Journal of Computational and Applied Mathematics 415 (2022) 114474

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Optimal rate convergence analysis of a numerical scheme for the ternary Cahn–Hilliard system with a Flory–Huggins–deGennes energy potential

Lixiu Dong [a], Cheng Wang [b,*], Steven M. Wise [c], Zhengru Zhang [d]

[a] College of Education for the Future, Beijing Normal University, Zhuhai 519087, China
[b] Department of Mathematics, The University of Massachusetts, North Dartmouth, MA 02747, USA
[c] Department of Mathematics, The University of Tennessee, Knoxville, TN 37996, USA
[d] Laboratory of Mathematics and Complex Systems, Ministry of Education and School of Mathematical Sciences, Beijing Normal University, Beijing, 100875, China

ARTICLE INFO

Article history:
Received 18 March 2022
Received in revised form 23 May 2022

MSC:
35K35
65M06
65M12

Keywords:
Ternary Cahn–Hilliard system
Flory–Huggins–deGennes energy
Energy stability
Positivity preserving
Optimal rate convergence analysis
Rough and refined error estimates

ABSTRACT

We present an error analysis for a fully discrete finite difference scheme for the three-component Macromolecular Microsphere Composite (MMC) hydrogels system, a ternary Cahn–Hilliard system with a Flory–Huggins–deGennes free energy potential. The numerical scheme was recently proposed, and the positivity-preserving property and unconditional energy stability were theoretically established. In this paper, we rigorously prove first order convergence in time and second order convergence in space for the numerical scheme, in the $L^\infty_{\Delta t}(0,T;H_h^{-1}) \cap L^2_{\Delta t}(0,T;H_h^1)$ norm. Many highly non-standard estimates have to be involved, due to the nonlinear and singular nature of the surface diffusion coefficients. The combination of (i) a higher order asymptotic expansion of the numerical solution (up to second order temporal accuracy); (ii) a rough error estimate (to establish the $L^\infty_{\Delta t}$ bound for the phase variables); (iii) and a refined error estimate have to be carried out to conclude such a convergence result. To our knowledge, it will be the first work to provide an optimal rate convergence estimate for a ternary phase field system with singular energy coefficients.

1. Introduction

Macromolecular microsphere composite (MMC) hydrogels, a class of polymeric materials, have attracted theoretical and experimental studies due to their well-defined network microstructures and high mechanical strength. A binary mathematical model was presented in [1] to describe the periodic structures and the phase transitions of the MMC hydrogels based on Boltzmann entropy theory. The corresponding model leads to the MMC-TDGL equation, with a similar structure to the Cahn–Hilliard equation. The binary Cahn–Hilliard equation – with either polynomial Ginzburg–Landau or singular Flory–Huggins-type free energy – models spinodal decomposition, phase separation, and coarsening in a two-phase fluid. There have been many theoretical analyses and numerical approximations for these kinds of gradient flows in the two-phase case [2–13]. The two-phase version of the MMC-TDGL equation, which is like the Cahn–Hilliard equation, but with certain singular gradient coefficients, is discussed in [14–17]. Also see the related works [18–22] for the hydrogel model.

* Corresponding author.
E-mail addresses: lxdong@bnu.edu.cn (L. Dong), cwang1@umassd.edu (C. Wang), swise1@utk.edu (S.M. Wise), zrzhang@bnu.edu.cn (Z. Zhang).

https://doi.org/10.1016/j.cam.2022.114474
0377-0427/

For the ternary Cahn–Hilliard system, the general framework is to adopt three independent phase variables (ϕ_1, ϕ_2, ϕ_3) while enforcing a mass conservation (or "no-voids") constraint $\phi_1 + \phi_2 + \phi_3 = 1$. See the related works [23–25]. A ternary system with Flory–Huggins–deGennes energy potential has been of great scientific interests, which turns out to be an improvement over the model proposed in [1], as it removes certain limiting assumptions. The singular Flory–Huggins–deGennes energy potential is as follows:

$$G_o(\phi_1, \phi_2, \phi_3) = \int_\Omega \left\{ S_o(\phi_1, \phi_2, \phi_3) + \frac{1}{36} \sum_{i=1}^{3} \frac{\varepsilon_i^2}{\phi_i} |\nabla \phi_i|^2 + H_o(\phi_1, \phi_2, \phi_3) \right\} d\mathbf{x},$$

where $S_o(\phi_1, \phi_2, \phi_3) + H_o(\phi_1, \phi_2, \phi_3)$ is the reticular (Flory–Huggins style) free energy density:

$$S_o(\phi_1, \phi_2, \phi_3) = \frac{\phi_1}{M_0} \ln \frac{\alpha \phi_1}{M_0} + \frac{\phi_2}{N_0} \ln \frac{\beta \phi_2}{N_0} + \phi_3 \ln \phi_3,$$
$$H_o(\phi_1, \phi_2, \phi_3) = \chi_{12}\phi_1\phi_2 + \chi_{13}\phi_1\phi_3 + \chi_{23}\phi_2\phi_3.$$

S_o is the ideal solution part and H_o is the entropy of mixing part. The domain $\Omega \subset \mathbb{R}^2$ is assumed open, bounded, and simply connected. We focus on the 2-D case for simplicity of presentation, while the extension to the 3-D gradient flow is straightforward. The mass-conservative phase variables ϕ_1, ϕ_2 and ϕ_3, represent the concentration of the macromolecular microsphere, the polymer chain, and the solvent, respectively. These three phase variables are subject to the "no-voids" constraint $\phi_1 + \phi_2 + \phi_3 = 1$. We denote by M_0 the relative volume of one macromolecular microsphere, and by N_0 the degree of polymerization of the polymer chains. The coefficient ε_i is called the statistical segment length of the ith component, which is always positive. The parameters α and β depend on M_0 and N_0:

$$\alpha = \pi \left(\left(\frac{M_0}{\pi} \right)^{\frac{1}{2}} + \frac{N_0}{2} \right)^2, \quad \beta = 2 \left(\frac{M_0}{\pi} \right)^{\frac{1}{2}} + N_0.$$

By χ_{12}, χ_{13}, and χ_{23} we denote the Huggins interaction parameters between (i) the macromolecular microspheres and polymer chains, (ii) the macromolecular microspheres and solvent, and (iii) the polymer chains and solvent, respectively. All these parameters are positive, and the following inequality is assumed to guarantee the concavity of the entropy of mixing H_0 term:

$$4\chi_{13}\chi_{23} - (\chi_{12} - \chi_{13} - \chi_{23})^2 > 0.$$

Making use of the no-voids constraint $\phi_3 = 1 - \phi_1 - \phi_2$, we can rewrite the energy functional as

$$G(\phi_1, \phi_2) = \int_\Omega \left\{ S(\phi_1, \phi_2) + \frac{\varepsilon_1^2 |\nabla \phi_1|^2}{36\phi_1} + \frac{\varepsilon_2^2 |\nabla \phi_2|^2}{36\phi_2} + \frac{\varepsilon_3^2 |\nabla (1 - \phi_1 - \phi_2)|^2}{36(1 - \phi_1 - \phi_2)} + H(\phi_1, \phi_2) \right\} d\mathbf{x}, \tag{1.1}$$

where, naturally,

$$S(\phi_1, \phi_2) = \frac{\phi_1}{M_0} \ln \frac{\alpha \phi_1}{M_0} + \frac{\phi_2}{N_0} \ln \frac{\beta \phi_2}{N_0} + (1 - \phi_1 - \phi_2) \ln(1 - \phi_1 - \phi_2),$$
$$H(\phi_1, \phi_2) = \chi_{12}\phi_1\phi_2 + \chi_{13}\phi_1(1 - \phi_1 - \phi_2) + \chi_{23}\phi_2(1 - \phi_1 - \phi_2).$$

The ternary MMC dynamic equations are H^{-1} gradient flows associated with the given energy functional (1.1):

$$\partial_t \phi_1 = \mathcal{M}_1 \Delta \mu_1, \quad \partial_t \phi_2 = \mathcal{M}_2 \Delta \mu_2, \tag{1.2}$$

where $\mathcal{M}_1, \mathcal{M}_2 > 0$ are mobilities, which are assumed to be positive constants. μ_1 and μ_2 are the chemical potentials with respect to ϕ_1 and ϕ_2, respectively, i.e.,

$$\begin{aligned} \mu_1 := \delta_{\phi_1} G = &\frac{1}{M_0} \ln \frac{\alpha \phi_1}{M_0} - \ln(1 - \phi_1 - \phi_2) - 2\chi_{13}\phi_1 + (\chi_{12} - \chi_{13} - \chi_{23})\phi_2 \\ &+ \chi_{13} + \frac{1}{M_0} - 1 - \frac{\varepsilon_1^2 |\nabla \phi_1|^2}{36\phi_1^2} - \nabla \cdot \left(\frac{\varepsilon_1^2 \nabla \phi_1}{18\phi_1} \right) \\ &+ \frac{\varepsilon_3^2 |\nabla (1 - \phi_1 - \phi_2)|^2}{36(1 - \phi_1 - \phi_2)^2} + \nabla \cdot \left(\frac{\varepsilon_3^2 \nabla (1 - \phi_1 - \phi_2)}{18(1 - \phi_1 - \phi_2)} \right), \end{aligned} \tag{1.3}$$

$$\begin{aligned} \mu_2 := \delta_{\phi_2} G = &\frac{1}{N_0} \ln \frac{\beta \phi_2}{N_0} - \ln(1 - \phi_1 - \phi_2) - 2\chi_{23}\phi_2 + (\chi_{12} - \chi_{13} - \chi_{23})\phi_1 \\ &+ \chi_{23} + \frac{1}{N_0} - 1 - \frac{\varepsilon_2^2 |\nabla \phi_2|^2}{36\phi_2^2} - \nabla \cdot \left(\frac{\varepsilon_2^2 \nabla \phi_2}{18\phi_2} \right) \\ &+ \frac{\varepsilon_3^2 |\nabla (1 - \phi_1 - \phi_2)|^2}{36(1 - \phi_1 - \phi_2)^2} + \nabla \cdot \left(\frac{\varepsilon_3^2 \nabla (1 - \phi_1 - \phi_2)}{18(1 - \phi_1 - \phi_2)} \right). \end{aligned} \tag{1.4}$$

For simplicity, periodic boundary conditions are assumed. These equations would reduce to the classical ternary Cahn–Hilliard system if the gradient energy coefficients $\varepsilon_i^2/(36\phi_i)$ were replaced by $\varepsilon_i^2/2$. In any case, it is then easy to see that the energy is non-increasing for the ternary MMC model. The evolution equations (1.2) are mass conservative; the mass fluxes are proportional to the gradients of the respective chemical potentials. Clearly the phase fields must satisfy $0 < \phi_1$, $0 < \phi_2$, and $0 < 1 - \phi_1 - \phi_2$ for the model to make sense physically and mathematically. We define the following *Gibbs Triangles* for use later:

$$\mathcal{G} := \left\{ (\phi_1, \phi_2) \in \mathbb{R}^2 \mid 0 < \phi_1,\ \phi_2,\ \phi_1 + \phi_2 < 1 \right\}, \tag{1.5}$$

and, for $\delta \geq 0$,

$$\mathcal{G}_\delta := \left\{ (\phi_1, \phi_2) \in \mathbb{R}^2 \mid \delta \leq \phi_1,\ \phi_2,\ \phi_1 + \phi_2 \leq 1 - \delta \right\}. \tag{1.6}$$

Of course, $\mathcal{G}_0 = \mathcal{G}$, and $\mathcal{G}_\delta \subseteq \mathcal{G}$, for each $\delta \geq 0$. If $(\phi_1(\,\cdot\,, t), \phi_2(\,\cdot\,, t)) \in \mathcal{G}$, point-wise, for all $t \geq 0$, we say that the *positivity-preserving property* holds for the equation. If, for some strictly positive $\delta > 0$, $(\phi_1(\,\cdot\,, t), \phi_2(\,\cdot\,, t)) \in \mathcal{G}_\delta$, point-wise, for all $t \geq 0$, we say that a *strict separation property* holds for the equation.

A numerical approximation to the ternary MMC system (1.2)–(1.4) turns out to be very challenging, due to the highly nonlinear and singular nature of both the Flory–Huggins logarithmic part and the singular surface diffusion terms. In particular, the positivity-preserving property and the energy stability are two important theoretical issues for any numerical algorithm. A fully discrete finite difference scheme has been proposed in a recent article [26], with both of these theoretical properties rigorously established. In more detail, implicit treatments are applied to the singular logarithmic term and the chemical potential terms associated with the nonlinear deGennes surface diffusion energy, while the linear expansive term is treated explicitly. The resulting scheme is proven to be uniquely solvable, positivity-preserving and unconditionally energy stable. In fact, the following key point plays a crucial role in the positivity-preserving analysis: the convex and the singular natures of the implicit nonlinear parts prevents the numerical solutions from approaching the boundary of the Gibbs triangle $\mathcal{G}$. Because of this subtle fact, an implicit treatment for the nonlinear terms is necessary to ensure these theoretical properties; also see the related works [14,27–37] for the corresponding analysis. By contrast, the invariant energy quadratization (IEQ) [38], scalar auxiliary variable (SAV) [39,40] or linear stabilization [41,42] approaches face serious difficulty to justify these theoretical properties for gradient flows with singular potential.

Several interesting numerical simulation results were presented in [26]. On the other hand, the convergence analysis for ternary system (1.2)–(1.4) remained an open problem. The primary difficulties are associated with the highly nonlinear and singular surface diffusion parts and logarithmic terms, in contrast with the analysis required for the ternary model with polynomial energy potential and constant diffuse interface coefficients [43]. In this article, we provide an optimal rate convergence analysis for the fully discrete scheme formulated in [26], which is shown to be first order accurate in time and second order in space. Because of the nonlinear structure for both the logarithmic and surface diffusion terms, such an error estimate has to be performed in the $L^\infty_{\Delta t}(0, T; H_h^{-1}) \cap L^2_{\Delta t}(0, T; H_h^1)$ space, to make use of the convex structure for these nonlinear terms. To overcome the well-known difficulties associated with the nonlinear and singular surface diffusion coefficients, many highly non-standard estimates have to be involved. A higher order asymptotic expansion, up to second order temporal accuracy, has to be performed with a careful linearization technique. Such a higher order asymptotic expansion enable one to obtain a rough error estimate, so that to the $L^\infty_{\Delta t}$ bound for all three phase variables could be derived. This $L^\infty_{\Delta t}$ estimate yields the upper and lower bounds of the two variables, and these bounds ensure a uniform distance between the numerical solution and the singular limit values, which will play a crucial role in the subsequent analysis. Finally, the refined error estimate is carried out to accomplish the desired convergence result. To our knowledge, this will be the first work to provide an optimal rate convergence estimate for a ternary phase field system with singular energy potential.

The rest of the article is organized as follows. In Section 2, we review the fully discrete finite difference scheme and state the main theoretical result. The optimal rate convergence analysis and error estimate are presented in Section 3. Finally, we give some concluding remarks in Section 4.

2. The fully discrete numerical scheme

2.1. The finite difference spatial discretization

We use the notation and results for some discrete functions and operators from [44–46]. Let $\Omega = (0, L_x) \times (0, L_y)$, where for simplicity, we assume $L_x = L_y =: L > 0$. Let $N \in \mathbb{N}$ be given, and define the grid spacing $h := \frac{L}{N}$, i.e., a uniform spatial mesh size is taken for simplicity of presentation. We define the following two uniform, infinite grids with grid spacing $h > 0$: $E := \{p_{i+1/2} \mid i \in \mathbb{Z}\}$, $C := \{p_i \mid i \in \mathbb{Z}\}$, where $p_i = p(i) := (i - 1/2) \cdot h$. Consider the following 2-D discrete N^2-periodic function spaces:

$$\mathcal{C}_{\rm per} := \left\{ \nu : C \times C \to \mathbb{R} \mid \nu_{i,j} = \nu_{i+\alpha N, j+\beta N},\ \forall\, i, j, \alpha, \beta, \in \mathbb{Z} \right\},$$
$$\mathcal{E}^{\rm x}_{\rm per} := \left\{ \nu : E \times C \to \mathbb{R} \mid \nu_{i+\frac{1}{2},j} = \nu_{i+\frac{1}{2}+\alpha N, j+\beta N},\ \forall\, i, j, \alpha, \beta \in \mathbb{Z} \right\},$$

in which identification $\nu_{i,j} = \nu(p_i, p_j)$ is taken. The space $\mathcal{E}^{\mathrm{y}}_{\mathrm{per}}$ is analogously defined. The functions of $\mathcal{C}_{\mathrm{per}}$ are called *cell centered functions*, and the functions of $\mathcal{E}^{\mathrm{x}}_{\mathrm{per}}$, $\mathcal{E}^{\mathrm{y}}_{\mathrm{per}}$ are called *east–west*, *north–south face-centered functions*, respectively. We also define the mean zero space $\mathring{\mathcal{C}}_{\mathrm{per}} := \{\nu \in \mathcal{C}_{\mathrm{per}} \,|\, 0 = \overline{\nu} := \frac{h^2}{|\Omega|}\sum_{i,j=1}^N \nu_{i,j}\}$, and denote $\vec{\mathcal{E}}_{\mathrm{per}} := \mathcal{E}^{\mathrm{x}}_{\mathrm{per}} \times \mathcal{E}^{\mathrm{y}}_{\mathrm{per}}$. The space $\vec{\mathcal{C}}^{\mathcal{G}}_{\mathrm{per}}$ is defined as

$$\vec{\mathcal{C}}^{\mathcal{G}}_{\mathrm{per}} := \left\{(u_1, u_2) \in \mathcal{C}_{\mathrm{per}} \times \mathcal{C}_{\mathrm{per}} \mid (u_{1i,j}, u_{2i,j}) \in \mathcal{G}, \quad i,j \in \mathbb{Z}\right\},$$

where $\mathcal{G}$ is the Gibbs Triangle (1.5). In addition, the following difference and average operators are introduced:

$$A_x\nu_{i+1/2,j} := \frac{1}{2}\left(\nu_{i+1,j} + \nu_{i,j}\right), \quad D_x\nu_{i+1/2,j} := \frac{1}{h}\left(\nu_{i+1,j} - \nu_{i,j}\right),$$
$$A_y\nu_{i,j+1/2} := \frac{1}{2}\left(\nu_{i,j+1} + \nu_{i,j}\right), \quad D_y\nu_{i,j+1/2} := \frac{1}{h}\left(\nu_{i,j+1} - \nu_{i,j}\right),$$

with $A_x,\ D_x : \mathcal{C}_{\mathrm{per}} \to \mathcal{E}^{\mathrm{x}}_{\mathrm{per}}$, $A_y,\ D_y : \mathcal{C}_{\mathrm{per}} \to \mathcal{E}^{\mathrm{y}}_{\mathrm{per}}$. Likewise,

$$a_x\nu_{i,j} := \frac{1}{2}\left(\nu_{i+1/2,j} + \nu_{i-1/2,j}\right), \quad d_x\nu_{i,j} := \frac{1}{h}\left(\nu_{i+1/2,j} - \nu_{i-1/2,j}\right),$$
$$a_y\nu_{i,j} := \frac{1}{2}\left(\nu_{i,j+1/2} + \nu_{i,j-1/2}\right), \quad d_y\nu_{i,j} := \frac{1}{h}\left(\nu_{i,j+1/2} - \nu_{i,j-1/2}\right),$$

with $a_x,\ d_x : \mathcal{E}^{\mathrm{x}}_{\mathrm{per}} \to \mathcal{C}_{\mathrm{per}}$, and $a_y,\ d_y : \mathcal{E}^{\mathrm{y}}_{\mathrm{per}} \to \mathcal{C}_{\mathrm{per}}$. The discrete gradient $\nabla_h : \mathcal{C}_{\mathrm{per}} \to \vec{\mathcal{E}}_{\mathrm{per}}$ and the discrete divergence $\nabla_h\cdot : \vec{\mathcal{E}}_{\mathrm{per}} \to \mathcal{C}_{\mathrm{per}}$ are given by

$$\nabla_h\nu_{i,j} = \left(D_x\nu_{i+1/2,j}, D_y\nu_{i,j+1/2}\right), \quad \nabla_h \cdot \vec{f}_{i,j} = d_x f^x_{i,j} + d_y f^y_{i,j},$$

where $\vec{f} = (f^x, f^y) \in \vec{\mathcal{E}}_{\mathrm{per}}$. The standard 2-D discrete Laplacian, $\Delta_h : \mathcal{C}_{\mathrm{per}} \to \mathcal{C}_{\mathrm{per}}$, becomes

$$\Delta_h\nu_{i,j} := d_x(D_x\nu)_{i,j} + d_y(D_y\nu)_{i,j} = \frac{1}{h^2}\left(\nu_{i+1,j} + \nu_{i-1,j} + \nu_{i,j+1} + \nu_{i,j-1} - 4\nu_{i,j}\right).$$

More generally, if $\mathcal{D}$ is a periodic *scalar* function that is defined at all of the face center points and $\vec{f} \in \vec{\mathcal{E}}_{\mathrm{per}}$, then $\mathcal{D}\vec{f} \in \vec{\mathcal{E}}_{\mathrm{per}}$, assuming point-wise multiplication, and we may define $\nabla_h \cdot \left(\mathcal{D}\vec{f}\right)_{i,j} = d_x\left(\mathcal{D}f^x\right)_{i,j} + d_y\left(\mathcal{D}f^y\right)_{i,j}$. Specifically, if $\nu \in \mathcal{C}_{\mathrm{per}}$, then $\nabla_h \cdot (\mathcal{D}\nabla_h\ \ ) : \mathcal{C}_{\mathrm{per}} \to \mathcal{C}_{\mathrm{per}}$ is defined point-wise via $\nabla_h \cdot \left(\mathcal{D}\nabla_h\nu\right)_{i,j} = d_x\left(\mathcal{D}D_x\nu\right)_{i,j} + d_y\left(\mathcal{D}D_y\nu\right)_{i,j}$. In particular, suppose that $\nu, \phi \in \mathcal{C}_{\mathrm{per}}$ are grid functions and $\sigma : \mathbb{R} \to \mathbb{R}$ is a continuous function. Then we define

$$\nabla_h \cdot \left(\sigma(\mathcal{A}_h\nu)\nabla_h\phi\right)_{i,j} := d_x\left(\sigma(A_x\nu)D_x\phi\right)_{i,j} + d_y\left(\sigma(A_y\nu)D_y\phi\right)_{i,j},$$

where $\mathcal{A}_h\nu$ is understood to be a periodic function defined at the edge centered points obtained by doing appropriate east–west and north–south averages.

In addition, the following grid inner products are defined:

$$\langle \nu, \xi\rangle := h^2\sum_{i,j=1}^N \nu_{i,j}\,\xi_{i,j}, \quad \nu,\ \xi \in \mathcal{C}_{\mathrm{per}}, \quad [\vec{f}_1, \vec{f}_2] := \left[f^x_1, f^x_2\right]_{\mathrm{x}} + \left[f^y_1, f^y_2\right]_{\mathrm{y}}, \quad \vec{f}_i = (f^x_i, f^y_i) \in \vec{\mathcal{E}}_{\mathrm{per}},$$
$$[\nu, \xi]_{\mathrm{x}} := \langle a_x(\nu\xi), 1\rangle, \quad \nu,\ \xi \in \mathcal{E}^{\mathrm{x}}_{\mathrm{per}}, \quad [\nu, \xi]_{\mathrm{y}} := \langle a_y(\nu\xi), 1\rangle, \quad \nu,\ \xi \in \mathcal{E}^{\mathrm{y}}_{\mathrm{per}}.$$

Subsequently, we define the following norms for cell-centered functions. If $\nu \in \mathcal{C}_{\mathrm{per}}$, then $\|\nu\|_2^2 := \langle\nu, \nu\rangle$; $\|\nu\|_p^p := \langle|\nu|^p, 1\rangle$, for $1 \le p < \infty$, and $\|\nu\|_\infty := \max_{1\le i,j\le N}\left|\nu_{i,j}\right|$. The gradient norms are introduced as follows:

$$\|\nabla_h\nu\|_2^2 := [\nabla_h\nu, \nabla_h\nu] = [D_x\nu, D_x\nu]_{\mathrm{x}} + \left[D_y\nu, D_y\nu\right]_{\mathrm{y}}, \quad \text{for } \nu \in \mathcal{C}_{\mathrm{per}},$$
$$\|\nabla_h\nu\|_p := \left(\left[|D_x\nu|^p, 1\right]_{\mathrm{x}} + \left[|D_y\nu|^p, 1\right]_{\mathrm{y}}\right)^{\frac{1}{p}}, \quad 1 \le p < \infty.$$

The discrete H^1 norm is defined as $\|\nu\|^2_{H^1_h} := \|\nu\|_2^2 + \|\nabla_h\nu\|_2^2$.

Lemma 2.1 ([46,47])**.** *Let $\mathcal{D}$ be an arbitrary periodic, scalar function defined on all of the face center points. For any $\psi, \nu \in \mathcal{C}_{\mathrm{per}}$ and any $\vec{f} \in \vec{\mathcal{E}}_{\mathrm{per}}$, the following summation by parts formulas are valid:*

$$\langle\psi, \nabla_h \cdot \vec{f}\rangle = -[\nabla_h\psi, \vec{f}], \quad \langle\psi, \nabla_h \cdot (\mathcal{D}\nabla_h\nu)\rangle = -[\nabla_h\psi, \mathcal{D}\nabla_h\nu]. \tag{2.1}$$

2.2. The fully discrete numerical scheme and the main theoretical results

The following numerical scheme is proposed in a recent work [26], based on a careful convex–concave decomposition of the physical energy (1.1):

$$\begin{aligned}\frac{\phi_1^{n+1}-\phi_1^n}{\Delta t} &= \mathcal{M}_1\Delta_h\Big(\frac{1}{M_0}\ln\frac{\alpha\phi_1^{n+1}}{M_0}-\ln(1-\phi_1^{n+1}-\phi_2^{n+1})-2\chi_{13}\phi_1^n+(\chi_{12}-\chi_{13}-\chi_{23})\phi_2^n\\ &\quad -\frac{\varepsilon_1^2}{36}\mathcal{A}_h\Big(\frac{|\nabla_h\phi_1^{n+1}|^2}{(\mathcal{A}_h\phi_1^{n+1})^2}\Big)-\frac{\varepsilon_1^2}{18}\nabla_h\cdot\Big(\frac{\nabla_h\phi_1^{n+1}}{\mathcal{A}_h\phi_1^{n+1}}\Big)\\ &\quad +\frac{\varepsilon_3^2}{36}\mathcal{A}_h\Big(\frac{|\nabla_h(1-\phi_1^{n+1}-\phi_2^{n+1})|^2}{(\mathcal{A}_h(1-\phi_1^{n+1}-\phi_2^{n+1}))^2}\Big)+\frac{\varepsilon_3^2}{18}\nabla_h\cdot\Big(\frac{\nabla_h(1-\phi_1^{n+1}-\phi_2^{n+1})}{\mathcal{A}_h(1-\phi_1^{n+1}-\phi_2^{n+1})}\Big)\Big),\end{aligned} \tag{2.2}$$

$$\begin{aligned}\frac{\phi_2^{n+1}-\phi_2^n}{\Delta t} &= \mathcal{M}_2\Delta_h\Big(\frac{1}{N_0}\ln\frac{\beta\phi_2^{n+1}}{N_0}-\ln(1-\phi_1^{n+1}-\phi_2^{n+1})-2\chi_{23}\phi_2^n+(\chi_{12}-\chi_{13}-\chi_{23})\phi_1^n\\ &\quad -\frac{\varepsilon_2^2}{36}\mathcal{A}_h\Big(\frac{|\nabla_h\phi_2^{n+1}|^2}{(\mathcal{A}_h\phi_2^{n+1})^2}\Big)-\frac{\varepsilon_2^2}{18}\nabla_h\cdot\Big(\frac{\nabla_h\phi_2^{n+1}}{\mathcal{A}_h\phi_2^{n+1}}\Big)\\ &\quad +\frac{\varepsilon_3^2}{36}\mathcal{A}_h\Big(\frac{|\nabla_h(1-\phi_1^{n+1}-\phi_2^{n+1})|^2}{(\mathcal{A}_h(1-\phi_1^{n+1}-\phi_2^{n+1}))^2}\Big)+\frac{\varepsilon_3^2}{18}\nabla_h\cdot\Big(\frac{\nabla_h(1-\phi_1^{n+1}-\phi_2^{n+1})}{\mathcal{A}_h(1-\phi_1^{n+1}-\phi_2^{n+1})}\Big)\Big),\end{aligned} \tag{2.3}$$

where

$$\begin{aligned}\mathcal{A}_h\left(\frac{|\nabla_h u|^2}{(\mathcal{A}_h u)^2}\right) &:= a_x\left(\frac{|D_x u|^2}{(A_x u)^2}\right)+a_y\left(\frac{|D_y u|^2}{(A_y u)^2}\right),\\ \nabla_h\cdot\left(\frac{\nabla_h u}{\mathcal{A}_h u}\right) &:= d_x\left(\frac{D_x u}{A_x u}\right)+d_y\left(\frac{D_y u}{A_y u}\right),\end{aligned}$$

for all $u\in\mathcal{C}_{\rm per}$, provided u does not vanish at any grid points.

The positivity-preserving property and unique solvability has been established in [26].

Theorem 2.1 ([26]). *Given $(\phi_1^n,\phi_2^n)\in\vec{\mathcal{C}}_{\rm per}^{\mathcal{G}}$, there exists a unique solution $(\phi_1^{n+1},\phi_2^{n+1})\in\vec{\mathcal{C}}_{\rm per}^{\mathcal{G}}$ and $\overline{\phi_1^{n+1}}=\overline{\phi_1^n}$, $\overline{\phi_2^{n+1}}=\overline{\phi_2^n}$. In addition, the numerical scheme (2.2)–(2.3) is unconditionally energy stable: $G_h(\phi_1^{n+1},\phi_2^{n+1})\le G_h(\phi_1^n,\phi_2^n)$, where the discrete energy $G_h(\phi_1,\phi_2):\vec{\mathcal{C}}_{\rm per}^{\mathcal{G}}\to\mathbb{R}$ is defined as*

$$\begin{aligned}G_h(\phi_1,\phi_2) :=& \langle S(\phi_1,\phi_2)+H(\phi_1,\phi_2),1\rangle\\ &+\langle a_x(\kappa(A_x\phi_1)(D_x\phi_1)^2)+a_y(\kappa(A_y\phi_1)(D_y\phi_1)^2),\varepsilon_1^2\rangle\\ &+\langle a_x(\kappa(A_x\phi_2)(D_x\phi_2)^2)+a_y(\kappa(A_y\phi_2)(D_y\phi_2)^2),\varepsilon_2^2\rangle\\ &+\langle a_x(\kappa(A_x(1-\phi_1-\phi_2))(D_x(1-\phi_1-\phi_2))^2),\varepsilon_3^2\rangle\\ &+\langle a_y(\kappa(A_y(1-\phi_1-\phi_2))(D_y(1-\phi_1-\phi_2))^2),\varepsilon_3^2\rangle,\end{aligned} \tag{2.4}$$

with $\kappa(\phi):=\frac{1}{36\phi}$.

Now we proceed into the convergence analysis. Let Φ_1, Φ_2 be the exact solution for the ternary MMC flow (1.2)–(1.4). With sufficiently regular initial data, we could assume that the exact solution has regularity of class $\mathcal{R}$:

$$\Phi_1,\Phi_2\in\mathcal{R}:=H^3\left(0,T;C_{\rm per}(\Omega)\right)\cap H^2\left(0,T;C^2_{\rm per}(\Omega)\right)\cap L^\infty\left(0,T;C^6_{\rm per}(\Omega)\right). \tag{2.5}$$

In addition, we assume that the following separation property is valid for the exact solution: for some δ,

$$(\Phi_1,\Phi_2)\in\mathcal{G}_\delta, \tag{2.6}$$

which is satisfied at a point-wise level, for all $t\in[0,T]$. Define $\Phi_{1,N}(\,\cdot\,,t):=\mathcal{P}_N\Phi_1(\,\cdot\,,t)$, $\Phi_{2,N}(\,\cdot\,,t):=\mathcal{P}_N\Phi_2(\,\cdot\,,t)$, the (spatial) Fourier projection of the exact solution into $\mathcal{B}^K$, the space of trigonometric polynomials of degree up to and including K (with $N=2K+1$). The following projection approximation is standard: if $\Phi_j\in L^\infty(0,T;H^\ell_{\rm per}(\Omega))$, for some $\ell\in\mathbb{N}$,

$$\left\|\Phi_{j,N}-\Phi_j\right\|_{L^\infty(0,T;H^k)}\le Ch^{\ell-k}\left\|\Phi_j\right\|_{L^\infty(0,T;H^\ell)},\quad\forall\, 0\le k\le\ell,\ j=1,2. \tag{2.7}$$

By $\Phi_{j,N}^m$, Φ_j^m we denote $\Phi_{j,N}(\,\cdot\,,t_m)$ and $\Phi_j(\,\cdot\,,t_m)$, respectively, with $t_m=m\cdot\Delta t$. Since $\Phi_{j,N}\in\mathcal{B}^K$, the mass conservative property is available at the discrete level:

$$\overline{\Phi_{j,N}^m}=\frac{1}{|\Omega|}\int_\Omega\Phi_{j,N}(\cdot,t_m)\,d\mathbf{x}=\frac{1}{|\Omega|}\int_\Omega\Phi_{j,N}(\cdot,t_{m-1})\,d\mathbf{x}=\overline{\Phi_{j,N}^{m-1}},\quad\forall\, m\in\mathbb{N}. \tag{2.8}$$

On the other hand, the solution of (2.2)–(2.3) is also mass conservative at the discrete level:

$$\overline{\phi_j^m} = \overline{\phi_j^{m-1}}, \quad \forall\, m \in \mathbb{N},\ j = 1, 2. \tag{2.9}$$

As indicated before, we use the mass conservative projection for the initial data: $\phi_j^0 = \mathcal{P}_h \Phi_{j,N}(\,\cdot\,, t = 0)$, that is

$$(\phi_1^0)_{i,j} := \Phi_{1,N}(p_i, p_j, t = 0), \ \ (\phi_2^0)_{i,j} := \Phi_{2,N}(p_i, p_j, t = 0). \tag{2.10}$$

The error grid function is defined as

$$e_1^m := \mathcal{P}_h \Phi_{1,N}^m - \phi_1^m, \ \ e_2^m := \mathcal{P}_h \Phi_{2,N}^m - \phi_2^m, \quad \forall\, m \in \{0, 1, 2, 3, \ldots\}\,. \tag{2.11}$$

Therefore, it follows that $\overline{e_j^m} = 0$, for any $m \in \{0, 1, 2, 3, \ldots\}$, $j = 1, 2$. Meanwhile, we need to introduce a discrete H^{-1} norm. For any $\varphi \in \mathring{\mathcal{C}}_{per}$, there exists a unique $\psi = (-\Delta_h)^{-1}\varphi \in \mathring{\mathcal{C}}_{per}$ that solves $-\Delta_h \psi = \varphi$, with $\overline{\psi} = 0$. In turn, the following norm is introduced:

$$\|\varphi\|_{-1,h} = \sqrt{\langle \varphi, (-\Delta_h)^{-1}\varphi\rangle}.$$

Therefore, the discrete norm $\|\cdot\|_{-1,h}$ is well defined for the error grid functions e_1^m and e_2^m.

The following theorem is the main result of this article.

Theorem 2.2. *Given initial data $\Phi_1(\,\cdot\,, t = 0), \Phi_2(\,\cdot\,, t = 0) \in C^6_{\rm per}(\Omega)$ and $\Phi_1(\,\cdot\,, t = 0), \Phi_2(\,\cdot\,, t = 0) \in \mathcal{G}$, point-wise, suppose the exact solution for ternary MMC flow (1.2)–(1.4) is of regularity class $\mathcal{R}$. Then, provided Δt and h are sufficiently small, and under the linear refinement requirement $C_1 h \le \Delta t \le C_2 h$, we have*

$$\frac{1}{\mathcal{M}_j}\|e_j^n\|_{-1,h} + \left(\frac{\varepsilon_0^2}{36}\Delta t \sum_{m=1}^{n} \|\nabla_h e_j^m\|_2^2\right)^{1/2} \le C(\Delta t + h^2), \quad \varepsilon_0 = \min(\varepsilon_1^2, \varepsilon_2^2, \varepsilon_3^2),\ \ j = 1, 2, \tag{2.12}$$

for all positive integers n, such that $t_n = n\Delta t \le T$, where $C > 0$ is independent of Δt and h.

Remark 2.1. The proposed numerical scheme (2.2)–(2.3) is based on the convex splitting for the free energy (1.1), which in turn leads to an implicit treatment for the highly singular and nonlinear terms. Meanwhile, many linear numerical schemes, such as the IEQ [48–52] and SAV [53–58] approaches, have been widely applied to various phase field models, either with two-component or three components, either with or without fluid motion coupling. For the ternary MMC gradient flow (1.2)–(1.4), the IEQ and SAV methods are expected to be applicable; an extension of the free energy is required if the phase variable takes a value outside the range of $(0, 1)$. The associated IEQ and SAV numerical schemes will be linear, and a modified energy stability is expected. However, a theoretical justification of the positivity preserving property will face a serious difficulty for these linear numerical schemes, due to the explicit treatment of the singular nonlinear terms. In contrast, an implicit treatment for the convex singular terms is necessary to ensure the positivity-preserving property of the phase variables; see the related nonlinear analysis in the related works [14,29,30,33,35,37], etc.

Remark 2.2. The finite difference spatial approximation is taken in proposed numerical scheme (2.2)–(2.3), which in turn gives second order spatial accuracy. Meanwhile, many high precision spatial discretization methods, such as Fourier Galerkin spectral or pseudo-spectral approximation, have been extensively applied to various Cahn–Hilliard and other related phase field models [6,48,49]. The advantage of the spectral method is associated with its exponential convergence with a limited spatial resolution, which has been verified by extensive numerical experiments. For the ternary MMC gradient flow (1.2)–(1.4), the Fourier spectral method is expected to be applicable. Meanwhile, due to the global nature of the spectral spatial discretization, the unique solvability and positivity-preserving analysis of the spectral method is expected to be much more challenging; in contrast, the positivity-preserving analysis for the finite difference scheme (2.2)–(2.3) replies heavily on the local difference stencil structure, as revealed in [26]. A more detailed analysis of the spectral numerical scheme will be reported in the future works.

3. Optimal rate convergence analysis in $L^\infty_{\Delta t}(0, T; H_h^{-1}) \cap L^2_{\Delta t}(0, T; H_h^1)$

3.1. Higher order consistency analysis of (2.2)–(2.3): asymptotic expansion of the numerical solution

By consistency, the projection solution $\Phi_{1,N}$, $\Phi_{2,N}$ solves the discrete equation (2.2)–(2.3) with a first order in time and second order in space local truncation error. However, we should point out that this leading local truncation error will not be enough to recover an a-priori $L^\infty_{\Delta t}$ bound for the numerical solution to recover the separation property. To remedy this, we use a higher order consistency analysis, via a perturbation argument, to recover such a bound in later analysis. In more detail, we need to construct supplementary fields, $\Phi_{j,\Delta t}$ and $\check{\Phi}_j$ satisfying

$$\check{\Phi}_j = \Phi_{j,N} + \Delta t \Phi_{j,\Delta t}, \quad j = 1, 2, \tag{3.1}$$

so that a higher $O(\Delta t^2+h^2)$ consistency is satisfied with the given numerical scheme (2.2)–(2.3). The constructed fields $\Phi_{j,\Delta t}$, which will be found using a perturbation expansion, will depend solely on the exact solution Φ_j.

In other words, we introduce a higher order approximate expansion of the exact solution, since a first order temporal consistency estimate is not able to control the discrete $L^\infty_{\Delta t}$ norm of the numerical solution. Instead of substituting the exact solution into the numerical scheme, a careful construction of an approximate profile is performed by adding $O(\Delta t)$ correction term to the projection solution to satisfy an $O(\Delta t^2)$ truncation error. In turn, we estimate the numerical error function between the constructed profile and the numerical solution, instead of a direct comparison between the numerical solution and projection solution. Such a higher order consistency enables us to derive a higher order convergence estimate in the $\|\cdot\|_{-1,h}$ norm, which in turn leads to a desired $\|\cdot\|_\infty$ bound of the numerical solution, via an application of inverse inequality. This approach has been reported for a wide class of nonlinear PDEs; see the related works for the incompressible fluid equation [59–65], various gradient equations [66–69], the porous medium equation based on the energetic variational approach [70,71], nonlinear wave equation [72], etc.

The following truncation error analysis for the temporal discretization can be obtained by using a straightforward Taylor expansion, as well as the estimate (2.7) for the projection solution:

$$
\begin{aligned}
\frac{\Phi_{1,N}^{n+1}-\Phi_{1,N}^n}{\Delta t} = \mathcal{M}_1\Delta\Bigg(&\frac{1}{M_0}\ln\frac{\alpha\Phi_{1,N}^{n+1}}{M_0}-\ln(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})-2\chi_{13}\Phi_{1,N}^n+(\chi_{12}-\chi_{13}-\chi_{23})\Phi_{2,N}^n\\
&-\frac{\varepsilon_1^2}{36}\frac{|\nabla\Phi_{1,N}^{n+1}|^2}{(\Phi_{1,N}^{n+1})^2}-\frac{\varepsilon_1^2}{18}\nabla\cdot\Big(\frac{\nabla\Phi_{1,N}^{n+1}}{\Phi_{1,N}^{n+1}}\Big)+\frac{\varepsilon_3^2}{36}\Big(\frac{|\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})|^2}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^2}\Big)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\Big(\frac{\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})}\Big)\Bigg)+\Delta t\mathbf{g}_1^{(0)}+O(\Delta t^2)+O(h^m),
\end{aligned}
\tag{3.2}
$$

$$
\begin{aligned}
\frac{\Phi_{2,N}^{n+1}-\Phi_{2,N}^n}{\Delta t} = \mathcal{M}_2\Delta\Bigg(&\frac{1}{N_0}\ln\frac{\beta\Phi_{2,N}^{n+1}}{N_0}-\ln(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})-2\chi_{23}\Phi_{2,N}^n+(\chi_{12}-\chi_{13}-\chi_{23})\Phi_{1,N}^n\\
&-\frac{\varepsilon_2^2}{36}\frac{|\nabla\Phi_{2,N}^{n+1}|^2}{(\Phi_{2,N}^{n+1})^2}-\frac{\varepsilon_2^2}{18}\nabla\cdot\Big(\frac{\nabla\Phi_{2,N}^{n+1}}{\Phi_{2,N}^{n+1}}\Big)+\frac{\varepsilon_3^2}{36}\Big(\frac{|\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})|^2}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^2}\Big)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\Big(\frac{\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})}\Big)\Bigg)+\Delta t\mathbf{g}_2^{(0)}+O(\Delta t^2)+O(h^m).
\end{aligned}
\tag{3.3}
$$

Here the function $\mathbf{g}_j^{(0)}$ is smooth enough in the sense that its derivatives are bounded in the $\|\cdot\|_{L^\infty}$ norm. In fact, $\mathbf{g}_j^{(0)}$ turns out to be only dependent on the higher order derivatives (both spatial and temporal) of the projection solution $(\Phi_{1,N},\Phi_{2,N})$, henceforth only dependent on the exact solution (Φ_1,Φ_2), as indicated by the Taylor expansion and the Fourier projection estimate.

The temporal correction function $\Phi_{j,\Delta t}$ is given by solving the following equations:

$$
\begin{aligned}
\partial_t\Phi_{1,\Delta t} = \mathcal{M}_1\Delta\Bigg(&\frac{1}{M_0}\frac{\Phi_{1,\Delta t}}{\Phi_{1,N}}+\frac{\Phi_{1,\Delta t}+\Phi_{2,\Delta t}}{(1-\Phi_{1,N}-\Phi_{2,N})}-2\chi_{13}\Phi_{1,\Delta t}+(\chi_{12}-\chi_{13}-\chi_{23})\Phi_{2,\Delta t}\\
&+\frac{\varepsilon_1^2}{36}\frac{2|\nabla\Phi_{1,N}|^2\Phi_{1,\Delta t}}{\Phi_{1,N}^3}-\frac{\varepsilon_1^2}{36}\frac{2\nabla\Phi_{1,N}\cdot\nabla\Phi_{1,\Delta t}}{\Phi_{1,N}^2}-\frac{\varepsilon_1^2}{18}\nabla\cdot\Big(\frac{\nabla\Phi_{1,\Delta t}}{\Phi_{1,N}}-\frac{\Phi_{1,\Delta t}\nabla\Phi_{1,N}}{\Phi_{1,N}^2}\Big)\\
&+\frac{\varepsilon_3^2}{36}\Big(\frac{2|\nabla(1-\Phi_{1,N}-\Phi_{2,N})|^2(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})}{(1-\Phi_{1,N}-\Phi_{2,N})^3}\\
&\qquad-\frac{2\nabla(1-\Phi_{1,N}-\Phi_{2,N})\cdot\nabla(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})}{(1-\Phi_{1,N}-\Phi_{2,N})^2}\Big)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\Big(\frac{-\nabla(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})}{(1-\Phi_{1,N}-\Phi_{2,N})}+\frac{(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})\nabla(1-\Phi_{1,N}-\Phi_{2,N})}{(1-\Phi_{1,N}-\Phi_{2,N})^2}\Big)\Bigg)-\mathbf{g}_1^{(0)},
\end{aligned}
\tag{3.4}
$$

$$
\begin{aligned}
\partial_t\Phi_{2,\Delta t} = \mathcal{M}_2\Delta\Bigg(&\frac{1}{N_0}\frac{\Phi_{2,\Delta t}}{\Phi_{2,N}}+\frac{\Phi_{1,\Delta t}+\Phi_{2,\Delta t}}{(1-\Phi_{1,N}-\Phi_{2,N})}-2\chi_{23}\Phi_{2,\Delta t}+(\chi_{12}-\chi_{13}-\chi_{23})\Phi_{1,\Delta t}\\
&+\frac{\varepsilon_1^2}{36}\frac{2|\nabla\Phi_{2,N}|^2\Phi_{2,\Delta t}}{\Phi_{2,N}^3}-\frac{\varepsilon_1^2}{36}\frac{2\nabla\Phi_{2,N}\cdot\nabla\Phi_{2,\Delta t}}{\Phi_{2,N}^2}-\frac{\varepsilon_1^2}{18}\nabla\cdot\Big(\frac{\nabla\Phi_{2,\Delta t}}{\Phi_{2,N}}-\frac{\Phi_{2,\Delta t}\nabla\Phi_{2,N}}{\Phi_{2,N}^2}\Big)\\
&+\frac{\varepsilon_3^2}{36}\Big(\frac{2|\nabla(1-\Phi_{1,N}-\Phi_{2,N})|^2(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})}{(1-\Phi_{1,N}-\Phi_{2,N})^3}
\end{aligned}
$$

$$
- \frac{2\nabla(1-\Phi_{1,N}-\Phi_{2,N})\cdot\nabla(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})}{(1-\Phi_{1,N}-\Phi_{2,N})^2}\Big)
+ \frac{\varepsilon_3^2}{18}\nabla\cdot\left(\frac{-\nabla(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})}{(1-\Phi_{1,N}-\Phi_{2,N})} + \frac{(\Phi_{1,\Delta t}+\Phi_{2,\Delta t})\nabla(1-\Phi_{1,N}-\Phi_{2,N})}{(1-\Phi_{1,N}-\Phi_{2,N})^2}\right)\Bigg) - \mathbf{g}_2^{(0)}. \tag{3.5}
$$

Existence of a solution of the above linear PDE system is straightforward. Note that the solution depends only on the projection solution $\Phi_{j,N}$. In addition, the derivatives of $\Phi_{j,\Delta t}$ of various orders are bounded. Of course, an application of the semi-implicit discretization (as given by (2.2)–(2.3)) to (3.4)–(3.5) implies that

$$
\begin{aligned}
&\frac{\Phi_{1,\Delta t}^{n+1}-\Phi_{1,\Delta t}^n}{\Delta t} \qquad (3.6)\\
=&\mathcal{M}_1\Delta\Bigg(\frac{1}{M_0}\frac{\Phi_{1,\Delta t}^{n+1}}{\Phi_{1,N}^{n+1}} + \frac{\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1}}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})} - 2\chi_{13}\Phi_{1,\Delta t}^n + (\chi_{12}-\chi_{13}-\chi_{23})\Phi_{2,\Delta t}^n\\
&+\frac{\varepsilon_1^2}{36}\frac{2|\nabla\Phi_{1,N}^{n+1}|^2\Phi_{1,\Delta t}^{n+1}}{(\Phi_{1,N}^{n+1})^3} - \frac{\varepsilon_1^2}{36}\frac{2\nabla\Phi_{1,N}^{n+1}\cdot\nabla\Phi_{1,\Delta t}^{n+1}}{(\Phi_{1,N}^{n+1})^2} - \frac{\varepsilon_1^2}{18}\nabla\cdot\left(\frac{\nabla\Phi_{1,\Delta t}^{n+1}}{\Phi_{1,N}^{n+1}} - \frac{\Phi_{1,\Delta t}^{n+1}\nabla\Phi_{1,N}^{n+1}}{(\Phi_{1,N}^{n+1})^2}\right)\\
&+\frac{\varepsilon_3^2}{36}\left(\frac{2|\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})|^2(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^3} - \frac{2\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})\cdot\nabla(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^2}\right)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\left(\frac{-\nabla(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})} + \frac{(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^2}\right)\Bigg) - \mathbf{g}_1^{(0)} + \Delta t\boldsymbol{h}_1^n,\\
&\frac{\Phi_{2,\Delta t}^{n+1}-\Phi_{2,\Delta t}^n}{\Delta t} \qquad (3.7)\\
=&\mathcal{M}_2\Delta\Bigg(\frac{1}{N_0}\frac{\Phi_{2,\Delta t}^{n+1}}{\Phi_{2,N}^{n+1}} + \frac{\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1}}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})} - 2\chi_{23}\Phi_{2,\Delta t}^n + (\chi_{12}-\chi_{13}-\chi_{23})\Phi_{1,\Delta t}^n\\
&+\frac{\varepsilon_1^2}{36}\frac{2|\nabla\Phi_{2,N}^{n+1}|^2\Phi_{2,\Delta t}^{n+1}}{(\Phi_{2,N}^{n+1})^3} - \frac{\varepsilon_1^2}{36}\frac{2\nabla\Phi_{2,N}^{n+1}\cdot\nabla\Phi_{2,\Delta t}^{n+1}}{(\Phi_{2,N}^{n+1})^2} - \frac{\varepsilon_1^2}{18}\nabla\cdot\left(\frac{\nabla\Phi_{2,\Delta t}^{n+1}}{\Phi_{2,N}^{n+1}} - \frac{\Phi_{2,\Delta t}^{n+1}\nabla\Phi_{2,N}^{n+1}}{(\Phi_{2,N}^{n+1})^2}\right)\\
&+\frac{\varepsilon_3^2}{36}\left(\frac{2|\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})|^2(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^3} - \frac{2\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})\cdot\nabla(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^2}\right)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\left(\frac{-\nabla(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})} + \frac{(\Phi_{1,\Delta t}^{n+1}+\Phi_{2,\Delta t}^{n+1})\nabla(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})}{(1-\Phi_{1,N}^{n+1}-\Phi_{2,N}^{n+1})^2}\right)\Bigg) - \mathbf{g}_2^{(0)} + \Delta t\boldsymbol{h}_2^n.
\end{aligned}
$$

Similarly, the function $\boldsymbol{h}_j$ is smooth enough in the sense that its derivatives are bounded in the $\|\cdot\|_{L^\infty}$ norm, and these functions are only dependent on the higher order derivatives of $\Phi_{j,\Delta t}$ and $\Phi_{j,N}$ ($j=1,2$), henceforth only dependent on the exact solution (Φ_1,Φ_2).

Therefore, a combination of (3.2)–(3.3) and (3.6)–(3.7) leads to the second order temporal truncation error for $\check{\Phi}_1$, $\check{\Phi}_2$ (given by (3.1)):

$$
\begin{aligned}
\frac{\check{\Phi}_1^{n+1}-\check{\Phi}_1^n}{\Delta t} =& \mathcal{M}_1\Delta\Bigg(\frac{1}{M_0}\ln\frac{\alpha\check{\Phi}_1^{n+1}}{M_0} - \ln(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1}) - 2\chi_{13}\check{\Phi}_1^n + (\chi_{12}-\chi_{13}-\chi_{23})\check{\Phi}_2^n\\
&-\frac{\varepsilon_1^2}{36}\frac{|\nabla\check{\Phi}_1^{n+1}|^2}{(\check{\Phi}_1^{n+1})^2} - \frac{\varepsilon_1^2}{18}\nabla\cdot\left(\frac{\nabla\check{\Phi}_1^{n+1}}{\check{\Phi}_1^{n+1}}\right) + \frac{\varepsilon_3^2}{36}\left(\frac{|\nabla(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})|^2}{(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})^2}\right)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\left(\frac{\nabla(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})}{(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})}\right)\Bigg) + O(\Delta t^2) + O(h^m),
\end{aligned} \tag{3.8}
$$

$$
\begin{aligned}
\frac{\check{\Phi}_2^{n+1}-\check{\Phi}_2^n}{\Delta t} =& \mathcal{M}_2\Delta\Bigg(\frac{1}{N_0}\ln\frac{\beta\check{\Phi}_2^{n+1}}{N_0}\ln(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1}) - 2\chi_{23}\check{\Phi}_2^n + (\chi_{12}-\chi_{13}-\chi_{23})\check{\Phi}_1^n\\
&-\frac{\varepsilon_2^2}{36}\frac{|\nabla\check{\Phi}_2^{n+1}|^2}{(\check{\Phi}_2^{n+1})^2} - \frac{\varepsilon_2^2}{18}\nabla\cdot\left(\frac{\nabla\check{\Phi}_2^{n+1}}{\check{\Phi}_2^{n+1}}\right) + \frac{\varepsilon_3^2}{36}\left(\frac{|\nabla(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})|^2}{(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})^2}\right)\\
&+\frac{\varepsilon_3^2}{18}\nabla\cdot\left(\frac{\nabla(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})}{(1-\check{\Phi}_1^{n+1}-\check{\Phi}_2^{n+1})}\right)\Bigg) + O(\Delta t^2) + O(h^m).
\end{aligned} \tag{3.9}
$$

In the derivation of (3.8)–(3.9), the following linearized expansions have been utilized:

$$
\begin{aligned}
&\ln \check{\Phi}_j = \ln(\Phi_{j,N} + \Delta t \Phi_{j,\Delta t}) = \ln \Phi_{j,N} + \frac{\Delta t \Phi_{j,\Delta t}}{\Phi_{j,N}} + O(\Delta t^2), \quad j = 1,2,\\
&\ln(1 - \check{\Phi}_1 - \check{\Phi}_2) = \ln(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t \Phi_{1,\Delta t} - \Delta t \Phi_{2,\Delta t})\\
&\quad = \ln(1 - \Phi_{1,N} - \Phi_{2,N}) - \Delta t \frac{\Phi_{1,\Delta t} + \Phi_{2,\Delta t}}{1 - \Phi_{1,N} - \Phi_{2,N}} + O(\Delta t^2),\\
&\frac{|\nabla \check{\Phi}_j|^2}{\check{\Phi}_j^2} = \frac{|\nabla(\Phi_{j,N} + \Delta t \Phi_{j,\Delta t})|^2}{(\Phi_{j,N} + \Delta t \Phi_{j,\Delta t})^2}\\
&\quad = \frac{|\nabla \Phi_{j,N}|^2}{\Phi_{j,N}^2} - 2\Delta t \frac{|\nabla \Phi_{j,N}|^2 \Phi_{j,\Delta t}}{\Phi_{j,N}^3} + 2\Delta t \frac{\nabla \Phi_{j,N} \cdot \nabla \Phi_{j,\Delta t}}{\Phi_{j,N}^2} + O(\Delta t^2), \quad j = 1,2,\\
&\frac{\nabla \check{\Phi}_j}{\check{\Phi}_j} = \frac{\nabla(\Phi_{j,N} + \Delta t \Phi_{j,\Delta t})}{\Phi_{j,N} + \Delta t \Phi_{j,\Delta t}} = \frac{\nabla \Phi_{j,N}}{\Phi_{j,N}} + \Delta t \frac{\nabla \Phi_{j,\Delta t}}{\Phi_{j,N}} - \Delta t \frac{\Phi_{j,\Delta t} \nabla \Phi_{j,N}}{\Phi_{j,N}^2} + O(\Delta t^2),\\
&\frac{|\nabla(1 - \check{\Phi}_1 - \check{\Phi}_2)|^2}{(1 - \check{\Phi}_1 - \check{\Phi}_2)^2} = \frac{|\nabla(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t \Phi_{1,\Delta t} - \Delta t \Phi_{2,\Delta t})|^2}{(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t \Phi_{1,\Delta t} - \Delta t \Phi_{2,\Delta t})^2}\\
&\quad = \frac{|\nabla(1 - \Phi_{1,N} - \Phi_{2,N})|^2}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} - \Delta t \frac{2\nabla(1 - \Phi_{1,N} - \Phi_{2,N}) \cdot \nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N})^2}\\
&\quad + \frac{2\Delta t |\nabla(1 - \Phi_{1,N} - \Phi_{2,N})|^2 (\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N})^3} + O(\Delta t^2),\\
&\frac{\nabla(1 - \check{\Phi}_1 - \check{\Phi}_2)}{(1 - \check{\Phi}_1 - \check{\Phi}_2)} = \frac{\nabla(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t \Phi_{1,\Delta t} - \Delta t \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t \Phi_{1,\Delta t} - \Delta t \Phi_{2,\Delta t})}\\
&\quad = \frac{\nabla(1 - \Phi_{1,N} - \Phi_{2,N})}{1 - \Phi_{1,N} - \Phi_{2,N}} - \Delta t \frac{\nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{1 - \Phi_{1,N} - \Phi_{2,N}}\\
&\quad + \Delta t \frac{(\Phi_{1,\Delta t} + \Phi_{2,\Delta t}) \nabla(1 - \Phi_{1,N} - \Phi_{2,N})}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} + O(\Delta t^2).
\end{aligned}
$$

Subsequently, we introduce $\check{\Phi}_{j,N}(\,\cdot\,, t) := \mathcal{P}_N \check{\Phi}_j(\,\cdot\,, t)$, the (spatial) Fourier projection of the constructed solution $\check{\Phi}_j$ into $\mathcal{B}^K$, $j = 1, 2$. A careful application of Taylor expansion in space yields the desired higher order consistency estimate for $\check{\Phi}_{1,N}$, $\check{\Phi}_{2,N}$ in the fully discrete scheme:

$$
\begin{aligned}
\frac{\check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{1,N}^n}{\Delta t} = {} & \mathcal{M}_1 \Delta_h \Big(\frac{1}{M_0} \ln \frac{\alpha \check{\Phi}_{1,N}^{n+1}}{M_0} - \ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - 2\chi_{13} \check{\Phi}_{1,N}^n + (\chi_{12} - \chi_{13} - \chi_{23}) \check{\Phi}_{2,N}^n\\
& - \frac{\varepsilon_1^2}{36} \mathcal{A}_h \Big(\frac{|\nabla_h \check{\Phi}_{1,N}^{n+1}|^2}{(\mathcal{A}_h \check{\Phi}_{1,N}^{n+1})^2} \Big) - \frac{\varepsilon_1^2}{18} \nabla_h \cdot \Big(\frac{\nabla_h \check{\Phi}_{1,N}^{n+1}}{\mathcal{A}_h \check{\Phi}_{1,N}^{n+1}} \Big)\\
& + \frac{\varepsilon_3^2}{36} \mathcal{A}_h \Big(\frac{|\nabla_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})|^2}{(\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}))^2} \Big) + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \Big(\frac{\nabla_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})}{\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})} \Big) \Big) + \tau_1^{n+1},
\end{aligned} \tag{3.10}
$$

$$
\begin{aligned}
\frac{\check{\Phi}_{2,N}^{n+1} - \check{\Phi}_{2,N}^n}{\Delta t} = {} & \mathcal{M}_2 \Delta_h \Big(\frac{1}{N_0} \ln \frac{\beta \check{\Phi}_{2,N}^{n+1}}{N_0} - \ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - 2\chi_{23} \check{\Phi}_{2,N}^n + (\chi_{12} - \chi_{13} - \chi_{23}) \check{\Phi}_{1,N}^n\\
& - \frac{\varepsilon_2^2}{36} \mathcal{A}_h \Big(\frac{|\nabla_h \check{\Phi}_{2,N}^{n+1}|^2}{(\mathcal{A}_h \check{\Phi}_{2,N}^{n+1})^2} \Big) - \frac{\varepsilon_2^2}{18} \nabla_h \cdot \Big(\frac{\nabla_h \check{\Phi}_{2,N}^{n+1}}{\mathcal{A}_h \check{\Phi}_{2,N}^{n+1}} \Big)\\
& + \frac{\varepsilon_3^2}{36} \mathcal{A}_h \Big(\frac{|\nabla_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})|^2}{(\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}))^2} \Big) + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \Big(\frac{\nabla_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})}{\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})} \Big) \Big) + \tau_2^{n+1},
\end{aligned} \tag{3.11}
$$

with $\|\tau_1^{n+1}\|_{-1,h}$, $\|\tau_2^{n+1}\|_{-1,h} \le C(\Delta t^2 + h^2)$.

Remark 3.1. Trivial initial data $\Phi_{j,\Delta t}(\cdot, t = 0) \equiv 0$ are given to $\Phi_{j,\Delta t}$ as (3.4)–(3.5). Therefore, using similar arguments as in (2.8)–(2.9), we conclude that

$$
\phi_j^0 \equiv \check{\Phi}_{j,N}^0, \quad \overline{\phi_j^k} = \overline{\phi_j^0}, \quad \forall k \ge 0, \tag{3.12}
$$

$$\overline{\check{\Phi}_{j,N}^k} = \frac{1}{|\Omega|}\int_\Omega \check{\Phi}_{j,N}(\cdot, t_k)\, d\mathbf{x} = \frac{1}{|\Omega|}\int_\Omega \check{\Phi}_j(\cdot, t_k)\, d\mathbf{x} = \frac{1}{|\Omega|}\int_\Omega \check{\Phi}_j^0\, d\mathbf{x} = \overline{\phi_j^0}, \quad \forall\, k \ge 0, \tag{3.13}$$

in which the first step of (3.13) is based on the fact that $\check{\Phi}_{j,N} \in \mathcal{B}^K$, the second step comes from the fact that $\check{\Phi}_{j,N}$ is the projection of $\check{\Phi}_j$ onto $\mathcal{B}^K$, and the third step comes from the mass conservative property of $\check{\Phi}_j$ at the continuous level. These two properties will be used in later analysis.

In addition, since $\check{\Phi}_{j,N}$ is mass conservative at a discrete level, as given by (3.13), we observe that the local truncation error τ_j has a similar property:

$$\overline{\tau_1^{n+1}} = \overline{\tau_2^{n+1}} = 0, \quad \forall n \ge 0, \;\; j = 1, 2. \tag{3.14}$$

Remark 3.2. Since the temporal correction function $\Phi_{j,\Delta t}$ is bounded, we recall the separation property (2.6) for the exact solution, and obtain a similar property for the constructed profile $\check{\Phi}_{j,N}$:

$$\check{\Phi}_{1,N} \ge \delta_0, \;\; \check{\Phi}_{2,N} \ge \delta_0, \;\; 1 - \check{\Phi}_{1,N} - \check{\Phi}_{2,N} \ge \delta_0, \quad \exists\, \delta_0 > 0, \tag{3.15}$$

in which the projection estimate (2.7) has been repeatedly used. Such a uniform bound will be used in the convergence analysis.

In addition, since the temporal correction function $\Phi_{j,\Delta t}$ only depends on $\Phi_{j,N}$ and the exact solution, its $W^{1,\infty}$ norm will stay bounded. In turn, we are able to obtain a discrete $W^{1,\infty}$ bound for the constructed profile $\check{\Phi}_{j,N}$:

$$\|\nabla_h \check{\Phi}_{j,N}\|_\infty \le C^*, \quad j = 1, 2. \tag{3.16}$$

Remark 3.3. The reason for such a higher order asymptotic expansion and truncation error estimate is to justify an a-priori $L^\infty_{\Delta t}$ bound of the numerical solution, which is needed to obtain the separation property, similarly formulated as (3.15) for the constructed approximate solution. With such a property valid for both the constructed approximate solution and the numerical solution, the nonlinear error term could be appropriately analyzed in the H^{-1} convergence estimate.

3.2. A rough error estimate

Instead of a direct analysis for the error function defined in (2.11), we introduce an alternate numerical error function:

$$\tilde{\phi}_1^m := \mathcal{P}_h \check{\Phi}_{1,N}^m - \phi_1^m, \;\; \tilde{\phi}_2^m := \mathcal{P}_h \check{\Phi}_{2,N}^m - \phi_2^m, \quad \forall\, m \in \{0, 1, 2, 3, \ldots\}. \tag{3.17}$$

The advantage of such a numerical error function is associated with its higher order accuracy, which comes from the higher order consistency estimate (3.8)–(3.9). Again, since $\overline{\tilde{\phi}_1^m} = \overline{\tilde{\phi}_2^m} = 0$, which comes from the fact (3.12)–(3.13), for any $m \ge 0$, we conclude that the discrete norm $\|\cdot\|_{-1,h}$ is well defined for the error grid function $\tilde{\phi}_j^m$, $j = 1, 2$.

In turn, subtracting the numerical scheme (2.2)–(2.3) from the consistency estimate (3.10)–(3.11) yields

$$\frac{\tilde{\phi}_1^{n+1} - \tilde{\phi}_1^n}{\Delta t} = \mathcal{M}_1 \Delta_h \tilde{\mu}_1^{n+1} + \tau_1^{n+1}, \tag{3.18}$$

$$\frac{\tilde{\phi}_2^{n+1} - \tilde{\phi}_2^n}{\Delta t} = \mathcal{M}_2 \Delta_h \tilde{\mu}_2^{n+1} + \tau_2^{n+1}, \tag{3.19}$$

with

$$\begin{aligned} \tilde{\mu}_1^{n+1} = {} & \frac{1}{M_0}(\ln \check{\Phi}_{1,N}^{n+1} - \ln \phi_1^{n+1}) - (\ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1})) \\ & - 2\chi_{13}\tilde{\phi}_1^n + (\chi_{12} - \chi_{13} - \chi_{23})\tilde{\phi}_2^n + \tilde{\mu}_{1,s}^{n+1} + \tilde{\mu}_{3,s}^{n+1}, \end{aligned} \tag{3.20}$$

$$\begin{aligned} \tilde{\mu}_2^{n+1} = {} & \frac{1}{N_0}(\ln \check{\Phi}_{2,N}^{n+1} - \ln \phi_2^{n+1}) - (\ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1})) \\ & - 2\chi_{23}\tilde{\phi}_2^n + (\chi_{12} - \chi_{13} - \chi_{23})\tilde{\phi}_1^n + \tilde{\mu}_{2,s}^{n+1} + \tilde{\mu}_{3,s}^{n+1}, \end{aligned} \tag{3.21}$$

$$\tilde{\mu}_{1,s}^{n+1} = \frac{\varepsilon_1^2}{36}\mathcal{A}_h\Big(\gamma^{(1)}\mathcal{A}_h\tilde{\phi}_1^{n+1} - \frac{\nabla_h(\check{\Phi}_{1,N}^{n+1} + \phi_1^{n+1}) \cdot \nabla_h \tilde{\phi}_1^{n+1}}{(\mathcal{A}_h \check{\Phi}_{1,N}^{n+1})^2}\Big) - \frac{\varepsilon_1^2}{18}\nabla_h \cdot \Big(\frac{\nabla_h \tilde{\phi}_1^{n+1}}{\mathcal{A}_h \phi_1^{n+1}} - \frac{\tilde{\phi}_1^{n+1}\nabla_h \check{\Phi}_{1,N}^{n+1}}{\mathcal{A}_h \phi_1^{n+1}\mathcal{A}_h \check{\Phi}_{1,N}^{n+1}}\Big), \tag{3.22}$$

$$\tilde{\mu}_{2,s}^{n+1} = \frac{\varepsilon_2^2}{36}\mathcal{A}_h\Big(\gamma^{(2)}\mathcal{A}_h\tilde{\phi}_2^{n+1} - \frac{\nabla_h(\check{\Phi}_{2,N}^{n+1} + \phi_2^{n+1}) \cdot \nabla_h \tilde{\phi}_2^{n+1}}{(\mathcal{A}_h \check{\Phi}_{2,N}^{n+1})^2}\Big) - \frac{\varepsilon_2^2}{18}\nabla_h \cdot \Big(\frac{\nabla_h \tilde{\phi}_2^{n+1}}{\mathcal{A}_h \phi_2^{n+1}} - \frac{\tilde{\phi}_2^{n+1}\nabla_h \check{\Phi}_{2,N}^{n+1}}{\mathcal{A}_h \phi_2^{n+1}\mathcal{A}_h \check{\Phi}_{2,N}^{n+1}}\Big), \tag{3.23}$$

$$\tilde{\mu}_{3,s}^{n+1} = \frac{\varepsilon_3^2}{36}\mathcal{A}_h\Big(\gamma^{(3)}\mathcal{A}_h(\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})\Big) - \frac{\varepsilon_3^2}{18}\nabla_h \cdot \Big(\frac{\nabla_h(\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})}{\mathcal{A}_h(1 - \phi_1^{n+1} - \phi_2^{n+1})}$$

$$
\begin{aligned}
&- \frac{\varepsilon_3^2}{36} \mathcal{A}_h \Big(\frac{\nabla_h (2 - \phi_1^{n+1} - \phi_2^{n+1} - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) \cdot \nabla_h (\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})}{(\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}))^2} \Big) \\
&- \frac{\varepsilon_3^2}{18} \nabla_h \cdot \Big(\frac{(\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}) \nabla_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})}{\mathcal{A}_h (1 - \phi_1^{n+1} - \phi_2^{n+1}) \mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})} \Big),
\end{aligned}
\tag{3.24}
$$

$$
\gamma^{(1)} = \frac{\mathcal{A}_h (\phi_1^{n+1} + \check{\Phi}_{1,N}^{n+1}) |\nabla_h \phi_1^{n+1}|^2}{(\mathcal{A}_h \phi_1^{n+1})^2 (\mathcal{A}_h \check{\Phi}_{1,N}^{n+1})^2}, \tag{3.25}
$$

$$
\gamma^{(2)} = \frac{\mathcal{A}_h (\phi_2^{n+1} + \check{\Phi}_{2,N}^{n+1}) |\nabla_h \phi_2^{n+1}|^2}{(\mathcal{A}_h \phi_2^{n+1})^2 (\mathcal{A}_h \check{\Phi}_{2,N}^{n+1})^2}, \tag{3.26}
$$

$$
\gamma^{(3)} = \frac{\mathcal{A}_h (2 - \phi_1^{n+1} - \phi_2^{n+1} - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) |\nabla_h (1 - \phi_1^{n+1} - \phi_2^{n+1})|^2}{(\mathcal{A}_h (1 - \phi_1^{n+1} - \phi_2^{n+1}))^2 (\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}))^2}. \tag{3.27}
$$

To proceed with the nonlinear analysis, we make the following a-priori assumption at the previous time step:

$$
\|\tilde{\phi}_j^n\|_{-1,h} \le \Delta t^{\frac{7}{4}} + h^{\frac{7}{4}}, \quad \|\tilde{\phi}_j^n\|_2 \le \Delta t^{\frac{5}{4}} + h^{\frac{5}{4}}, \quad j = 1, 2. \tag{3.28}
$$

Such an a-priori assumption will be recovered by the optimal rate convergence analysis at the next time step, as will be demonstrated later.

Taking a discrete inner product with (3.18), (3.19) by $\tilde{\mu}_1^{n+1}$, $\tilde{\mu}_2^{n+1}$, respectively, leads to

$$
\begin{aligned}
&\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle + \Delta t (\mathcal{M}_1 \|\nabla_h \tilde{\mu}_1^{n+1}\|_2^2 + \mathcal{M}_2 \|\nabla_h \tilde{\mu}_2^{n+1}\|_2^2) \\
&= \langle \tilde{\phi}_1^n, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^n, \tilde{\mu}_2^{n+1} \rangle + \Delta t (\langle \tau_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tau_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle).
\end{aligned}
\tag{3.29}
$$

Because of the mean-zero property (3.14) for the local truncation error terms, the following estimate is available:

$$
\langle \tau_j^{n+1}, \tilde{\mu}_j^{n+1} \rangle \le \|\tau_j^{n+1}\|_{-1,h} \cdot \|\nabla_h \tilde{\mu}_j^{n+1}\|_2 \le \frac{1}{2\mathcal{M}_j} \|\tau_j^{n+1}\|_{-1,h}^2 + \frac{\mathcal{M}_j}{2} \|\nabla_h \tilde{\mu}_j^{n+1}\|_2^2, \quad j = 1, 2. \tag{3.30}
$$

For the two terms $\langle \tilde{\phi}_1^n, \tilde{\mu}_1^{n+1} \rangle$ and $\langle \tilde{\phi}_2^n, \tilde{\mu}_2^{n+1} \rangle$, an application of the Cauchy inequality reveals that

$$
\langle \tilde{\phi}_j^n, \tilde{\mu}_j^{n+1} \rangle \le \|\tilde{\phi}_j^n\|_{-1,h} \cdot \|\nabla_h \tilde{\mu}_j^{n+1}\|_2 \le \frac{1}{2\mathcal{M}_j \Delta t} \|\tilde{\phi}_j^n\|_{-1,h}^2 + \frac{\mathcal{M}_j}{2} \Delta t \|\nabla_h \tilde{\mu}_j^{n+1}\|_2^2, \quad j = 1, 2. \tag{3.31}
$$

Going back (3.29), we get

$$
\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle \le \frac{1}{2\mathcal{M}_* \Delta t} (\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) + \frac{\Delta t}{2\mathcal{M}_*} (\|\tau_1^{n+1}\|_{-1,h}^2 + \|\tau_2^{n+1}\|_{-1,h}^2), \tag{3.32}
$$

which $\mathcal{M}_* = \min(\mathcal{M}_1, \mathcal{M}_2)$. On the other hand, the detailed expansions in (3.20)–(3.21) reveal the following identity:

$$
\begin{aligned}
&\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle \\
&= \frac{1}{M_0} \langle (\ln \check{\Phi}_{1,N}^{n+1} - \ln \phi_1^{n+1}), \tilde{\phi}_1^{n+1} \rangle + \frac{1}{N_0} \langle (\ln \check{\Phi}_{2,N}^{n+1} - \ln \phi_2^{n+1}), \tilde{\phi}_2^{n+1} \rangle \\
&- \langle (\ln (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln (1 - \phi_1^{n+1} - \phi_2^{n+1})), \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle \\
&- 2\chi_{13} \langle \tilde{\phi}_1^n, \tilde{\phi}_1^{n+1} \rangle - 2\chi_{23} \langle \tilde{\phi}_2^n, \tilde{\phi}_2^{n+1} \rangle + (\chi_{12} - \chi_{13} - \chi_{23}) (\langle \tilde{\phi}_2^n, \tilde{\phi}_1^{n+1} \rangle + \langle \tilde{\phi}_1^n, \tilde{\phi}_2^{n+1} \rangle) \\
&+ \langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1} \rangle + \langle \tilde{\mu}_{2,s}^{n+1}, \tilde{\phi}_2^{n+1} \rangle + \langle \tilde{\mu}_{3,s}^{n+1}, \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle.
\end{aligned}
\tag{3.33}
$$

For the first nonlinear inner product on the right hand side, we begin with the following observation:

$$
\ln \check{\Phi}_{1,N}^{n+1} - \ln \phi_1^{n+1} = \frac{1}{\xi} \tilde{\phi}_1^{n+1}, \quad \text{with } 0 < \xi < 1 \text{ between } \phi_1^{n+1} \text{ and } \check{\Phi}_{1,N}^{n+1},
$$

which comes from an application of intermediate value theorem. Since the bound $0 < \xi < 1$ is available at a point-wise level, we conclude that

$$
\langle (\ln \check{\Phi}_{1,N}^{n+1} - \ln \phi_1^{n+1}), \tilde{\phi}_1^{n+1} \rangle \ge \|\tilde{\phi}_1^{n+1}\|_2^2. \tag{3.34}
$$

Using similar arguments, we also obtain

$$
\langle (\ln \check{\Phi}_{2,N}^{n+1} - \ln \phi_2^{n+1}), \tilde{\phi}_2^{n+1} \rangle \ge \|\tilde{\phi}_2^{n+1}\|_2^2, \tag{3.35}
$$

$$
-\langle (\ln (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln (1 - \phi_1^{n+1} - \phi_2^{n+1})), \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle \ge \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_2^2. \tag{3.36}
$$

Moreover, since the discrete surface energy functional presented in (2.4) is convex, we conclude that

$$\langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1} \rangle + \langle \tilde{\mu}_{2,s}^{n+1}, \tilde{\phi}_2^{n+1} \rangle + \langle \tilde{\mu}_{3,s}^{n+1}, \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle \geq 0. \tag{3.37}$$

Going back (3.33), we arrive at

$$\begin{aligned}
&\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle \\
\geq\ & \frac{1}{M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 + \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_2^2 - 4\chi_{13}^2 M_0 \|\tilde{\phi}_1^n\|_2^2 - \frac{1}{4M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 \\
& -4\chi_{23}^2 N_0 \|\tilde{\phi}_2^n\|_2^2 - \frac{1}{4N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 - \frac{1}{4M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 - \frac{1}{4N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 \\
& -(\chi_{12} - \chi_{13} - \chi_{23})^2 (M_0 \|\tilde{\phi}_2^n\|_2^2 + N_0 \|\tilde{\phi}_1^n\|_2^2) \\
\geq\ & \frac{1}{2M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{2N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 - (4\chi_{13}^2 M_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 N_0) \|\tilde{\phi}_1^n\|_2^2 \\
& -(4\chi_{23}^2 N_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 M_0) \|\tilde{\phi}_2^n\|_2^2.
\end{aligned} \tag{3.38}$$

In turn, its substitution into (3.32) yields

$$\begin{aligned}
& \frac{1}{2M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{2N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 \\
\leq\ & (4\chi_{13}^2 M_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 N_0) \|\tilde{\phi}_1^n\|_2^2 + (4\chi_{23}^2 N_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 M_0) \|\tilde{\phi}_2^n\|_2^2 \\
& + \frac{1}{2\mathcal{M}_* \Delta t} (\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) + \frac{\Delta t}{2\mathcal{M}_*} (\|\tau_1^{n+1}\|_{-1,h}^2 + \|\tau_2^{n+1}\|_{-1,h}^2).
\end{aligned} \tag{3.39}$$

Furthermore, a substitution of the a-priori error bound (3.28) at the previous time step results in a rough error estimate for $\tilde{\phi}_1^{n+1}$, $\tilde{\phi}_2^{n+1}$:

$$\|\tilde{\phi}_1^{n+1}\|_2 + \|\tilde{\phi}_2^{n+1}\|_2 \leq \hat{C} (\Delta t^{\frac{5}{4}} + h^{\frac{5}{4}}), \tag{3.40}$$

under the linear refinement requirement $C_1 h \leq \Delta t \leq C_2 h$, with $\hat{C}$ dependent on M_0, N_0, χ_{12}, χ_{13} and χ_{23}. Subsequently, an application of 2-D inverse inequality implies that

$$\|\tilde{\phi}_1^{n+1}\|_\infty + \|\tilde{\phi}_2^{n+1}\|_\infty \leq \frac{C(\|\tilde{\phi}_1^{n+1}\|_2 + \|\tilde{\phi}_2^{n+1}\|_2)}{h} \leq \hat{C}_1 (\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}), \quad \text{with } \hat{C}_1 = C\hat{C}, \tag{3.41}$$

under the same linear refinement requirement. Because of the accuracy order, we could take Δt and h sufficient small so that

$$\hat{C}_1 (\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}) \leq \frac{\delta_0}{4}, \quad \text{so that } \|\tilde{\phi}_1^{n+1}\|_\infty + \|\tilde{\phi}_2^{n+1}\|_\infty \leq \frac{\delta_0}{4}. \tag{3.42}$$

Its combination with (3.15), the separation property for the constructed approximate solution, leads to a similar property for the numerical solution:

$$\phi_1^{n+1} \geq \frac{\delta_0}{2}, \ \ \phi_2^{n+1} \geq \frac{\delta_0}{2}, \ \ 1 - \phi_1^{n+1} - \phi_2^{n+1} \geq \frac{\delta_0}{2}, \quad \text{for } \delta_0 > 0. \tag{3.43}$$

Such a uniform $\|\cdot\|_\infty$ bound will play a very important role in the refined error estimate.

Remark 3.4. In the rough error estimate (3.40), we see that the accuracy order is lower than the one given by the a-priori-assumption (3.28). Therefore, such a rough estimate could not be used for a global induction analysis. Instead, the purpose of such an estimate is to establish a uniform $\|\cdot\|_\infty$ bound, via the technique of inverse inequality, so that a discrete separation property becomes available for the numerical solution. With such a property established for the numerical solution, the refined error analysis will yield much sharper estimates.

3.3. The refined error estimate

Taking a discrete inner product with (3.18), (3.19) by $(-\Delta_h)^{-1}\tilde{\phi}_1^{n+1}$, $(-\Delta_h)^{-1}\tilde{\phi}_2^{n+1}$, respectively, leads to

$$\begin{aligned}
& \frac{1}{\mathcal{M}_1} \langle \tilde{\phi}_1^{n+1} - \tilde{\phi}_1^n, \tilde{\phi}_1^{n+1} \rangle_{-1,h} + \frac{1}{\mathcal{M}_2} \langle \tilde{\phi}_2^{n+1} - \tilde{\phi}_2^n, \tilde{\phi}_2^{n+1} \rangle_{-1,h} + \Delta t (\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle) \\
=\ & \frac{\Delta t}{\mathcal{M}_1} \langle \tau_1^{n+1}, \tilde{\phi}_1^{n+1} \rangle_{-1,h} + \frac{\Delta t}{\mathcal{M}_2} \langle \tau_2^{n+1}, \tilde{\phi}_2^{n+1} \rangle_{-1,h},
\end{aligned} \tag{3.44}$$

with the summation by parts formulas applied. The following identities are available for the temporal approximation terms:

$$\frac{1}{\mathcal{M}_j} \langle \tilde{\phi}_j^{n+1} - \tilde{\phi}_j^n, \tilde{\phi}_j^{n+1} \rangle_{-1,h} = \frac{1}{2\mathcal{M}_j} (\|\tilde{\phi}_j^{n+1}\|_{-1,h}^2 - \|\tilde{\phi}_j^n\|_{-1,h}^2 + \|\tilde{\phi}_j^{n+1} - \tilde{\phi}_j^n\|_{-1,h}^2), \quad j = 1, 2. \tag{3.45}$$

For the local truncation error terms, similar estimates could be derived:

$$\frac{1}{\mathcal{M}_j}\langle \tau_j^{n+1}, \tilde{\phi}_j^{n+1}\rangle_{-1,h} \le \frac{1}{2\mathcal{M}_j}(\|\tau_j^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_j^{n+1}\|_{-1,h}^2), \quad j=1,2. \tag{3.46}$$

For the term $\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1}\rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1}\rangle$, the expansion (3.33), as well as the inequalities (3.34)–(3.36), are still valid. For the inner product associated with the concave terms, a standard Cauchy inequality is applied:

$$\begin{aligned}&-2\chi_{13}\langle \tilde{\phi}_1^n, \tilde{\phi}_1^{n+1}\rangle \ge -2\chi_{13}\|\tilde{\phi}_1^n\|_{-1,h}\|\nabla_h\tilde{\phi}_1^{n+1}\|_2\\ &\ge -\frac{144\chi_{13}^2}{\varepsilon_0^2}\|\tilde{\phi}_1^n\|_{-1,h}^2 - \frac{\varepsilon_0^2}{144}\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^2,\end{aligned} \tag{3.47}$$

$$\begin{aligned}&-2\chi_{23}\langle \tilde{\phi}_2^n, \tilde{\phi}_2^{n+1}\rangle \ge -2\chi_{23}\|\tilde{\phi}_2^n\|_{-1,h}\|\nabla_h\tilde{\phi}_2^{n+1}\|_2\\ &\ge -\frac{144\chi_{23}^2}{\varepsilon_0^2}\|\tilde{\phi}_2^n\|_{-1,h}^2 - \frac{\varepsilon_0^2}{144}\|\nabla_h\tilde{\phi}_2^{n+1}\|_2^2,\end{aligned} \tag{3.48}$$

$$\begin{aligned}&(\chi_{12}-\chi_{13}-\chi_{23})(\langle \tilde{\phi}_2^n, \tilde{\phi}_1^{n+1}\rangle + \langle \tilde{\phi}_1^n, \tilde{\phi}_2^{n+1}\rangle)\\ &\ge -\frac{36(\chi_{12}-\chi_{13}-\chi_{23})^2}{\varepsilon_0^2}(\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) - \frac{\varepsilon_0^2}{144}(\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h\tilde{\phi}_2^{n+1}\|_2^2).\end{aligned} \tag{3.49}$$

The rest works are focused on the estimates for the error terms associated with the nonlinear surface diffusion, as given by $\langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1}\rangle$, $\langle \tilde{\mu}_{2,s}^{n+1}, \tilde{\phi}_2^{n+1}\rangle$, $\langle \tilde{\mu}_{3,s}^{n+1}, \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\rangle$, the last three terms in (3.33). First, we look at the expansion for $\langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1}\rangle$, which comes from the expression (3.22):

$$\begin{aligned}&\langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1}\rangle = I_1 + I_2 + I_3 + I_4, \quad \text{with}\\ &I_1 := \frac{\varepsilon_1^2}{36}\langle \mathcal{A}_h(\gamma^{(1)}\mathcal{A}_h\tilde{\phi}_1^{n+1}), \tilde{\phi}_1^{n+1}\rangle, \quad I_2 := -\frac{\varepsilon_1^2}{36}\Big\langle \mathcal{A}_h\Big(\frac{\nabla_h(\check{\Phi}_{1,N}^{n+1} + \phi_1^{n+1})\cdot\nabla_h\tilde{\phi}_1^{n+1}}{(\mathcal{A}_h\check{\Phi}_{1,N}^{n+1})^2}\Big), \tilde{\phi}_1^{n+1}\Big\rangle\\ &I_3 := -\frac{\varepsilon_1^2}{18}\Big\langle \nabla_h\cdot\Big(\frac{\nabla_h\tilde{\phi}_1^{n+1}}{\mathcal{A}_h\phi_1^{n+1}}\Big), \tilde{\phi}_1^{n+1}\Big\rangle, \quad I_4 := \frac{\varepsilon_1^2}{18}\Big\langle \nabla_h\cdot\Big(\frac{\tilde{\phi}_1^{n+1}\nabla_h\check{\Phi}_{1,N}^{n+1}}{\mathcal{A}_h\phi_1^{n+1}\mathcal{A}_h\check{\Phi}_{1,N}^{n+1}}\Big), \tilde{\phi}_1^{n+1}\Big\rangle.\end{aligned} \tag{3.50}$$

It is clear that I_1 stays non-negative:

$$I_1 = \frac{\varepsilon_1^2}{36}\langle \gamma^{(1)}\mathcal{A}_h\tilde{\phi}_1^{n+1}, \mathcal{A}_h\tilde{\phi}_1^{n+1}\rangle \ge 0, \tag{3.51}$$

in which the summation by parts formula is applied in the first step, while the fact that $\gamma^{(1)} \ge 0$ (given by (3.25)) is used in the second step. Similarly, for the third part I_3, an application of summation by parts reveals that

$$I_3 = \frac{\varepsilon_1^2}{18}\Big[\frac{\nabla_h\tilde{\phi}_1^{n+1}}{\mathcal{A}_h\phi_1^{n+1}}, \nabla_h\tilde{\phi}_1^{n+1}\Big] \ge \frac{\varepsilon_1^2}{18}\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^2, \tag{3.52}$$

in which the point-wise estimate $0 < \phi_1^{n+1} < 1$ has been used in the second step. For the fourth part I_4, an application of summation by parts formula gives

$$\begin{aligned}-I_4 &= \frac{\varepsilon_1^2}{18}\Big[\frac{\tilde{\phi}_1^{n+1}\nabla_h\check{\Phi}_{1,N}^{n+1}}{\mathcal{A}_h\phi_1^{n+1}\mathcal{A}_h\check{\Phi}_{1,N}^{n+1}}, \nabla_h\tilde{\phi}_1^{n+1}\Big]\\ &\le \frac{\varepsilon_1^2}{18}\Big\|\frac{1}{\mathcal{A}_h\phi_1^{n+1}}\Big\|_\infty\cdot\Big\|\frac{1}{\mathcal{A}_h\check{\Phi}_{1,N}^{n+1}}\Big\|_\infty\cdot\|\nabla_h\check{\Phi}_{1,N}^{n+1}\|_\infty\cdot\|\tilde{\phi}_1^{n+1}\|_2\cdot\|\nabla_h\tilde{\phi}_1^{n+1}\|_2\\ &\le \frac{C^*\varepsilon_1^2}{18}\cdot 2(\delta_0)^{-2}\|\tilde{\phi}_1^{n+1}\|_2\cdot\|\nabla_h\tilde{\phi}_1^{n+1}\|_2\\ &\le \frac{C^*\varepsilon_1^2(\delta_0)^{-2}}{9}\|\tilde{\phi}_1^{n+1}\|_{-1,h}^{\frac{1}{2}}\cdot\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^{\frac{3}{2}}\\ &\le C(C^*)^4(\delta_0)^{-8}\varepsilon_1^2\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{\varepsilon_1^2}{72}\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^2.\end{aligned} \tag{3.53}$$

In more details, the preliminary estimate (3.16) has been applied in the third step, combined the separation properties (3.15), (3.43); the Sobolev interpolation formula, $\|\tilde{\phi}_1^{n+1}\|_2 \le \|\tilde{\phi}_1^{n+1}\|_{-1,h}^{\frac{1}{2}}\cdot\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^{\frac{1}{2}}$, has been used in the fourth step; the Young's inequality has been applied in the last step. For the second term I_2, we begin with the following summation by parts:

$$-I_2 = \frac{\varepsilon_1^2}{36}\Big[\frac{\nabla_h(\check{\Phi}_{1,N}^{n+1} + \phi_1^{n+1})\cdot\nabla_h\tilde{\phi}_1^{n+1}}{(\mathcal{A}_h\check{\Phi}_{1,N}^{n+1})^2}, \mathcal{A}_h\tilde{\phi}_1^{n+1}\Big]. \tag{3.54}$$

Meanwhile, because of the fact $\phi_1^{n+1} = \check{\Phi}_{1,N}^{n+1} - \tilde{\phi}_1^{n+1}$, we are able to decompose $-I_2$ into two parts:

$$-I_2 = -I_{2,1} - I_{2,2}, \quad \text{with } -I_{2,1} := \frac{\varepsilon_1^2}{18}\Big[\frac{\nabla_h \check{\Phi}_{1,N}^{n+1} \cdot \nabla_h \tilde{\phi}_1^{n+1}}{(\mathcal{A}_h \check{\Phi}_{1,N}^{n+1})^2}, \mathcal{A}_h \tilde{\phi}_1^{n+1}\Big], \tag{3.55}$$

$$-I_{2,2} := -\frac{\varepsilon_1^2}{36}\Big[\frac{|\nabla_h \tilde{\phi}_1^{n+1}|^2}{(\mathcal{A}_h \check{\Phi}_{1,N}^{n+1})^2}, \mathcal{A}_h \tilde{\phi}_1^{n+1}\Big]. \tag{3.56}$$

The bound for $-I_{2,1}$ could be obtained in a similar style as (3.53):

$$\begin{aligned}
-I_{2,1} &\le \frac{\varepsilon_1^2}{18}\Big\|\frac{1}{\mathcal{A}_h \check{\Phi}_{1,N}^{n+1}}\Big\|_\infty^2 \cdot \|\nabla_h \check{\Phi}_{1,N}^{n+1}\|_\infty \cdot \|\mathcal{A}_h \tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\
&\le \frac{C^* \varepsilon_1^2}{18} \cdot (\delta_0)^{-2} \|\mathcal{A}_h \tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \le \frac{C^* \varepsilon_1^2}{18} \cdot (\delta_0)^{-2} \|\tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\
&\le \frac{C^* \varepsilon_1^2 (\delta_0)^{-2}}{18} \|\tilde{\phi}_1^{n+1}\|_{-1,h}^{\frac{1}{2}} \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^{\frac{3}{2}} \\
&\le C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{\varepsilon_1^2}{144} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2.
\end{aligned} \tag{3.57}$$

For the other part $-I_{2,2}$, we recall the $\|\cdot\|_\infty$ rough estimate (3.41) and the separation inequality (3.15), and arrive at

$$\begin{aligned}
-I_{2,2} &\le \frac{\varepsilon_1^2}{36}\Big\|\frac{1}{\mathcal{A}_h \check{\Phi}_{1,N}^{n+1}}\Big\|_\infty^2 \cdot \|\mathcal{A}_h \tilde{\phi}_1^{n+1}\|_\infty \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 \\
&\le \frac{\varepsilon_1^2}{36} \cdot (\delta_0)^{-2} \cdot \hat{C}_1 (\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}) \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2.
\end{aligned} \tag{3.58}$$

In turn, if Δt and h are sufficiently small so that

$$\frac{\hat{C}_1 (\delta_0)^{-2}}{36} (\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}) \le \frac{1}{144}, \tag{3.59}$$

we obtain a useful bound

$$-I_{2,2} \le \frac{\varepsilon_1^2}{144} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \tag{3.60}$$

A substitution of (3.57)–(3.60) into (3.54) leads to

$$-I_2 \le C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{\varepsilon_1^2}{72} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \tag{3.61}$$

Finally, a combination of (3.51)–(3.53) and (3.61) results in

$$\langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1} \rangle \ge \frac{\varepsilon_1^2}{36} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 - 2C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2. \tag{3.62}$$

The two other nonlinear surface diffusion error terms could be analyzed in the same style. The results are stated below; the technical details are skipped for the sake of brevity.

$$\langle \tilde{\mu}_{2,s}^{n+1}, \tilde{\phi}_2^{n+1} \rangle \ge \frac{\varepsilon_2^2}{36} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 - 2C(C^*)^4 (\delta_0)^{-8} \varepsilon_2^2 \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2, \tag{3.63}$$

$$\begin{aligned}
\langle \tilde{\mu}_{3,s}^{n+1}, \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle &\ge \frac{\varepsilon_3^2}{36} \|\nabla_h (\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})\|_2^2 - 2C(C^*)^4 (\delta_0)^{-8} \varepsilon_3^2 \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_{-1,h}^2 \\
&\ge \frac{\varepsilon_3^2}{36} \|\nabla_h (\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})\|_2^2 \\
&\quad -4C(C^*)^4 (\delta_0)^{-8} \varepsilon_3^2 (\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2).
\end{aligned} \tag{3.64}$$

A substitution of (3.34)–(3.36), (3.47)–(3.49), (3.62)–(3.64) into (3.33) results in

$$\begin{aligned}
&\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle \\
\ge\ & \frac{\varepsilon_0^2}{72} (\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2) - 4C(C^*)^4 (\delta_0)^{-8} (\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2)(\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2) \\
&- \frac{144}{\varepsilon_0^2} (\chi_{13}^2 + \chi_{23}^2 + (\chi_{12} - \chi_{13} - \chi_{23})^2)(\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2).
\end{aligned} \tag{3.65}$$

A combination of (3.44)–(3.46) and (3.65) gives

$$\begin{aligned}
&\left(\frac{1}{\mathcal{M}_1}\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2+\frac{1}{\mathcal{M}_2}\|\tilde{\phi}_2^{n+1}\|_{-1,h}^2\right)-\left(\frac{1}{\mathcal{M}_1}\|\tilde{\phi}_1^{n}\|_{-1,h}^2+\frac{1}{\mathcal{M}_2}\|\tilde{\phi}_2^{n}\|_{-1,h}^2\right)\\
&+\frac{\varepsilon_0^2}{36}\Delta t(\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^2+\|\nabla_h\tilde{\phi}_2^{n+1}\|_2^2)\\
\le{}& \kappa^{(1)}\Delta t(\|\tilde{\phi}_1^{n}\|_{-1,h}^2+\|\tilde{\phi}_2^{n}\|_{-1,h}^2)+\kappa^{(2)}\Delta t(\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2+\|\tilde{\phi}_2^{n+1}\|_{-1,h}^2)\\
&+\Delta t\left(\frac{1}{\mathcal{M}_1}\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2+\frac{1}{\mathcal{M}_2}\|\tilde{\phi}_2^{n+1}\|_{-1,h}^2\right)+\Delta t\left(\frac{1}{\mathcal{M}_1}\|\tau_1^{n+1}\|_{-1,h}^2+\frac{1}{\mathcal{M}_2}\|\tau_2^{n+1}\|_{-1,h}^2\right),\\
&\text{with}\quad \kappa^{(1)}=\frac{288}{\varepsilon_0^2}(\chi_{13}^2+\chi_{23}^2+(\chi_{12}-\chi_{13}-\chi_{23})^2),\ \kappa^{(2)}=8C(C^*)^4(\delta_0)^{-8}(\varepsilon_1^2+\varepsilon_2^2+\varepsilon_3^2).
\end{aligned} \tag{3.66}$$

In other words, we have

$$\begin{aligned}
&\left(\frac{1}{\mathcal{M}_1}\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2+\frac{1}{\mathcal{M}_2}\|\tilde{\phi}_2^{n+1}\|_{-1,h}^2\right)-\left(\frac{1}{\mathcal{M}_1}\|\tilde{\phi}_1^{n}\|_{-1,h}^2+\frac{1}{\mathcal{M}_2}\|\tilde{\phi}_2^{n}\|_{-1,h}^2\right)\\
&+\frac{\varepsilon_0^2}{36}\Delta t(\|\nabla_h\tilde{\phi}_1^{n+1}\|_2^2+\|\nabla_h\tilde{\phi}_2^{n+1}\|_2^2)\\
\le{}& \kappa^{(1)}\Delta t(\|\tilde{\phi}_1^{n}\|_{-1,h}^2+\|\tilde{\phi}_2^{n}\|_{-1,h}^2)+\left(\kappa^{(2)}+\frac{\mathcal{M}_1+\mathcal{M}_2}{\mathcal{M}_1\mathcal{M}_2}\right)\Delta t(\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2+\|\tilde{\phi}_2^{n+1}\|_{-1,h}^2)\\
&+\frac{\mathcal{M}_1+\mathcal{M}_2}{\mathcal{M}_1\mathcal{M}_2}\Delta t\left(\|\tau_1^{n+1}\|_{-1,h}^2+\|\tau_2^{n+1}\|_{-1,h}^2\right),
\end{aligned} \tag{3.67}$$

Therefore, an application of discrete Gronwall inequality leads to the desired higher order convergence estimate

$$\frac{1}{\mathcal{M}_j^{1/2}}\|\tilde{\phi}_j^{n+1}\|_{-1,h}+\left(\frac{\varepsilon_0^2}{36}\Delta t\sum_{m=1}^{n+1}\|\nabla_h\tilde{\phi}_j^m\|_2^2\right)^{1/2}\le\hat{C}_2(\Delta t^2+h^2),\quad j=1,2, \tag{3.68}$$

based on the higher order truncation error accuracy, $\|\tau_1^{n+1}\|_{-1,h}$, $\|\tau_2^{n+1}\|_{-1,h}\le C(\Delta t^2+h^2)$. This completes the refined error estimate.

Recovery of the a-priori assumption (3.28)

With the higher order error estimate (3.68) at hand, we notice that the first a-priori assumption in (3.28) is satisfied at the next time step t^{n+1}:

$$\|\tilde{\phi}_j^{n+1}\|_{-1,h}\le C\hat{C}_2(\Delta t^2+h^2)\le\Delta t^{\frac{7}{4}}+h^{\frac{7}{4}},\quad \text{if } \Delta t \text{ and } h \text{ are sufficiently small,} \tag{3.69}$$

for $j=1,2$. For the second assumption in (3.28), we observe that the $L^2_{\Delta t}(0,T;H_h^1)$ error estimate in (3.68) implies that

$$\|\nabla_h\tilde{\phi}_j^{n+1}\|_2\le\frac{C\hat{C}_2(\Delta t^2+h^2)}{\Delta t^{\frac{1}{2}}}\le C\hat{C}_2(\Delta t^{\frac{3}{2}}+h^{\frac{3}{2}}), \tag{3.70}$$

in which we have used the linear refinement $C_1h\le\Delta t\le C_2h$ in the second step. Moreover, since $\overline{\tilde{\phi}_1^{n+1}}=\overline{\tilde{\phi}_2^{n+1}}=0$, an application of discrete Poincaré inequality implies that

$$\|\tilde{\phi}_j^{n+1}\|_2\le C\|\nabla_h\tilde{\phi}_j^{n+1}\|_2\le C^2\hat{C}_2(\Delta t^{\frac{3}{2}}+h^{\frac{3}{2}})\le\Delta t^{\frac{5}{4}}+h^{\frac{5}{4}},\quad j=1,2, \tag{3.71}$$

provided that Δt and h are sufficiently small. Therefore, both a-priori assumptions in (3.28) are satisfied, so that an induction analysis could be applied. This finishes the second order convergence analysis.

Finally, the convergence estimate (2.12) is a direct consequence of (3.68), combined with the definition (3.1) of the constructed approximate solution $\check{\Phi}_j$, as well as the projection estimate (2.7). This completes the proof of Theorem 2.2.

4. Concluding remarks

In this paper, we have established the convergence analysis and error estimate of a fully discrete finite difference scheme for the three-component Macromolecular Microsphere Composite (MMC) hydrogels system, a ternary Cahn–Hilliard system with a Flory–Huggins–deGennes free energy potential. The numerical scheme, proposed in [26], is based on a convex–concave decomposition of the ternary phase field energy, with its positivity-preserving property and energy stability available. The first order convergence in time and second order convergence in space have been proved in the $L^\infty_{\Delta t}(0,T;H_h^{-1})\cap L^2_{\Delta t}(0,T;H_h^1)$ norm. To overcome a well-known difficulty associated with the highly nonlinear and singular surface diffusion coefficient, many non-standard estimates have to be involved in the analysis. The higher order asymptotic expansion, up to second order temporal accuracy, has to be performed with a careful linearization technique. Such a higher order asymptotic expansion enables one to obtain a rough error estimate, so that to the $L^\infty_{\Delta t}$ bound for the phase variables could be derived. This $L^\infty_{\Delta t}$ estimate yields the upper and lower bounds of the two variables, and these bounds ensure a uniform distance between the numerical solution and the singular limit values, which has played a crucial role in the subsequent analysis. Finally, the refined error estimate are carried out to accomplish the desired convergence result. It is the first work to provide an optimal rate convergence estimate for a ternary phase field system with singular energy potential.

Acknowledgments

L.X. Dong is partially supported by the Guangdong Basic and Applied Basic Research Foundation No. 2022A1515010222 and the China Scholarship Council (CSC) during her visit in the University of Tennessee at Knoxville. Z.R. Zhang is partially supported by the NSFC No. 11871105 and Science Challenge Project No. TZ2018002. C. Wang is partially supported by the NSF, USA DMS-2012269. S.M. Wise is partially supported by the NSF, USA DMS-1719854, DMS-2012634. In addition, L.X. Dong also thanks the University of Tennessee at Knoxville for the generous support and hospitality during her visit.

References

[1] D. Zhai, H. Zhang, Investigation on the application of the TDGL equation in macromolecular microsphere composite hydrogel, Soft Matter 9 (2012) 820–825.
[2] W. Chen, W. Feng, Y. Liu, C. Wang, S. Wise, A second order energy stable scheme for the Cahn-Hilliard-Hele-Shaw equation, Disc. Cont. Dyn. Sys. B 24 (2019) 149–182.
[3] W. Chen, Y. Liu, C. Wang, S. Wise, An optimal-rate convergence analysis of a fully discrete finite difference scheme for Cahn-Hilliard-Hele-Shaw equation, Math. Comp. 85 (2016) 2231–2257.
[4] Y. Chen, J.S. Lowengrub, J. Shen, C. Wang, S.M. Wise, Efficient energy stable schemes for isotropic and strongly anisotropic Cahn-Hilliard systems with the Willmore regularization, J. Comput. Phys. 365 (2018) 57–73.
[5] K. Cheng, W. Feng, C. Wang, S.M. Wise, An energy stable fourth order finite difference scheme for the Cahn-Hilliard equation, J. Comput. Appl. Math. 362 (2019) 574–595.
[6] K. Cheng, C. Wang, S.M. Wise, X. Yue, A second-order, weakly energy-stable pseudo-spectral scheme for the Cahn-Hilliard equation and its solution by the homogeneous linear iteration method, J. Sci. Comput. 69 (2016) 1083–1114.
[7] A. Diegel, X. Feng, S. Wise, Convergence analysis of an unconditionally stable method for a Cahn-Hilliard-Stokes system of equations, SIAM J. Numer. Anal. 53 (2015) 127–152.
[8] A. Diegel, C. Wang, X. Wang, S. Wise, Convergence analysis and error estimates for a second order accurate finite element method for the Cahn-Hilliard-Navier-Stokes system, Numer. Math. 137 (2017) 495–534.
[9] A. Diegel, C. Wang, S.M. Wise, Stability and convergence of a second order mixed finite element method for the Cahn-Hilliard equation, IMA J. Numer. Anal. 36 (2016) 1867–1897.
[10] W. Feng, C. Wang, S.M. Wise, Z. Zhang, A second-order energy stable backward differentiation formula method for the epitaxial thin film equation with slope selection, Numer. Methods Partial Differ. Equ. 34 (6) (2018) 1975–2007.
[11] D. Han, X. Wang, A second order in time, uniquely solvable, unconditionally stable numerical scheme for Cahn-Hilliard-Navier-Stokes equation, J. Comput. Phys. 290 (2015) 139–156.
[12] Y. Liu, W. Chen, C. Wang, S. Wise, Error analysis of a mixed finite element method for a Cahn-Hilliard-Hele-Shaw system, Numer. Math. 135 (2017) 679–709.
[13] Y. Yan, W. Chen, C. Wang, S. Wise, A second-order energy stable BDF numerical scheme for the Cahn-Hilliard equation, Commun. Comput. Phys. 23 (2018) 572–602.
[14] L. Dong, C. Wang, H. Zhang, Z. Zhang, A positivity-preserving, energy stable and convergent numerical scheme for the Cahn-Hilliard equation with a Flory-Huggins-deGennes energy, Commun. Math. Sci. 17 (2019) 921–939.
[15] X. Li, G. Ji, H. Zhang, Phase transitions of macromolecular microsphere composite hydrogels based on the stochastic Cahn-Hilliard equation, J. Comput. Phys. 283 (2015) 81–97.
[16] X. Li, Z. Qiao, H. Zhang, An unconditionally energy stable finite difference scheme for a stochastic Cahn-Hilliard equation, Sci. China. Math. 59 (2016) 1815–1834.
[17] X. Li, Z. Qiao, H. Zhang, A second-order convex-splitting scheme for a Cahn-Hilliard equation with variable interfacial parameters, J. Comput. Math. 35 (2017) 693–710.
[18] J.L. Drury, D.J. Mooney, Hydrogels for tissue engineering: scaffold design variables and applications, Biomaterials 24 (24) (2003) 4337–4351.
[19] U. Edlund, Ryberg, Y. Zhu, A. Albertsson, Barrier films from renewable forestry waste, Biomacromolecules 11 (9) (2010) 2532–2538.
[20] T. Huang, H. Xu, K. Jiao, L. Zhu, H. Brown, H. Wang, A novel hydrogel with high mechanical strength: A macromolecular microsphere composite hydrogel, Adv. Mater. 19 (12) (2007) 1622–1626.
[21] G. Ji, Y. Yang, H. Zhang, Modeling and simulation of a ternary system for macromolecular microsphere composite hydrogels, East Asian J. Appl. Math. 11 (1) (2021) 93–118.
[22] J. Johnson, N. Turro, J. Koberstein, J. Mark, Some hydrogels having novel molecular structures, Prog. Polym. Sci. 35 (3) (2010) 332–337.
[23] F. Boyer, C. Lapuerta, Study of a three component Cahn-Hilliard flow model, M2AN Math. Model. Numer. Anal. 40 (2006) 653–687.
[24] F. Boyer, S. Minjeaud, Numerical schemes for a three component Cahn-Hilliard model, M2AN Math. Model. Numer. Anal. 45 (2011) 697–738.
[25] X. Yang, J. Zhao, Q. Wang, J. Shen, Numerical approximations for a three-component Cahn–Hilliard phase-field model based on the invariant energy quadratization method, Math. Models Methods Appl. Sci. (2017) 1–38.
[26] L. Dong, C. Wang, S. Wise, Z. Zhang, A positivity-preserving, energy stable scheme for a ternary Cahn-Hilliard system with the singular interfacial parameters, J. Comput. Phys. 442 (2021) 110451.
[27] W. Chen, J. Jing, C. Wang, X. Wang, A positivity preserving, energy stable finite difference scheme for the Flory-Huggins-Cahn-Hilliard-Navier-Stokes system, J. Sci. Comput. 92 (2022) 31.
[28] W. Chen, J. Jing, C. Wang, X. Wang, S.M. Wise, A modified Crank-Nicolson scheme for the Flory-Huggin Cahn-Hilliard model, Commun. Comput. Phys. 31 (1) (2022) 60–93.
[29] W. Chen, C. Wang, X. Wang, S. Wise, Positivity-preserving, energy stable numerical schemes for the Cahn-Hilliard equation with logarithmic potential, J. Comput. Phys. X 3 (2019) 100031.
[30] L. Dong, C. Wang, H. Zhang, Z. Zhang, A positivity-preserving second-order BDF scheme for the Cahn-Hilliard equation with variable interfacial parameters, Commun. Comput. Phys. 28 (3) (2020) 967–998.

[31] C. Liu, C. Wang, Y. Wang, A structure-preserving, operator splitting scheme for reaction-diffusion equations with detailed balance, J. Comput. Phys. 436 (2021) 110253.
[32] C. Liu, C. Wang, Y. Wang, S.M. Wise, Convergence analysis of the variational operator splitting scheme for a reaction-diffusion system with detailed balance, SIAM J. Numer. Anal. 60 (2) (2022) 781–803.
[33] C. Liu, C. Wang, S.M. Wise, X. Yue, S. Zhou, A positivity-preserving, energy stable and convergent numerical scheme for the Poisson-Nernst-Planck system, Math. Comp. 90 (2021) 2071–2106.
[34] C. Liu, C. Wang, S.M. Wise, X. Yue, S. Zhou, An iteration solver for the Poisson-Nernst-Planck system and its convergence analysis, J. Comput. Appl. Math. 406 (2022) 114017.
[35] M. Yuan, W. Chen, C. Wang, S. Wise, Z. Zhang, An energy stable finite element scheme for the three-component Cahn-Hilliard-type model for macromolecular microsphere composite hydrogels, J. Sci. Comput. 87 (2021) 78.
[36] M. Yuan, W. Chen, C. Wang, S. Wise, Z. Zhang, A second order accurate in time, energy stable finite element scheme for the Flory-Huggins-Cahn-Hilliard equation, Adv. Appl. Math. Mech. (2022) http://dx.doi.org/10.4208/aamm.OA-2021-0331.
[37] J. Zhang, C. Wang, S.M. Wise, Z. Zhang, Structure-preserving, energy stable numerical schemes for a liquid thin film coarsening model, SIAM J. Sci. Comput. 43 (2) (2021) A1248–A1272.
[38] F. Guillén-González, G. Tierra, Second order schemes and time-step adaptivity for Allen-Cahn and Cahn-Hilliard models, Comput. Math. Appl. 68 (8) (2014) 821–846.
[39] J. Shen, J. Xu, Convergence and error analysis for the scalar auxiliary variable (SAV) schemes to gradient flows, SIAM J. Numer. Anal. 56 (2018) 2895–2912.
[40] J. Shen, J. Xu, J. Yang, The scalar auxiliary variable (SAV) approach for gradient flows, J. Comput. Phys. 353 (2018) 407–416.
[41] D. Li, Z. Qiao, On second order semi-implicit Fourier spectral methods for 2D Cahn-Hilliard equations, J. Sci. Comput. 70 (2017) 301–341.
[42] D. Li, Z. Qiao, T. Tang, Characterizing the stabilization size for semi-implicit Fourier-spectral method to phase field equations, SIAM J. Numer. Anal. 54 (2016) 1653–1681.
[43] W. Chen, C. Wang, S. Wang, X. Wang, S. Wise, Energy stable numerical schemes for a ternary Cahn-Hilliard system, J. Sci. Comput. 84 (2020) 27.
[44] J. Guo, C. Wang, S. Wise, An H^2 convergence of a second-order convex-splitting, finite difference scheme for the three-dimensional Cahn-Hilliard equation, Commu. Math. Sci. 14 (2016) 489–515.
[45] S. Wise, Unconditionally stable finite difference, nonlinear multigrid simulation of the Cahn-Hilliard-Hele-Shaw system of equations, J. Sci. Comput. 44 (2010) 38–68.
[46] S.M. Wise, C. Wang, J. Lowengrub, An energy stable and convergent finite-difference scheme for the phase field crystal equation, SIAM J. Numer. Anal. 47 (2009) 2269–2288.
[47] C. Wang, S. Wise, An energy stable and convergent finite-difference scheme for the modified phase field crystal equation, SIAM J. Numer. Anal. 49 (2011) 945–969.
[48] J. Cao, J. Zhang, X. Yang, Fully-discrete spectral-Galerkin scheme with second-order time-accuracy and unconditionally energy stability for the volume-conserved phase-field lipid vesicle model, J. Comput. Appl. Math. 406 (2022) 113988.
[49] X. Yang, Fully-discrete spectral-Galerkin scheme with decoupled structure and second-order time accuracy for the anisotropic phase-field dendritic crystal growth model, Int. J. Heat Mass Transfer 180 (2021) 121750.
[50] X. Yang, A novel fully-decoupled scheme with second-order time accuracy and unconditional energy stability for the Navier-Stokes equations coupled with mass-conserved Allen-Cahn phase-field model of two-phase incompressible flow, Internat. J. Numer. Methods Engrg. 122 (2021) 1283–1306.
[51] X. Yang, X. He, A fully-discrete decoupled finite element method for the conserved allen-cahn type phase-field model of three-phase fluid flow system, Comput. Methods Appl. Mech. Engrg. 389 (2022) 114376.
[52] G.-D. Zhang, X. He, X. Yang, A fully decoupled linearized finite element method with second-order temporal accuracy and unconditional energy stability for incompressible MHD equations, J. Comput. Phys. 448 (2022) 110752.
[53] C. Chen, X. Yang, Fully-discrete finite element numerical scheme with decoupling structure and energy stability for the Cahn-Hilliard phase-field model of two-phase incompressible flow system with variable density and viscosity, M2AN Math. Model. Numer. Anal. 55 (2021) 2323–2347.
[54] X. Yang, A new efficient fully-decoupled and second-order time-accurate scheme for Cahn-Hilliard phase-field model of three-phase incompressible flow, Comput. Methods Appl. Mech. Engrg. 376 (2021) 13589.
[55] X. Yang, A novel fully-decoupled, second-order and energy stable numerical scheme of the conserved Allen-Cahn type flow-coupled binary surfactant model, Comput. Methods Appl. Mech. Engrg. 373 (2021) 113502.
[56] X. Yang, Numerical approximations of the Navier-Stokes equation coupled with volume-conserved multi-phase-field vesicles system: fully-decoupled, linear, unconditionally energy stable and second-order time-accurate numerical scheme, Comput. Methods Appl. Mech. Engrg. 375 (2021) 113600.
[57] X. Yang, On a novel full decoupling, linear, second-order accurate, and unconditionally energy stable numerical scheme for the anisotropic phase-field dendritic crystal growth model, Internat. J. Numer. Methods Engrg. 122 (2021) 4129–4153.
[58] X. Yang, A novel fully-decoupled, second-order time-accurate, unconditionally energy stable scheme for a flow-coupled volume-conserved phase-field elastic bending energy model, J. Comput. Phys. 432 (2021) 110015.
[59] W. E., J.-G. Liu, Projection method I: Convergence and numerical boundary layers, SIAM J. Numer. Anal. 32 (1995) 1017–1057.
[60] W. E., J.-G. Liu, Projection method III. Spatial discretization on the staggered grid, Math. Comp. 71 (2002) 27–47.
[61] R. Samelson, R. Temam, C. Wang, S. Wang, Surface pressure Poisson equation formulation of the primitive equations: Numerical schemes, SIAM J. Numer. Anal. 41 (2003) 1163–1194.
[62] R. Samelson, R. Temam, C. Wang, S. Wang, A fourth order numerical method for the planetary geostrophic equations with inviscid geostrophic balance, Numer. Math. 107 (2007) 669–705.
[63] C. Wang, J.-G. Liu, Convergence of gauge method for incompressible flow, Math. Comp. 69 (2000) 1385–1407.
[64] C. Wang, J.-G. Liu, Analysis of finite difference schemes for unsteady Navier-Stokes equations in vorticity formulation, Numer. Math. 91 (2002) 543–576.
[65] C. Wang, J.-G. Liu, H. Johnston, Analysis of a fourth order finite difference method for incompressible Boussinesq equations, Numer. Math. 97 (2004) 555–594.
[66] A. Baskaran, J. Lowengrub, C. Wang, S.M. Wise, Convergence analysis of a second order convex splitting scheme for the modified phase field crystal equation, SIAM J. Numer. Anal. 51 (2013) 2851–2873.
[67] Z. Guan, J.S. Lowengrub, C. Wang, Convergence analysis for second order accurate schemes for the periodic nonlocal Allen-Cahn and Cahn-Hilliard equations, Math. Methods Appl. Sci. 40 (18) (2017) 6836–6863.
[68] Z. Guan, C. Wang, S.M. Wise, A convergent convex splitting scheme for the periodic nonlocal Cahn-Hilliard equation, Numer. Math. 128 (2014) 377–406.
[69] X. Li, Z. Qiao, C. Wang, Convergence analysis for a stabilized linear semi-implicit numerical scheme for the nonlocal Cahn-Hilliard equation, Math. Comp. 90 (2021) 171–188.

[70] C. Duan, W. Chen, C. Liu, C. Wang, X. Yue, A second order accurate numerical scheme for the porous medium equation by an energetic variational approach, Commun. Math. Sci. 20 (4) (2022) 987–1024.
[71] C. Duan, C. Liu, C. Wang, X. Yue, Convergence analysis of a numerical scheme for the porous medium equation by an energetic variational approach, Numer. Math. Theor. Meth. Appl. 13 (2020) 1–18.
[72] L. Wang, W. Chen, C. Wang, An energy-conserving second order numerical scheme for nonlinear hyperbolic equation with an exponential nonlinear term, J. Comput. Appl. Math. 280 (2015) 347–366.