, \forall t \in (0, T),
\]

where \(\frac{d}{dt}\) denotes the partial time derivative.
and integrating (3.3) over \( \Gamma \), we have

\[
\frac{d}{dt} \int_\Gamma \psi(\cdot, t) dS - \int_\Gamma J \cdot n dS = 0, \forall t \in (0, T).
\]

Combining (3.5) with (3.6) and the flux \( J = \phi u \), we obtain the total mass conservation law, see (3.4).

Then we show the energy law of the KLLM model, where the total free energy (sum of the bulk and surface free energies) is decreasing in time. Precisely, multiplying the first equation of (1.15) by \( \mu \) and integrating over \( \Omega \), we get

\[
(\phi_t, \mu)_\Omega = (\Delta \mu, \mu)_\Omega = (\partial_{\mu \mu}, \mu)_\Gamma - \|\nabla \mu\|_{L^2(\Omega)}^2.
\]

Since

\[
(\phi_t, \mu)_\Omega = (\phi_t, -\varepsilon \Delta \phi + \frac{1}{\varepsilon} F'(\phi))_\Omega,
\]

\[
(\phi_t, -\varepsilon \Delta \phi)_\Omega = -(\varepsilon \partial_{\mu \phi}, \phi_t) + \frac{\varepsilon}{2} \frac{d}{dt} \int_\Omega |\nabla \phi|^2 d\Omega,
\]

we arrive that

\[
\frac{d}{dt} \int_\Omega \frac{1}{\varepsilon} F(\phi) d\Omega + \frac{\varepsilon}{2} \int_\Omega |\nabla \phi|^2 d\Omega - (\varepsilon \partial_{\mu \phi}, \phi_t) = (\partial_{\mu \mu}, \mu)_\Gamma - \|\nabla \mu\|_{L^2(\Omega)}^2.
\]

Multiplying the boundary equation in (1.15) by \( \mu_t \) and integrating over \( \Gamma \), we get

\[
(\psi_t, \mu_t)_\Gamma = (\Delta_{\Gamma} \mu_t, \mu_t)_\Gamma - (\partial_{\mu \mu}, \mu)_\Gamma = -\|\nabla_{\Gamma} \mu_t\|_{L^2(\Gamma)}^2 - (\partial_{\mu \mu}, \mu_t)_\Gamma.
\]

Since

\[
(\psi_t, \mu_t)_\Gamma = (\psi_t, -\delta \kappa \Delta_{\Gamma} \psi + \frac{1}{\delta} G'(\psi) + \varepsilon \partial_{\mu \phi})_\Gamma,
\]

\[
(\psi_t, -\delta \kappa \Delta_{\Gamma} \psi)_\Gamma = \frac{\delta \kappa}{2} \frac{d}{dt} \int_\Gamma |\nabla_{\Gamma} \psi|^2 dS,
\]

we arrive that

\[
\frac{d}{dt} \int_\Gamma \frac{1}{\delta} G(\psi) dS + \frac{\delta \kappa}{2} \int_\Gamma |\nabla_{\Gamma} \psi|^2 dS + (\varepsilon \partial_{\mu \phi}, \psi_t)_\Gamma = - (\partial_{\mu \mu}, \mu_t)_\Gamma - \|\nabla_{\Gamma} \mu_t\|_{L^2(\Gamma)}^2.
\]

Adding (3.7) and (3.8) together, we get

\[
\frac{d}{dt} \left( \int_\Gamma \frac{1}{\varepsilon} F(\phi) dS + \frac{\delta \kappa}{2} \int_\Gamma |\nabla \phi|^2 dS + \int_\Gamma \frac{1}{\delta} G(\psi) + \frac{\delta \kappa}{2} |\nabla_{\Gamma} \psi|^2 dS \right) = -\|\nabla \mu\|_{L^2(\Omega)}^2 - \|\nabla_{\Gamma} \mu_t\|_{L^2(\Gamma)}^2 + (\partial_{\mu \mu}, \mu - \mu_t)_\Gamma
\]

\[
= -\|\nabla \mu\|_{L^2(\Omega)}^2 - \|\nabla_{\Gamma} \mu_t\|_{L^2(\Gamma)}^2 - K\|\partial_{\mu \mu}\|_{L^2(\Gamma)}^2.
\]
Since $K > 0$, we arrive at
\[
\frac{d}{dt} \left( \int_\Omega \frac{1}{e} F(\phi) + \frac{\mu}{2} |\nabla \phi|^2 \, dx + \int_\Gamma \frac{1}{\delta} G(\psi) + \frac{\delta \kappa}{2} |\nabla_\Gamma \psi|^2 \, dS \right) \leq 0,
\]
namely,
\[
\frac{d}{dt} \left[ E^{\text{bulk}}(\phi) + E^{\text{surf}}(\psi) \right] \leq 0.
\]

Now we present the numerical scheme for the KLLM model (namely, Eq. (1.15)). The scheme can be written as follows,

\[
\begin{align*}
\phi^{n+1} - \phi^n &= \Delta \mu^{n+1}, \quad \text{in } \Omega, \\
\mu^{n+1} &= -\varepsilon \Delta \phi^{n+1} + \frac{1}{e} F'(\phi^n) + s_1(\phi^{n+1} - \phi^n), \quad \text{in } \Omega, \\
K \partial_n \mu^{n+1} &= \mu^{n+1} - \mu^{n+1}, \quad \text{on } \Gamma, \\
\phi^{n+1} \big|_\Gamma &= \psi^{n+1}, \quad \text{on } \Gamma, \\
\psi^{n+1} - \psi^n &= \Delta \Gamma \psi^{n+1} - \partial_n \mu^{n+1}, \quad \text{on } \Gamma, \\
\mu^{n+1} \big|_\Gamma &= -\delta \kappa \Delta \psi^{n+1} + \frac{1}{\delta} G'(\psi^n) + \varepsilon \partial_n \phi^{n+1} + s_2(\psi^{n+1} - \psi^n), \quad \text{on } \Gamma.
\end{align*}
\]

Here, $T$ is an arbitrary and fixed time, $N$ is the number of time steps and $\tau = T/N$ is the step size.

**Remark 3.1.** The parameters $s_1, s_2 > 0$. And the stabilization terms $s_1(\phi^{n+1} - \phi^n)$ and $s_2(\psi^{n+1} - \psi^n)$ are added in the bulk and on the boundary to enhance the stability, respectively.

**Remark 3.2.** For the Liu-Wu model, we need to modify Eq. (3.12) to be
\[
\partial_n \mu^{n+1} = 0, \quad \text{on } \Gamma,
\]
and the last term $\partial_n \mu^{n+1}$ in (3.14) vanishes. For the GMS model, Eq. (3.12) is modified to be
\[
\mu^{n+1} \big|_\Gamma = \mu^{n+1}, \quad \text{on } \Gamma.
\]

We have the energy stability as follows.

**Theorem 3.3.** Assume that $s_1 \geq \frac{1}{2\varepsilon} \max_{\xi \in \mathbb{R}} F''(\xi), s_2 \geq \frac{1}{2\delta} \max_{\eta \in \mathbb{R}} G''(\eta)$, the scheme (3.10)-(3.15) is energy stable in the sense that

\[
\frac{E(\phi^{n+1}, \psi^{n+1}) - E(\phi^n, \psi^n)}{\tau} \leq -\|\nabla \mu^{n+1}\|_{L^2(\Omega)}^2 - \|\nabla_\Gamma \mu^{n+1}\|_{L^2(\Gamma)}^2 - \frac{1}{K} \|\mu^{n+1} - \mu^{n+1}\|_{L^2(\Gamma)}^2,
\]

where

\[
E(\phi, \psi) = \int_\Omega \frac{1}{e} F(\phi) + \frac{\mu}{2} |\nabla \phi|^2 \, dx + \int_\Gamma \frac{1}{\delta} G(\psi) + \frac{\delta \kappa}{2} |\nabla_\Gamma \psi|^2 \, dS
\]
Proof. By taking inner product of (3.10) with $\mu^{n+1}$ in $\Omega$, we have

$$
\langle \frac{\phi^{n+1} - \phi^n}{\tau}, \mu^{n+1} \rangle_\Omega = (\Delta \mu^{n+1}, \mu^{n+1})_\Omega = (\partial_n \mu^{n+1}, \mu^{n+1})_\Gamma - \|\nabla \mu^{n+1}\|_{L^2(\Omega)}^2. 
$$

For the boundary integral term, by using (3.12), we have

$$
(\partial_n \mu^{n+1}, \mu^{n+1})_\Gamma = \frac{1}{K}(\mu_{\Omega}^{n+1} - \mu^{n+1}, \mu^{n+1})_\Gamma.
$$

By using (3.11), we have

$$
\langle \frac{\phi^{n+1} - \phi^n}{\tau}, \mu^{n+1} \rangle_\Omega = \langle \frac{\phi^{n+1} - \phi^n}{\tau}, -\varepsilon \Delta \phi^{n+1} + \frac{1}{\varepsilon} F'(\phi^n) + s_1(\phi^{n+1} - \phi^n) \rangle_\Omega,
$$

and

$$
\langle \frac{\phi^{n+1} - \phi^n}{\tau}, -\varepsilon \Delta \phi^{n+1} \rangle_\Omega = -\varepsilon (\partial_n \phi^{n+1}, \phi^{n+1} - \phi^n)_\Gamma + \varepsilon (\nabla \phi^{n+1}, \nabla \phi^{n+1} - \nabla \phi^n)_\Omega.
$$

For the boundary integral term in (3.20), by taking the inner product of (3.14) with $\mu^{n+1}_\Gamma$ on $\Gamma$, we obtain

$$
(\frac{\psi^{n+1} - \psi^n}{\tau}, \mu^{n+1}_\Gamma)_\Gamma = (\Delta \mu^{n+1}_\Gamma, \mu^{n+1}_\Gamma)_\Gamma - (\partial_n \mu^{n+1}_\Gamma, \mu^{n+1}_\Gamma)_\Gamma
= -\|\nabla \mu^{n+1}_\Gamma\|^2_{L^2(\Gamma)} - (\partial_n \mu^{n+1}_\Gamma, \mu^{n+1}_\Gamma)_\Gamma.
$$

By using (3.15), we have

$$
(\frac{\psi^{n+1} - \psi^n}{\tau}, \mu^{n+1}_\Gamma)_\Gamma = (\frac{\psi^{n+1} - \psi^n}{\tau}, -\delta_k \Delta \mu^{n+1}_\Gamma + \frac{1}{\delta} G'(\phi^n) + \varepsilon \partial_n \phi^{n+1} + s_2(\phi^{n+1} - \phi^n))_\Gamma,
$$

and

$$
(\frac{\psi^{n+1} - \psi^n}{\tau}, -\delta_k \Delta \mu^{n+1}_\Gamma)_\Gamma = (\frac{\nabla \mu^{n+1}_\Gamma - \nabla \mu^{n}_\Gamma}{\tau}, \delta_k \nabla \mu^{n+1}_\Gamma)_\Gamma.
$$

To handle the nonlinear term associated with $F'$ and $G'$ in (3.19) and (3.22), we need the following identities

$$
F'(\phi^n)(\phi^{n+1} - \phi^n) = F(\phi^{n+1}) - F(\phi^n) - \frac{F''(\eta)}{2}(\phi^{n+1} - \phi^n)^2,
$$

$$
G'(\phi^n)(\phi^{n+1} - \phi^n) = G(\phi^{n+1}) - G(\phi^n) - \frac{G''(\zeta)}{2}(\phi^{n+1} - \phi^n)^2.
$$

Combining the equations mentioned above, we get

$$
\langle \frac{\phi^{n+1} - \phi^n}{\tau}, \mu^{n+1} \rangle_\Omega + (\frac{\psi^{n+1} - \psi^n}{\tau}, \mu^{n+1}_\Gamma)_\Gamma
= (\partial_n \mu^{n+1}, \mu^{n+1})_\Gamma - ||\nabla \mu^{n+1}\|^2_{L^2(\Omega)} - ||\nabla \mu^{n+1}_\Gamma||^2_{L^2(\Gamma)} - (\partial_n \mu^{n+1}, \mu^{n+1})_\Gamma
= -||\nabla \mu^{n+1}\|^2_{L^2(\Omega)} - ||\nabla \mu^{n+1}_\Gamma||^2_{L^2(\Gamma)} - \frac{1}{K}||\mu^{n+1} - \mu^{n+1}_\Gamma||^2_{L^2(\Gamma)},
$$

$$
(\frac{\psi^{n+1} - \psi^n}{\tau}, \mu^{n+1}_\Gamma)_\Gamma
= (\Delta \mu^{n+1}_\Gamma, \mu^{n+1}_\Gamma)_\Gamma - (\partial_n \mu^{n+1}_\Gamma, \mu^{n+1}_\Gamma)_\Gamma
= -||\nabla \mu^{n+1}_\Gamma||^2_{L^2(\Gamma)} - (\partial_n \mu^{n+1}_\Gamma, \mu^{n+1}_\Gamma)_\Gamma.
$$
and
\[
\begin{align*}
\left( \frac{\phi^{n+1} - \phi^n}{\tau}, \mu^{n+1} \right) - (\xi^{n+1} - \xi^n) + \left( \frac{\psi^{n+1} - \psi^n}{\tau}, \phi^{n+1} \right) & = 0. \\
\left( \frac{\phi^{n+1} - \phi^n}{\tau}, \nabla \phi^{n+1} - \nabla \phi^n \right) + \frac{1}{\varepsilon} (F'(\phi^n) - F'(\phi^n)) & = \frac{1}{\varepsilon} (F(\phi^{n+1}) - F(\phi^n)) \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (F''(\xi^n) - F''(\xi^n)) \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n)
\end{align*}
\]
Thus, we have
\[
\begin{align*}
\left( \frac{\phi^{n+1} - \phi^n}{\tau}, \mu^{n+1} \right) - (\xi^{n+1} - \xi^n) + \left( \frac{\psi^{n+1} - \psi^n}{\tau}, \phi^{n+1} \right) & = 0. \\
& = -\frac{1}{\varepsilon} [E(\phi^{n+1}, \psi^{n+1}) - E(\phi^n, \psi^n)] - \frac{1}{\varepsilon} [E(\phi^{n+1}, \psi^{n+1}) - E(\phi^n, \psi^n)] \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) \\
& + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n) + \frac{1}{\varepsilon} (\phi^{n+1} - \phi^n)
\end{align*}
\]

Therefore, under the conditions that
\[
s_1 \geq \frac{1}{2\varepsilon} \max_{\xi \in \mathbb{R}} F''(\xi)
\]
and
\[
s_2 \geq \frac{1}{2\delta} \max_{\eta \in \mathbb{R}} G''(\eta),
\]
we have
\[
\frac{1}{\tau} [E(\phi^{n+1}, \psi^{n+1}) - E(\phi^n, \psi^n)] \leq 0,
\]

namely, the scheme (3.10)-(3.15) is energy stable. \quad \square
4 Error estimates for the stabilized semi-discrete scheme

In this section, we establish the error estimates for the phase functions \( \phi \) and \( \psi \) for the numerical scheme (3.10)-(3.15). During the estimate, the mathematics induction is utilized and the trace theorem is applied to estimate the boundary terms.

Assume that the Lipschitz properties hold for \( F'' \) and \( G'' \), and \( F'' \) and \( G'' \) are bounded:

\[
\begin{align*}
\text{(4.1)} \quad \max_{\phi \in \mathbb{R}} |F''(\phi)| &\leq L_1, \\
\text{(4.2)} \quad \max_{\psi \in \mathbb{R}} |G''(\psi)| &\leq L_2,
\end{align*}
\]

which are necessary for error estimates.

Remark 4.1. One example of the functionals \( F \) and \( G \), satisfying the assumptions mentioned above, is the modified double-well potential:

\[
\text{(4.3)} \quad F(\phi) = G(\phi) = \begin{cases} 
(\phi - 1)^2 & \phi > 1, \\
\frac{1}{4}(\phi^2 - 1)^2 & -1 \leq \phi < 1, \\
(\phi + 1)^2 & \phi \leq -1.
\end{cases}
\]

The Lipschitz property holds for \( F'' \) and \( G'' \) and

\[
\text{(4.4)} \quad \max_{\phi \in \mathbb{R}} |F''(\phi)| = \max_{\psi \in \mathbb{R}} |G''(\psi)| \leq 2.
\]

The PDE system (1.15) can be rewritten as the following truncated form,

\[
\begin{align*}
\phi(t^{n+1}) - \phi(t^n) &= \Delta \mu(t^{n+1}) + R_{\phi}^{n+1}, \quad \text{in } \Omega, \\
\mu(t^{n+1}) &= -\varepsilon \Delta \phi(t^n) + \frac{1}{\varepsilon} F'(\phi(t^n)) + s_1(t^{n+1}) - \phi(t^n) + R_{\mu}^{n+1}, \quad \text{in } \Omega, \\
K \partial_n \mu(t^{n+1}) &= \mu(\Gamma, t^{n+1}) - \mu(t^{n+1}) \quad \text{on } \Gamma, \\
\phi(t^{n+1})|_{\Gamma} &= \psi(t^{n+1}), \quad \text{on } \Gamma, \\
\psi(t^{n+1}) - \psi(t^n) &= \Delta \mu(t^{n+1}) - \partial_n \mu(t^{n+1}) + R_{\psi}^{n+1}, \quad \text{on } \Gamma, \\
\mu(\Gamma, t^{n+1}) &= -\delta \kappa \Delta \phi(t^{n+1}) + \frac{1}{\delta} G'(\psi(t^n)) + \varepsilon \partial_n \phi(t^{n+1}) \\
&\quad + s_2(t^{n+1}) - \psi(t^n) + R_{\mu}^{n+1}, \quad \text{on } \Gamma,
\end{align*}
\]

where

\[
\begin{align*}
R_{\phi}^{n+1} &= \frac{\phi(t^{n+1}) - \phi(t^n)}{\tau} - \phi(t^{n+1}), \\
R_{\psi}^{n+1} &= \frac{\psi(t^{n+1}) - \psi(t^n)}{\tau} - \psi(t^{n+1}),
\end{align*}
\]
Obviously, we have \( e^n_\phi = \phi(t^n) - \phi^n \), \( e^n_\mu = \mu(t^n) - \mu^n \), \( e^n_\psi = \psi(t^n) - \psi^n \), \( e^n_\Gamma = \Gamma(t^n) - \Gamma^n \). The corresponding sequence of error functions are denoted as \( e_{\phi,\tau} \), \( e_{\psi,\tau} \), \( e_{\mu,\tau} \) and \( e_{\Gamma,\tau} \).

Thus we can establish the estimates for the scheme (3.10)-(3.15) as follows.
**Theorem 4.3.** Provided that the exact solutions are sufficiently smooth, then for $0 \leq m \leq \left\lfloor \frac{T}{\tau} \right\rfloor - 1$, the solution $(\phi^m, \psi^m)$ of the scheme (3.10)-(3.15) satisfy the following error estimates

\begin{equation}
\|e_{\phi,\tau}\|_{n^1(H^{1}Ω)} + \|e_{\psi,\tau}\|_{n^1(H^{1}(Γ))} \leq \tau.
\end{equation}

**Proof.** We use the mathematical induction to prove this theorem. When $m = 0$, we have $e_0^\phi = e_0^\psi = \nabla e_0^\phi = \nabla e_0^\psi = 0$. Obviously, (4.25) holds. Assuming that (4.25) holds for all $n \leq m$, we need to show that (4.25) holds for $e_{\phi,\tau}^{m+1}$ and $e_{\psi,\tau}^{m+1}$. In the following, we use the letter $C$ to denote generic positive constants independent of $\tau, n, m$ and $T$, which can change values from line to line.  

For each $n \leq m$, by taking the $L^2$ inner product of (4.18) with $\tau e_{\phi,\tau}^{n+1}$ in $Ω$, we obtain

\begin{equation}
(e_{\phi}^{n+1} - e_{\phi}^{n}, e_{\mu}^{n+1})_Ω + \tau \|
abla e_{\psi}^{n+1}\|_{Ω}^2 = \tau (\partial_n e_{\phi}^{n+1}, e_{\mu}^{n+1})_Γ + \tau (R_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ.
\end{equation}

By taking the $L^2$ inner product of (4.18) with $\varepsilon e_{\phi}^{n+1}$ in $Ω$, we obtain

\begin{equation}
\frac{ε}{2} (\|e_{\phi}^{n+1}\|_{Ω}^2 - \|e_{\phi}^{n}\|_{Ω}^2 + \|e_{\phi}^{n+1} - e_{\phi}^{n}\|_{Ω}^2) = -ε \tau (\nabla e_{\phi}^{n+1}, \nabla e_{\phi}^{n+1})_Ω + \varepsilon \tau (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ + \varepsilon \tau (R_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ.
\end{equation}

By taking the $L^2$ inner product of (4.19) with $-e_{\phi}^{n+1} - e_{\phi}^{n}$ in $Ω$, we obtain

\begin{equation}
-e_{\phi}^{n+1} + e_{\phi}^{n} + \frac{ε}{2} (\|\nabla e_{\phi}^{n+1}\|_{Ω}^2 - \|\nabla e_{\phi}^{n}\|_{Ω}^2 + \|\nabla e_{\phi}^{n+1} - \nabla e_{\phi}^{n}\|_{Ω}^2) + s_1 \|e_{\phi}^{n+1} - e_{\phi}^{n}\|_{Ω}^2 = \varepsilon (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ - \frac{ε}{2} (F'(\phi(t^n)) - F'(\phi^n), e_{\phi}^{n+1} - e_{\phi}^{n})_Ω - (R_{\phi}^{n+1}, e_{\phi}^{n+1} - e_{\phi}^{n})_Ω.
\end{equation}

By combining the equations above, we derive

\begin{equation}
\frac{ε}{2} (\|\nabla e_{\phi}^{n+1}\|_{Ω}^2 - \|\nabla e_{\phi}^{n}\|_{Ω}^2 + \|\nabla e_{\phi}^{n+1} - \nabla e_{\phi}^{n}\|_{Ω}^2) + s_1 \|e_{\phi}^{n+1} - e_{\phi}^{n}\|_{Ω}^2 + \varepsilon \tau \|
abla e_{\phi}^{n+1}\|_{Ω}^2 \\
= \tau (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ + \tau (R_{\phi}^{n+1}, e_{\phi}^{n+1})_Ω - ε \tau (\nabla e_{\phi}^{n+1}, \nabla e_{\phi}^{n+1})_Ω + \varepsilon \tau (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ + \varepsilon \tau (R_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ + \varepsilon (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ - e_{\phi}^{n})_Γ \nonumber \\
- \frac{ε}{2} (F'(\phi(t^n)) - F'(\phi^n), e_{\phi}^{n+1} - e_{\phi}^{n})_Ω - (R_{\phi}^{n+1}, e_{\phi}^{n+1} - e_{\phi}^{n})_Ω.
\end{equation}

For the boundary term, by taking the $L^2$ inner product of (4.22) with $\tau e_{\phi,\tau}^{n+1}$ on $Γ$, we obtain

\begin{equation}
(e_{\phi}^{n+1} - e_{\phi}^{n}, e_{\mu}^{n+1})_Γ + \tau \|
abla e_{\psi}^{n+1}\|_{Γ}^2 = \tau (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ = (R_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ.
\end{equation}

By taking the $L^2$ inner product of (4.22) with $\varepsilon e_{\phi}^{n+1}$ on $Γ$, we obtain

\begin{equation}
\frac{ε}{2} (\|e_{\phi}^{n+1}\|_{Γ}^2 - \|e_{\phi}^{n}\|_{Γ}^2 + \|e_{\phi}^{n+1} - e_{\phi}^{n}\|_{Γ}^2) = -ε \tau (\nabla e_{\phi}^{n+1}, \nabla e_{\phi}^{n+1})_Γ + \varepsilon \tau (\partial_n e_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ + \varepsilon \tau (R_{\phi}^{n+1}, e_{\phi}^{n+1})_Γ.
\end{equation}
where the boundary terms vanish due to $\Gamma$ is closed. By taking the $L^2$ inner product of (4.23) with $-(e^{n+1}_\psi - e^n_\psi)$ on $\Gamma$, we obtain
\begin{align*}
- (e^{n+1}_\psi, e^{n+1}_\psi - e^n_\psi)_{\Gamma} + \frac{\delta \kappa}{2} (\|\nabla \Gamma e^{n+1}_\psi\|^2_{\Gamma} - \|\nabla \Gamma e^n_\psi\|^2_{\Gamma}) + \|\nabla \Gamma e^{n+1}_\psi - \nabla \Gamma e^n_\psi\|^2_{\Gamma}) + s_2 \|e^{n+1}_\psi - e^n_\psi\|^2_{\Gamma}
= -\varepsilon (\partial_n e^{n+1}_\psi, e^{n+1}_\psi - e^n_\psi)_{\Gamma} - \frac{1}{\delta} (G'(\psi(t^n)) - G'(\psi^n), e^{n+1}_\psi - e^n_\psi)_{\Gamma} - (R^{n+1}_\Gamma, e^{n+1}_\psi - e^n_\psi)_{\Gamma}.
\end{align*}

By combining the equations above, we derive
\begin{align*}
\frac{\delta \kappa}{2} (\|\nabla \Gamma e^{n+1}_\psi\|^2_{\Gamma} - \|\nabla \Gamma e^n_\psi\|^2_{\Gamma}) + \|\nabla \Gamma e^{n+1}_\psi - \nabla \Gamma e^n_\psi\|^2_{\Gamma}) + s_2 \|e^{n+1}_\psi - e^n_\psi\|^2_{\Gamma}
+ \frac{\varepsilon}{2} (\|e^{n+1}_\psi\|^2 - \|e^n_\psi\|^2 + \|e^{n+1}_\psi - e^n_\psi\|^2) + \tau \|\nabla \Gamma e^{n+1}_\psi\|^2_{\Gamma} + \tau (\partial_n e^{n+1}_\psi, e^{n+1}_\psi)_{\Gamma}

= \tau (R^{n+1}_\psi, e^{n+1}_\psi)_{\Omega} - \varepsilon \tau (\nabla \Gamma e^{n+1}_\psi, \nabla \Gamma e^n_\psi)_{\Omega} - \varepsilon \tau (\partial_n e^{n+1}_\psi, e^n_\psi)_{\Omega}

+ \tau (R^{n+1}_e, e^{n+1}_e)_{\Omega} - \frac{1}{\delta} (G'(\psi(t^n)) - G'(\psi^n), e^{n+1}_\psi - e^n_\psi)_{\Gamma}

- \varepsilon (\partial_n e^{n+1}_\psi, e^{n+1}_\psi - e^n_\psi)_{\Gamma} - (R^{n+1}_\Gamma, e^{n+1}_\psi - e^n_\psi)_{\Gamma}.
\end{align*}

By combining (4.26) and (4.27) together, we derive
\begin{align*}
\frac{\delta \kappa}{2} (\|\nabla \Gamma e^{n+1}_\phi\|^2_{\Omega} - \|\nabla \Gamma e^n_\phi\|^2_{\Omega}) + \|\nabla \Gamma e^{n+1}_\phi - \nabla \Gamma e^n_\phi\|^2_{\Omega}) + \frac{\varepsilon}{2} (\|e^{n+1}_\phi\|^2_{\Omega} - \|e^n_\phi\|^2_{\Omega} + \|e^{n+1}_\phi - e^n_\phi\|^2)

+ \frac{\delta \kappa}{2} (\|\nabla \Gamma e^{n+1}_e\|^2_{\Gamma} - \|\nabla \Gamma e^n_e\|^2_{\Gamma}) + \|\nabla \Gamma e^{n+1}_e - \nabla \Gamma e^n_e\|^2_{\Gamma})

+ \frac{\varepsilon}{2} (\|e^{n+1}_\psi\|^2 - \|e^n_\psi\|^2 + \|e^{n+1}_\psi - e^n_\psi\|^2) + s_1 \|e^{n+1}_\psi - e^n_\psi\|^2_{\Omega} + s_2 \|e^{n+1}_\psi - e^n_\psi\|^2_{\Gamma}

+ \tau \|\nabla e^{n+1}_\psi\|^2_{\Omega} + \tau (\nabla \Gamma e^{n+1}_\psi)_{\Omega} + K \tau (\partial_n e^{n+1}_\psi)_{\Omega}^2

= \varepsilon \tau (R^{n+1}_\phi, e^{n+1}_\phi)_{\Omega} + \tau (R^{n+1}_e, e^{n+1}_e)_{\Omega} \quad (:= \text{term A}_1)

+ \tau (R^{n+1}_\psi, e^{n+1}_\psi)_{\Omega} + \tau (R^{n+1}_\psi, e^{n+1}_\psi)_{\Gamma} \quad (:= \text{term A}_2)

- \varepsilon \tau (\nabla e^{n+1}_\psi, \nabla e^{n+1}_\psi)_{\Omega} - \varepsilon \tau (\nabla \Gamma e^{n+1}_\psi, \nabla \Gamma e^n_\psi)_{\Omega} \quad (:= \text{term A}_3)

- \frac{1}{\varepsilon} (F'(\phi(t^n)) - F'(\phi^n), e^{n+1}_\phi - e^n_\phi)_{\Omega} - (R^{n+1}_\mu, e^{n+1}_\phi - e^n_\phi)_{\Omega} \quad (:= \text{term A}_4)

- \frac{1}{\delta} (G'(\psi(t^n)) - G'(\psi^n), e^{n+1}_\phi - e^n_\phi)_{\Gamma} - (R^{n+1}_\Gamma, e^{n+1}_\phi - e^n_\phi)_{\Gamma} \quad (:= \text{term A}_5).
\end{align*}

For the term A1, we have
\begin{align*}
\varepsilon \tau (R^{n+1}_\phi, e^{n+1}_\phi)_{\Omega} + \tau (R^{n+1}_\psi, e^{n+1}_\psi)_{\Gamma}
\leq \varepsilon \tau \|R^{n+1}_\phi\|_{\Omega} \|e^{n+1}_\phi\|_{\Omega} + \varepsilon \tau \|R^{n+1}_\psi\|_{\Gamma} \|e^{n+1}_\psi\|_{\Gamma}
\leq \frac{\varepsilon \tau}{2} \|e^{n+1}_\phi\|^2_{\Omega} + \frac{\varepsilon \tau}{2} \|e^{n+1}_\psi\|^2_{\Gamma} + \varepsilon \tau^3,
\end{align*}

where we use the estimates for the truncation terms $R^{n+1}_\phi$ and $R^{n+1}_\psi$.

In this section, we define $H^n = F'(\phi(t^n)) - F'(\phi^n)$ for simplicity. It can be rewritten as
\begin{align*}
H^n = e^n_\phi \int_0^1 F''(s\phi(t^n)) + (1 - s)\phi^n)ds.
\end{align*}
Then we have \( \|H^n\|_\Omega \leq \|e^{\phi}_n\|_\Omega \) since \( F'' \) is bounded. By taking the gradient of \( H^n \), we have

\[
\nabla H^n = F''(\phi(t^n))\nabla \phi(t^n) - F''(\phi(t^n))\nabla \phi^n = (F''(\phi(t^n)) - F''(\phi(t^n)))\nabla \phi(t^n) + F''(\phi(t^n))\nabla e^\phi_n.
\]

Since \( F'' \) is bounded and Lipschitz and \( \phi \in L^\infty(0, T; H^{m_1}(\Omega)) \) with \( m_1 \) sufficiently large, we have

\[
\|\nabla H^n\|_\Omega \leq \|e^{\phi}_n\|_\Omega + \|\nabla e^\phi_n\|_\Omega.
\]

Similarly, we define \( \tilde{H}^n = G'(\psi(t^n)) - G'(\psi^n) \). Since \( G'' \) is bounded and Lipschitz and \( \psi \in L^\infty(0, T; H^{m_{m-1/2}}(\Gamma)) \) with \( m_1 \) sufficiently large, we have

\[
\|\tilde{H}^n\|_\Gamma \leq \|e^{\psi}_n\|_\Gamma, \quad \|\nabla_{\Gamma}\tilde{H}^n\|_\Gamma \leq \|e^{\psi}_n\|_\Gamma + \|\nabla_{\Gamma} e^\psi_n\|_\Gamma.
\]

For the term \( A_2 \), we have

\[
\tau(R^{n+1}_\phi, e^{n+1}_\phi) + \tau(R^{n+1}_\psi, e^{n+1}_\psi)\Gamma
\]

\[
= \tau(R^{n+1}_\phi, -\varepsilon\Delta e^{n+1}_\phi + \frac{1}{e}H^n + s_1(e^{n+1}_\phi - e^n_\phi) + R^{n+1}_\phi)\Omega
\]

\[
+ \tau(R^{n+1}_\psi, \delta\varepsilon_e \nabla e^{n+1}_\psi + s_2(e^{n+1}_\phi - e^n_\phi) + R^{n+1}_\psi)\Gamma
\]

\[
= \varepsilon\tau(\nabla R^{n+1}_\phi, \nabla e^{n+1}_\phi)\Omega - \varepsilon\tau(\nabla R^{n+1}_\psi, \nabla e^{n+1}_\psi)\Gamma + \frac{\tau}{\varepsilon}(H^n, R^{n+1}_\phi)\Omega + s_1\tau(R^{n+1}_\phi, e^{n+1}_\phi - e^n_\phi)\Omega
\]

\[
+ \tau(R^{n+1}_\psi, R^{n+1}_\psi)\Omega + \tau(\varepsilon(\nabla R^{n+1}_\phi, \nabla e^{n+1}_\psi)\Omega + \frac{\tau}{\varepsilon}(H^n, R^{n+1}_\phi)\Omega + s_1\tau(R^{n+1}_\phi, e^{n+1}_\phi - e^n_\phi)\Omega
\]

\[
+ s_2\tau(R^{n+1}_\psi, R^{n+1}_\psi)\Gamma + \tau(\varepsilon(\nabla R^{n+1}_\phi, \nabla e^{n+1}_\psi)\Gamma + \frac{\tau}{\varepsilon}(H^n, R^{n+1}_\phi)\Gamma)
\]

\[
\leq \varepsilon\tau(\nabla R^{n+1}_\phi, \nabla e^{n+1}_\phi)\Omega + s_1\tau(R^{n+1}_\phi, e^{n+1}_\phi - e^n_\phi)\Omega
\]

\[
+ \tau(R^{n+1}_\phi, R^{n+1}_\phi)\Omega + \tau(\varepsilon(\nabla R^{n+1}_\phi, \nabla e^{n+1}_\psi)\Omega + s_1\tau(R^{n+1}_\phi, e^{n+1}_\phi - e^n_\phi)\Omega
\]

\[
+ \tau(R^{n+1}_\psi, R^{n+1}_\psi)\Gamma + \tau(\varepsilon(\nabla R^{n+1}_\phi, \nabla e^{n+1}_\psi)\Gamma + s_1\tau(R^{n+1}_\phi, e^{n+1}_\phi - e^n_\phi)\Omega
\]

\[
\leq \tau(\nabla e^{n+1}_\phi, R^{n+1}_\phi)\Omega + \tau(\nabla e^{n+1}_\psi, R^{n+1}_\psi)\Gamma
\]

\[
\leq C\tau + \frac{\varepsilon}{2}\|\nabla e^{n+1}\|_\Omega + C\tau\|e^{n+1}\|_\Omega + \frac{s_1\tau}{2}\|e^{n+1}_\phi - e^n_\phi\|_\Omega
\]

\[
+ \frac{\tau\delta\varepsilon_e}{2}\|\nabla e^{n+1}\|_\Omega + \tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Gamma
\]

\[
\leq 2\varepsilon\tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Omega + \frac{\tau}{8}\|\nabla e^{n+1}_\phi\|_\Omega + 2\varepsilon\tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Gamma
\]

\[
+ \frac{\tau}{8}\|\nabla e^{n+1}_\phi\|_\Gamma.
\]

where we use the estimates for \( H^n \) and \( \tilde{H}^n \) and the truncation terms \( R^{n+1}_\phi, R^{n+1}_\psi, R^{n+1}_\mu \) and \( R^{n+1}_\Gamma \). The fact that \( R^{n+1}_\phi |_{\Gamma} = \gamma(R^{n+1}_\phi) = R^{n+1}_\psi \) is also applied, where \( \gamma \) is the trace operator.

We estimate \( A_3 \) as follows

\[
- \varepsilon\tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Omega - \varepsilon\tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Gamma
\]

\[
\leq 2\varepsilon\tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Omega + \frac{\tau}{8}\|\nabla e^{n+1}_\phi\|_\Omega + 2\varepsilon\tau(\nabla e^{n+1}_\phi, \nabla e^{n+1}_\psi)\Gamma + \frac{\tau}{8}\|\nabla e^{n+1}_\phi\|_\Gamma.
\]
For the first term in $A_4$, we have

\begin{equation}
- \frac{1}{\varepsilon} (F'(\phi(\eta)) - F'(\phi^n), e^\eta_{\phi} - e^n_{\phi})_\Omega \\
= - \frac{\tau}{\varepsilon} (H^n, e^\eta_{\phi} - e^n_{\phi})_\Omega = - \frac{\tau}{\varepsilon} (H^n, \Delta e^\eta_{\phi} + R^\eta_{\phi})_\Omega \\
= \frac{\tau}{\varepsilon} (\nabla H^n, \nabla e^\eta_{\phi})_\Omega - \frac{\tau}{\varepsilon} (H^n, \partial_ne^\eta_{\phi})_\Gamma - \frac{\tau}{\varepsilon} (H^n, R^\eta_{\phi})_\Omega \\
\leq \frac{\tau}{\varepsilon} \|\nabla H^n\|_\Omega \|\nabla e^\eta_{\phi}\|_\Omega + \frac{\tau}{\varepsilon} \|H^n\|_\Gamma \|\partial_ne^\eta_{\phi}\|_\Gamma + \frac{\tau}{\varepsilon} \|H^n\|_\Omega \|R^\eta_{\phi}\|_\Omega.
\end{equation}

Applying the trace theorem,

\[ \|H^n\|_\Gamma = \|\gamma H^n\|_\Gamma \leq \|H^n\|_{H^1(\Omega)} \leq \|H^n\|_\Omega + \|\nabla H^n\|_\Omega \leq \|e^n_{\phi}\|_\Omega + \|\nabla e^n_{\phi}\|_\Omega \leq \tau, \]

where we use the assumption that $e^n_{\phi}$ satisfies the error estimate (4.25), we obtain

\begin{equation}
\begin{aligned}
&- \frac{1}{\varepsilon} (H^n, e^\eta_{\phi} - e^n_{\phi})_\Omega \\
&\leq C \tau (\|e^\eta_{\phi}\|_\Omega + \|\nabla e^\eta_{\phi}\|_\Omega) \|\nabla e^\eta_{\phi}\|_\Omega + C \tau (\|e^n_{\phi}\|_\Omega + \|\nabla e^n_{\phi}\|_\Omega) \|\partial_ne^\eta_{\phi}\|_\Gamma \\
&+ C \tau (\|e^n_{\phi}\|_\Omega \|R^\eta_{\phi}\|_\Omega) \\
&\leq C \tau^3 + \frac{\tau}{4} \|\nabla e^\eta_{\phi}\|_\Omega^2 + \frac{K \tau}{16} ||\partial_n e^\eta_{\phi}\|_\Omega^2.
\end{aligned}
\end{equation}

Here, we use the estimates for $H^n$ and $R^\eta_{\phi}$.

For the second term in $A_4$, we have

\begin{equation}
\begin{aligned}
&-(R^\eta_{\mu}, e^\eta_{\phi} - e^n_{\phi})_\Omega = -\tau (R^\eta_{\mu}, e^\eta_{\phi} - e^n_{\phi})_\Omega \\
&= -\tau (R^\eta_{\mu}, \Delta e^\eta_{\phi} + R^\eta_{\phi})_\Omega \\
&= \tau (\nabla R^\eta_{\mu}, \nabla e^\eta_{\phi})_\Omega - \tau (R^\eta_{\mu}, \partial_n e^\eta_{\phi})_\Gamma - \tau (R^\eta_{\mu}, R^\eta_{\phi})_\Omega \\
&\leq \tau \|\nabla R^\eta_{\mu}\|_\Omega \|\nabla e^\eta_{\phi}\|_\Omega + \tau \|R^\eta_{\mu}\|_\Gamma \|\partial_ne^\eta_{\phi}\|_\Gamma + \tau \|R^\eta_{\phi}\|_\Omega \|R^\eta_{\phi}\|_\Omega \\
&\leq 2 \tau \|\nabla R^\eta_{\mu}\|_\Omega^2 + \frac{\tau}{8} \|\nabla e^\eta_{\phi}\|_\Omega^2 + \frac{8 \tau}{K} \|R^\eta_{\mu}\|_\Gamma^2 + \frac{K \tau}{32} \|\partial_n e^\eta_{\phi}\|_\Gamma^2 \\
&+ \frac{\tau}{2} \|R^\eta_{\phi}\|_\Omega^2 + \frac{\tau}{2} \|R^\eta_{\phi}\|_\Omega^2 \\
&\leq C \tau^3 + \frac{\tau}{8} \|\nabla e^\eta_{\phi}\|_\Omega^2 + \frac{K \tau}{32} \|\partial_n e^\eta_{\phi}\|_\Gamma^2.
\end{aligned}
\end{equation}

Here, we apply the trace theorem that

\[ \|R^\eta_{\mu}\|_\Gamma = \|\gamma R^\eta_{\mu}\|_\Gamma \leq \|R^\eta_{\mu}\|_{H^1(\Omega)} \leq \|R^\eta_{\mu}\|_\Omega + \|\nabla R^\eta_{\mu}\|_\Omega \leq \tau, \]

and use the estimates for $R^\eta_{\mu}$ and $R^\eta_{\phi}$. 
Similarly, for the first term in $A_5$, we have

$$\begin{align*}
- \frac{1}{\delta}(G'(\psi(t^n)) - G'(\psi^n), e^n_{\psi} - e^n_{\phi})_\Gamma &= -\frac{\tau}{\delta}(\tilde{H}^n, \Delta \tilde{H}^n e_{\psi}^{n+1} + \partial_n e_{\mu}^{n+1} + R_{\psi}^{n+1})_\Gamma \\
&= -\frac{\tau}{\delta}(\tilde{H}^n, \Delta \tilde{H}^n e_{\psi}^{n+1} + \partial_n e_{\mu}^{n+1} + R_{\psi}^{n+1})_\Gamma \\
&= -\frac{\tau}{\delta}(\nabla_{\Gamma} \tilde{H}^n, \nabla_{\Gamma} e^{n+1})_\Gamma + \frac{\tau}{\delta}(\tilde{H}^n, \partial_n e_{\mu}^{n+1})_\Gamma - \frac{\tau}{\delta}(\tilde{H}^n, R_{\psi}^{n+1})_\Gamma \\
&\leq \frac{\tau}{\delta}(\tilde{H}^n, \nabla_{\Gamma} e^{n+1})_\Gamma + \frac{\tau}{\delta}(\tilde{H}^n, \partial_n e_{\mu}^{n+1})_\Gamma + \frac{\tau}{\delta}(\tilde{H}^n, R_{\psi}^{n+1})_\Gamma \\
&\leq C\tau(\|e_{\psi}^n\|_\Gamma + \|\nabla_{\Gamma} e_{\psi}^n\|_\Gamma||\nabla_{\Gamma} e^{n+1}\|_\Gamma + C\tau\|e_{\psi}^n\|_\Gamma||\partial_n e_{\mu}^{n+1}\|_\Gamma + C\tau\|e_{\psi}^n\|_\Gamma||R_{\psi}^{n+1}\|_\Gamma \\
&\leq C\tau^3 + \frac{\tau}{4}\|\nabla_{\Gamma} e^{n+1}\|_\Gamma^2 + \frac{K\tau}{32}\|\partial_n e_{\mu}^{n+1}\|_\Gamma^2.
\end{align*}$$

(4.39)

Here, we use the assumption that $e_{\psi}^n$ satisfies the error estimate (4.25) and use the estimate for $R_{\psi}^{n+1}$.

For the second term in $A_5$, we have

$$\begin{align*}
-(R_{\psi}^{n+1}, e_{\psi}^{n+1} - e_{\phi}^n)_\Gamma &= -\tau(R_{\psi}^{n+1}, \frac{e_{\psi}^{n+1} - e_{\phi}^n}{\tau})_\Gamma \\
&= -\tau(R_{\psi}^{n+1}, \Delta \tilde{H}^{n+1} e_{\psi}^{n+1} + \partial_n e_{\mu}^{n+1} + R_{\psi}^{n+1})_\Gamma \\
&= \tau(\nabla_{\Gamma} R_{\psi}^{n+1}, \nabla_{\Gamma} e_{\psi}^{n+1})_\Gamma + \tau(R_{\psi}^{n+1}, \partial_n e_{\mu}^{n+1})_\Gamma - \tau(R_{\psi}^{n+1}, R_{\psi}^{n+1})_\Gamma \\
&\leq 2\tau\|\nabla_{\Gamma} R_{\psi}^{n+1}\|_\Gamma^2 + \frac{\tau}{8}\|\nabla_{\Gamma} e_{\psi}^{n+1}\|_\Gamma^2 + \frac{\tau}{2}\|\partial_n e_{\mu}^{n+1}\|_\Gamma^2 + \frac{\tau}{2}\|R_{\psi}^{n+1}\|_\Gamma^2 \\
&+ \frac{8\tau}{K}\|R_{\psi}^{n+1}\|_\Gamma^2 + \frac{\tau K}{32}\|\partial_n e_{\mu}^{n+1}\|_\Gamma^2 \\
&\leq C\tau^3 + \frac{\tau}{8}\|\nabla_{\Gamma} e_{\psi}^{n+1}\|_\Gamma^2 + \frac{\tau K}{32}\|\partial_n e_{\mu}^{n+1}\|_\Gamma^2,
\end{align*}$$

where we use the estimates for $R_{\psi}^{n+1}$ and $R_{\psi}^{n+1}$.

Combine (4.28) with (4.29), (4.34), (4.35), (4.37), (4.38), (4.39) and (4.40), we derive

$$\begin{align*}
\frac{E}{2}(\|\nabla e_{\psi}^{n+1}\|_\Omega^2 - \|\nabla e_{\phi}^n\|_\Omega^2 + \|\nabla e_{\psi}^{n+1} - e_{\phi}^n\|_\Omega^2) + \frac{\delta K}{2}(\|\nabla_{\Gamma} e_{\psi}^{n+1}\|_\Gamma^2 - \|\nabla_{\Gamma} e_{\phi}^n\|_\Gamma^2 + \|\nabla_{\Gamma} e_{\psi}^{n+1} - \nabla_{\Gamma} e_{\phi}^n\|_\Gamma^2) + \frac{E}{2}(\|e_{\phi}^{n+1}\|_\Omega^2 - \|e_{\phi}^n\|_\Omega^2 + \|e_{\phi}^{n+1} - e_{\phi}^n\|_\Omega^2) \\
+ \frac{\delta K}{2}(\|\nabla_{\Gamma} e_{\phi}^{n+1}\|_\Gamma^2 - \|\nabla_{\Gamma} e_{\phi}^n\|_\Gamma^2 + \|\nabla_{\Gamma} e_{\phi}^{n+1} - \nabla_{\Gamma} e_{\phi}^n\|_\Gamma^2) \\
+ \frac{E}{2}(\|e_{\phi}^{n+1}\|_\Omega^2 - \|e_{\phi}^n\|_\Omega^2 + \|e_{\phi}^{n+1} - e_{\phi}^n\|_\Omega^2 + s_1\|e_{\psi}^{n+1} - e_{\phi}^n\|_\Omega^2 + s_2\|e_{\psi}^{n+1} - e_{\phi}^n\|_\Omega^2) \\
+ \frac{\tau}{2}\|\nabla_{\Gamma} e_{\phi}^{n+1}\|_\Gamma^2 + \frac{\tau}{2}\|\nabla_{\Gamma} e_{\phi}^n\|_\Gamma^2 + \frac{27K\tau}{32}\|\partial_n e_{\mu}^{n+1}\|_\Gamma^2 \\
&\leq \tau^3 + \tau(\|\nabla e_{\psi}^{n+1}\|_\Omega^2 + \|e_{\phi}^{n+1}\|_\Omega^2 + \|e_{\phi}^{n+1} - e_{\phi}^n\|_\Omega^2 \\
&+ \|\nabla_{\Gamma} e_{\phi}^{n+1}\|_\Gamma^2 + \|e_{\psi}^{n+1}\|_\Gamma^2 + \|e_{\psi}^{n+1} - e_{\phi}^n\|_\Gamma^2).
\end{align*}$$

(4.41)

Summing (4.41) together for $n = 0$ to $m$, we derive
5 Numerical simulations

In this section, we present numerical experiments of the KLLM model (Eq. (1.15)) by implementing the developed scheme (3.10)-(3.15). The numerical examples include the comparison with the numerical results in [18], accuracy tests with respect to the time step size, and the convergence of discrete solutions for $K \to \infty$ and $K \to 0$.

In this section, we present the numerical simulations in two dimensions. For the spatial operators, we use the second-order central finite difference method to discretize them over a uniform spatial grid.
5.1 Comparison with former work

We consider the domain \( \Omega = (0, 1)^2 \subset \mathbb{R}^2 \) and place a square shaped droplet with center at (0.5, 0.25) and the length of each side is 0.5 (see Fig. 1). The phase inside the droplet is set to be 1 and outside the droplet to be -1. \( F \) and \( G \) are chosen to be of the regular double-well form:

\[
F(x) = G(x) = \frac{1}{4}(x^2 - 1)^2, \quad x \in \mathbb{R}.
\]

And the parameters are set as \( \varepsilon = \delta = 0.02, \kappa = 0.25, s_1 = s_2 = 50 \).

We simulate the behaviour of the droplet from \( t = 0 \) to \( T = 0.2 \) with the time step \( \tau = 2 \times 10^{-4} \) and the spatial step size \( h = 0.01 \).

The evolution of the droplet is plotted in Fig. 5.1 for different \( K (K = 0, 0.1, 1, 10, \infty) \). The conservation of mass and energy is plotted in Fig. 3 and Fig. 4. In the case of the Liu-Wu model, namely, the case of \( K = \infty \), the bulk mass \( \int_{\Omega} \phi dx \) and the surface mass \( \int_{\Gamma} \psi dS \) are conserved respectively (see the green continuous line in Fig. 3). Hence, in that case, the contact area on the boundary can not change. However, the square shaped droplet still evolves to attain the circular shape with constant mean curvature (see the last row in Fig. 2). When \( K < \infty \), the conservation law of both the bulk and the boundary mass is relaxed and only the total mass \( \int_{\Omega} \phi dx + \int_{\Gamma} \psi dS \) is conserved. Therefore, the contact area is allowed to grow (see the first four rows in Fig. 2) and the droplet’s bulk mass is reduced. This phenomenon is intensifies when \( K \) is decreasing. Meanwhile, the square shaped droplet also evolves to attain the circular shape when \( K < \infty \). In addition, although we don’t explicitly show the evolution of the total mass, we emphasize here that in our numerical experiments, the total mass is conserved for different \( K (K = 0, 0.1, 1, 10, \infty) \).

The time evolutions of the total free energy is plotted in Fig. 4, indicating that our numerical scheme is energy stable. For different \( K \), we observe that an initial drop occurs for different \( K \). After the initial drop, the evolution of the free energy greatly depends on \( K \). When the energy in the case of \( K = \infty \) stops decreasing and arrives at a stationary state, the energy still decreases for \( K < \infty \). The results are consistent with the numerical results in [18].

Then we check the experimental order of convergence (EOC) of \( \phi \) for \( K \rightarrow 0 \) and \( K \rightarrow \infty \). Define \( \phi_{\text{EOC}} \) as the discrete solution under the case of \( K = 0, \phi_{\text{EOC}} \) as the solution under the case of
Numerical approximations of the Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions

Figure 2: Phase-field at $t = 0.004$, $t = 0.02$, $t = 0.1$ and $t = 0.2$. From top to bottom: $K = 0$, $K = 0.1$, $K = 1$, $K = 10$ and $K = \infty$. 
Figure 3: Time evolution of the bulk mass and the surface mass with different $K$.

Figure 4: Time evolution of the total energy with different $K$. 
Numerical approximations of the Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions

\[ \| \phi_{K_i} - \phi_0 \|_{L^2(0,T;L^2(\Omega))} \]

Table 1: Comparison of \( \phi \) for different \( K \) with the solution for \( K = 0 \)(left) and \( K = \infty \)(right).

\[
| K | \| \phi_{K_i} - \phi_0 \|_{L^2(0,T;L^2(\Omega))} | \text{EOC} | \| \phi_{K_i} - \phi_{\infty} \|_{L^2(0,T;L^2(\Omega))} | \text{EOC} |
\]

| 1e-4 | 4.1965e-06 | - | 1e4 | 1.0445e-05 | - |
| 2*1e-4 | 8.3917e-06 | 0.9998 | 5000 | 2.0886e-05 | -0.9997 |
| 5*1e-4 | 2.0963e-05 | 0.9992 | 2500 | 4.1755e-05 | -0.9994 |
| 1e-3 | 4.1876e-05 | 0.9983 | 2000 | 5.2182e-05 | -0.9990 |
| 0.01 | 4.1058e-04 | 0.9910 | 1000 | 1.0425e-04 | -0.9819 |
| 0.1 | 0.0036 | 0.9429 | 100 | 0.0010 | -0.9819 |
| 1 | 0.0333 | 0.9661 | 10 | 0.0086 | -0.9345 |

Table 2: Comparison of \( \psi \) for different \( K \) with the solution for \( K = 0 \)(left) and \( K = \infty \)(right).

\[
| K | \| \psi_{K_i} - \psi_0 \|_{L^2(0,T;L^2(\Gamma))} | \text{EOC} | \| \psi_{K_i} - \psi_{\infty} \|_{L^2(0,T;L^2(\Gamma))} | \text{EOC} |
\]

| 1e-4 | 3.5417e-07 | - | 1e4 | 5.1383e-07 | - |
| 2*1e-4 | 7.0798e-07 | 0.9993 | 5000 | 1.0276e-06 | -0.9999 |
| 5*1e-4 | 1.7681e-06 | 0.9976 | 2500 | 2.0549e-06 | -0.9998 |
| 1e-3 | 3.5303e-06 | 0.9996 | 2000 | 2.5684e-06 | -0.9996 |
| 0.01 | 3.4392e-05 | 0.9966 | 1000 | 5.1343e-05 | -0.9966 |
| 0.1 | 2.9145e-04 | 0.9958 | 100 | 5.0937e-05 | -0.9958 |
| 1 | 0.0023 | 0.9819 | 10 | 5.0450e-04 | -0.9958 |

\( K = \infty \) and \( \phi_{K_i} \) as the solution under the case of \( K_i \). First we compare the discrete solutions \( \phi_{K_i} \) with \( \phi_0 \) for different \( K_i \). The corresponding error is defined as

\[ Err_{i,0} = \| \phi_{K_i} - \phi_0 \|_{L^2(0,T;L^2(\Omega))} \]

where the time integral is approximated using the trapezoidal rule with time increment \( \tilde{\tau} = 1e - 3 \).

The experimental order is defined as

\[ EOC_{K_i} = \frac{\ln (Err_{i+1,0})}{\ln (Err_{i,0})} \]

Similarly, we can define the corresponding error and the experimental order for the case of \( K \to \infty \).

The results for the convergence of \( \phi \) and \( \psi \) are shown in Table 1 and Table 2, indicating that for \( K \leq 1e - 3 \) and \( K \geq 1e3 \), the convergence rate is almost 1. The convergence rate obtained here is the same as that in [18].

5.2 Accuracy test

In this section, we present numerical accuracy tests using the scheme (3.10)-(3.15) to support our error analysis. Let \( \Omega \) to be the unit square, the spatial step size \( h = 0.01 \) and the parameters are chosen as \( \varepsilon = \delta = 0.02, \kappa = 1 \) and \( s_1 = s_2 = 50 \). The initial data is set to be zero in the bulk and set to be one on the boundary. In this section, we choose \( F \) and \( G \) to be the modified double-well potential (4.3), and thus, the Lipschitz property holds for their derivatives

\[ \max_{\phi \in \mathbb{R}} |F''(\phi)| = \max_{\psi \in \mathbb{R}} |G''(\psi)| \leq 2. \]
Figure 5: The $H^1$ numerical errors for $\phi$ and $\psi$ at $T = 1$. 

The errors are calculated as the difference between the solution of the coarse time step and that of the reference time step $\tau^* = 10^{-4}$. In Fig. 5, we plot the $H^1$ errors of $\phi$ and $\psi$ between the numerical solution and the reference solution at $T = 1$ with different time step sizes in the cases of $K = 1$ and $K = 100$. The results show clearly that the convergence rate of the numerical scheme is asymptotically first-order temporally for $\phi$ and $\psi$, which is consistent with our numerical analysis in Section 4.

6 Conclusions

In the present work, we consider numerical approximations and error analysis for the Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions (P. Knopf et. al., arXiv, 2020). This model can be interpreted as an interpolation between the Liu-Wu model (C. Liu et. al., Arch. Rational Mech. Anal., 2019) and the GMS model (G.R. Goldstein et. al., Physica D, 2011).

A first-order in time, linear and energy stable scheme for solving this model is proposed, which also allows us to simulate the two limit models – the Liu-Wu model and the GMS model. The stabilization terms are utilized to enhance the stability of the scheme. To the best of the authors’ knowledge, this is the first linear and energy stable scheme for solving this new model. The semi-discretized-in-time error estimates for the scheme are also derived.

The numerical experiments are constructed in the two-dimensional space to validate the accuracy of the proposed scheme by comparing with the former work. Moreover, the accuracy tests with respect to the time step size validate our error analysis. The convergence results for $K \to 0$ and $K \to \infty$ are also illustrated, which is consistent with the former work.

Acknowledgment

The authors would like to thank Prof. Chun Liu for some useful discussions on the subject of this article. X. Bao is thankful to Prof. Chun Liu, Prof. Yiwei Wang, Prof. Qing Cheng and Prof. Tengfei Zhang for some stimulating discussions during the visit of Illinois Institute of Technology. X. Bao is partially supported by China Scholarship Council (No. 201906040019). H. Zhang is
Numerical approximations of the Cahn-Hilliard equation with reaction rate dependent dynamic boundary conditions partially supported by the National Natural Science Foundation of China (Nos. 11971002 and 11471046).

References

[1] X. Bao and H. Zhang, Numerical approximations and error analysis of the Cahn-Hilliard equation with dynamic boundary conditions, Preprint: arXiv:2006.05391 [math.NA], 2020.

[2] J.W. Cahn and J.E. Hilliard, Free energy of a nonuniform system I. Interfacial free energy, J. Chem. Phys., 2:205-245, 1958.

[3] L. Cherfils, M. Petcu and M. Pierre, A numerical analysis of the Cahn-Hilliard equation with dynamic boundary conditions, Discrete Contin. Dyn. Syst., 27: 1511-1533, 2010.

[4] L. Cherfils and M. Petcu, A numerical analysis of the Cahn-Hilliard equation with non-permeable walls, Numer. Math., 128: 517-549, 2014.

[5] P. Colli and T. Fukao, Cahn-Hilliard equation with dynamic boundary conditions and mass constraint on the boundary, J. Math. Anal. Appl., 429: 1190-1213, 2015.

[6] P. Colli, G. Gilardi, R. Nakayashiki, and K. Shirakawa, A class of quasi-linear Allen-Cahn type equations with dynamic boundary conditions, Nonlinear Anal., 158:32-59, 2017.

[7] H.P. Fischer, P. Maass, and W. Dieterich, Novel Surface Modes in Spinodal Decomposition, Phys. Rev. Lett., 79:893-896, 1997.

[8] H.P. Fischer, J. Reinhard, W. Dieterich, J. F. Gouyet, P. Maass, A. Majhofer, and D. Reinel, Timedependent density functional theory and the kinetics of lattice gas systems in contact with a wall, J. Chem. Phys., 108(7):3028-3037, 1998.

[9] T. Fukao, S. Yoshikawa and S. Wada, Structure-preserving finite difference schemes for the Cahn-Hilliard equation with dynamic boundary conditions in the one-dimensional case, Commun. Pure Applied Anal., 16: 1915-1938, 2017.

[10] C.G. Gal. A Cahn-Hilliard model in bounded domains with permeable walls, Math. Methods Appl.Sci., 29:2009-2036, 2006.

[11] H. Garcke and P. Knopf, Weak Solutions of the Cahn-Hilliard System with Dynamic Boundary Conditions: A Gradient Flow Approach, SIAM J. Math. Anal., 52(1):340-369, 2020.

[12] G.R. Goldstein, A. Miranville, and G. Schimperna, A Cahn-Hilliard model in a domain with nonpermeable walls, Physica D, 240:754-766, 2011.

[13] G. Grün, On convergent schemes for diffuse interface models for two-phase flow of incompressible fluids with general mass densities, SIAM J. Numer. Anal., 51(6): 3036-3061, 2013.

[14] Y.N. He, Y.X. Liu and T. Tang, On large time-stepping methods for the Cahn-Hilliard equation, Appl. Numer. Math., 57: 616-628, 2007.
[15] H. Israel, A. Miranville and M. Petcu, Numerical analysis of a Cahn-Hilliard type equation with dynamic boundary conditions, Ricerche Mat., 64: 25-50, 2015.

[16] R. Kenzler, F. Eurich, P. Maass, B. Rinn, J. Schropp, E. Bohl, and W. Dietrich, Phase separation in confined geometries: Solving the Cahn-Hilliard equation with generic boundary conditions, Comp. Phys. Comm., 133:139-157, 2001.

[17] P. Knopf and K.F. Lam, Convergence of a Robin boundary approximation for a Cahn-Hilliard system with dynamic boundary conditions, Accepted in Nonlinearity, Preprint: arXiv:1908.06124 [math.AP], 2019.

[18] P. Knopf, K. F. Lam, C. Liu and S. Metzger, Phase-field dynamics with transfer of materials: The Cahn–Hillard equation with reaction rate dependent dynamic boundary conditions, Preprint: arXiv:2003.12983 [math.AP], 2020.

[19] C. Liu and H. Wu, An energetic variational approach for the Cahn-Hilliard equation with dynamic boundary condition: model derivation and mathematical analysis, Arch. Ration. Mech. Anal., 233(1):167-247, 2019.

[20] S. Metzger. An efficient and convergent finite element scheme for Cahn-Hilliard equations with dynamic boundary conditions, Preprint arXiv: 1908.04910 [math.NA], 2019.

[21] R.M. Mininni, A. Miranville, and S. Romanelli. Higher-order Cahn-Hilliard equations with dynamic boundary conditions, J. Math. Anal. Appl., 449:1321-1339, 2017.

[22] R. Racke and S. Zheng, The Cahn-Hilliard equation with dynamic boundary conditions, Adv. Differential Equations, 8:83-110, 2003.

[23] J. Shen, C. Wang, X. M. Wang and S. M. Wise, Second-order convex splitting schemes for gradient flows with Ehrlich-Schwoebel type energy: application to thin film epitaxy, SIAM J. Numer. Anal., 50(1): 105-125, 2012.

[24] J. Shen, J. Xu and J. Yang, The scalar auxiliary variable (SAV) approach for gradient flows, J. Comput. Phys., 353: 407-416, 2018.

[25] P.A. Thompson and M.O. Robbins, Simulations of contact-line motion: slip and the dynamic contact angle, Phys. Rev. Lett., 63:766-769, 1989.

[26] D. Trautwein, Finite-Elemente Approximation der Cahn-Hilliard-Gleichung mit Neumann- und dynamischen Randbedingungen, Bachelor thesis, University of Regensburg, 2018.

[27] H. Wu and S. Zheng, Convergence to equilibrium for the Cahn-Hilliard equation with dynamic boundary conditions, J. Differential Equations, 204:511-531, 2004.

[28] X. F. Yang, Linear, first and second-order, unconditionally energy stable numerical schemes for the phase field model of homopolymer blends, J. Comput. Phys., 327: 294-316, 2016.

[29] X. F. Yang, J. Zhao and X. M. He, Linear, second order and unconditionally energy stable schemes for the viscous Cahn-Hilliard equation with hyperbolic relaxation using the invariant energy quadratization method, J. Comput. Appl. Math., 343: 80-97, 2018.