



A positivity-preserving, second-order energy stable and convergent numerical scheme for a ternary system of macromolecular microsphere composite hydrogels

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ABSTRACT

A second order accurate numerical scheme is proposed and analyzed for the periodic three-component Macromolecular Microsphere Composite(MMC) hydrogels system, a ternary Cahn-Hilliard system with a Flory–Huggins–deGennes free energy potential. This numerical scheme with energy stability is based on the Backward Differentiation Formula(BDF) method in time derivation combining with Douglas-Dupont regularization term, combined the finite difference method in space. We provide a theoretical justification of positivity-preserving property for all the singular terms, i.e., not only the two phase variables are always between 0 and 1, but also the sum of the two phase variables is between 0 and 1, at a point-wise level. In addition, an optimal rate convergence analysis is provided in this paper, in which a higher order asymptotic expansion of the numerical solution, the rough error estimate and refined error estimate techniques have to be included to accomplish such an analysis. This paper will be the first to combine the following theoretical properties for a second order accurate numerical scheme for the ternary MMC system: (i) unique solvability and positivity-preserving property; (ii) energy stability; (iii) and optimal rate convergence. A few numerical results are also presented.

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, but with certain singular gradient coefficients, is discussed in [2–5]. Also see the related works [6–10] for the hydrogel model. 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 [11–18].

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 [19–22]. A ternary system with

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Flory–Huggins–deGennes energy potential [9] 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:

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

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 i th 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_o 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

$$G(\phi_1, \phi_2) = \int_{\Omega} \left\{ S(\phi_1, \phi_2) + \frac{\epsilon_1^2 |\nabla \phi_1|^2}{36\phi_1} + \frac{\epsilon_2^2 |\nabla \phi_2|^2}{36\phi_2} + \frac{\epsilon_3^2 |\nabla (1 - \phi_1 - \phi_2)|^2}{36(1 - \phi_1 - \phi_2)} + H(\phi_1, \phi_2) \right\} d\mathbf{x}, \quad (1.1)$$

where

$$S(\phi_1, \phi_2) = \frac{\phi_1}{M_0} \ln \frac{\alpha \phi_1}{M_0} + \frac{\phi_2}{N_0} \ln \frac{\beta \phi_2}{N_0} + (1 - \phi_1 - \phi_2) \ln(1 - \phi_1 - \phi_2),$$

$$H(\phi_1, \phi_2) = \chi_{12} \phi_1 \phi_2 + \chi_{13} \phi_1 (1 - \phi_1 - \phi_2) + \chi_{23} \phi_2 (1 - \phi_1 - \phi_2).$$

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

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

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

$$\begin{aligned} \mu_1 := \delta_{\phi_1} G = & \frac{1}{M_0} \ln \frac{\alpha \phi_1}{M_0} - \ln(1 - \phi_1 - \phi_2) - 2\chi_{13}\phi_1 + (\chi_{12} - \chi_{13} - \chi_{23})\phi_2 \\ & + \chi_{13} + \frac{1}{M_0} - 1 - \frac{\epsilon_1^2 |\nabla \phi_1|^2}{36\phi_1^2} - \nabla \cdot \left(\frac{\epsilon_1^2 \nabla \phi_1}{18\phi_1} \right) \\ & + \frac{\epsilon_3^2 |\nabla (1 - \phi_1 - \phi_2)|^2}{36(1 - \phi_1 - \phi_2)^2} + \nabla \cdot \left(\frac{\epsilon_3^2 \nabla (1 - \phi_1 - \phi_2)}{18(1 - \phi_1 - \phi_2)} \right), \end{aligned} \quad (1.3)$$

$$\begin{aligned} \mu_2 := \delta_{\phi_2} G = & \frac{1}{N_0} \ln \frac{\beta \phi_2}{N_0} - \ln(1 - \phi_1 - \phi_2) - 2\chi_{23}\phi_2 + (\chi_{12} - \chi_{13} - \chi_{23})\phi_1 \\ & + \chi_{23} + \frac{1}{N_0} - 1 - \frac{\epsilon_2^2 |\nabla \phi_2|^2}{36\phi_2^2} - \nabla \cdot \left(\frac{\epsilon_2^2 \nabla \phi_2}{18\phi_2} \right) \\ & + \frac{\epsilon_3^2 |\nabla (1 - \phi_1 - \phi_2)|^2}{36(1 - \phi_1 - \phi_2)^2} + \nabla \cdot \left(\frac{\epsilon_3^2 \nabla (1 - \phi_1 - \phi_2)}{18(1 - \phi_1 - \phi_2)} \right). \end{aligned} \quad (1.4)$$

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

physically and mathematically. We define the following *Gibbs Triangles* for use later:

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

and, for $\delta \geq 0$,

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

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.

There have been some numerical works for the ternary MMC system, while most existing works have focused on first order accurate (in time) algorithms. Such as the recent literature [23,24], the authors presented a first order discrete finite difference numerical scheme based on the convex splitting method of the free energy with logarithmic potential, established a theoretical justification of the positivity property and convergence analysis. Also see the related finite element work [22]. One well-known drawback of the first order convex splitting approach is that an extra dissipation added to ensure unconditional stability also introduces a significant amount of numerical error [25]. Due to this fact, second-order energy stable methods have been highly desirable, which preserves all important theoretical features, i.e., unique solvability, positivity preserving, mass conversation, energy stability and convergence analysis.

The goal of this paper is to extend the convex-splitting framework to develop a second order in both time and space for the ternary MMC system. We propose and analyze a numerical scheme with four theoretical properties justified: unique solvability and positivity-preserving, mass conservation, energy stability and convergence analysis. This scheme is based on the 2nd BDF temporal approximation and the finite difference method in space for the ternary MMC system. Based on the idea of convex splitting, we treat the convex part implicitly and the linear part explicitly using the second-order Adams–Bashforth extrapolation formula. In addition, a second order Douglas-Dupont regularization of the form $A_i \Delta t \Delta_h (\phi_i^{n+1} - \phi_i^n)$ is specifically introduced to ensure the energy stability in this paper, this technique is similar in [13,18,26,27]. Moreover, the highly nonlinear and singular nature of the surface diffusion coefficients makes the system turn to be a very challenging issue. In this paper, we will adopt similar techniques in [23,28] to estimate the positivity property. First, the fully discrete numerical scheme is equivalent to a minimization of a strictly convex discrete energy functional, so we can transform the positivity preserving problem of the numerical solution into the problem that the minimizer of this functional could not occur on the boundary points. A more careful analysis reveals that, the convex and the singular natures of these implicit nonlinear parts prevent the numerical solutions approach the singular limit values of 0 and 1, so that the phase variables are always between 0 and 1. At the same time, the sum of these two phase variables is between 0 and 1, at a point-wise level. Although the extra term $A_i \Delta t \Delta_h (\phi_i^{n+1} - \phi_i^n)$ is added into the numerical scheme, it does not matter because the logarithmic function always changes faster than the linear function as the phase variable approaches the boundary points. For convergence analysis, to control the explicit part of the extra regularization term, a higher order asymptotic expansion (up to third order temporal accuracy and fourth order spatial accuracy) has to be involved. To overcome the highly nonlinear and singular nature of the surface diffusion coefficients, a rough error estimate has to be performed, so that the $\mathcal{C}^\infty$ bound for ϕ_i could be derived. This $\mathcal{C}^\infty$ estimate yields the upper and lower bounds of the three variables, and these bounds play a crucial role in the subsequent analysis. Finally, the refined error estimate is carried out to accomplish the desired convergence result.

The rest part of this paper is organized as follows. In Section 2, we present a finite difference scheme based on the 2nd BDF method and the idea of convex splitting method of the energy functional. In Section 3, the unique solvability and the positivity preserving property of the numerical solutions are analyzed. The energy stability analysis is provided in Section 4. The detailed convergence analysis is given by Section 5. Some numerical results are presented in Section 6. Finally, concluding remarks are made in Section 7.

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 [13,29,30]. 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:

$$C_{\text{per}} := \left\{ v : C \times C \rightarrow \mathbb{R} \mid v_{i,j} = v_{i+\alpha N, j+\beta N}, \forall i, j, \alpha, \beta \in \mathbb{Z} \right\},$$

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

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

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

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

$$A_x v_{i+1/2,j} := \frac{1}{2} (v_{i+1,j} + v_{i,j}), \quad D_x v_{i+1/2,j} := \frac{1}{h} (v_{i+1,j} - v_{i,j}),$$

$$A_y v_{i,j+1/2} := \frac{1}{2} (v_{i,j+1} + v_{i,j}), \quad D_y v_{i,j+1/2} := \frac{1}{h} (v_{i,j+1} - v_{i,j}),$$

with $A_x, D_x : C_{\text{per}} \rightarrow \mathcal{E}_{\text{per}}^x$, $A_y, D_y : C_{\text{per}} \rightarrow \mathcal{E}_{\text{per}}^y$. Likewise,

$$a_x v_{i,j} := \frac{1}{2} (v_{i+1/2,j} + v_{i-1/2,j}), \quad d_x v_{i,j} := \frac{1}{h} (v_{i+1/2,j} - v_{i-1/2,j}),$$

$$a_y v_{i,j} := \frac{1}{2} (v_{i,j+1/2} + v_{i,j-1/2}), \quad d_y v_{i,j} := \frac{1}{h} (v_{i,j+1/2} - v_{i,j-1/2}),$$

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

$$\nabla_h v_{i,j} = (D_x v_{i+1/2,j}, D_y v_{i,j+1/2}), \quad \nabla_h \cdot \vec{f}_{i,j} = d_x f_{i,j}^x + d_y f_{i,j}^y,$$

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

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

More generally, if D is a periodic scalar function that is defined at all of the face-centered points and $\vec{f} \in \vec{\mathcal{E}}_{\text{per}}$, then $D\vec{f} \in \vec{\mathcal{E}}_{\text{per}}$, assuming point-wise multiplication, and we may define $\nabla_h \cdot (D\vec{f})_{i,j} = d_x (Df^x)_{i,j} + d_y (Df^y)_{i,j}$. Specifically, if $v \in C_{\text{per}}$, then $\nabla_h \cdot (D\nabla_h v) : C_{\text{per}} \rightarrow C_{\text{per}}$ is defined point-wise via $\nabla_h \cdot (D\nabla_h v)_{i,j} = d_x (DD_x v)_{i,j} + d_y (DD_y v)_{i,j}$. In particular, suppose that $v, \phi \in C_{\text{per}}$ are grid functions and $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ is a continuous function. Then we define

$$\nabla_h \cdot (\sigma(A_h v) \nabla_h \phi)_{i,j} := d_x (\sigma(A_x v) D_x v)_{i,j} + d_y (\sigma(A_y v) D_y v)_{i,j},$$

where $A_h v$ is understood to be a periodic function defined at the face-centered points obtained by doing appropriate east-west and north-south averages.

In addition, the following grid inner products are defined:

$$\langle v, \xi \rangle := h^2 \sum_{i,j=1}^N v_{i,j} \xi_{i,j}, \quad v, \xi \in C_{\text{per}}, \quad [\vec{f}_1, \vec{f}_2] := [f_1^x, f_2^x]_x + [f_1^y, f_2^y]_y, \quad \vec{f}_i = (f_i^x, f_i^y) \in \vec{\mathcal{E}}_{\text{per}},$$

$$[v, \xi]_x := \langle a_x(v\xi), 1 \rangle, \quad v, \xi \in \mathcal{E}_{\text{per}}^x, \quad [v, \xi]_y := \langle a_y(v\xi), 1 \rangle, \quad v, \xi \in \mathcal{E}_{\text{per}}^y.$$

Subsequently, we define the following norms for cell-centered functions. If $v \in C_{\text{per}}$, then $\|v\|_2^2 := \langle v, v \rangle$; $\|v\|_p^p := \langle |v|^p, 1 \rangle$, for $1 \leq p < \infty$, and $\|v\|_\infty := \max_{1 \leq i,j \leq N} |v_{i,j}|$. The gradient norms are introduced as follows:

$$\|\nabla_h v\|_2^2 := [\nabla_h v, \nabla_h v] = [D_x v, D_x v]_x + [D_y v, D_y v]_y, \quad \text{for } v \in C_{\text{per}},$$

$$\|\nabla_h v\|_p := \left([|D_x v|^p, 1]_x + [|D_y v|^p, 1]_y \right)^{\frac{1}{p}}, \quad 1 \leq p < \infty.$$

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

Lemma 2.1 ([30,31]). Let D be an arbitrary periodic, scalar function defined on all of the face center points. For any $\psi, v \in C_{\text{per}}$ and any $\vec{f} \in \vec{\mathcal{E}}_{\text{per}}$, the following summation by parts formulas are valid:

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

To facilitate the analysis, we need to introduce a discrete analogue of the space $H_{\text{per}}^{-1}(\Omega)$, as outlined in [31]. Suppose that D is a positive, periodic scalar function defined at edge-center points. For any $\phi \in C_{\text{per}}$, there exists a unique $\psi \in \mathring{C}_{\text{per}}$ that solves

$$\mathcal{L}_D(\psi) := -\nabla_h \cdot (D\nabla_h \psi) = \phi - \bar{\phi},$$

where $\bar{\phi} := |\Omega|^{-1} \langle \phi, 1 \rangle$. We equip this space with a bilinear form: for any $\phi_1, \phi_2 \in \mathring{C}_{\text{per}}$, define

$$\langle \phi_1, \phi_2 \rangle_{\mathcal{L}_D^{-1}} := [D\nabla_h \psi_1, \nabla_h \psi_2],$$

where $\psi_i \in \mathring{C}_{\text{per}}$ is the unique solution to

$$\mathcal{L}_D(\psi_i) := -\nabla_h \cdot (D\nabla_h \psi_i) = \phi_i, \quad i = 1, 2.$$

The following identity [31] is easy to prove via summation-by-parts:

$$\langle \phi_1, \phi_2 \rangle_{\mathcal{L}_D^{-1}} = \langle \phi_1, \mathcal{L}_D^{-1}(\phi_2) \rangle = \langle \mathcal{L}_D^{-1}(\phi_1), \phi_2 \rangle,$$

and since $\mathcal{L}_D$ is symmetric positive definite, $\langle \cdot, \cdot \rangle_{\mathcal{L}_D^{-1}}$ is an inner product on $\mathring{C}_{\text{per}}$. When $D \equiv 1$, we drop the subscript and write $\mathcal{L}_1 = \mathcal{L} = -\Delta_h$, and introduce the notation $\langle \cdot, \cdot \rangle_{\mathcal{L}_D^{-1}} =: \langle \cdot, \cdot \rangle_{-1,h}$. In the general setting, the norm associated to this inner product is denoted $\|\phi\|_{\mathcal{L}_D^{-1}} := \sqrt{\langle \phi, \phi \rangle_{\mathcal{L}_D^{-1}}}$, for all $\phi \in \mathring{C}_{\text{per}}$, but, if $D \equiv 1$, we write $\|\cdot\|_{\mathcal{L}_D^{-1}} =: \|\cdot\|_{-1,h}$.

2.2. A convex-concave decomposition of the discrete energy

In this section, we will recall a convex-concave decomposition of the energy (1.1). The detailed proof of the following preliminary and lemma results could be found in the work [23].

Define $\kappa(\phi) := \frac{1}{36\phi}$. The discrete energy $G_h(\phi_1, \phi_2) : \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}} \rightarrow \mathbb{R}$ is introduced as

$$\begin{aligned} G_h(\phi_1, \phi_2) = & \langle S(\phi_1, \phi_2) + H(\phi_1, \phi_2), 1 \rangle \\ & + \langle a_x(\kappa(A_x\phi_1)(D_x\phi_1)^2) + a_y(\kappa(A_y\phi_1)(D_y\phi_1)^2), \varepsilon_1^2 \rangle \\ & + \langle a_x(\kappa(A_x\phi_2)(D_x\phi_2)^2) + a_y(\kappa(A_y\phi_2)(D_y\phi_2)^2), \varepsilon_2^2 \rangle \\ & + \langle a_x(\kappa(A_x(1-\phi_1-\phi_2))(D_x(1-\phi_1-\phi_2))^2), \varepsilon_3^2 \rangle \\ & + \langle a_y(\kappa(A_y(1-\phi_1-\phi_2))(D_y(1-\phi_1-\phi_2))^2), \varepsilon_3^2 \rangle. \end{aligned} \quad (2.1)$$

Lemma 2.2 (Existence of a Convex-Concave Decomposition). Suppose $(\phi_1, \phi_2) \in \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}}$. The functions

$$G_{h,c}(\phi_1, \phi_2) := \langle S(\phi_1, \phi_2), 1 \rangle \quad (2.2)$$

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

$$G_{h,e}(\phi_1, \phi_2) := -\langle H(\phi_1, \phi_2), 1 \rangle, \quad (2.3)$$

where $G_{h,c}$ and $G_{h,e}$ are linear combination of certain convex functions. Therefore, $G_h(\phi_1, \phi_2) = G_{h,c}(\phi_1, \phi_2) - G_{h,e}(\phi_1, \phi_2)$ is a convex-concave decomposition of the discrete energy.

Proposition 2.1. Suppose $(\phi_1, \phi_2) \in \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}}$. The variational derivatives of $G_{h,c}$ and $G_{h,e}$ with respect to ϕ_1 and ϕ_2 are grid functions satisfying

$$\begin{aligned} \delta_{\phi_i} G_{h,c}(\phi_1, \phi_2) = & \frac{\partial}{\partial \phi_i} S(\phi_1, \phi_2) \\ & + \varepsilon_i^2 a_x(\kappa'(A_x\phi_i)(D_x\phi_i)^2) - 2\varepsilon_i^2 d_x(\kappa(A_x\phi_i)D_x\phi_i) \\ & + \varepsilon_i^2 a_y(\kappa'(A_y\phi_i)(D_y\phi_i)^2) - 2\varepsilon_i^2 d_y(\kappa(A_y\phi_i)D_y\phi_i) \\ & - \varepsilon_3^2 a_x(\kappa'(A_x(1-\phi_1-\phi_2))(D_x(1-\phi_1-\phi_2))^2) \\ & + 2\varepsilon_3^2 d_x(\kappa(A_x(1-\phi_1-\phi_2))D_x(1-\phi_1-\phi_2)) \\ & - \varepsilon_3^2 a_y(\kappa'(A_y(1-\phi_1-\phi_2))(D_y(1-\phi_1-\phi_2))^2) \\ & + 2\varepsilon_3^2 d_y(\kappa(A_y(1-\phi_1-\phi_2))D_y(1-\phi_1-\phi_2)), \\ \delta_{\phi_i} G_{h,e}(\phi_1, \phi_2) = & -\frac{\partial}{\partial \phi_i} H(\phi_1, \phi_2), \end{aligned}$$

for $i = 1, 2$.

Lemma 2.3. Suppose that $\vec{\phi}, \vec{\psi} \in \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}}$. Consider the canonical convex splitting of the energy $G_h(\vec{\phi})$ in (2.1) into $G_h = G_{h,c} - G_{h,e}$ given by (2.2)–(2.3). The following inequality is available

$$\begin{aligned} G_h(\vec{\phi}) - G_h(\vec{\psi}) \leq & \langle \delta_{\phi_1} G_{h,c}(\vec{\phi}) - \delta_{\phi_1} G_{h,e}(\vec{\psi}), \phi_1 - \psi_1 \rangle \\ & + \langle \delta_{\phi_2} G_{h,c}(\vec{\phi}) - \delta_{\phi_2} G_{h,e}(\vec{\psi}), \phi_2 - \psi_2 \rangle. \end{aligned}$$

Using the idea of the convex splitting and the backward differentiation formula, we consider the following semi-implicit, fully discrete scheme: for $n \geq 1$, given $(\phi_1^n, \phi_2^n) \in \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}}$, $(\phi_1^{n-1}, \phi_2^{n-1}) \in \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}}$, find $(\phi_1^{n+1}, \phi_2^{n+1}) \in \tilde{\mathcal{C}}_{\text{per}}^{\mathcal{G}}$ such that

$$\begin{aligned} \frac{3\phi_1^{n+1} - 4\phi_1^n + \phi_1^{n-1}}{2\Delta t} & = \mathcal{M}_1 \Delta_h \mu_1^{n+1}, \\ \mu_1^{n+1} := & \delta_{\phi_1} G_{h,c}(\phi_1^{n+1}, \phi_2^{n+1}) - \delta_{\phi_1} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n) - A_1 \Delta t \Delta_h (\phi_1^{n+1} - \phi_1^n) \\ & = \frac{1}{M_0} \ln \frac{\alpha \phi_1^{n+1}}{M_0} - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1}) - 2\chi_{13} \hat{\phi}_1^n + (\chi_{12} - \chi_{13} - \chi_{23}) \hat{\phi}_2^n \\ & - \frac{\varepsilon_1^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h \phi_1^{n+1}|^2}{(\mathcal{A}_h \phi_1^{n+1})^2} \right) - \frac{\varepsilon_1^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \phi_1^{n+1}}{\mathcal{A}_h \phi_1^{n+1}} \right) - A_1 \Delta t \Delta_h (\phi_1^{n+1} - \phi_1^n) \end{aligned} \quad (2.4)$$

$$+ \frac{\varepsilon_3^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h(1 - \phi_1^{n+1} - \phi_2^{n+1})|^2}{(\mathcal{A}_h(1 - \phi_1^{n+1} - \phi_2^{n+1}))^2} \right) + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h(1 - \phi_1^{n+1} - \phi_2^{n+1})}{\mathcal{A}_h(1 - \phi_1^{n+1} - \phi_2^{n+1})} \right), \quad (2.5)$$

$$\frac{3\phi_2^{n+1} - 4\phi_2^n + \phi_2^{n-1}}{2\Delta t} = \mathcal{M}_2 \Delta_h \mu_2^{n+1}, \quad (2.6)$$

$$\begin{aligned} \mu_2^{n+1} &:= \delta_{\phi_2} G_{h,c}(\phi_1^{n+1}, \phi_2^{n+1}) - \delta_{\phi_2} G_{h,c}(\hat{\phi}_1^n, \hat{\phi}_2^n) - A_2 \Delta t \Delta_h(\phi_2^{n+1} - \phi_2^n) \\ &= \frac{1}{N_0} \ln \frac{\beta \phi_2^{n+1}}{N_0} - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1}) - 2\chi_{23} \hat{\phi}_2^n + (\chi_{12} - \chi_{13} - \chi_{23}) \hat{\phi}_1^n \\ &\quad - \frac{\varepsilon_2^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h \phi_2^{n+1}|^2}{(\mathcal{A}_h \phi_2^{n+1})^2} \right) - \frac{\varepsilon_2^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \phi_2^{n+1}}{\mathcal{A}_h \phi_2^{n+1}} \right) - A_2 \Delta t \Delta_h(\phi_2^{n+1} - \phi_2^n) \\ &\quad + \frac{\varepsilon_3^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h(1 - \phi_1^{n+1} - \phi_2^{n+1})|^2}{(\mathcal{A}_h(1 - \phi_1^{n+1} - \phi_2^{n+1}))^2} \right) + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h(1 - \phi_1^{n+1} - \phi_2^{n+1})}{\mathcal{A}_h(1 - \phi_1^{n+1} - \phi_2^{n+1})} \right), \end{aligned} \quad (2.7)$$

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 $u \in C_{\text{per}}$, provided u does not vanish at any grid points. And $\hat{u}^n := 2u^n - u^{n-1}$.

The initialization step comes from a combination of convex splitting and a second order numerical correction:

$$\begin{aligned} \frac{\phi_1^1 - \phi_1^0}{\Delta t} &= \mathcal{M}_1 \Delta_h \mu_1^1, \\ \mu_1^1 &:= \frac{1}{2} \left(\delta_{\phi_1} G_{h,c}(\phi_1^1, \phi_2^1) + \delta_{\phi_1} G_{h,c}(\phi_1^0, \phi_2^0) \right) + \frac{\partial}{\partial \phi_1} H(\phi_1^0, \phi_2^0) + \frac{\Delta t}{2} \frac{\partial^2}{\partial \phi_1^2} H(\phi_1^0, \phi_2^0) (\phi_1)_t^0, \\ \frac{\phi_2^1 - \phi_2^0}{\Delta t} &= \mathcal{M}_2 \Delta_h \mu_2^1, \\ \mu_2^1 &:= \frac{1}{2} \left(\delta_{\phi_2} G_{h,c}(\phi_1^1, \phi_2^1) + \delta_{\phi_2} G_{h,c}(\phi_1^0, \phi_2^0) \right) + \frac{\partial}{\partial \phi_2} H(\phi_1^0, \phi_2^0) + \frac{\Delta t}{2} \frac{\partial^2}{\partial \phi_2^2} H(\phi_1^0, \phi_2^0) (\phi_2)_t^0. \end{aligned} \quad (2.8)$$

The local truncation error of this initialization step is second order, which matches the overall second-order accuracy of the scheme and is consistent with the high order consistency analysis, as will be shown in later sections. In addition, this initialization step method satisfies the positivity-preserving property and energy stability.

Remark 2.1. The construction of a second order accurate, positivity-preserving and energy stable numerical scheme for the ternary MMC system turns out to be more challenging than the first order accurate algorithm [23,24]. Because of the complicated structure of the nonlinear and singular surface diffusion energy, as well as its functional derivatives, a Crank–Nicolson style approximation could hardly ensure both the positivity-preserving and energy stability properties. In turn, such a numerical effort has to be focused on the BDF style approach. With the BDF2 approximation, the nonlinear and singular terms could be treated in a similar manner as in the first order numerical method, while the computation of the concave and expansive terms becomes more tricky. Because of the negative eigenvalues in the concave expansive terms, an explicit treatment is necessary for the sake of both the unique solvability and energy stability. In the first order numerical method, an explicit treatment to the concave terms is able to ensure a dissipation of the associated energy; however, a direct application of second order Adams–Bashforth extrapolation for the concave terms would not enforce such an energy stability at a theoretical level. To remedy this numerical effort, we have to add artificial regularization terms, for both ϕ_1 and ϕ_2 , to establish such a theoretical analysis of energy stability, as will be demonstrated in the later section. Moreover, since a multi-step approach is applied in the second order accurate scheme, the initialization step turns out to be more challenging, and a careful computation in the initial step, as given by (2.8), is needed to ensure the theoretical properties at the initial time step.

3. Unique solvability and positivity-preserving property

The proof of the following lemma can be found in [28].

Lemma 3.1. Suppose that $\phi_1, \phi_2 \in C_{\text{per}}$, with $\langle \phi_1 - \phi_2, 1 \rangle = 0$, that is, $\phi_1 - \phi_2 \in \mathring{C}_{\text{per}}$, and assume that $\|\phi_1\|_\infty < 1$, $\|\phi_2\|_\infty \leq M$. Then, we have the following estimate:

$$\left\| (-\Delta_h)^{-1} (\phi_1 - \phi_2) \right\|_\infty \leq C_1,$$

where $C_1 > 0$ depends only upon M and Ω . In particular, C_1 is independent of the mesh size h .

In fact, in the ternary MMC model, all the phase variables have to stay within $(0, 1)$, due to the positivity-preserving property, i.e., $0 < \phi_1, \phi_2, 1 - \phi_1 - \phi_2 < 1$, at a point-wise level. Therefore, we could take $M = 1$ to justify an application of this lemma, and appropriate functional space could be set to enforce such a point-wise bound. The following theorem is the main result of this section.

Theorem 3.1. Given $(\phi_1^k, \phi_2^k) \in \tilde{C}_{\text{per}}^{\mathcal{G}}$, $k = n-1, n$, and $(\overline{\phi_1^n}, \overline{\phi_2^n}), (\overline{\phi_1^{n-1}}, \overline{\phi_2^{n-1}}) \in \mathcal{G}$, then there exists a unique solution $(\phi_1^{n+1}, \phi_2^{n+1}) \in \tilde{C}_{\text{per}}^{\mathcal{G}}$ to (2.4)–(2.7), with $\overline{\phi_1^n} = \phi_1^{n+1}$ and $\overline{\phi_2^n} = \phi_2^{n+1}$.

3.1. The equivalent form of solving (2.4)–(2.7)

For bookkeeping, we introduce the following notation:

$$\delta_{\phi_1} G_{h,c}(\phi_1, \phi_2) = \sum_{\ell=1}^9 Q_{\ell}(\phi_1, \phi_2),$$

where

$$\begin{aligned} Q_1(\phi_1, \phi_2) &:= \frac{\partial}{\partial \phi_1} S(\phi_1, \phi_2), \\ Q_2(\phi_1, \phi_2) &:= \varepsilon_1^2 a_x (\kappa'(A_x \phi_1) (D_x \phi_1)^2), \\ Q_3(\phi_1, \phi_2) &:= -2\varepsilon_1^2 d_x (\kappa(A_x \phi_1) D_x \phi_1), \\ Q_4(\phi_1, \phi_2) &:= \varepsilon_1^2 a_y (\kappa'(A_y \phi_1) (D_y \phi_1)^2), \\ Q_5(\phi_1, \phi_2) &:= -2\varepsilon_1^2 d_y (\kappa(A_y \phi_1) D_y \phi_1), \\ Q_6(\phi_1, \phi_2) &:= -\varepsilon_3^2 a_x (\kappa'(A_x (1 - \phi_1 - \phi_2)) (D_x (1 - \phi_1 - \phi_2))^2), \\ Q_7(\phi_1, \phi_2) &:= 2\varepsilon_3^2 d_x (\kappa(A_x (1 - \phi_1 - \phi_2)) D_x (1 - \phi_1 - \phi_2)), \\ Q_8(\phi_1, \phi_2) &:= -\varepsilon_3^2 a_y (\kappa'(A_y (1 - \phi_1 - \phi_2)) (D_y (1 - \phi_1 - \phi_2))^2), \\ Q_9(\phi_1, \phi_2) &:= 2\varepsilon_3^2 d_y (\kappa(A_y (1 - \phi_1 - \phi_2)) D_y (1 - \phi_1 - \phi_2)). \end{aligned}$$

The numerical solution of (2.4)–(2.7) is a minimizer of the following discrete energy functional:

$$\begin{aligned} \mathcal{J}_h^n(\phi_1, \phi_2) &= \frac{1}{12\mathcal{M}_1 \Delta t} \|3\phi_1 - 4\phi_1^n + \phi_1^{n-1}\|_{-1,h}^2 + \frac{1}{12\mathcal{M}_2 \Delta t} \|3\phi_2 - 4\phi_2^n + \phi_2^{n-1}\|_{-1,h}^2 \\ &\quad + \langle S(\phi_1, \phi_2), 1 \rangle + \langle a_x (\kappa(A_x \phi_1) (D_x \phi_1)^2) + a_y (\kappa(A_y \phi_1) (D_y \phi_1)^2), \varepsilon_1^2 \rangle \\ &\quad + \langle a_x (\kappa(A_x \phi_2) (D_x \phi_2)^2) + a_y (\kappa(A_y \phi_2) (D_y \phi_2)^2), \varepsilon_2^2 \rangle \\ &\quad + \langle a_x (\kappa(A_x (1 - \phi_1 - \phi_2)) (D_x (1 - \phi_1 - \phi_2))^2) \\ &\quad \quad + a_y (\kappa(A_y (1 - \phi_1 - \phi_2)) (D_y (1 - \phi_1 - \phi_2))^2), \varepsilon_3^2 \rangle \\ &\quad + \langle \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_1 \rangle + \langle \frac{\partial}{\partial \phi_2} H(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_2 \rangle \\ &\quad + \frac{A_1 \Delta t}{2} \|\nabla_h(\phi_1 - \phi_1^n)\|_2^2 + \frac{A_2 \Delta t}{2} \|\nabla_h(\phi_2 - \phi_2^n)\|_2^2, \end{aligned}$$

over the admissible set

$$A_h := \left\{ (\phi_1, \phi_2) \in \tilde{C}_{\text{per}}^{\mathcal{G}} \mid \langle \phi_1, 1 \rangle = |\Omega| \overline{\phi_1^0}, \quad \langle \phi_2, 1 \rangle = |\Omega| \overline{\phi_2^0} \right\} \subset \mathbb{R}^{2N^2}.$$

It is clear that $\mathcal{J}_h^n$ is a strictly convex functional.

3.2. Proof by contradiction

Now, consider the following closed domain:

$$\begin{aligned} A_{h,\delta} &:= \left\{ (\phi_1, \phi_2) \in C_{\text{per}} \times C_{\text{per}} \mid \phi_1, \phi_2 \geq g(\delta), \quad \delta \leq \phi_1 + \phi_2 \leq 1 - \delta, \right. \\ &\quad \left. \langle \phi_1, 1 \rangle = |\Omega| \overline{\phi_1^0}, \quad \langle \phi_2, 1 \rangle = |\Omega| \overline{\phi_2^0} \right\} \subset \mathbb{R}^{2N^2}, \end{aligned}$$

where $g(\delta) > 0$ will be given later. Define the hyperplane

$$V := \left\{ (\phi_1, \phi_2) \mid \langle \phi_1, 1 \rangle = |\Omega| \overline{\phi_1^0}, \quad \langle \phi_2, 1 \rangle = |\Omega| \overline{\phi_2^0} \right\} \subset \mathbb{R}^{2N^2}.$$

Since $A_{h,\delta}$ is a bounded, compact, and convex subset of V , there exists (not necessarily unique) a minimizer of $\mathcal{J}_h^n(\phi_1, \phi_2)$ over $A_{h,\delta}$. The key point of the positivity analysis is that, such a minimizer could not occur at a boundary point of $A_{h,\delta}$, if δ and $g(\delta)$ are sufficiently small. Assume the minimizer of $\mathcal{J}_h^n(\phi_1, \phi_2)$ over $A_{h,\delta}$ occurs at a boundary point of $A_{h,\delta}$.

3.2.1. The minimizer $(\phi_1^*, \phi_2^*) \in A_{h,\delta}$ could not occur at $\phi_1^* = g(\delta)$.

We suppose the minimizer $(\phi_1^*, \phi_2^*) \in A_{h,\delta}$, satisfies $(\phi_1^*)_{\vec{a}_0} = g(\delta)$, for some grid point $\vec{a}_0 := (i_0, j_0)$. Assume that ϕ_1^* reaches its maximum value at the grid point $\vec{a}_1 := (i_1, j_1)$. It is obvious that $(\phi_1^*)_{\vec{a}_1} \geq \overline{\phi_1^*} = \overline{\phi_1^0}$. A careful calculation gives the following directional derivative

$$\begin{aligned} & d_s \mathcal{J}_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} \\ &= \frac{1}{2\mathcal{M}_1 \Delta t} \langle (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1}), \psi \rangle - A_1 \Delta t \langle \Delta_h(\phi_1^* - \phi_1^n), \psi \rangle \\ & \quad + \langle \delta_{\phi_1} G_{h,c}(\phi_1^*, \phi_2^*), \psi \rangle + \langle \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n), \psi \rangle, \end{aligned}$$

for any $\psi \in \hat{C}_{\text{per}}$. Let us pick the direction

$$\psi_{i,j} = \delta_{i,i_0} \delta_{j,j_0} - \delta_{i,i_1} \delta_{j,j_1},$$

where $\delta_{i,j}$ is the Dirac delta function. Note that ψ is of mean zero. The derivative may be expressed as

$$\begin{aligned} \frac{1}{h^2} d_s \mathcal{J}_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} &= \frac{1}{2\mathcal{M}_1 \Delta t} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\vec{a}_0} \\ & \quad - \frac{1}{2\mathcal{M}_1 \Delta t} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\vec{a}_1} \\ & \quad + Q_\ell(\phi_1^*, \phi_2^*)_{\vec{a}_0} - Q_\ell(\phi_1^*, \phi_2^*)_{\vec{a}_1} \\ & \quad + \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\vec{a}_0} - \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\vec{a}_1} \\ & \quad - A_1 \Delta t \left(\Delta_h(\phi_1^* - \phi_1^n)_{\vec{a}_0} - \Delta_h(\phi_1^* - \phi_1^n)_{\vec{a}_1} \right). \end{aligned} \quad (3.1)$$

For the first and second terms appearing in the right hand side of (3.1), we apply Lemma 3.1 and obtain

$$-\frac{8C_1}{\mathcal{M}_1} \leq \frac{1}{\mathcal{M}_1} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\vec{a}_0} - \frac{1}{\mathcal{M}_1} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\vec{a}_1} \leq \frac{8C_1}{\mathcal{M}_1}. \quad (3.2)$$

For the Q_1 terms, the following inequality is available:

$$\begin{aligned} & Q_1(\phi_1^*, \phi_2^*)_{\vec{a}_0} - Q_1(\phi_1^*, \phi_2^*)_{\vec{a}_1} \\ &= \frac{\partial}{\partial \phi_1} S(\phi_1^*, \phi_2^*)|_{\vec{a}_0} - \frac{\partial}{\partial \phi_1} S(\phi_1^*, \phi_2^*)|_{\vec{a}_1} \\ &= \left(\frac{1}{M_0} \ln \frac{\alpha \phi_1^*}{M_0} - \ln(1 - \phi_1^* - \phi_2^*) \right) |_{\vec{a}_0} - \left(\frac{1}{M_0} \ln \frac{\alpha \phi_1^*}{M_0} - \ln(1 - \phi_1^* - \phi_2^*) \right) |_{\vec{a}_1} \\ &= \left(\ln \frac{(\phi_1^*)^{1/M_0}}{1 - \phi_1^* - \phi_2^*} \right) |_{\vec{a}_0} - \left(\ln \frac{(\phi_1^*)^{1/M_0}}{1 - \phi_1^* - \phi_2^*} \right) |_{\vec{a}_1} \\ &\leq \ln \frac{(g(\delta))^{1/M_0}}{\delta} - \ln \frac{(\phi_1^0)^{1/M_0}}{1 - \delta} \\ &\leq \ln \frac{(g(\delta))^{1/M_0}}{\delta} - \frac{1}{M_0} \ln \overline{\phi_1^0}. \end{aligned} \quad (3.3)$$

Using the logarithm property $\ln(ab) = \ln a + \ln b$, we have eliminated the constant $\frac{1}{M_0} \ln \frac{\alpha}{M_0}$. The next-to-last step comes from the facts that $(\phi_1^*)_{\vec{a}_0} = g(\delta)$, $(\phi_1^*)_{\vec{a}_1} \geq \overline{\phi_1^0}$ and $\delta \leq \phi_1 + \phi_2 \leq 1 - \delta$. The last step comes from the inequality that $\ln(1 - \delta) < 0$. For the Q_2 terms, we have

$$\begin{aligned} & Q_2(\phi_1^*, \phi_2^*)_{\vec{a}_0} - Q_2(\phi_1^*, \phi_2^*)_{\vec{a}_1} \\ &= \varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\vec{a}_0} - \varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\vec{a}_1} \\ &\leq -\varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\vec{a}_1} \\ &\leq \frac{\varepsilon_1^2}{9h^2}. \end{aligned} \quad (3.4)$$

The second step above comes from the fact that

$$\varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\vec{a}_0} \leq 0,$$

since $\kappa'(\phi) = -\frac{1}{36\phi^2} < 0$. The last step is based on the definitions of $\kappa'(\phi)$, a_x , A_x , and D_x , as well as the fact that $|\frac{a-b}{a+b}| < 1$, $\forall a > 0, b > 0$. In details, we observe the following expansion

$$-\varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\vec{a}_1} = \frac{\varepsilon_1^2}{18h^2} \left[\frac{(\phi_1^*)_{i_1+1,j_1} - (\phi_1^*)_{i_1,j_1}}{(\phi_1^*)_{i_1+1,j_1} + (\phi_1^*)_{i_1,j_1}} \right]^2$$

$$\begin{aligned}
& + \frac{\varepsilon_1^2}{18h^2} \left[\frac{(\phi_1^*)_{i_1,j_1} - (\phi_1^*)_{i_1-1,j_1}}{(\phi_1^*)_{i_1-1,j_1} + (\phi_1^*)_{i_1,j_1}} \right]^2 \\
& \leq \frac{\varepsilon_1^2}{9h^2}.
\end{aligned}$$

The Q_4 terms can be similarly handled:

$$\begin{aligned}
Q_4(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_4(\phi_1^*, \phi_2^*)_{\bar{a}_1} &= \varepsilon_1^2 a_y (\kappa'(A_y \phi_1^*) (D_y \phi_1^*)^2)_{\bar{a}_0} \\
&\quad - \varepsilon_1^2 a_y (\kappa'(A_y \phi_1^*) (D_y \phi_1^*)^2)_{\bar{a}_1} \\
&\leq \frac{\varepsilon_1^2}{9h^2}.
\end{aligned} \tag{3.5}$$

For the Q_3 terms, we see that

$$\begin{aligned}
Q_3(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_3(\phi_1^*, \phi_2^*)_{\bar{a}_1} &= -2\varepsilon_1^2 d_x (\kappa(A_x \phi_1^*) D_x \phi_1^*)_{\bar{a}_0} \\
&\quad + 2\varepsilon_1^2 d_x (\kappa(A_x \phi_1^*) D_x \phi_1^*)_{\bar{a}_1} \\
&\leq 0,
\end{aligned} \tag{3.6}$$

in which the last step comes from the fact that $(D_x \phi_1^*)_{i_0-1/2,j_0} \leq 0$, $(D_x \phi_1^*)_{i_0+1/2,j_0} \geq 0$, $(D_x \phi_1^*)_{i_1-1/2,j_1} \geq 0$, and $(D_x \phi_1^*)_{i_1+1/2,j_1} \leq 0$.

A bound for the Q_5 terms could be similarly derived:

$$\begin{aligned}
Q_5(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_5(\phi_1^*, \phi_2^*)_{\bar{a}_1} &= -2\varepsilon_1^2 d_y (\kappa(A_y \phi_1^*) D_y \phi_1^*)_{\bar{a}_0} \\
&\quad + 2\varepsilon_1^2 d_y (\kappa(A_y \phi_1^*) D_y \phi_1^*)_{\bar{a}_1} \\
&\leq 0.
\end{aligned} \tag{3.7}$$

Use a technique similar to that used for Q_2 , the Q_6 terms could be controlled as follows:

$$\begin{aligned}
& Q_6(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_6(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
&= -\varepsilon_3^2 a_x (\kappa'(A_x(1 - \phi_1^* - \phi_2^*)) (D_x(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_0} \\
&\quad + \varepsilon_3^2 a_x (\kappa'(A_x(1 - \phi_1^* - \phi_2^*)) (D_x(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_1} \\
&\leq -\varepsilon_3^2 a_x (\kappa'(A_x(1 - \phi_1^* - \phi_2^*)) (D_x(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_0} \\
&\leq \frac{\varepsilon_3^2}{9h^2}.
\end{aligned} \tag{3.8}$$

A similar inequality could be derived for the Q_8 terms:

$$\begin{aligned}
& Q_8(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_8(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
&= -\varepsilon_3^2 a_y (\kappa'(A_y(1 - \phi_1^* - \phi_2^*)) (D_y(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_0} \\
&\quad + \varepsilon_3^2 a_y (\kappa'(A_y(1 - \phi_1^* - \phi_2^*)) (D_y(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_1} \\
&\leq -\varepsilon_3^2 a_y (\kappa'(A_y(1 - \phi_1^* - \phi_2^*)) (D_y(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_0} \\
&\leq \frac{\varepsilon_3^2}{9h^2}.
\end{aligned} \tag{3.9}$$

For the Q_7 terms, we have

$$\begin{aligned}
& Q_7(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_7(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
&= 2\varepsilon_3^2 d_x (\kappa(A_x(1 - \phi_1^* - \phi_2^*)) D_x(1 - \phi_1^* - \phi_2^*))_{\bar{a}_0} \\
&\quad - 2\varepsilon_3^2 d_x (\kappa(A_x(1 - \phi_1^* - \phi_2^*)) D_x(1 - \phi_1^* - \phi_2^*))_{\bar{a}_1} \\
&= \frac{\varepsilon_3^2}{18h} \left(\frac{D_x(1 - \phi_1^* - \phi_2^*)}{A_x(1 - \phi_1^* - \phi_2^*)} \right)_{i_0+1/2,j_0} - \frac{\varepsilon_3^2}{18h} \left(\frac{D_x(1 - \phi_1^* - \phi_2^*)}{A_x(1 - \phi_1^* - \phi_2^*)} \right)_{i_0-1/2,j_0} \\
&\quad - \frac{\varepsilon_3^2}{18h} \left(\frac{D_x(1 - \phi_1^* - \phi_2^*)}{A_x(1 - \phi_1^* - \phi_2^*)} \right)_{i_1+1/2,j_1} + \frac{\varepsilon_3^2}{18h} \left(\frac{D_x(1 - \phi_1^* - \phi_2^*)}{A_x(1 - \phi_1^* - \phi_2^*)} \right)_{i_1-1/2,j_1} \\
&\leq \frac{4\varepsilon_3^2}{9h^2}.
\end{aligned} \tag{3.10}$$

The last step above is based on the definitions of A_x and D_x , as well as the fact that $|\frac{a-b}{a+b}| < 1$, $\forall a > 0, b > 0$.

Similarly, for the Q_9 terms, we have

$$\begin{aligned}
Q_9(\phi_1^*, \phi_2^*)_{\vec{a}_0} - Q_9(\phi_1^*, \phi_2^*)_{\vec{a}_1} &= 2\epsilon_3^2 d_y (\kappa(A_y(1 - \phi_1^* - \phi_2^*)) D_y(1 - \phi_1^* - \phi_2^*))_{\vec{a}_0} \\
&\quad - 2\epsilon_3^2 d_y (\kappa(A_y(1 - \phi_1^* - \phi_2^*)) D_y(1 - \phi_1^* - \phi_2^*))_{\vec{a}_1} \\
&\leq \frac{4\epsilon_3^2}{9h^2}.
\end{aligned} \tag{3.11}$$

For the numerical solution ϕ_i^n, ϕ_i^{n-1} at the previous time step, the a-priori assumption $0 < \phi_i^n < 1$ indicates that

$$-1 \leq (\phi_i^n)_{\vec{a}_0} - (\phi_i^n)_{\vec{a}_1} \leq 1, \quad -1 \leq (\phi_i^{n-1})_{\vec{a}_0} - (\phi_i^{n-1})_{\vec{a}_1} \leq 1, \quad i = 1, 2, \tag{3.12}$$

then, we have

$$-3 \leq (\hat{\phi}_i^n)_{\vec{a}_0} - (\hat{\phi}_i^n)_{\vec{a}_1} \leq 3, \quad i = 1, 2. \tag{3.13}$$

For the fifth and sixth terms appearing in (3.1), we see that

$$\begin{aligned}
&\frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\vec{a}_0} - \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\vec{a}_1} \\
&= -2\chi_{13}[(\hat{\phi}_1^n)_{\vec{a}_0} - (\hat{\phi}_1^n)_{\vec{a}_1}] + (\chi_{12} - \chi_{13} - \chi_{23})[(\hat{\phi}_2^n)_{\vec{a}_0} - (\hat{\phi}_2^n)_{\vec{a}_1}] \\
&\leq 3(\chi_{12} + 3\chi_{13} + \chi_{23}).
\end{aligned} \tag{3.14}$$

For the last term appearing in the right hand of (3.1), we see that

$$\Delta_h(\phi_1^*)_{\vec{a}_0} - \Delta_h(\phi_1^*)_{\vec{a}_1} \geq 0, \quad -\frac{8}{h^2} \leq \Delta_h(\phi_1^n)_{\vec{a}_0} - \Delta_h(\phi_1^n)_{\vec{a}_1} \leq \frac{8}{h^2}, \tag{3.15}$$

this means

$$-A_1 \Delta t \left(\Delta_h(\phi_1^* - \phi_1^n)_{\vec{a}_0} - \Delta_h(\phi_1^* - \phi_1^n)_{\vec{a}_1} \right) \leq \frac{8A_1 \Delta t}{h^2}. \tag{3.16}$$

Putting every terms together, we have

$$\begin{aligned}
\frac{1}{h^2} d_s J_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} &\leq \ln \frac{(g(\delta))^{1/M_0}}{\delta} - \frac{1}{M_0} \ln \overline{\phi_1^0} + \frac{4C_1}{\mathcal{M}_1 \Delta t} \\
&\quad + \frac{2\epsilon_1^2}{9h^2} + \frac{10\epsilon_3^2}{9h^2} + 3(\chi_{12} + 3\chi_{13} + \chi_{23}) + \frac{8A_1 \Delta t}{h^2}.
\end{aligned}$$

The following quantity is introduced:

$$D_0 := -\frac{1}{M_0} \ln \overline{\phi_1^0} + \frac{4C_1}{\mathcal{M}_1 \Delta t} + \frac{2\epsilon_1^2}{9h^2} + \frac{10\epsilon_3^2}{9h^2} + 3(\chi_{12} + 3\chi_{13} + \chi_{23}) + \frac{8A_1 \Delta t}{h^2}.$$

Notice that D_0 is a constant for a fixed $\Delta t, h$, while it becomes singular as $\Delta t, h \rightarrow 0$. For any fixed $\Delta t, h$, we could choose $g(\delta)$ small enough so that

$$\ln \frac{(g(\delta))^{1/M_0}}{\delta} + D_0 < 0. \tag{3.17}$$

In particular, we can choose

$$g(\delta) := (\delta \exp(-D_0 - 1))^{M_0}.$$

This in turn shows that

$$\frac{1}{h^2} d_s J_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} < 0,$$

provided that $g(\delta)$ satisfies (3.17). But, this contradicts the assumption that J_h^n has a minimum at (ϕ_1^*, ϕ_2^*) , since the directional derivative is negative in a direction pointing into $(A_{h,\delta})^o$, the interior of $A_{h,\delta}$.

3.2.2. The minimizer $(\phi_1^*, \phi_2^*) \in A_{h,\delta}$ could not occur at $\phi_2^* = g(\delta)$

Using similar arguments to Section 3.2.1, we are able to prove that, the global minimum of J_h^n over $A_{h,\delta}$ could not occur on the boundary section where $(\phi_2^*)_{\vec{a}_0} = g(\delta)$, if $g(\delta)$ is small enough, for any grid index $\vec{a}_0$.

3.2.3. The minimizer $(\phi_1^*, \phi_2^*) \in A_{h,\delta}$ could not occur at $\phi_1^* + \phi_2^* = 1 - \delta$

Suppose the minimum point (ϕ_1^*, ϕ_2^*) satisfies

$$(\phi_1^*)_{\vec{a}_0} + (\phi_2^*)_{\vec{a}_0} = 1 - \delta,$$

with $\vec{a}_0 := (i_0, j_0)$. We could choose $\delta \in (0, 1/3)$. Without loss of generality, it is assumed that $(\phi_1^*)_{\vec{a}_0} \geq \frac{1}{3}$. In addition, we see that

$$\frac{1}{N^2} \sum_{i,j=1}^N (\phi_1^* + \phi_2^*)_{i,j} = \overline{\phi_1^*} + \overline{\phi_2^*}.$$

There exists one grid point $\vec{a}_1 := (i_1, j_1)$, so that $\phi_1^* + \phi_2^*$ reaches the minimum value at $\vec{a}_1$. Then it is obvious that $(\phi_1^*)_{\vec{a}_1} + (\phi_2^*)_{\vec{a}_1} \leq \overline{\phi_1^*} + \overline{\phi_2^*} = \phi_1^0 + \phi_2^0$. In turn, the following directional derivative could be derived:

$$\begin{aligned}
& d_s \mathcal{J}_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} \\
&= \frac{1}{2\mathcal{M}_1 \Delta t} \langle (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1}), \psi \rangle - A_1 \Delta t \langle \Delta_h(\phi_1^* - \phi_1^n), \psi \rangle \\
&+ \langle \delta_{\phi_1} G_{n,c}(\phi_1^*, \phi_2^*), \psi \rangle + \langle \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n), \psi \rangle,
\end{aligned}$$

for any $\psi \in \tilde{C}_{\text{per}}$. Setting the direction as

$$\psi_{i,j} = \delta_{i,i_0} \delta_{j,j_0} - \delta_{i,i_1} \delta_{j,j_1},$$

then the derivative may be expanded as

$$\begin{aligned}
\frac{1}{h^2} d_s \mathcal{J}_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} &= \frac{1}{2\mathcal{M}_1 \Delta t} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\bar{a}_0} \\
&- \frac{1}{2\mathcal{M}_1 \Delta t} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\bar{a}_1} \\
&+ Q_\ell(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_\ell(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
&+ \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\bar{a}_0} - \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\bar{a}_1} \\
&- A_1 \Delta t \left(\Delta_h(\phi_1^* - \phi_1^n)_{\bar{a}_0} - \Delta_h(\phi_1^* - \phi_1^n)_{\bar{a}_1} \right).
\end{aligned} \tag{3.18}$$

For the first and second terms appearing in (3.18), we apply Lemma 3.1 and obtain

$$-\frac{8C_1}{\mathcal{M}_1} \leq \frac{1}{\mathcal{M}_1} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\bar{a}_0} - \frac{1}{\mathcal{M}_1} (-\Delta_h)^{-1} (3\phi_1^* - 4\phi_1^n + \phi_1^{n-1})_{\bar{a}_1} \leq \frac{8C_1}{\mathcal{M}_1}. \tag{3.19}$$

For the Q_1 terms, we have

$$\begin{aligned}
& Q_1(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_1(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
&= \left(\ln \frac{(\phi_1^*)^{1/M_0}}{1 - \phi_1^* - \phi_2^*} \right)_{\bar{a}_0} - \left(\ln \frac{(\phi_1^*)^{1/M_0}}{1 - \phi_1^* - \phi_2^*} \right)_{\bar{a}_1} \\
&\geq \ln \frac{(\frac{1}{3})^{1/M_0}}{\delta} - \ln \frac{1}{1 - \phi_1^0 - \phi_2^0}.
\end{aligned} \tag{3.20}$$

The last step above comes from the facts that $(\phi_1^*)_{\bar{a}_0} \geq \frac{1}{3}$, $(\phi_1^*)_{\bar{a}_1} + (\phi_2^*)_{\bar{a}_1} \leq \overline{\phi_1^0} + \overline{\phi_2^0}$, and $(\phi_1^*)_{\bar{a}_1} < 1$.

For the Q_2 terms, we have

$$\begin{aligned}
& Q_2(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_2(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
&= \varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\bar{a}_0} - \varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\bar{a}_1} \\
&\geq \varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\bar{a}_0} \\
&\geq -\frac{\varepsilon_1^2}{9h^2},
\end{aligned} \tag{3.21}$$

in which the second step comes from the fact that $-\varepsilon_1^2 a_x (\kappa'(A_x \phi_1^*) (D_x \phi_1^*)^2)_{\bar{a}_1} \geq 0$, since $\kappa'(\phi) = -\frac{1}{36\phi^2} < 0$, and the last step is based on the definitions of $\kappa'(\phi)$, a_x , A_x , and D_x , as well as the fact that $|\frac{a-b}{a+b}| < 1$, $\forall a > 0, b > 0$.

For the Q_4 terms, similarly, we get

$$\begin{aligned}
& Q_4(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_4(\phi_1^*, \phi_2^*)_{\bar{a}_1} = \varepsilon_1^2 a_y (\kappa'(A_y \phi_1^*) (D_y \phi_1^*)^2)_{\bar{a}_0} \\
&- \varepsilon_1^2 a_y (\kappa'(A_y \phi_1^*) (D_y \phi_1^*)^2)_{\bar{a}_1} \\
&\geq -\frac{\varepsilon_1^2}{9h^2}.
\end{aligned} \tag{3.22}$$

The Q_3 and Q_5 terms could be analyzed as follows

$$\begin{aligned}
& Q_3(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_3(\phi_1^*, \phi_2^*)_{\bar{a}_1} = -2\varepsilon_1^2 d_x (\kappa(A_x \phi_1^*) D_x \phi_1^*)_{\bar{a}_0} \\
&+ 2\varepsilon_1^2 d_x (\kappa(A_x \phi_1^*) D_x \phi_1^*)_{\bar{a}_1} \\
&\geq -\frac{4\varepsilon_1^2}{9h^2},
\end{aligned} \tag{3.23}$$

$$\begin{aligned}
& Q_5(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_5(\phi_1^*, \phi_2^*)_{\bar{a}_1} = -2\varepsilon_1^2 d_y (\kappa(A_y \phi_1^*) D_y \phi_1^*)_{\bar{a}_0} \\
&+ 2\varepsilon_1^2 d_y (\kappa(A_y \phi_1^*) D_y \phi_1^*)_{\bar{a}_1} \\
&\geq -\frac{4\varepsilon_1^2}{9h^2}.
\end{aligned} \tag{3.24}$$

The estimates for the Q_6 and Q_8 terms are similar:

$$\begin{aligned}
 & Q_6(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_6(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
 &= -\varepsilon_3^2 a_x (\kappa'(A_x(1 - \phi_1^* - \phi_2^*))(D_x(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_0} \\
 &\quad + \varepsilon_3^2 a_x (\kappa'(A_x(1 - \phi_1^* - \phi_2^*))(D_x(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_1} \\
 &\geq \varepsilon_3^2 a_x (\kappa'(A_x(1 - \phi_1^* - \phi_2^*))(D_x(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_1} \\
 &\geq -\frac{\varepsilon_3^2}{9h^2},
 \end{aligned} \tag{3.25}$$

$$\begin{aligned}
 & Q_8(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_8(\phi_1^*, \phi_2^*)_{\bar{a}_1} \\
 &= -\varepsilon_3^2 a_y (\kappa'(A_y(1 - \phi_1^* - \phi_2^*))(D_y(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_0} \\
 &\quad + \varepsilon_3^2 a_y (\kappa'(A_y(1 - \phi_1^* - \phi_2^*))(D_y(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_1} \\
 &\geq \varepsilon_3^2 a_y (\kappa'(A_y(1 - \phi_1^* - \phi_2^*))(D_y(1 - \phi_1^* - \phi_2^*))^2)_{\bar{a}_1} \\
 &\geq -\frac{\varepsilon_3^2}{9h^2}.
 \end{aligned} \tag{3.26}$$

For the Q_7 terms, we see that

$$\begin{aligned}
 Q_7(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_7(\phi_1^*, \phi_2^*)_{\bar{a}_1} &= 2\varepsilon_3^2 d_x (\kappa(A_x(1 - \phi_1^* - \phi_2^*))D_x(1 - \phi_1^* - \phi_2^*))_{\bar{a}_0} \\
 &\quad - 2\varepsilon_3^2 d_x (\kappa(A_x(1 - \phi_1^* - \phi_2^*))D_x(1 - \phi_1^* - \phi_2^*))_{\bar{a}_1} \\
 &\geq 0.
 \end{aligned} \tag{3.27}$$

The last step above comes from the fact that

$$\begin{aligned}
 (D_x(1 - \phi_1^* - \phi_2^*))_{i_0-1/2, j_0} &\leq 0, \\
 (D_x(1 - \phi_1^* - \phi_2^*))_{i_0+1/2, j_0} &\geq 0, \\
 (D_x(1 - \phi_1^* - \phi_2^*))_{i_1-1/2, j_1} &\geq 0, \\
 (D_x(1 - \phi_1^* - \phi_2^*))_{i_1+1/2, j_1} &\leq 0.
 \end{aligned}$$

Similarly, for the Q_9 terms, we see that

$$\begin{aligned}
 Q_9(\phi_1^*, \phi_2^*)_{\bar{a}_0} - Q_9(\phi_1^*, \phi_2^*)_{\bar{a}_1} &= 2\varepsilon_3^2 d_y (\kappa(A_y(1 - \phi_1^* - \phi_2^*))D_y(1 - \phi_1^* - \phi_2^*))_{\bar{a}_0} \\
 &\quad - 2\varepsilon_3^2 d_y (\kappa(A_y(1 - \phi_1^* - \phi_2^*))D_y(1 - \phi_1^* - \phi_2^*))_{\bar{a}_1} \\
 &\geq 0.
 \end{aligned} \tag{3.28}$$

For the numerical solution ϕ_i^{n-1}, ϕ_i^n at the previous time step, similar bounds could be derived for the fifth and sixth terms appearing in (3.18), we have

$$\begin{aligned}
 & \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\bar{a}_0} - \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n)|_{\bar{a}_1} \\
 &= -2\chi_{13}[(\hat{\phi}_1^n)_{\bar{a}_0} - (\hat{\phi}_1^n)_{\bar{a}_1}] + (\chi_{12} - \chi_{13} - \chi_{23})[(\hat{\phi}_2^n)_{\bar{a}_0} - (\hat{\phi}_2^n)_{\bar{a}_1}] \\
 &\geq -3(\chi_{12} + 3\chi_{13} + \chi_{23}).
 \end{aligned} \tag{3.29}$$

For the last term appearing in (3.18), similar bounds could be derived

$$-A_1 \Delta t \left(\Delta_h(\phi_1^* - \phi_1^n)_{\bar{a}_0} - \Delta_h(\phi_1^* - \phi_1^n)_{\bar{a}_1} \right) \geq -\frac{16A_1 \Delta t}{h^2}. \tag{3.30}$$

Putting estimates together, we arrive at

$$\begin{aligned}
 \frac{1}{h^2} d_s J_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} &\geq \ln \frac{(\frac{1}{3})^{1/M_0}}{\delta} - \ln \frac{1}{1 - \phi_1^0 - \phi_2^0} - \frac{4C_1}{\mathcal{M}_1 \Delta t} \\
 &\quad - \frac{10\varepsilon_1^2}{9h^2} - \frac{2\varepsilon_3^2}{9h^2} - 3(\chi_{12} + 3\chi_{13} + \chi_{23}) - \frac{16A_1 \Delta t}{h^2}.
 \end{aligned}$$

The following quantity is introduced:

$$D_1 := \frac{1}{M_0} \ln 3 + \ln \frac{1}{1 - \phi_1^0 - \phi_2^0} + \frac{4C_1}{\mathcal{M}_1 \Delta t} + \frac{10\varepsilon_1^2}{9h^2} + \frac{2\varepsilon_3^2}{9h^2} + 3(\chi_{12} + 3\chi_{13} + \chi_{23}) + \frac{16A_1 \Delta t}{h^2}. \tag{3.31}$$

For any fixed $\Delta t, h$, we could choose δ small enough so that

$$-\ln \delta - D_1 > 0, \tag{3.32}$$

in particular, $\delta = \min\{\exp(-D_1 - 1), 1/3\}$. This in turn shows that

$$\frac{1}{h^2} d_s J_h^n(\phi_1^* + s\psi, \phi_2^*)|_{s=0} > 0,$$

provided that δ satisfies (3.32). This contradicts the assumption that J_h^n has a minimum at (ϕ_1^*, ϕ_2^*) .

3.2.4. The minimizer $(\phi_1^*, \phi_2^*) \in A_{h,\delta}$ could not occur at $\phi_1^* + \phi_2^* = \delta$

Using similar arguments to Section 3.2.3, we can also prove that, the global minimum of J_h^n over $A_{h,\delta}$ could not occur on the boundary section where $(\phi_1^*)_{\tilde{\alpha}_0} + (\phi_2^*)_{\tilde{\alpha}_0} = \delta$, if δ is small enough, for any grid index $\tilde{\alpha}_0$. The details are left to the interested readers.

Finally, a combination of these four cases reveals that, the global minimizer of $J_h^n(\phi_1, \phi_2)$ could only possibly occur at interior point of $(A_{h,\delta})^0 \subset (A_h)^0$. We conclude that there must be a solution $(\phi_1, \phi_2) \in (A_h)^0$ that minimizes $J_h^n(\phi_1, \phi_2)$ over A_h , which is equivalent to the numerical solution of (2.4)–(2.7). The existence of the numerical solution is established.

In addition, since $J_h^n(\phi_1, \phi_2)$ is a strictly convex function over A_h , the uniqueness analysis for this numerical solution is straightforward. Using similar argument, the positivity-preserving property is established for the initialization step, the details are left to the interested readers. The proof of Theorem 3.1 is complete.

4. Energy stability

Due to the fully discrete scheme (2.4)–(2.7) is three-level scheme, here, we define the modified discrete energy as

$$\begin{aligned} E_h^{n+1,n} := & G_h(\phi_1^{n+1}, \phi_2^{n+1}) + \frac{\Delta t}{4\mathcal{M}_1} \left\| \frac{\phi_1^{n+1} - \phi_1^n}{\Delta t} \right\|_{-1,h}^2 + \frac{\Delta t}{4\mathcal{M}_2} \left\| \frac{\phi_2^{n+1} - \phi_2^n}{\Delta t} \right\|_{-1,h}^2 \\ & + \frac{2\chi_{12} + 3\chi_{13} + \chi_{23}}{2} \|\phi_1^{n+1} - \phi_1^n\|_2^2 + \frac{2\chi_{12} + \chi_{13} + 3\chi_{23}}{2} \|\phi_2^{n+1} - \phi_2^n\|_2^2, \end{aligned}$$

in which $n \geq 0$.

Theorem 4.1 (Energy Stability). When $n \geq 1$, $A_1 \geq \frac{\mathcal{M}_1(3\chi_{13} + 3\chi_{23} + 2\chi_{12})^2}{4}$, $A_2 \geq \frac{\mathcal{M}_2(3\chi_{13} + 3\chi_{23} + 2\chi_{12})^2}{4}$, the fully discrete scheme (2.4)–(2.7) has the energy-decay property

$$E_h^{n+1,n} \leq E_h^{n,n-1}.$$

Proof. Due to the mass conservation, $\mathcal{L}^{-1}(\phi_i^{n+1} - \phi_i^n)$ is well-defined. Taking a discrete inner product with (2.4) by $\frac{1}{\mathcal{M}_1} \mathcal{L}^{-1}(\phi_1^{n+1} - \phi_1^n)$, with (2.5) by $\phi_1^{n+1} - \phi_1^n$, with (2.6) by $\frac{1}{\mathcal{M}_2} \mathcal{L}^{-1}(\phi_2^{n+1} - \phi_2^n)$, with (2.7) by $\phi_2^{n+1} - \phi_2^n$ yields

$$\begin{aligned} 0 = & \frac{1}{2\mathcal{M}_1 \Delta t} \langle 3\phi_1^{n+1} - 4\phi_1^n + \phi_1^{n-1}, \mathcal{L}^{-1}(\phi_1^{n+1} - \phi_1^n) \rangle + \langle \mu_1^{n+1}, \phi_1^{n+1} - \phi_1^n \rangle \\ & + \frac{1}{2\mathcal{M}_2 \Delta t} \langle 3\phi_2^{n+1} - 4\phi_2^n + \phi_2^{n-1}, \mathcal{L}^{-1}(\phi_2^{n+1} - \phi_2^n) \rangle + \langle \mu_2^{n+1}, \phi_2^{n+1} - \phi_2^n \rangle. \end{aligned}$$

The equivalent form is the following identity

$$\begin{aligned} 0 = & \frac{1}{2\mathcal{M}_1 \Delta t} \langle 3\phi_1^{n+1} - 4\phi_1^n + \phi_1^{n-1}, \mathcal{L}^{-1}(\phi_1^{n+1} - \phi_1^n) \rangle + A_1 \Delta t \|\nabla_h(\phi_1^{n+1} - \phi_1^n)\|_2^2 \\ & + \langle \delta_{\phi_1} G_{h,c}(\phi_1^{n+1}, \phi_2^{n+1}) - \delta_{\phi_1} G_{h,c}(\phi_1^n, \phi_2^n), \phi_1^{n+1} - \phi_1^n \rangle \\ & + \langle \delta_{\phi_1} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n) - \delta_{\phi_1} G_{h,e}(\hat{\phi}_1^{n-1}, \hat{\phi}_2^{n-1}), \phi_1^{n+1} - \phi_1^n \rangle \\ & + \frac{1}{2\mathcal{M}_2 \Delta t} \langle 3\phi_2^{n+1} - 4\phi_2^n + \phi_2^{n-1}, \mathcal{L}^{-1}(\phi_2^{n+1} - \phi_2^n) \rangle + A_2 \Delta t \|\nabla_h(\phi_2^{n+1} - \phi_2^n)\|_2^2 \\ & + \langle \delta_{\phi_2} G_{h,c}(\phi_1^{n+1}, \phi_2^{n+1}) - \delta_{\phi_2} G_{h,c}(\phi_1^n, \phi_2^n), \phi_2^{n+1} - \phi_2^n \rangle \\ & + \langle \delta_{\phi_2} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n) - \delta_{\phi_2} G_{h,e}(\hat{\phi}_1^{n-1}, \hat{\phi}_2^{n-1}), \phi_2^{n+1} - \phi_2^n \rangle. \end{aligned} \quad (4.1)$$

For the first and fifth term of the right hand side of (4.1), we have

$$\begin{aligned} & \frac{1}{2\mathcal{M}_i \Delta t} \langle 3\phi_i^{n+1} - 4\phi_i^n + \phi_i^{n-1}, \mathcal{L}^{-1}(\phi_i^{n+1} - \phi_i^n) \rangle \\ = & \frac{\Delta t}{\mathcal{M}_i} \left(\frac{5}{4} \left\| \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \right\|_{-1,h}^2 - \frac{1}{4} \left\| \frac{\phi_i^n - \phi_i^{n-1}}{\Delta t} \right\|_{-1,h}^2 \right) \\ & + \frac{\Delta t^3}{4\mathcal{M}_i} \left\| \frac{\phi_i^{n+1} - 2\phi_i^n + \phi_i^{n-1}}{\Delta t^2} \right\|_{-1,h}^2 \\ \geq & \frac{\Delta t}{\mathcal{M}_i} \left(\frac{5}{4} \left\| \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \right\|_{-1,h}^2 - \frac{1}{4} \left\| \frac{\phi_i^n - \phi_i^{n-1}}{\Delta t} \right\|_{-1,h}^2 \right), \quad i = 1, 2. \end{aligned} \quad (4.2)$$

For the third and seventh term of the right hand side of (4.1), using Lemma 2.3, we have

$$\begin{aligned} & \langle \delta_{\phi_1} G_{h,c}(\phi_1^{n+1}, \phi_2^{n+1}) - \delta_{\phi_1} G_{h,c}(\phi_1^n, \phi_2^n), \phi_1^{n+1} - \phi_1^n \rangle \\ & + \langle \delta_{\phi_2} G_{h,c}(\phi_1^{n+1}, \phi_2^{n+1}) - \delta_{\phi_2} G_{h,c}(\phi_1^n, \phi_2^n), \phi_2^{n+1} - \phi_2^n \rangle \\ & \geq G_h(\phi_1^{n+1}, \phi_2^{n+1}) - G_h(\phi_1^n, \phi_2^n). \end{aligned}$$

For the fourth term of the right hand side of (4.1), we have

$$\begin{aligned} & \langle \delta_{\phi_1} G_{h,e}(\phi_1^n, \phi_2^n) - \delta_{\phi_1} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_1^{n+1} - \phi_1^n \rangle \\ & = - \langle \frac{\partial}{\partial \phi_1} H(\phi_1^n, \phi_2^n) - \frac{\partial}{\partial \phi_1} H(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_1^{n+1} - \phi_1^n \rangle \\ & = (2\chi_{13}(\phi_1^n - \hat{\phi}_1^n) - (\chi_{12} - \chi_{13} - \chi_{23})(\phi_2^n - \hat{\phi}_2^n), \phi_1^{n+1} - \phi_1^n) \\ & = -2\chi_{13}(\phi_1^n - \phi_1^{n-1}, \phi_1^{n+1} - \phi_1^n) + (\chi_{12} - \chi_{13} - \chi_{23})(\phi_2^n - \phi_2^{n-1}, \phi_1^{n+1} - \phi_1^n) \\ & \geq -\chi_{13}(\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2) \\ & \quad + \frac{\chi_{12} - \chi_{13} - \chi_{23}}{2} (\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2 - \|\phi_2^n - \phi_2^{n-1} - \phi_1^{n+1} + \phi_1^n\|_2^2) \\ & \geq -\chi_{13}(\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2) \\ & \quad - \frac{\chi_{13} + \chi_{23}}{2} (\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2) - \frac{\chi_{12}}{2} \|\phi_2^n - \phi_2^{n-1} - \phi_1^{n+1} + \phi_1^n\|_2^2 \\ & \geq -\chi_{13}(\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2) \\ & \quad - \frac{\chi_{13} + \chi_{23}}{2} (\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2) \\ & \quad - \chi_{12}(\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2) \\ & = -\chi_{13}\|\phi_1^n - \phi_1^{n-1}\|_2^2 - \frac{3\chi_{13} + \chi_{23} + 2\chi_{12}}{2} \|\phi_1^{n+1} - \phi_1^n\|_2^2 \\ & \quad - \frac{2\chi_{12} + \chi_{13} + \chi_{23}}{2} \|\phi_2^n - \phi_2^{n-1}\|_2^2, \end{aligned}$$

in which the fourth step is based on the formula $2ab \leq a^2 + b^2$, $2ab = a^2 + b^2 - (a - b)^2$, the next-to-last step comes from inequality $(a - b)^2 \leq 2(a^2 + b^2)$.

For the last term of the right hand side of (4.1), similarly, we have

$$\begin{aligned} & \langle \delta_{\phi_2} G_{h,e}(\phi_1^n, \phi_2^n) - \delta_{\phi_2} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_2^{n+1} - \phi_2^n \rangle \\ & = - \langle \frac{\partial}{\partial \phi_2} H(\phi_1^n, \phi_2^n) - \frac{\partial}{\partial \phi_2} H(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_2^{n+1} - \phi_2^n \rangle \\ & = (2\chi_{23}(\phi_2^n - \hat{\phi}_2^n) - (\chi_{12} - \chi_{13} - \chi_{23})(\phi_1^n - \hat{\phi}_1^n), \phi_2^{n+1} - \phi_2^n) \\ & = -2\chi_{23}(\phi_2^n - \phi_2^{n-1}, \phi_2^{n+1} - \phi_2^n) + (\chi_{12} - \chi_{13} - \chi_{23})(\phi_1^n - \phi_1^{n-1}, \phi_2^{n+1} - \phi_2^n) \\ & \geq -\chi_{23}(\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2) \\ & \quad + \frac{\chi_{12} - \chi_{13} - \chi_{23}}{2} (\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2 - \|\phi_1^n - \phi_1^{n-1} - \phi_2^{n+1} + \phi_2^n\|_2^2) \\ & \geq -\chi_{23}(\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2) \\ & \quad - \frac{\chi_{13} + \chi_{23}}{2} (\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2) - \frac{\chi_{12}}{2} \|\phi_1^n - \phi_1^{n-1} - \phi_2^{n+1} + \phi_2^n\|_2^2 \\ & \geq -\chi_{23}(\|\phi_2^n - \phi_2^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2) \\ & \quad - \frac{\chi_{13} + \chi_{23}}{2} (\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2) \\ & \quad - \chi_{12}(\|\phi_1^n - \phi_1^{n-1}\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2) \\ & = -\chi_{23}\|\phi_2^n - \phi_2^{n-1}\|_2^2 - \frac{\chi_{13} + 3\chi_{23} + 2\chi_{12}}{2} \|\phi_2^{n+1} - \phi_2^n\|_2^2 \\ & \quad - \frac{2\chi_{12} + \chi_{13} + \chi_{23}}{2} \|\phi_1^n - \phi_1^{n-1}\|_2^2. \end{aligned}$$

Going back (4.1) and by simple calculation, we arrive at

$$\begin{aligned} & \frac{\Delta t}{\mathcal{M}_1} \left(\frac{5}{4} \left\| \frac{\phi_1^{n+1} - \phi_1^n}{\Delta t} \right\|_{-1,h}^2 - \frac{1}{4} \left\| \frac{\phi_1^n - \phi_1^{n-1}}{\Delta t} \right\|_{-1,h}^2 \right) + A_1 \Delta t \left\| \nabla_h(\phi_1^{n+1} - \phi_1^n) \right\|_2^2 \\ & + \frac{\Delta t}{\mathcal{M}_2} \left(\frac{5}{4} \left\| \frac{\phi_2^{n+1} - \phi_2^n}{\Delta t} \right\|_{-1,h}^2 - \frac{1}{4} \left\| \frac{\phi_2^n - \phi_2^{n-1}}{\Delta t} \right\|_{-1,h}^2 \right) + A_2 \Delta t \left\| \nabla_h(\phi_2^{n+1} - \phi_2^n) \right\|_2^2 \\ & + G_h(\phi_1^{n+1}, \phi_2^{n+1}) - G_h(\phi_1^n, \phi_2^n) \end{aligned}$$

$$\begin{aligned}
& -\frac{2\chi_{12}+3\chi_{13}+\chi_{23}}{2}(\|\phi_1^n-\phi_1^{n-1}\|_2^2-\|\phi_1^{n+1}-\phi_1^n\|_2^2) \\
& -\frac{\chi_{13}+3\chi_{23}+2\chi_{12}}{2}(\|\phi_2^n-\phi_2^{n-1}\|_2^2-\|\phi_2^{n+1}-\phi_2^n\|_2^2) \\
& \leq (3\chi_{13}+3\chi_{23}+2\chi_{12})\left(\|\phi_1^{n+1}-\phi_1^n\|_2^2+\|\phi_2^{n+1}-\phi_2^n\|_2^2\right).
\end{aligned} \tag{4.3}$$

For the right hand side of (4.3), we have

$$\|\phi_1^{n+1}-\phi_1^n\|_2^2 \leq \frac{\Delta t}{2\alpha} \|\nabla_h(\phi_1^{n+1}-\phi_1^n)\|_2^2 + \frac{\alpha\Delta t}{2} \left\| \frac{\phi_1^{n+1}-\phi_1^n}{\Delta t} \right\|_{-1,h}^2,$$

and

$$\|\phi_2^{n+1}-\phi_2^n\|_2^2 \leq \frac{\Delta t}{2\beta} \|\nabla_h(\phi_2^{n+1}-\phi_2^n)\|_2^2 + \frac{\beta\Delta t}{2} \left\| \frac{\phi_2^{n+1}-\phi_2^n}{\Delta t} \right\|_{-1,h}^2.$$

Let $\alpha = \frac{3\chi_{13}+3\chi_{23}+2\chi_{12}}{2A_1}$, $\beta = \frac{3\chi_{13}+3\chi_{23}+2\chi_{12}}{2A_2}$, when $A_1 \geq \frac{\mathcal{M}_1(3\chi_{13}+3\chi_{23}+2\chi_{12})^2}{4}$, $A_2 \geq \frac{\mathcal{M}_2(3\chi_{13}+3\chi_{23}+2\chi_{12})^2}{4}$, we have $E_h^{n+1,n} \leq E_h^{n,n-1}$.

This completes the proof. $\square$

In fact, for the fourth term of the right hand side of (4.1), it can be analyzed in another way:

$$\begin{aligned}
& \langle \delta_{\phi_1} G_{h,e}(\phi_1^n, \phi_2^n) - \delta_{\phi_1} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_1^{n+1} - \phi_1^n \rangle \\
& = -2\chi_{13} \langle \phi_1^n - \phi_1^{n-1}, \phi_1^{n+1} - \phi_1^n \rangle + (\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_2^n - \phi_2^{n-1}, \phi_1^{n+1} - \phi_1^n \rangle \\
& = (\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_2^n - \phi_2^{n-1}, \phi_1^{n+1} - \phi_1^n \rangle \\
& \quad - \chi_{13} (\|\phi_1^n - \phi_1^{n-1}\|_2^2 - \|\phi_1^{n+1} - \phi_1^n\|_2^2 + \|\phi_1^{n+1} - \phi_1^n\|_2^2).
\end{aligned} \tag{4.4}$$

Similarly, the following estimate is valid for ϕ_2 :

$$\begin{aligned}
& \langle \delta_{\phi_2} G_{h,e}(\phi_1^n, \phi_2^n) - \delta_{\phi_2} G_{h,e}(\hat{\phi}_1^n, \hat{\phi}_2^n), \phi_2^{n+1} - \phi_2^n \rangle \\
& = (\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_1^n - \phi_1^{n-1}, \phi_2^{n+1} - \phi_2^n \rangle \\
& \quad - \chi_{23} (\|\phi_2^n - \phi_2^{n-1}\|_2^2 - \|\phi_2^{n+1} - \phi_2^n\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2).
\end{aligned} \tag{4.5}$$

Meanwhile, the following vector norms are introduced:

$$\begin{aligned}
\|\phi^{n+1} - \phi^n\|_{-1,h}^2 & := \|\phi_1^{n+1} - \phi_1^n\|_{-1,h}^2 + \|\phi_2^{n+1} - \phi_2^n\|_{-1,h}^2, \\
\|\phi^{n+1} - \phi^n\|_2^2 & := \|\phi_1^{n+1} - \phi_1^n\|_2^2 + \|\phi_2^{n+1} - \phi_2^n\|_2^2.
\end{aligned}$$

For simplify, we set the mobility parameters $\mathcal{M}_1 = \mathcal{M}_2 = 1$ in the model. Substituting (4.2), (4.4) and (4.5) into (4.1), and applying Lemma 2.2, we obtain

$$\begin{aligned}
& \frac{1}{\Delta t} \left(\frac{5}{4} \|\phi^{n+1} - \phi^n\|_{-1,h}^2 - \frac{1}{4} \|\phi^n - \phi^{n-1}\|_{-1,h}^2 \right) + G_h(\phi_1^{n+1}, \phi_2^{n+1}) - G_h(\phi_1^n, \phi_2^n) \\
& + A_1 \Delta t \|\nabla_h(\phi_1^{n+1} - \phi_1^n)\|_2^2 + A_2 \Delta t \|\nabla_h(\phi_2^{n+1} - \phi_2^n)\|_2^2 \\
& - \chi_{13} (\|\phi_1^n - \phi_1^{n-1}\|_2^2 - \|\phi_1^{n+1} - \phi_1^n\|_2^2) - \chi_{23} (\|\phi_2^n - \phi_2^{n-1}\|_2^2 - \|\phi_2^{n+1} - \phi_2^n\|_2^2) \\
& \leq -(\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_2^n - \phi_2^{n-1}, \phi_1^{n+1} - \phi_1^n \rangle - (\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_1^n - \phi_1^{n-1}, \phi_2^{n+1} - \phi_2^n \rangle \\
& + 2\chi_{13} \|\phi_1^{n+1} - \phi_1^n\|_2^2 + 2\chi_{23} \|\phi_2^{n+1} - \phi_2^n\|_2^2.
\end{aligned} \tag{4.6}$$

For the first term of the right hand of (4.6), it is observed that

$$\begin{aligned}
& -(\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_2^n - \phi_2^{n-1}, \phi_1^{n+1} - \phi_1^n \rangle \\
& \leq |\chi_{12} - \chi_{13} - \chi_{23}| \left(\frac{\Delta t}{2\beta_1} \|\nabla_h(\phi_1^{n+1} - \phi_1^n)\|_2^2 + \frac{\beta_1}{2\Delta t} \|\phi_2^n - \phi_2^{n-1}\|_{-1,h}^2 \right).
\end{aligned} \tag{4.7}$$

Similarly, for the second term of the right hand of (4.6), the following inequality is available:

$$\begin{aligned}
& -(\chi_{12} - \chi_{13} - \chi_{23}) \langle \phi_1^n - \phi_1^{n-1}, \phi_2^{n+1} - \phi_2^n \rangle \\
& \leq |\chi_{12} - \chi_{13} - \chi_{23}| \left(\frac{\Delta t}{2\beta_2} \|\nabla_h(\phi_2^{n+1} - \phi_2^n)\|_2^2 + \frac{\beta_2}{2\Delta t} \|\phi_1^n - \phi_1^{n-1}\|_{-1,h}^2 \right).
\end{aligned} \tag{4.8}$$

For the third term of the right hand of (4.6), we see that

$$2\chi_{13} \|\phi_1^{n+1} - \phi_1^n\|_2^2 \leq \chi_{13} \left(\frac{\Delta t}{\alpha_1} \|\nabla_h(\phi_1^{n+1} - \phi_1^n)\|_2^2 + \frac{\alpha_1}{\Delta t} \|\phi_1^{n+1} - \phi_1^n\|_{-1,h}^2 \right). \tag{4.9}$$

A similar estimate could also be derived for the fourth term of the right hand of (4.6):

$$2\chi_{23}\|\phi_2^{n+1} - \phi_2^n\|_2^2 \leq \chi_{23} \left(\frac{\Delta t}{\alpha_2} \|\nabla_h(\phi_2^{n+1} - \phi_2^n)\|_2^2 + \frac{\alpha_2}{\Delta t} \|\phi_2^{n+1} - \phi_2^n\|_{-1,h}^2 \right). \quad (4.10)$$

Subsequently, the following constant quantities are denoted:

$$\alpha_1 = \frac{1}{2\chi_{13}}, \quad \beta_2 = \frac{1}{|\chi_{12} - \chi_{13} - \chi_{23}|},$$

$$\alpha_2 = \frac{1}{2\chi_{23}}, \quad \beta_1 = \frac{1}{|\chi_{12} - \chi_{13} - \chi_{23}|},$$

and

$$A_1 = \frac{\chi_{13}}{\alpha_1} + \frac{|\chi_{12} - \chi_{13} - \chi_{23}|}{2\beta_1}, \quad A_2 = \frac{\chi_{23}}{\alpha_2} + \frac{|\chi_{12} - \chi_{13} - \chi_{23}|}{2\beta_2}.$$

A careful calculation reveals that

$$A_1 = 2\chi_{13}^2 + 0.5(\chi_{12} - \chi_{13} - \chi_{23})^2, \quad A_2 = 2\chi_{23}^2 + 0.5(\chi_{12} - \chi_{13} - \chi_{23})^2.$$

In turn, with an introduction of the following quantity

$$F_h^{n+1} := G_h(\phi_1^{n+1}, \phi_2^{n+1}) + \frac{3}{4\Delta t} \left(\|\phi_1^{n+1} - \phi_1^n\|_{-1,h}^2 + \|\phi_2^{n+1} - \phi_2^n\|_{-1,h}^2 \right) \\ + \chi_{13}\|\phi_1^{n+1} - \phi_1^n\|_2^2 + \chi_{23}\|\phi_2^{n+1} - \phi_2^n\|_2^2,$$

a substitution of (4.7)–(4.10) into (4.6) results in

$$F_h^{n+1} \leq F_h^n.$$

5. Optimal rate convergence analysis in $\mathcal{L}^\infty(0, T; H_h^{-1}) \cap \mathcal{L}^2(0, T; H_h^1)$

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

$$\Phi_1, \Phi_2 \in \mathcal{R} := H^5(0, T; C_{\text{per}}(\Omega)) \cap H^4(0, T; C_{\text{per}}^2(\Omega)) \cap L^\infty(0, T; C_{\text{per}}^6(\Omega)).$$

In addition, we assume that the following separation property is valid for the exact solution: for some δ_0 ,

$$(\Phi_1, \Phi_2) \in \mathcal{G}_{\delta_0}, \quad (5.1)$$

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 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 $\Phi_j \in L^\infty(0, T; H_{\text{per}}^\ell(\Omega))$, for some $\ell \in \mathbb{N}$,

$$\|\Phi_{j,N} - \Phi_j\|_{L^\infty(0,T;H^k)} \leq Ch^{\ell-k} \|\Phi_j\|_{L^\infty(0,T;H^\ell)}, \quad \forall 0 \leq k \leq \ell, \quad j = 1, 2. \quad (5.2)$$

By $\Phi_{j,N}^m, \Phi_j^m$ we denote $\Phi_{j,N}(\cdot, t_m)$ and $\Phi_j(\cdot, t_m)$, respectively, with $t_m = m \cdot \Delta t$, $j = 1, 2$.

Since the exact solution has regularity of class $\mathcal{R}$, the separation property (5.1) for the exact solution and the projection approximation (5.2), we are able to obtain a discrete $W^{1,\infty}$ bound and the separation property for the projection of the exact solution:

$$\|\nabla_h \Phi_{j,N}\|_\infty \leq C^*, \quad j = 1, 2, \quad (\Phi_{1,N}, \Phi_{2,N}) \in \mathcal{G}_{\delta_0}.$$

Since $\Phi_{j,N} \in B^K$, the mass conservative property is available at the discrete level:

$$\overline{\Phi_{j,N}^m} = \frac{1}{|\Omega|} \int_\Omega \Phi_{j,N}(\cdot, t_m) d\mathbf{x} = \frac{1}{|\Omega|} \int_\Omega \Phi_{j,N}(\cdot, t_{m-1}) d\mathbf{x} = \overline{\Phi_{j,N}^{m-1}}, \quad \forall m \in \mathbb{N}. \quad (5.3)$$

On the other hand, the solution of (2.4)–(2.8) is also mass conservative at the discrete level:

$$\overline{\phi_j^m} = \overline{\phi_j^{m-1}}, \quad \forall m \in \mathbb{N}, \quad j = 1, 2. \quad (5.4)$$

Defined the grid projection operator, $\mathcal{P}_h : C_{\text{per}}^0(\Omega) \rightarrow C_{\text{per}}$, by $\mathcal{P}_h f_{i,j} = f(p_i, p_j)$, for all $f \in C_{\text{per}}^0(\Omega)$. For the initial data, we have $\phi_j^0 = \mathcal{P}_h \Phi_{j,N}(\cdot, t = 0)$, that is

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

The error grid function is defined as

$$e_1^m := \mathcal{P}_h \Phi_{1,N}^m - \phi_1^m, \quad e_2^m := \mathcal{P}_h \Phi_{2,N}^m - \phi_2^m, \quad \forall m \in \{0, 1, 2, 3, \dots\}. \quad (5.5)$$

Therefore, it follows that $\overline{e_j^m} = 0$, for any $m \in \{0, 1, 2, 3, \dots\}$, $j = 1, 2$, so the discrete norm $\|\cdot\|_{-1,h}$ is well defined for the error grid functions e_1^m and e_2^m . Before proceeding into the convergence analysis, we introduce a new norm $\|\cdot\|_{-1,G}$ [32]. Let Ω be an arbitrary bounded domain and $\mathbf{p} = [u, v]^T \in [L^2(\Omega)]^2$. We define $\|\cdot\|_{-1,G}$ to be a weighted inner product

$$\|\mathbf{p}\|_{-1,G}^2 = (\mathbf{p}, G(-\Delta_h)^{-1}\mathbf{p}), \quad G = \begin{pmatrix} \frac{1}{2} & -1 \\ -1 & \frac{5}{2} \end{pmatrix}.$$

Since G is symmetric positive definite, the norm is well-defined. Moreover,

$$G = \begin{pmatrix} \frac{1}{2} & -1 \\ -1 & \frac{5}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -1 \\ -1 & 2 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} =: G_1 + G_2.$$

By the positive semi-definiteness of G_1 , we immediately have

$$\|\mathbf{p}\|_{-1,G}^2 = (\mathbf{p}, (G_1 + G_2)(-\Delta_h)^{-1}\mathbf{p}) \geq (\mathbf{p}, G_2(-\Delta_h)^{-1}\mathbf{p}) = \frac{1}{2} \|v\|_{-1,h}^2.$$

In addition, for any $v_i \in \mathcal{C}_{\text{per}}^3$, $i = 1, 2$, the following equality is valid:

$$\begin{aligned} & \left\langle \frac{3}{2} v_i^{n+1} - 2v_i^n + \frac{1}{2} v_i^{n-1}, (-\Delta_h)^{-1} v_i^{n+1} \right\rangle \\ &= \frac{1}{2} (\|\mathbf{p}_i^{n+1}\|_{-1,G}^2 - \|\mathbf{p}_i^n\|_{-1,G}^2) + \frac{\|v_i^{n+1} - 2v_i^n + v_i^{n-1}\|_{-1,h}^2}{4}, \end{aligned} \quad (5.6)$$

with $\mathbf{p}_i^{n+1} = [v_i^n, v_i^{n+1}]^T$, $\mathbf{p}_i^n = [v_i^{n-1}, v_i^n]^T$.

The optimal rate convergence result is stated in the following theorem.

Theorem 5.1. Given initial data $\Phi_j(\cdot, t = 0) \in C_{\text{per}}^6(\Omega)$ and $\Phi_j(\cdot, t = 0) \in G$, point-wise, suppose the exact solution for ternary MMC flow (1.2)–(1.4) is of regularity class R . Then, provided Δt and h are sufficiently small, and under the linear refinement requirement $C_1 h \leq \Delta t \leq C_2 h$, we have

$$\|e_j^n\|_{-1,h} + \left(\frac{\epsilon_0^2}{36} \Delta t \sum_{m=1}^n \|\nabla_h e_j^m\|_2^2 \right)^{1/2} \leq C(\Delta t^2 + h^2), \quad \epsilon_0 = \min(\epsilon_1^2, \epsilon_2^2, \epsilon_3^2), \quad j = 1, 2, \quad (5.7)$$

for all positive integers n , such that $t_n = n\Delta t \leq T$, where $n \geq 1$. $C > 0$ is independent of Δt and h .

5.1. Higher order consistency analysis

A direct substitution of the projection solution $\Phi_{j,N}$ into the numerical scheme (2.4)–(2.7) gives the second order accuracy in both time and space. However, due to the explicit part of the extra regularization term, this leading local truncation error will not be sufficient to recover an $L_{\Delta t}^\infty$ bound of the discrete temporal derivative of the numerical solution, which is needed in the nonlinear convergence analysis. This technique has been reported for a wide class of nonlinear PDEs, such as incompressible fluid flow, various gradient models, the porous medium equation based on the energetic variational approach, nonlinear wave equation, et cetera. Such a higher order consistency result and the detailed proof is stated below.

Proposition 5.1. Given the exact solution Φ_j for the ternary MMC system (1.2)–(1.4) and its Fourier projection $\Phi_{j,N}$. There exist auxiliary fields, $\check{\Phi}_{j,\Delta t}, \check{\Phi}_{j,h}$, so that the following

$$\check{\Phi}_j = \Phi_{j,N} + \mathcal{P}_N(\Delta t^2 \Phi_{j,\Delta t} + h^2 \Phi_{j,h}), \quad j = 1, 2, \quad (5.8)$$

satisfies the numerical scheme up to a higher $O(\Delta t^3 + h^4)$ consistency:

$$\begin{aligned} & \frac{3\check{\Phi}_1^{n+1} - 4\check{\Phi}_1^n + \check{\Phi}_1^{n-1}}{2\Delta t} \\ &= \mathcal{M}_1 \mathcal{A}_h \left(\frac{1}{M_0} \ln \frac{\alpha \check{\Phi}_1^{n+1}}{M_0} - \ln(1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1}) - 2\chi_{13}(2\check{\Phi}_1^n - \check{\Phi}_1^{n-1}) \right. \\ & \quad + (\chi_{12} - \chi_{13} - \chi_{23})(2\check{\Phi}_2^n - \check{\Phi}_2^{n-1}) - \frac{\epsilon_1^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h \check{\Phi}_1^{n+1}|^2}{(\mathcal{A}_h \check{\Phi}_1^{n+1})^2} \right) \\ & \quad - \frac{\epsilon_1^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \check{\Phi}_1^{n+1}}{\mathcal{A}_h \check{\Phi}_1^{n+1}} \right) + \frac{\epsilon_3^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h(1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1})|^2}{(\mathcal{A}_h(1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1}))^2} \right) \\ & \quad + \frac{\epsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h(1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1})}{\mathcal{A}_h(1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1})} \right) + A_1 \Delta t \mathcal{A}_h(\check{\Phi}_1^{n+1} - \check{\Phi}_1^n) \\ & \quad + \tau_1^{n+1}, \\ & \frac{3\check{\Phi}_2^{n+1} - 4\check{\Phi}_2^n + \check{\Phi}_2^{n-1}}{2\Delta t} \\ &= \mathcal{M}_2 \mathcal{A}_h \left(\frac{1}{N_0} \ln \frac{\beta \check{\Phi}_2^{n+1}}{N_0} - \ln(1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1}) - 2\chi_{23}(2\check{\Phi}_2^n - \check{\Phi}_2^{n-1}) \right. \end{aligned} \quad (5.9)$$

$$\begin{aligned}
& + (\chi_{12} - \chi_{13} - \chi_{23})(2\check{\Phi}_1^n - \check{\Phi}_1^{n-1}) - \frac{\varepsilon_2^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h \check{\Phi}_2^{n+1}|^2}{(\mathcal{A}_h \check{\Phi}_2^{n+1})^2} \right) \\
& - \frac{\varepsilon_2^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \check{\Phi}_2^{n+1}}{\mathcal{A}_h \check{\Phi}_2^{n+1}} \right) + \frac{\varepsilon_3^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h (1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1})|^2}{(\mathcal{A}_h (1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1}))^2} \right) \\
& + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h (1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1})}{\mathcal{A}_h (1 - \check{\Phi}_1^{n+1} - \check{\Phi}_2^{n+1})} \right) + A_2 \Delta t \Delta_h (\check{\Phi}_2^{n+1} - \check{\Phi}_2^n) \\
& + \tau_2^{n+1}.
\end{aligned} \tag{5.10}$$

with $\|\tau_1^{n+1}\|_{-1,h}, \|\tau_2^{n+1}\|_{-1,h} \leq C(\Delta t^3 + h^4)$, $n \geq 1$. The constructed functions, $\Phi_{j,\Delta t}, \Phi_{j,h}$, depend solely on the exact solution Φ_j , and their derivatives are bounded. For the initialization step, we have

$$\check{\Phi}_j^0 = \Phi_{j,N}^0, \quad \check{\Phi}_j^1 = \Phi_{j,N}^1.$$

Proof. In terms of the temporal discretization, the following local truncation error can be derived by a Taylor expansion in time, combined with the projection estimate (5.2):

$$\begin{aligned}
& \frac{3\Phi_{1,N}^{n+1} - 4\Phi_{1,N}^n + \Phi_{1,N}^{n-1}}{2\Delta t} \\
& = \mathcal{M}_1 \Delta \left(\frac{1}{M_0} \ln \frac{\alpha \Phi_{1,N}^{n+1}}{M_0} - \ln(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}) - 2\chi_{13} \hat{\Phi}_{1,N}^n \right. \\
& \quad + (\chi_{12} - \chi_{13} - \chi_{23}) \hat{\Phi}_{2,N}^n - \frac{\varepsilon_1^2}{36} \frac{|\nabla \Phi_{1,N}^{n+1}|^2}{(\Phi_{1,N}^{n+1})^2} - \frac{\varepsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{1,N}^{n+1}}{\Phi_{1,N}^{n+1}} \right) \\
& \quad + \frac{\varepsilon_3^2}{36} \left(\frac{|\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})|^2}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^2} \right) + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})} \right) \\
& \quad \left. + A_1 \Delta t \Delta(\Phi_{1,N}^{n+1} - \Phi_{1,N}^n) \right) + \Delta t^2 g_1^{(0)} + O(\Delta t^3) + O(h^m),
\end{aligned} \tag{5.11}$$

$$\begin{aligned}
& \frac{3\Phi_{2,N}^{n+1} - 4\Phi_{2,N}^n + \Phi_{2,N}^{n-1}}{2\Delta t} \\
& = \mathcal{M}_2 \Delta \left(\frac{1}{N_0} \ln \frac{\beta \Phi_{2,N}^{n+1}}{N_0} - \ln(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}) - 2\chi_{23} \hat{\Phi}_{2,N}^n \right. \\
& \quad + (\chi_{12} - \chi_{13} - \chi_{23}) \hat{\Phi}_{1,N}^n - \frac{\varepsilon_2^2}{36} \frac{|\nabla \Phi_{2,N}^{n+1}|^2}{(\Phi_{2,N}^{n+1})^2} - \frac{\varepsilon_2^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{2,N}^{n+1}}{\Phi_{2,N}^{n+1}} \right) \\
& \quad + \frac{\varepsilon_3^2}{36} \left(\frac{|\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})|^2}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^2} \right) + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})}{1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}} \right) \\
& \quad \left. + A_2 \Delta t \Delta(\Phi_{2,N}^{n+1} - \Phi_{2,N}^n) \right) + \Delta t^2 g_2^{(0)} + O(\Delta t^3) + O(h^m).
\end{aligned} \tag{5.12}$$

with the projection accuracy order $m \geq 4$. In fact, the spatial functions $g_1^{(0)}, g_2^{(0)}$ are smooth enough in the sense that their derivatives are bounded.

Subsequently, the leading order temporal correction function $\Phi_{j,\Delta t}$ turns out to be the solution of the following equations:

$$\begin{aligned}
& \partial_t \Phi_{1,\Delta t} \\
& = \mathcal{M}_1 \Delta \left(\frac{1}{M_0} \frac{\Phi_{1,\Delta t}}{\Phi_{1,N}} + \frac{\Phi_{1,\Delta t} + \Phi_{2,\Delta t}}{1 - \Phi_{1,N} - \Phi_{2,N}} - 2\chi_{13} \Phi_{1,\Delta t} + (\chi_{12} - \chi_{13} - \chi_{23}) \Phi_{2,\Delta t} \right. \\
& \quad + \frac{\varepsilon_1^2}{36} \frac{2|\nabla \Phi_{1,N}|^2 \Phi_{1,\Delta t}}{\Phi_{1,N}^3} - \frac{\varepsilon_1^2}{36} \frac{2\nabla \Phi_{1,N} \cdot \nabla \Phi_{1,\Delta t}}{\Phi_{1,N}^2} - \frac{\varepsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{1,\Delta t}}{\Phi_{1,N}} - \frac{\Phi_{1,\Delta t} \nabla \Phi_{1,N}}{\Phi_{1,N}^2} \right) \\
& \quad + \frac{\varepsilon_3^2}{36} \left(\frac{2|\nabla(1 - \Phi_{1,N} - \Phi_{2,N})|^2 (\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N})^3} \right. \\
& \quad \left. - \frac{2\nabla(1 - \Phi_{1,N} - \Phi_{2,N}) \cdot \nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} \right) \\
& \quad \left. + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{-\nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{1 - \Phi_{1,N} - \Phi_{2,N}} + \frac{(\Phi_{1,\Delta t} + \Phi_{2,\Delta t}) \nabla(1 - \Phi_{1,N} - \Phi_{2,N})}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} \right) \right) - g_1^{(0)}.
\end{aligned} \tag{5.13}$$

$$\begin{aligned}
& \partial_t \Phi_{2,\Delta t} \\
= & \mathcal{M}_2 \Delta \left(\frac{1}{N_0} \frac{\Phi_{2,\Delta t}}{\Phi_{2,N}} + \frac{\Phi_{1,\Delta t} + \Phi_{2,\Delta t}}{1 - \Phi_{1,N} - \Phi_{2,N}} - 2\chi_{23}\Phi_{2,\Delta t} + (\chi_{12} - \chi_{13} - \chi_{23})\Phi_{1,\Delta t} \right. \\
& + \frac{\varepsilon_1^2}{36} \frac{2|\nabla \Phi_{2,N}|^2 \Phi_{2,\Delta t}}{\Phi_{2,N}^3} - \frac{\varepsilon_1^2}{36} \frac{2\nabla \Phi_{2,N} \cdot \nabla \Phi_{2,\Delta t}}{\Phi_{2,N}^2} - \frac{\varepsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{2,\Delta t}}{\Phi_{2,N}} - \frac{\Phi_{2,\Delta t} \nabla \Phi_{2,N}}{\Phi_{2,N}^2} \right) \\
& + \frac{\varepsilon_3^2}{36} \left(\frac{2|\nabla(1 - \Phi_{1,N} - \Phi_{2,N})|^2 (\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N})^3} \right. \\
& \quad \left. - \frac{2\nabla(1 - \Phi_{1,N} - \Phi_{2,N}) \cdot \nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} \right) \\
& \left. + \frac{\varepsilon_2^2}{18} \nabla \cdot \left(\frac{-\nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{1 - \Phi_{1,N} - \Phi_{2,N}} + \frac{(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})\nabla(1 - \Phi_{1,N} - \Phi_{2,N})}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} \right) \right) - \mathbf{g}_2^{(0)}. \tag{5.14}
\end{aligned}$$

Initial data $\Phi_{j,\Delta t}(\cdot, t=0) \equiv 0$. In fact, existence of a solution of the above linear PDE system is straightforward. It depends only on the projection solution $\Phi_{j,N}$. And also, the derivatives of $\Phi_{j,\Delta t}$ in various orders are bounded. In turn, when $n \geq 1$, an application of the semi-implicit discretization to (5.13)–(5.14) gives

$$\begin{aligned}
& \frac{3\Phi_{1,\Delta t}^{n+1} - 4\Phi_{1,\Delta t}^n + \Phi_{1,\Delta t}^{n-1}}{2\Delta t} \\
= & \mathcal{M}_1 \Delta \left(\frac{1}{M_0} \frac{\Phi_{1,\Delta t}^{n+1}}{\Phi_{1,N}^{n+1}} + \frac{\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1}}{1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}} - 2\chi_{13}(2\Phi_{1,\Delta t}^n - \Phi_{1,\Delta t}^{n-1}) \right. \\
& + (\chi_{12} - \chi_{13} - \chi_{23})(2\Phi_{2,\Delta t}^n - \Phi_{2,\Delta t}^{n-1}) + \frac{\varepsilon_1^2}{36} \frac{2|\nabla \Phi_{1,N}^{n+1}|^2 \Phi_{1,\Delta t}^{n+1}}{(\Phi_{1,N}^{n+1})^3} - \frac{\varepsilon_1^2}{36} \frac{2\nabla \Phi_{1,N}^{n+1} \cdot \nabla \Phi_{1,\Delta t}^{n+1}}{(\Phi_{1,N}^{n+1})^2} \\
& - \frac{\varepsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{1,\Delta t}^{n+1}}{\Phi_{1,N}^{n+1}} - \frac{\Phi_{1,\Delta t}^{n+1} \nabla \Phi_{1,N}^{n+1}}{(\Phi_{1,N}^{n+1})^2} \right) + A_1 \Delta t \Delta (\Phi_{1,\Delta t}^{n+1} - \Phi_{1,\Delta t}^n) \\
& + \frac{\varepsilon_3^2}{36} \left(\frac{2|\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})|^2 (\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^3} - \frac{2\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}) \cdot \nabla(\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^2} \right) \\
& + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{-\nabla(\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})}{1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}} + \frac{(\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^2} \right) \\
& \left. - \mathbf{g}_1^{(0)} + \Delta t^2 \mathbf{h}_1^n + O(\Delta t^3), \right. \\
& \frac{3\Phi_{2,\Delta t}^{n+1} - 4\Phi_{2,\Delta t}^n + \Phi_{2,\Delta t}^{n-1}}{2\Delta t} \tag{5.15}
\end{aligned}$$

$$\begin{aligned}
& \frac{3\Phi_{2,\Delta t}^{n+1} - 4\Phi_{2,\Delta t}^n + \Phi_{2,\Delta t}^{n-1}}{2\Delta t} \\
= & \mathcal{M}_2 \Delta \left(\frac{1}{N_0} \frac{\Phi_{2,\Delta t}^{n+1}}{\Phi_{2,N}^{n+1}} + \frac{\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1}}{1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}} - 2\chi_{23}(2\Phi_{2,\Delta t}^n - \Phi_{2,\Delta t}^{n-1}) \right. \\
& + (\chi_{12} - \chi_{13} - \chi_{23})(2\Phi_{1,\Delta t}^n - \Phi_{1,\Delta t}^{n-1}) + \frac{\varepsilon_1^2}{36} \frac{2|\nabla \Phi_{2,N}^{n+1}|^2 \Phi_{2,\Delta t}^{n+1}}{(\Phi_{2,N}^{n+1})^3} - \frac{\varepsilon_1^2}{36} \frac{2\nabla \Phi_{2,N}^{n+1} \cdot \nabla \Phi_{2,\Delta t}^{n+1}}{(\Phi_{2,N}^{n+1})^2} \\
& - \frac{\varepsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{2,\Delta t}^{n+1}}{\Phi_{2,N}^{n+1}} - \frac{\Phi_{2,\Delta t}^{n+1} \nabla \Phi_{2,N}^{n+1}}{(\Phi_{2,N}^{n+1})^2} \right) + A_2 \Delta t \Delta (\Phi_{2,\Delta t}^{n+1} - \Phi_{2,\Delta t}^n) \\
& + \frac{\varepsilon_3^2}{36} \left(\frac{2|\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})|^2 (\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^3} - \frac{2\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}) \cdot \nabla(\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^2} \right) \\
& + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{-\nabla(\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})}{1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1}} + \frac{(\Phi_{1,\Delta t}^{n+1} + \Phi_{2,\Delta t}^{n+1})\nabla(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})}{(1 - \Phi_{1,N}^{n+1} - \Phi_{2,N}^{n+1})^2} \right) \\
& \left. - \mathbf{g}_2^{(0)} + \Delta t^2 \mathbf{h}_2^n + O(\Delta t^3). \right. \tag{5.16}
\end{aligned}$$

The initial data $\Phi_{j,\Delta t}^0 = \Phi_{j,\Delta t}^1 \equiv 0$. A combination of (5.11)–(5.12) and (5.15)–(5.16) results in the third order temporal truncation error for $\check{\Phi}_{j,1} = \Phi_{j,N} + \Delta t^2 \mathcal{P}_N \Phi_{j,\Delta t}$, $j = 1, 2$, when $n \geq 1$:

$$\frac{3\Phi_{1,1}^{n+1} - 4\Phi_{1,1}^n + \Phi_{1,1}^{n-1}}{2\Delta t}$$

$$\begin{aligned}
&= \mathcal{M}_1 \Delta \left(\frac{1}{M_0} \ln \frac{\alpha \check{\Phi}_{1,1}^{n+1}}{M_0} - \ln(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}) - 2\chi_{13}(2\check{\Phi}_{1,1}^n - \check{\Phi}_{1,1}^{n-1}) \right. \\
&\quad + (\chi_{12} - \chi_{13} - \chi_{23})(2\check{\Phi}_{2,1}^n - \check{\Phi}_{2,1}^{n-1}) - \frac{\varepsilon_1^2}{36} \frac{|\nabla \check{\Phi}_{1,1}^{n+1}|^2}{(\check{\Phi}_{1,1}^{n+1})^2} \\
&\quad - \frac{\varepsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \check{\Phi}_{1,1}^{n+1}}{\check{\Phi}_{1,1}^{n+1}} \right) + \frac{\varepsilon_3^2}{36} \frac{|\nabla(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})|^2}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^2} \\
&\quad + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{\nabla(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})}{1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}} \right) + A_1 \Delta t \Delta(\check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{1,1}^n) \\
&\quad + O(\Delta t^3) + O(h^m), \\
&\quad \frac{3\check{\Phi}_{2,1}^{n+1} - 4\check{\Phi}_{2,1}^n + \check{\Phi}_{2,1}^{n-1}}{2\Delta t}
\end{aligned} \tag{5.17}$$

$$\begin{aligned}
&= \mathcal{M}_2 \Delta \left(\frac{1}{N_0} \ln \frac{\beta \check{\Phi}_{2,1}^{n+1}}{N_0} - \ln(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}) - 2\chi_{23}(2\check{\Phi}_{2,1}^n - \check{\Phi}_{2,1}^{n-1}) \right. \\
&\quad + (\chi_{12} - \chi_{13} - \chi_{23})(2\check{\Phi}_{1,1}^n - \check{\Phi}_{1,1}^{n-1}) - \frac{\varepsilon_2^2}{36} \frac{|\nabla \check{\Phi}_{2,1}^{n+1}|^2}{(\check{\Phi}_{2,1}^{n+1})^2} \\
&\quad - \frac{\varepsilon_2^2}{18} \nabla \cdot \left(\frac{\nabla \check{\Phi}_{2,1}^{n+1}}{\check{\Phi}_{2,1}^{n+1}} \right) + \frac{\varepsilon_3^2}{36} \frac{|\nabla(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})|^2}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^2} \\
&\quad + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{\nabla(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})}{1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}} \right) + A_2 \Delta t \Delta(\check{\Phi}_{2,1}^{n+1} - \check{\Phi}_{2,1}^n) \\
&\quad + O(\Delta t^3) + O(h^m),
\end{aligned} \tag{5.18}$$

in which the initial data is $\check{\Phi}_{j,1}^0 = \Phi_{j,N}^0$, $\check{\Phi}_{j,1}^1 = \Phi_{j,N}^1$. In the derivation of (5.17)–(5.18), the following linearized expansions have been utilized

$$\begin{aligned}
\ln \check{\Phi}_{j,1} &= \ln(\Phi_{j,N} + \Delta t^2 \Phi_{j,\Delta t}) = \ln \Phi_{j,N} + \frac{\Delta t^2 \Phi_{j,\Delta t}}{\Phi_{j,N}} + O(\Delta t^4), \quad j = 1, 2, \\
\ln(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}) &= \ln(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t^2 \Phi_{1,\Delta t} - \Delta t^2 \Phi_{2,\Delta t}) \\
&= \ln(1 - \Phi_{1,N} - \Phi_{2,N}) - \Delta t^2 \frac{\Phi_{1,\Delta t} + \Phi_{2,\Delta t}}{1 - \Phi_{1,N} - \Phi_{2,N}} + O(\Delta t^4), \\
\frac{|\nabla \check{\Phi}_{j,1}|^2}{\check{\Phi}_{j,1}^2} &= \frac{|\nabla(\Phi_{j,N} + \Delta t^2 \Phi_{j,\Delta t})|^2}{(\Phi_{j,N} + \Delta t^2 \Phi_{j,\Delta t})^2} \\
&= \frac{|\nabla \Phi_{j,N}|^2}{\Phi_{j,N}^2} - 2\Delta t^2 \frac{|\nabla \Phi_{j,N}|^2 \Phi_{j,\Delta t}}{\Phi_{j,N}^3} + 2\Delta t^2 \frac{\nabla \Phi_{j,N} \cdot \nabla \Phi_{j,\Delta t}}{\Phi_{j,N}^2} + O(\Delta t^4), \quad j = 1, 2, \\
\frac{\nabla \check{\Phi}_{j,1}}{\check{\Phi}_{j,1}} &= \frac{\nabla(\Phi_{j,N} + \Delta t^2 \Phi_{j,\Delta t})}{\Phi_{j,N} + \Delta t^2 \Phi_{j,\Delta t}} = \frac{\nabla \Phi_{j,N}}{\Phi_{j,N}} + \Delta t^2 \frac{\nabla \Phi_{j,\Delta t}}{\Phi_{j,N}} - \Delta t^2 \frac{\Phi_{j,\Delta t} \nabla \Phi_{j,N}}{\Phi_{j,N}^2} + O(\Delta t^4), \\
\frac{|\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})|^2}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^2} &= \frac{|\nabla(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t^2 \Phi_{1,\Delta t} - \Delta t^2 \Phi_{2,\Delta t})|^2}{(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t^2 \Phi_{1,\Delta t} - \Delta t^2 \Phi_{2,\Delta t})^2} \\
&= \frac{|\nabla(1 - \Phi_{1,N} - \Phi_{2,N})|^2}{(1 - \Phi_{1,N} - \Phi_{2,N})^2} - \Delta t^2 \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^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} + O(\Delta t^4), \\
\frac{\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})} &= \frac{\nabla(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t^2 \Phi_{1,\Delta t} - \Delta t^2 \Phi_{2,\Delta t})}{(1 - \Phi_{1,N} - \Phi_{2,N} - \Delta t^2 \Phi_{1,\Delta t} - \Delta t^2 \Phi_{2,\Delta t})} \\
&= \frac{\nabla(1 - \Phi_{1,N} - \Phi_{2,N})}{1 - \Phi_{1,N} - \Phi_{2,N}} - \Delta t^2 \frac{\nabla(\Phi_{1,\Delta t} + \Phi_{2,\Delta t})}{1 - \Phi_{1,N} - \Phi_{2,N}} \\
&\quad + \Delta t^2 \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^4).
\end{aligned}$$

For the sake of representation, the operator $\mathcal{P}_N$ is omitted from the above formulas.

In terms of spatial discretization, we construct the spatial correction term $\Phi_{j,h}$ to improve the spatial accuracy order when $n \geq 1$. The following truncation error estimate for the spatial discretization is available, by using a straightforward Taylor expansion for the constructed profile $\check{\Phi}^{n+1}_{1,1}$:

$$\begin{aligned} & \frac{3\check{\Phi}^{n+1}_{1,1} - 4\check{\Phi}^n_{1,1} + \check{\Phi}^{n-1}_{1,1}}{2\Delta t} \\ &= \mathcal{M}_1 \Delta_h \left(\frac{1}{M_0} \ln \frac{\alpha \check{\Phi}^{n+1}_{1,1}}{M_0} - \ln(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1}) - 2\chi_{13}(2\check{\Phi}^n_{1,1} - \check{\Phi}^{n-1}_{1,1}) \right. \\ & \quad + (\chi_{12} - \chi_{13} - \chi_{23})(2\check{\Phi}^n_{2,1} - \check{\Phi}^{n-1}_{2,1}) - \frac{\epsilon_1^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h \check{\Phi}^{n+1}_{1,1}|^2}{(\mathcal{A}_h \check{\Phi}^{n+1}_{1,1})^2} \right) \\ & \quad - \frac{\epsilon_1^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \check{\Phi}^{n+1}_{1,1}}{\mathcal{A}_h \check{\Phi}^{n+1}_{1,1}} \right) + \frac{\epsilon_3^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1})|^2}{(\mathcal{A}_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1}))^2} \right) \\ & \quad + \frac{\epsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1})}{\mathcal{A}_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1})} \right) + A_1 \Delta t \Delta_h (\check{\Phi}^{n+1}_{1,1} - \check{\Phi}^n_{1,1}) \\ & \quad \left. + h^2 H_1^{(0)} + O(\Delta t^3 + h^4), \right. \end{aligned} \quad (5.19)$$

$$\begin{aligned} & \frac{3\check{\Phi}^{n+1}_{2,1} - 4\check{\Phi}^n_{2,1} + \check{\Phi}^{n-1}_{2,1}}{2\Delta t} \\ &= \mathcal{M}_2 \Delta_h \left(\frac{1}{N_0} \ln \frac{\beta \check{\Phi}^{n+1}_{2,1}}{N_0} - \ln(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1}) - 2\chi_{23}(2\check{\Phi}^n_{2,1} - \check{\Phi}^{n-1}_{2,1}) \right. \\ & \quad + (\chi_{12} - \chi_{13} - \chi_{23})(2\check{\Phi}^n_{1,1} - \check{\Phi}^{n-1}_{1,1}) - \frac{\epsilon_2^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h \check{\Phi}^{n+1}_{2,1}|^2}{(\mathcal{A}_h \check{\Phi}^{n+1}_{2,1})^2} \right) \\ & \quad - \frac{\epsilon_2^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \check{\Phi}^{n+1}_{2,1}}{\mathcal{A}_h \check{\Phi}^{n+1}_{2,1}} \right) + \frac{\epsilon_3^2}{36} \mathcal{A}_h \left(\frac{|\nabla_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1})|^2}{(\mathcal{A}_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1}))^2} \right) \\ & \quad + \frac{\epsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1})}{\mathcal{A}_h(1 - \check{\Phi}^{n+1}_{1,1} - \check{\Phi}^{n+1}_{2,1})} \right) + A_2 \Delta t \Delta_h (\check{\Phi}^{n+1}_{2,1} - \check{\Phi}^n_{2,1}) \\ & \quad \left. + h^2 H_2^{(0)} + O(\Delta t^3 + h^4). \right. \end{aligned} \quad (5.20)$$

Similarly, the spatially discrete functions $H_j^{(0)}$ are smooth enough in the sense that their derivatives are bounded. Because of the symmetry in the centered finite difference approximation, there is no $O(h^3)$ truncation error term. In turn, the spatial correction function $\Phi_{j,h}$ is determined by solving the following linear PDE system:

$$\begin{aligned} & \partial_t \Phi_{1,h} \\ &= \mathcal{M}_1 \Delta \left(\frac{1}{M_0} \frac{\Phi_{1,h}}{\check{\Phi}_{1,1}} + \frac{\Phi_{1,h} + \Phi_{2,h}}{1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}} - 2\chi_{13} \Phi_{1,h} + (\chi_{12} - \chi_{13} - \chi_{23}) \Phi_{2,h} \right. \\ & \quad + \frac{\epsilon_1^2}{36} \frac{2|\nabla \check{\Phi}_{1,1}|^2 \Phi_{1,h}}{\check{\Phi}_{1,1}^3} - \frac{\epsilon_1^2}{36} \frac{2\nabla \check{\Phi}_{1,1} \cdot \nabla \Phi_{1,h}}{\check{\Phi}_{1,1}^2} - \frac{\epsilon_1^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{1,h}}{\check{\Phi}_{1,1}} - \frac{\Phi_{1,h} \nabla \check{\Phi}_{1,1}}{\check{\Phi}_{1,1}^2} \right) \\ & \quad + \frac{\epsilon_3^2}{36} \left(\frac{2|\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})|^2 (\Phi_{1,h} + \Phi_{2,h})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^3} \right. \\ & \quad \left. - \frac{2\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}) \cdot \nabla (\Phi_{1,h} + \Phi_{2,h})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^2} \right) \\ & \quad \left. + \frac{\epsilon_3^2}{18} \nabla \cdot \left(\frac{-\nabla (\Phi_{1,h} + \Phi_{2,h})}{1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}} + \frac{(\Phi_{1,h} + \Phi_{2,h}) \nabla (1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^2} \right) \right) - H_1^{(0)}. \end{aligned} \quad (5.21)$$

$$\begin{aligned} & \partial_t \Phi_{2,h} \\ &= \mathcal{M}_2 \Delta \left(\frac{1}{N_0} \frac{\Phi_{2,h}}{\check{\Phi}_{2,1}} + \frac{\Phi_{1,h} + \Phi_{2,h}}{1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}} - 2\chi_{23} \Phi_{2,h} + (\chi_{12} - \chi_{13} - \chi_{23}) \Phi_{1,h} \right. \\ & \quad + \frac{\epsilon_2^2}{36} \frac{2|\nabla \check{\Phi}_{2,1}|^2 \Phi_{2,h}}{\check{\Phi}_{2,1}^3} - \frac{\epsilon_2^2}{36} \frac{2\nabla \check{\Phi}_{2,1} \cdot \nabla \Phi_{2,h}}{\check{\Phi}_{2,1}^2} - \frac{\epsilon_2^2}{18} \nabla \cdot \left(\frac{\nabla \Phi_{2,h}}{\check{\Phi}_{2,1}} - \frac{\Phi_{2,h} \nabla \check{\Phi}_{2,1}}{\check{\Phi}_{2,1}^2} \right) \end{aligned}$$

$$\begin{aligned}
& + \frac{\varepsilon_3^2}{36} \left(\frac{2|\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})|^2 (\Phi_{1,h} + \Phi_{2,h})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^3} \right. \\
& \quad \left. - \frac{2\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}) \cdot \nabla(\Phi_{1,h} + \Phi_{2,h})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^2} \right) \\
& + \frac{\varepsilon_3^2}{18} \nabla \cdot \left(\frac{-\nabla(\Phi_{1,h} + \Phi_{2,h})}{1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1}} + \frac{(\Phi_{1,h} + \Phi_{2,h})\nabla(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})}{(1 - \check{\Phi}_{1,1} - \check{\Phi}_{2,1})^2} \right) - H_2^{(0)}, \tag{5.22}
\end{aligned}$$

in which the initial data $\Phi_{j,h}(\cdot, t = 0) = 0$. Again, the solution depends only on the exact solution Φ_j , with the divided differences of various orders stay bounded. In turn an application of a full discretization to (5.21)–(5.22) leads to

$$\begin{aligned}
& \frac{3\Phi_{1,h}^{n+1} - 4\Phi_{1,h}^n + \Phi_{1,h}^{n-1}}{2\Delta t} \\
= & \mathcal{M}_1 \Delta_h \left(\frac{1}{M_0} \frac{\Phi_{1,h}^{n+1}}{\check{\Phi}_{1,1}^{n+1}} + \frac{\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1}}{1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}} - 2\chi_{13}(2\Phi_{1,h}^n - \Phi_{1,h}^{n-1}) \right. \\
& + (\chi_{12} - \chi_{13} - \chi_{23})(2\Phi_{2,h}^n - \Phi_{2,h}^{n-1}) + \frac{\varepsilon_1^2}{36} \frac{2|\nabla_h \check{\Phi}_{1,1}^{n+1}|^2 \Phi_{1,h}^{n+1}}{(\check{\Phi}_{1,1}^{n+1})^3} \\
& - \frac{\varepsilon_1^2}{36} \frac{2\nabla_h \check{\Phi}_{1,1}^{n+1} \cdot \nabla_h \Phi_{1,h}^{n+1}}{(\check{\Phi}_{1,1}^{n+1})^2} - \frac{\varepsilon_1^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \Phi_{1,h}^{n+1}}{\check{\Phi}_{1,1}^{n+1}} - \frac{\Phi_{1,h}^{n+1} \nabla_h \check{\Phi}_{1,1}^{n+1}}{(\check{\Phi}_{1,1}^{n+1})^2} \right) \\
& + \frac{\varepsilon_3^2}{36} \frac{2|\nabla_h(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})|^2 (\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^3} + A_1 \Delta t \Delta_h (\Phi_{1,h}^{n+1} - \Phi_{1,h}^n) \\
& - \frac{\varepsilon_3^2}{36} \frac{2\nabla_h(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}) \cdot \nabla_h (\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^2} \\
& + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{-\nabla_h (\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})}{1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}} + \frac{(\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})\nabla_h(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^2} \right) \\
& \left. - H_1^{(0)} + O(\Delta t^2 + h^2), \right. \tag{5.23}
\end{aligned}$$

$$\begin{aligned}
& \frac{3\Phi_{2,h}^{n+1} - 4\Phi_{2,h}^n + \Phi_{2,h}^{n-1}}{2\Delta t} \\
= & \mathcal{M}_2 \Delta_h \left(\frac{1}{N_0} \frac{\Phi_{2,h}^{n+1}}{\check{\Phi}_{2,1}^{n+1}} + \frac{\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1}}{1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}} - 2\chi_{23}(2\Phi_{2,h}^n - \Phi_{2,h}^{n-1}) \right. \\
& + (\chi_{12} - \chi_{13} - \chi_{23})(2\Phi_{1,h}^n - \Phi_{1,h}^{n-1}) + \frac{\varepsilon_1^2}{36} \frac{2|\nabla_h \check{\Phi}_{2,1}^{n+1}|^2 \Phi_{2,h}^{n+1}}{(\check{\Phi}_{2,1}^{n+1})^3} \\
& - \frac{\varepsilon_1^2}{36} \frac{2\nabla_h \check{\Phi}_{2,1}^{n+1} \cdot \nabla_h \Phi_{2,h}^{n+1}}{(\check{\Phi}_{2,1}^{n+1})^2} - \frac{\varepsilon_1^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \Phi_{2,h}^{n+1}}{\check{\Phi}_{2,1}^{n+1}} - \frac{\Phi_{2,h}^{n+1} \nabla_h \check{\Phi}_{2,1}^{n+1}}{(\check{\Phi}_{2,1}^{n+1})^2} \right) \\
& + \frac{\varepsilon_3^2}{36} \frac{2|\nabla_h(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})|^2 (\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^3} + A_2 \Delta t \Delta_h (\Phi_{2,h}^{n+1} - \Phi_{2,h}^n) \\
& - \frac{\varepsilon_3^2}{36} \frac{2\nabla_h(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}) \cdot \nabla_h (\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^2} \\
& + \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{-\nabla_h (\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})}{1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1}} + \frac{(\Phi_{1,h}^{n+1} + \Phi_{2,h}^{n+1})\nabla_h(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})}{(1 - \check{\Phi}_{1,1}^{n+1} - \check{\Phi}_{2,1}^{n+1})^2} \right) \\
& \left. - H_2^{(0)} + O(\Delta t^2 + h^2), \right. \tag{5.24}
\end{aligned}$$

in which $\Phi_{j,h}^0 = \Phi_{j,h}^1 = 0$. Finally, a combination of (5.19)–(5.20) and (5.23)–(5.24) yields the higher order spatial truncation error for $\check{\Phi}_j$, as given by (5.9)–(5.10). Of course, the linear expansions have been extensively utilized. $\square$

Remark 5.1. Trivial initial data $\Phi_{j,\Delta t}(\cdot, t = 0) = \Phi_{j,h}(\cdot, t = 0) \equiv 0$ are given to $\Phi_{j,\Delta t}, \Phi_{j,h}$ as (5.13)–(5.14) and (5.21)–(5.22). Therefore, using similar arguments as in (5.3)–(5.4), we conclude that

$$\begin{aligned}
\phi_j^0 & \equiv \check{\Phi}_{j,N}^0, \quad \bar{\phi}_j^k = \bar{\phi}_j^0, \quad \forall k \geq 0, \\
\bar{\check{\Phi}}_{j,N}^k & = \bar{\phi}_j^0, \quad \forall k \geq 0,
\end{aligned}$$

$$\overline{\tau_1^{n+1}} = \overline{\tau_2^{n+1}} = 0, \quad \forall n \geq 0, \quad j = 1, 2.$$

Remark 5.2. Since the correction function $\Phi_{j,\Delta t}, \Phi_{j,h}$ is bounded, we recall the separation property (5.1) for the exact solution, and obtain a similar property for the constructed profile $\check{\Phi}_{j,N}$:

$$\check{\Phi}_{1,N} \geq \delta_0, \quad \check{\Phi}_{2,N} \geq \delta_0, \quad 1 - \check{\Phi}_{1,N} - \check{\Phi}_{2,N} \geq \delta_0, \quad \exists \delta_0 > 0, \quad (5.25)$$

in which the projection estimate (5.2) has been repeatedly used. Such a uniform bound will be used in the convergence analysis.

In addition, since the correction function $\Phi_{j,\Delta t}, \Phi_{j,h}$ 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 $\check{\Phi}_{j,N}$:

$$\|\nabla_h \check{\Phi}_{j,N}\|_\infty \leq C^*, \quad j = 1, 2. \quad (5.26)$$

5.2. A rough error estimate

Instead of a direct analysis for the error function defined in (5.5), we introduce an alternate numerical error function:

$$\check{\phi}_1^m := P_h \check{\Phi}_{1,N}^m - \phi_1^m, \quad \check{\phi}_2^m := P_h \check{\Phi}_{2,N}^m - \phi_2^m, \quad \forall m \in \{0, 1, 2, 3, \dots\}. \quad (5.27)$$

The advantage of such a numerical error function is associated with its higher order accuracy, which comes from the higher order consistency estimate (5.9)–(5.10). Again, since $\check{\phi}_1^m = \check{\phi}_2^m = 0$. Obviously, we have

$$e_j^0 = \check{\phi}_j^0, \quad e_j^1 = \check{\phi}_j^1, \quad j = 1, 2. \quad (5.28)$$

When $n \geq 1$, a careful consistent analysis indicates the following truncation error estimate:

$$\frac{3\check{\phi}_1^{n+1} - 4\check{\phi}_1^n + \check{\phi}_1^{n-1}}{2\Delta t} = \mathcal{M}_1 \Delta_h \check{\mu}_1^{n+1} + \tau_1^{n+1}, \quad (5.29)$$

$$\frac{3\check{\phi}_2^{n+1} - 4\check{\phi}_2^n + \check{\phi}_2^{n-1}}{2\Delta t} = \mathcal{M}_2 \Delta_h \check{\mu}_2^{n+1} + \tau_2^{n+1}, \quad (5.30)$$

with $\|\tau_i^{n+1}\|_{-1,h} \leq C(\Delta t^3 + h^4)$, and

$$\begin{aligned} \check{\mu}_1^{n+1} = & \frac{1}{M_0} (\ln \check{\Phi}_{1,N}^{n+1} - \ln \phi_1^{n+1}) - \left(\ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1}) \right) \\ & - 2\chi_{13} \check{\phi}_1^n + (\chi_{12} - \chi_{13} - \chi_{23}) \check{\phi}_2^n + \check{\mu}_{1,s}^{n+1} + \check{\mu}_{3,s}^{n+1} - A_1 \Delta t \Delta_h (\check{\phi}_1^{n+1} - \check{\phi}_1^n), \end{aligned} \quad (5.31)$$

$$\begin{aligned} \check{\mu}_2^{n+1} = & \frac{1}{N_0} (\ln \check{\Phi}_{2,N}^{n+1} - \ln \phi_2^{n+1}) - \left(\ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1}) \right) \\ & - 2\chi_{23} \check{\phi}_2^n + (\chi_{12} - \chi_{13} - \chi_{23}) \check{\phi}_1^n + \check{\mu}_{2,s}^{n+1} + \check{\mu}_{3,s}^{n+1} - A_2 \Delta t \Delta_h (\check{\phi}_2^{n+1} - \check{\phi}_2^n), \end{aligned} \quad (5.32)$$

$$\begin{aligned} \check{\mu}_{1,s}^{n+1} = & \frac{\varepsilon_1^2}{36} \mathcal{A}_h \left(\gamma^{(1)} \mathcal{A}_h \check{\phi}_1^{n+1} - \frac{\nabla_h (\check{\Phi}_{1,N}^{n+1} + \phi_1^{n+1}) \cdot \nabla_h \check{\phi}_1^{n+1}}{(\mathcal{A}_h \check{\Phi}_{1,N}^{n+1})^2} \right) \\ & - \frac{\varepsilon_1^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \check{\phi}_1^{n+1}}{\mathcal{A}_h \phi_1^{n+1}} - \frac{\check{\phi}_1^{n+1} \nabla_h \check{\Phi}_{1,N}^{n+1}}{\mathcal{A}_h \check{\Phi}_{1,N}^{n+1} \mathcal{A}_h \check{\Phi}_{1,N}^{n+1}} \right), \end{aligned} \quad (5.33)$$

$$\begin{aligned} \check{\mu}_{2,s}^{n+1} = & \frac{\varepsilon_2^2}{36} \mathcal{A}_h \left(\gamma^{(2)} \mathcal{A}_h \check{\phi}_2^{n+1} - \frac{\nabla_h (\check{\Phi}_{2,N}^{n+1} + \phi_2^{n+1}) \cdot \nabla_h \check{\phi}_2^{n+1}}{(\mathcal{A}_h \check{\Phi}_{2,N}^{n+1})^2} \right) \\ & - \frac{\varepsilon_2^2}{18} \nabla_h \cdot \left(\frac{\nabla_h \check{\phi}_2^{n+1}}{\mathcal{A}_h \phi_2^{n+1}} - \frac{\check{\phi}_2^{n+1} \nabla_h \check{\Phi}_{2,N}^{n+1}}{\mathcal{A}_h \check{\Phi}_{2,N}^{n+1} \mathcal{A}_h \check{\Phi}_{2,N}^{n+1}} \right), \\ \check{\mu}_{3,s}^{n+1} = & \frac{\varepsilon_3^2}{36} \mathcal{A}_h \left(\gamma^{(3)} \mathcal{A}_h (\check{\phi}_1^{n+1} + \check{\phi}_2^{n+1}) \right) - \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{\nabla_h (\check{\phi}_1^{n+1} + \check{\phi}_2^{n+1})}{\mathcal{A}_h (1 - \phi_1^{n+1} - \phi_2^{n+1})} \right) \\ & - \frac{\varepsilon_3^2}{36} \mathcal{A}_h \left(\frac{\nabla_h (2 - \phi_1^{n+1} - \phi_2^{n+1} - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) \cdot \nabla_h (\check{\phi}_1^{n+1} + \check{\phi}_2^{n+1})}{(\mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}))^2} \right) \\ & - \frac{\varepsilon_3^2}{18} \nabla_h \cdot \left(\frac{(\check{\phi}_1^{n+1} + \check{\phi}_2^{n+1}) \nabla_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})}{\mathcal{A}_h (1 - \phi_1^{n+1} - \phi_2^{n+1}) \mathcal{A}_h (1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1})} \right), \end{aligned}$$

$$\begin{aligned}
\gamma^{(1)} &= \frac{\mathcal{A}_h(\phi_1^{n+1} + \check{\phi}_{1,N}^{n+1})|\nabla_h \phi_1^{n+1}|^2}{(\mathcal{A}_h \phi_1^{n+1})^2 (\mathcal{A}_h \check{\phi}_{1,N}^{n+1})^2}, \\
\gamma^{(2)} &= \frac{\mathcal{A}_h(\phi_2^{n+1} + \check{\phi}_{2,N}^{n+1})|\nabla_h \phi_2^{n+1}|^2}{(\mathcal{A}_h \phi_2^{n+1})^2 (\mathcal{A}_h \check{\phi}_{2,N}^{n+1})^2}, \\
\gamma^{(3)} &= \frac{\mathcal{A}_h(2 - \phi_1^{n+1} - \phi_2^{n+1} - \check{\phi}_{1,N}^{n+1} - \check{\phi}_{2,N}^{n+1})|\nabla_h(1 - \phi_1^{n+1} - \phi_2^{n+1})|^2}{(\mathcal{A}_h(1 - \phi_1^{n+1} - \phi_2^{n+1}))^2 (\mathcal{A}_h(1 - \check{\phi}_{1,N}^{n+1} - \check{\phi}_{2,N}^{n+1}))^2}.
\end{aligned} \tag{5.34}$$

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

$$\|\tilde{\phi}_j^k\|_2 \leq \Delta t^{\frac{7}{4}} + h^{\frac{7}{4}}, \quad k = n-1, n, \quad j = 1, 2. \tag{5.35}$$

Then, based on the fact that $\|f\|_{-1,h} \leq C\|f\|_2$, we have

$$\|\tilde{\phi}_j^k\|_{-1,h} \leq C(\Delta t^{\frac{7}{4}} + h^{\frac{7}{4}}), \quad \|\nabla_h \tilde{\phi}_j^k\|_2 \leq C \frac{\|\tilde{\phi}_j^k\|_2}{h} \leq C(\Delta t^{\frac{3}{4}} + h^{\frac{3}{4}}), \quad k = n-1, n. \tag{5.36}$$

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

$$\|\tilde{\phi}_j^n\|_2^2 = \|2\tilde{\phi}_j^n - \tilde{\phi}_j^{n-1}\|_2^2 \leq 6\|\tilde{\phi}_j^n\|_2^2 + 3\|\tilde{\phi}_j^{n-1}\|_2^2 \leq 9C(\Delta t^{\frac{7}{2}} + h^{\frac{7}{2}}), \quad j = 1, 2.$$

Taking a discrete inner product with (5.29), (5.30) by $\tilde{\mu}_1^{n+1}$, $\tilde{\mu}_2^{n+1}$, respectively, leads to

$$\begin{aligned}
&3\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + 3\langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle + 2\Delta t(\mathcal{M}_1 \|\nabla_h \tilde{\mu}_1^{n+1}\|_2^2 + \mathcal{M}_2 \|\nabla_h \tilde{\mu}_2^{n+1}\|_2^2) \\
&= \langle 4\tilde{\phi}_1^n - \tilde{\phi}_1^{n-1}, \tilde{\mu}_1^{n+1} \rangle + \langle 4\tilde{\phi}_2^n - \tilde{\phi}_2^{n-1}, \tilde{\mu}_2^{n+1} \rangle + 2\Delta t(\langle \tau_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tau_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle).
\end{aligned} \tag{5.37}$$

For the two terms $\langle 4\tilde{\phi}_1^n - \tilde{\phi}_1^{n-1}, \tilde{\mu}_1^{n+1} \rangle$ and $\langle 4\tilde{\phi}_2^n - \tilde{\phi}_2^{n-1}, \tilde{\mu}_2^{n+1} \rangle$ of the right hand side of (5.37), an application of the Cauchy inequality reveals that

$$\langle \tilde{\phi}_j^n, \tilde{\mu}_j^{n+1} \rangle \leq \|\tilde{\phi}_j^n\|_{-1,h} \cdot \|\nabla_h \tilde{\mu}_j^{n+1}\|_2 \leq \frac{2}{\mathcal{M}_j \Delta t} \|\tilde{\phi}_j^n\|_{-1,h}^2 + \frac{\mathcal{M}_j}{8} \Delta t \|\nabla_h \tilde{\mu}_j^{n+1}\|_2^2, \quad j = 1, 2,$$

$$|\langle \tilde{\phi}_j^{n-1}, \tilde{\mu}_j^{n+1} \rangle| \leq \|\tilde{\phi}_j^{n-1}\|_{-1,h} \cdot \|\nabla_h \tilde{\mu}_j^{n+1}\|_2 \leq \frac{1}{2\mathcal{M}_j \Delta t} \|\tilde{\phi}_j^{n-1}\|_{-1,h}^2 + \frac{\mathcal{M}_j}{2} \Delta t \|\nabla_h \tilde{\mu}_j^{n+1}\|_2^2,$$

that means

$$\langle 4\tilde{\phi}_j^n - \tilde{\phi}_j^{n-1}, \tilde{\mu}_j^{n+1} \rangle \leq \left(\frac{8}{\mathcal{M}_j \Delta t} \|\tilde{\phi}_j^n\|_{-1,h}^2 + \frac{1}{2\mathcal{M}_j \Delta t} \|\tilde{\phi}_j^{n-1}\|_{-1,h}^2 \right) + \mathcal{M}_j \Delta t \|\nabla_h \tilde{\mu}_j^{n+1}\|_2^2.$$

For the local truncation error terms, the following estimate is available:

$$\langle \tau_j^{n+1}, \tilde{\mu}_j^{n+1} \rangle \leq \|\tau_j^{n+1}\|_{-1,h} \cdot \|\nabla_h \tilde{\mu}_j^{n+1}\|_2 \leq \frac{1}{2\mathcal{M}_j} \|\tau_j^{n+1}\|_{-1,h}^2 + \frac{\mathcal{M}_j}{2} \|\nabla_h \tilde{\mu}_j^{n+1}\|_2^2.$$

Going back (5.37), we get

$$\begin{aligned}
3\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + 3\langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle &\leq \frac{8}{\mathcal{M}_* \Delta t} (\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) \\
&+ \frac{1}{2\mathcal{M}_* \Delta t} (\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n-1}\|_{-1,h}^2) \\
&+ \frac{\Delta t}{\mathcal{M}_*} (\|\tau_1^{n+1}\|_{-1,h}^2 + \|\tau_2^{n+1}\|_{-1,h}^2),
\end{aligned} \tag{5.38}$$

which $\mathcal{M}_* = \min(\mathcal{M}_1, \mathcal{M}_2)$. On the other hand, the detailed expansions in (5.31)–(5.32) reveal the following identity:

$$\begin{aligned}
&\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle \\
&= \frac{1}{M_0} \langle (\ln \check{\phi}_{1,N}^{n+1} - \ln \phi_1^{n+1}), \tilde{\phi}_1^{n+1} \rangle + \frac{1}{N_0} \langle (\ln \check{\phi}_{2,N}^{n+1} - \ln \phi_2^{n+1}), \tilde{\phi}_2^{n+1} \rangle \\
&\quad - \langle (\ln(1 - \check{\phi}_{1,N}^{n+1} - \check{\phi}_{2,N}^{n+1}) - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1})), \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle \\
&\quad - 2\chi_{13} \langle \tilde{\phi}_1^n, \tilde{\phi}_1^{n+1} \rangle - 2\chi_{23} \langle \tilde{\phi}_2^n, \tilde{\phi}_2^{n+1} \rangle + (\chi_{12} - \chi_{13} - \chi_{23}) \langle \tilde{\phi}_2^n, \tilde{\phi}_1^{n+1} \rangle + \langle \tilde{\phi}_1^n, \tilde{\phi}_2^{n+1} \rangle \\
&\quad + A_1 \Delta t \langle \nabla_h(\tilde{\phi}_1^{n+1} - \tilde{\phi}_1^n), \nabla_h \tilde{\phi}_1^{n+1} \rangle + A_2 \Delta t \langle \nabla_h(\tilde{\phi}_2^{n+1} - \tilde{\phi}_2^n), \nabla_h \tilde{\phi}_2^{n+1} \rangle \\
&\quad + \langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1} \rangle + \langle \tilde{\mu}_{2,s}^{n+1}, \tilde{\phi}_2^{n+1} \rangle + \langle \tilde{\mu}_{3,s}^{n+1}, \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle.
\end{aligned} \tag{5.39}$$

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

$$\langle (\ln \check{\Phi}_{1,N}^{n+1} - \ln \phi_1^{n+1}), \tilde{\phi}_1^{n+1} \rangle \geq \|\tilde{\phi}_1^{n+1}\|_2^2. \quad (5.40)$$

Using similar arguments, we also obtain

$$\langle (\ln \check{\Phi}_{2,N}^{n+1} - \ln \phi_2^{n+1}), \tilde{\phi}_2^{n+1} \rangle \geq \|\tilde{\phi}_2^{n+1}\|_2^2, \quad (5.41)$$

$$-\langle (\ln(1 - \check{\Phi}_{1,N}^{n+1} - \check{\Phi}_{2,N}^{n+1}) - \ln(1 - \phi_1^{n+1} - \phi_2^{n+1})), \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle \geq \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_2^2. \quad (5.42)$$

Moreover, since the discrete surface energy functional presented in (2.2) is convex, we conclude that

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

For the artificial term, we have

$$2\langle \nabla_h(\tilde{\phi}_i^{n+1} - \tilde{\phi}_i^n), \nabla_h \tilde{\phi}_i^{n+1} \rangle = \|\nabla_h \tilde{\phi}_i^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_i^n\|_2^2 + \|\nabla_h(\tilde{\phi}_i^{n+1} - \tilde{\phi}_i^n)\|_2^2.$$

Going back (5.39), we arrive at

$$\begin{aligned} & \langle \tilde{\phi}_1^{n+1}, \check{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \check{\mu}_2^{n+1} \rangle \\ & \geq \frac{1}{M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 + \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_2^2 - 4\chi_{13}^2 M_0 \|\tilde{\phi}_1^n\|_2^2 - \frac{1}{4M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 \\ & \quad - 4\chi_{23}^2 N_0 \|\tilde{\phi}_2^n\|_2^2 - \frac{1}{4N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 - \frac{1}{4M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 - \frac{1}{4N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 \\ & \quad - (\chi_{12} - \chi_{13} - \chi_{23})^2 (M_0 \|\tilde{\phi}_2^n\|_2^2 + N_0 \|\tilde{\phi}_1^n\|_2^2) \\ & \quad + \frac{A_1 \Delta t}{2} \left(\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_1^n\|_2^2 \right) + \frac{A_2 \Delta t}{2} \left(\|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_2^n\|_2^2 \right) \\ & \geq \frac{1}{2M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{2N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 - (4\chi_{13}^2 M_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 N_0) \|\tilde{\phi}_1^n\|_2^2 \\ & \quad - (4\chi_{23}^2 N_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 M_0) \|\tilde{\phi}_2^n\|_2^2 \\ & \quad + \frac{A_1 \Delta t}{2} \left(\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_1^n\|_2^2 \right) + \frac{A_2 \Delta t}{2} \left(\|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_2^n\|_2^2 \right). \end{aligned}$$

In turn, its substitution into (5.38) yields

$$\begin{aligned} & \frac{1}{2M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{2N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 + \frac{A_1 \Delta t}{2} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \frac{A_2 \Delta t}{2} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 \\ & \leq (4\chi_{13}^2 M_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 N_0) \|\tilde{\phi}_1^n\|_2^2 + (4\chi_{23}^2 N_0 + (\chi_{12} - \chi_{13} - \chi_{23})^2 M_0) \|\tilde{\phi}_2^n\|_2^2 \\ & \quad + \frac{8}{3\mathcal{M}_* \Delta t} (\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) + \frac{1}{6\mathcal{M}_* \Delta t} (\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n-1}\|_{-1,h}^2) \\ & \quad + \frac{\Delta t}{3\mathcal{M}_*} (\|\tau_1^{n+1}\|_{-1,h}^2 + \|\tau_2^{n+1}\|_{-1,h}^2) + \frac{A_1 \Delta t}{2} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \frac{A_2 \Delta t}{2} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2. \end{aligned}$$

Furthermore, a substitution of the a-priori error bound (5.35) and (5.36) at the previous time step results in a rough error estimate for $\tilde{\phi}_1^{n+1}, \tilde{\phi}_2^{n+1}$:

$$\|\tilde{\phi}_1^{n+1}\|_2 + \|\tilde{\phi}_2^{n+1}\|_2 \leq \hat{C}(\Delta t^{\frac{5}{4}} + h^{\frac{5}{4}}), \quad (5.43)$$

under the linear refinement requirement $C_1 h \leq \Delta t \leq C_2 h$, with $\hat{C}$ dependent on $M_0, N_0, \chi_{12}, \chi_{13}, \chi_{23}, A_1$ and A_2 . Subsequently, an application of 2-D inverse inequality implies that

$$\|\tilde{\phi}_1^{n+1}\|_\infty + \|\tilde{\phi}_2^{n+1}\|_\infty \leq \frac{C(\|\tilde{\phi}_1^{n+1}\|_2 + \|\tilde{\phi}_2^{n+1}\|_2)}{h} \leq \hat{C}_1(\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}), \quad \text{with } \hat{C}_1 = C\hat{C}, \quad (5.44)$$

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

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

Its combination with the separation property (5.25) leads to a similar property for the numerical solution:

$$\phi_1^{n+1} \geq \frac{\delta_0}{2}, \quad \phi_2^{n+1} \geq \frac{\delta_0}{2}, \quad 1 - \phi_1^{n+1} - \phi_2^{n+1} \geq \frac{\delta_0}{2}, \quad \text{for } \delta_0 > 0. \quad (5.45)$$

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

Remark 5.3. In the rough error estimate (5.43), we see that the accuracy order is lower than the one given by the a-priori assumption (5.35). 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.

5.3. The refined error estimate

Taking a discrete inner product with (5.29), (5.30) by $\frac{2\Delta t}{\mathcal{M}_1}(-\Delta_h)^{-1}\tilde{\phi}_1^{n+1}$, $\frac{2\Delta t}{\mathcal{M}_2}(-\Delta_h)^{-1}\tilde{\phi}_2^{n+1}$, respectively, leads to

$$\begin{aligned} & \frac{1}{\mathcal{M}_1} \langle 3\tilde{\phi}_1^{n+1} - 4\tilde{\phi}_1^n + \tilde{\phi}_1^{n-1}, \tilde{\phi}_1^{n+1} \rangle_{-1,h} + \frac{1}{\mathcal{M}_2} \langle 3\tilde{\phi}_2^{n+1} - 4\tilde{\phi}_2^n + \tilde{\phi}_2^{n-1}, \tilde{\phi}_2^{n+1} \rangle_{-1,h} \\ & + 2\Delta t (\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle) \\ & = \frac{2\Delta t}{\mathcal{M}_1} \langle \tau_1^{n+1}, \tilde{\phi}_1^{n+1} \rangle_{-1,h} + \frac{2\Delta t}{\mathcal{M}_2} \langle \tau_2^{n+1}, \tilde{\phi}_2^{n+1} \rangle_{-1,h}, \end{aligned} \quad (5.46)$$

with the summation by parts formula applied. The following identities are available for the temporal approximation terms using (5.6):

$$\begin{aligned} & \frac{1}{\mathcal{M}_j} \langle 3\tilde{\phi}_j^{n+1} - 4\tilde{\phi}_j^n + \tilde{\phi}_j^{n-1}, \tilde{\phi}_j^{n+1} \rangle_{-1,h} \\ & = \frac{1}{\mathcal{M}_j} (\|\mathbf{p}_j^{n+1}\|_{-1,h}^2 - \|\mathbf{p}_j^n\|_{-1,h}^2) + \frac{\|\tilde{\phi}_j^{n+1} - 2\tilde{\phi}_j^n + \tilde{\phi}_j^{n-1}\|_{-1,h}^2}{2\mathcal{M}_j}, \end{aligned} \quad (5.47)$$

where $\mathbf{p}_j^{n+1} = [\tilde{\phi}_j^n, \tilde{\phi}_j^{n+1}]^T$.

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

$$\frac{2\Delta t}{\mathcal{M}_j} \langle \tau_j^{n+1}, \tilde{\phi}_j^{n+1} \rangle_{-1,h} \leq \frac{\Delta t}{\mathcal{M}_j} (\|\tau_j^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_j^{n+1}\|_{-1,h}^2), \quad j = 1, 2. \quad (5.48)$$

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 (5.39), as well as the inequalities (5.40)–(5.42), are still valid. For the inner product associated with the concave terms, a standard Cauchy inequality is applied:

$$\begin{aligned} & -2\chi_{13} \langle \tilde{\phi}_1^n, \tilde{\phi}_1^{n+1} \rangle \geq -2\chi_{13} \|\tilde{\phi}_1^n\|_{-1,h} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\ & \geq -\frac{144\chi_{13}^2}{\varepsilon_0^2} \|\tilde{\phi}_1^n\|_{-1,h}^2 - \frac{\varepsilon_0^2}{144} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 \\ & \geq -\frac{144\chi_{13}^2}{\varepsilon_0^2} \left(6\|\tilde{\phi}_1^n\|_{-1,h}^2 + 3\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 \right) - \frac{\varepsilon_0^2}{144} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2, \end{aligned} \quad (5.49)$$

$$\begin{aligned} & -2\chi_{23} \langle \tilde{\phi}_2^n, \tilde{\phi}_2^{n+1} \rangle \geq -2\chi_{23} \|\tilde{\phi}_2^n\|_{-1,h} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2 \\ & \geq -\frac{144\chi_{23}^2}{\varepsilon_0^2} \|\tilde{\phi}_2^n\|_{-1,h}^2 - \frac{\varepsilon_0^2}{144} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 \\ & \geq -\frac{144\chi_{23}^2}{\varepsilon_0^2} \left(6\|\tilde{\phi}_2^n\|_{-1,h}^2 + 3\|\tilde{\phi}_2^{n-1}\|_{-1,h}^2 \right) - \frac{\varepsilon_0^2}{144} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2, \end{aligned} \quad (5.50)$$

$$\begin{aligned} & (\chi_{12} - \chi_{13} - \chi_{23}) \langle \tilde{\phi}_2^n, \tilde{\phi}_1^{n+1} \rangle + \langle \tilde{\phi}_1^n, \tilde{\phi}_2^{n+1} \rangle \\ & \geq -\frac{36(\chi_{12} - \chi_{13} - \chi_{23})^2}{\varepsilon_0^2} (\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) - \frac{\varepsilon_0^2}{144} (\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2) \\ & \geq -\frac{36(\chi_{12} - \chi_{13} - \chi_{23})^2}{\varepsilon_0^2} \left(6(\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) + 3(\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n-1}\|_{-1,h}^2) \right) \\ & \quad - \frac{\varepsilon_0^2}{144} (\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2). \end{aligned} \quad (5.51)$$

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 (5.39). 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 (5.33):

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

It is clear that I_1 stays non-negative:

$$I_1 = \frac{\varepsilon_1^2}{36} \langle \gamma^{(1)} \mathcal{A}_h \tilde{\phi}_1^{n+1}, \mathcal{A}_h \tilde{\phi}_1^{n+1} \rangle \geq 0, \quad (5.52)$$

in which the summation by parts formula is applied in the first step, while the fact that $\gamma^{(1)} \geq 0$ (given by (5.34)) is used in the second step. Similarly, for the third part I_3 , an application of summation by parts formula reveals that

$$I_3 = \frac{\varepsilon_1^2}{18} \left[\frac{\nabla_h \tilde{\phi}_1^{n+1}}{\mathcal{A}_h \phi_1^{n+1}}, \nabla_h \tilde{\phi}_1^{n+1} \right] \geq \frac{\varepsilon_1^2}{18} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2, \quad (5.53)$$

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

$$\begin{aligned} -I_4 &= \frac{\varepsilon_1^2}{18} \left[\frac{\tilde{\phi}_1^{n+1} \nabla_h \check{\phi}_{1,N}^{n+1}}{\mathcal{A}_h \phi_1^{n+1} \mathcal{A}_h \check{\phi}_{1,N}^{n+1}}, \nabla_h \tilde{\phi}_1^{n+1} \right] \\ &\leq \frac{\varepsilon_1^2}{18} \left\| \frac{1}{\mathcal{A}_h \phi_1^{n+1}} \right\|_\infty \cdot \left\| \frac{1}{\mathcal{A}_h \check{\phi}_{1,N}^{n+1}} \right\|_\infty \cdot \|\nabla_h \check{\phi}_{1,N}^{n+1}\|_\infty \cdot \|\tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\ &\leq \frac{C^* \varepsilon_1^2}{18} \cdot 2(\delta_0)^{-2} \|\tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\ &\leq \frac{C^* \varepsilon_1^2 (\delta_0)^{-2}}{9} \|\tilde{\phi}_1^{n+1}\|_{-1,h}^{\frac{1}{2}} \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^{\frac{3}{2}} \\ &\leq C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{\varepsilon_1^2}{72} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \end{aligned} \quad (5.54)$$

In more details, the preliminary estimate (5.26) has been applied in the third step, combined the separation properties (5.45); the Sobolev interpolation formula, $\|\tilde{\phi}_1^{n+1}\|_2 \leq \|\tilde{\phi}_1^{n+1}\|_{-1,h}^{\frac{1}{2}} \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^{\frac{1}{2}}$, 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:

$$-I_2 = \frac{\varepsilon_1^2}{36} \left[\frac{\nabla_h (\check{\phi}_{1,N}^{n+1} + \phi_1^{n+1}) \cdot \nabla_h \tilde{\phi}_1^{n+1}}{(\mathcal{A}_h \check{\phi}_{1,N}^{n+1})^2}, \mathcal{A}_h \tilde{\phi}_1^{n+1} \right]. \quad (5.55)$$

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

$$\begin{aligned} -I_2 &= -I_{2,1} - I_{2,2}, \quad \text{with } -I_{2,1} := \frac{\varepsilon_1^2}{18} \left[\frac{\nabla_h \check{\phi}_{1,N}^{n+1} \cdot \nabla_h \tilde{\phi}_1^{n+1}}{(\mathcal{A}_h \check{\phi}_{1,N}^{n+1})^2}, \mathcal{A}_h \tilde{\phi}_1^{n+1} \right], \\ -I_{2,2} &:= -\frac{\varepsilon_1^2}{36} \left[\frac{|\nabla_h \tilde{\phi}_1^{n+1}|^2}{(\mathcal{A}_h \check{\phi}_{1,N}^{n+1})^2}, \mathcal{A}_h \tilde{\phi}_1^{n+1} \right]. \end{aligned}$$

The bound for $-I_{2,1}$ could be obtained in a similar style as (5.54):

$$\begin{aligned} -I_{2,1} &\leq \frac{\varepsilon_1^2}{18} \left\| \frac{1}{\mathcal{A}_h \check{\phi}_{1,N}^{n+1}} \right\|_\infty^2 \cdot \|\nabla_h \check{\phi}_{1,N}^{n+1}\|_\infty \cdot \|\mathcal{A}_h \tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\ &\leq \frac{C^* \varepsilon_1^2}{18} \cdot (\delta_0)^{-2} \|\mathcal{A}_h \tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \leq \frac{C^* \varepsilon_1^2}{18} \cdot (\delta_0)^{-2} \|\tilde{\phi}_1^{n+1}\|_2 \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2 \\ &\leq \frac{C^* \varepsilon_1^2 (\delta_0)^{-2}}{18} \|\tilde{\phi}_1^{n+1}\|_{-1,h}^{\frac{1}{2}} \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^{\frac{3}{2}} \\ &\leq C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{\varepsilon_1^2}{144} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \end{aligned} \quad (5.56)$$

For the other part $-I_{2,2}$, we recall the $\|\cdot\|_\infty$ rough estimate (5.44) and the separation inequality (5.26), and arrive at

$$\begin{aligned} -I_{2,2} &\leq \frac{\varepsilon_1^2}{36} \left\| \frac{1}{\mathcal{A}_h \check{\phi}_{1,N}^{n+1}} \right\|_\infty^2 \cdot \|\mathcal{A}_h \tilde{\phi}_1^{n+1}\|_\infty \cdot \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 \\ &\leq \frac{\varepsilon_1^2}{36} \cdot (\delta_0)^{-2} \cdot \hat{C}_1 (\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}) \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \end{aligned} \quad (5.57)$$

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

$$\frac{\hat{C}_1 (\delta_0)^{-2}}{36} (\Delta t^{\frac{1}{4}} + h^{\frac{1}{4}}) \leq \frac{1}{144}, \quad (5.58)$$

we obtain a useful bound

$$-I_{2,2} \leq \frac{\varepsilon_1^2}{144} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \quad (5.59)$$

A substitution of (5.56)–(5.59) into (5.55) leads to

$$-I_2 \leq C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{\varepsilon_1^2}{72} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2. \quad (5.60)$$

Finally, a combination of (5.52)–(5.54) and (5.60) results in

$$\langle \tilde{\mu}_{1,s}^{n+1}, \tilde{\phi}_1^{n+1} \rangle \geq \frac{\varepsilon_1^2}{36} \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 - 2C(C^*)^4 (\delta_0)^{-8} \varepsilon_1^2 \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2. \quad (5.61)$$

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.

$$\begin{aligned} & \langle \tilde{\mu}_{2,s}^{n+1}, \tilde{\phi}_2^{n+1} \rangle \\ & \geq \frac{\varepsilon_2^2}{36} \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 - 2C(C^*)^4 (\delta_0)^{-8} \varepsilon_2^2 \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2, \end{aligned} \quad (5.62)$$

$$\begin{aligned} & \langle \tilde{\mu}_{3,s}^{n+1}, \tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1} \rangle \\ & \geq \frac{\varepsilon_3^2}{36} \|\nabla_h (\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})\|_2^2 - 2C(C^*)^4 (\delta_0)^{-8} \varepsilon_3^2 \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_{-1,h}^2 \\ & \geq \frac{\varepsilon_3^2}{36} \|\nabla_h (\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1})\|_2^2 \\ & \quad - 4C(C^*)^4 (\delta_0)^{-8} \varepsilon_3^2 (\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2). \end{aligned} \quad (5.63)$$

A substitution of (5.40)–(5.42), (5.49)–(5.51), (5.61)–(5.63) into (5.39) results in

$$\begin{aligned} & \langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle \\ & \geq \frac{\varepsilon_0^2}{72} (\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2) - 4C(C^*)^4 (\delta_0)^{-8} (\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2) (\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2) \\ & \quad - \frac{144}{\varepsilon_0^2} (\chi_{13}^2 + \chi_{23}^2 + \frac{1}{4} (\chi_{12} - \chi_{13} - \chi_{23})^2) \left[6(\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) \right. \\ & \quad \left. + 3(\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n-1}\|_{-1,h}^2) \right] \\ & \quad + \frac{1}{M_0} \|\tilde{\phi}_1^{n+1}\|_2^2 + \frac{1}{N_0} \|\tilde{\phi}_2^{n+1}\|_2^2 + \|\tilde{\phi}_1^{n+1} + \tilde{\phi}_2^{n+1}\|_2^2 \\ & \quad + \frac{A_1 \Delta t}{2} \left(\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_1^n\|_2^2 \right) + \frac{A_2 \Delta t}{2} \left(\|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 - \|\nabla_h \tilde{\phi}_2^n\|_2^2 \right). \end{aligned} \quad (5.64)$$

A combination of (5.46)–(5.48) and (5.64) gives

$$\begin{aligned} & \left(\frac{1}{\mathcal{M}_1} \|\mathbf{p}_1^{n+1}\|_{-1,G}^2 + \frac{1}{\mathcal{M}_2} \|\mathbf{p}_2^{n+1}\|_{-1,G}^2 \right) - \left(\frac{1}{\mathcal{M}_1} \|\mathbf{p}_1^n\|_{-1,G}^2 + \frac{1}{\mathcal{M}_2} \|\mathbf{p}_2^n\|_{-1,G}^2 \right) \\ & + \frac{\varepsilon_0^2}{36} \Delta t (\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2) + \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 \right) \\ & - \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^n\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^n\|_2^2 \right) \\ & \leq \kappa^{(1)} \Delta t \left[6(\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) + 3(\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n-1}\|_{-1,h}^2) \right] \\ & \quad + \kappa^{(2)} \Delta t (\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2) + \Delta t \left(\frac{1}{\mathcal{M}_1} \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \frac{1}{\mathcal{M}_2} \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2 \right) \\ & \quad + \Delta t \left(\frac{1}{\mathcal{M}_1} \|\tau_1^{n+1}\|_{-1,h}^2 + \frac{1}{\mathcal{M}_2} \|\tau_2^{n+1}\|_{-1,h}^2 \right), \end{aligned} \quad (5.65)$$

with

$$\begin{aligned} \kappa^{(1)} &= \frac{288}{\varepsilon_0^2} (\chi_{13}^2 + \chi_{23}^2 + \frac{1}{4} (\chi_{12} - \chi_{13} - \chi_{23})^2), \\ \kappa^{(2)} &= 8C(C^*)^4 (\delta_0)^{-8} (\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2). \end{aligned}$$

In other words, we have

$$\begin{aligned} & \left(\frac{1}{\mathcal{M}_1} \|\mathbf{p}_1^{n+1}\|_{-1,G}^2 + \frac{1}{\mathcal{M}_2} \|\mathbf{p}_2^{n+1}\|_{-1,G}^2 \right) - \left(\frac{1}{\mathcal{M}_1} \|\mathbf{p}_1^n\|_{-1,G}^2 + \frac{1}{\mathcal{M}_2} \|\mathbf{p}_2^n\|_{-1,G}^2 \right) \\ & + \frac{\varepsilon_0^2}{36} \Delta t (\|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2) + \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 \right) \\ & - \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^n\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^n\|_2^2 \right) \\ & \leq \kappa^{(1)} \Delta t \left[6(\|\tilde{\phi}_1^n\|_{-1,h}^2 + \|\tilde{\phi}_2^n\|_{-1,h}^2) + 3(\|\tilde{\phi}_1^{n-1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n-1}\|_{-1,h}^2) \right] \end{aligned}$$

$$\begin{aligned}
& + \left(\kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \right) \Delta t (\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2) \\
& + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \Delta t \left(\|\tau_1^{n+1}\|_{-1,h}^2 + \|\tau_2^{n+1}\|_{-1,h}^2 \right).
\end{aligned} \tag{5.66}$$

Now we observe that $\|\mathbf{p}_i^1\|_{-1,G}^2 = \frac{5}{2} \|\tilde{\phi}_i^1\|_{-1,h}^2$, $\|\tilde{\phi}_i^0\|_{-1,h}^2 = 0$.

Summing both sides of (5.66) with respect to n gives

$$\begin{aligned}
& \left(\frac{1}{\mathcal{M}_1} \|\mathbf{p}_1^{n+1}\|_{-1,G}^2 + \frac{1}{\mathcal{M}_2} \|\mathbf{p}_2^{n+1}\|_{-1,G}^2 \right) + \frac{\varepsilon_0^2}{36} \Delta t \sum_{k=1}^n (\|\nabla_h \tilde{\phi}_1^{k+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{k+1}\|_2^2) \\
& + \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^{n+1}\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^{n+1}\|_2^2 \right) \\
& \leq \left(\kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \right) \Delta t (\|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 + \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2) \\
& + \frac{5}{2} \left(\frac{1}{\mathcal{M}_1} \|\tilde{\phi}_1^1\|_{-1,h}^2 + \frac{1}{\mathcal{M}_2} \|\tilde{\phi}_2^1\|_{-1,h}^2 \right) \\
& + \left(9\kappa^{(1)} + \kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \right) \Delta t \sum_{k=1}^n (\|\tilde{\phi}_1^k\|_{-1,h}^2 + \|\tilde{\phi}_2^k\|_{-1,h}^2) \\
& + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \Delta t \sum_{k=1}^n (\|\tau_1^{k+1}\|_{-1,h}^2 + \|\tau_2^{k+1}\|_{-1,h}^2) \\
& + \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^1\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^1\|_2^2 \right).
\end{aligned}$$

We observe $\|\mathbf{p}_i^{n+1}\|_{-1,G}^2 \geq \frac{1}{2} \|\tilde{\phi}_i^{n+1}\|_{-1,h}^2$. This means that

$$\begin{aligned}
& \left(\frac{1}{2\mathcal{M}_1} - \left(\kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \right) \Delta t \right) \|\tilde{\phi}_1^{n+1}\|_{-1,h}^2 \\
& + \left(\frac{1}{2\mathcal{M}_2} - \left(\kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \right) \Delta t \right) \|\tilde{\phi}_2^{n+1}\|_{-1,h}^2 \\
& + \frac{\varepsilon_0^2}{36} \Delta t \sum_{k=1}^n (\|\nabla_h \tilde{\phi}_1^{k+1}\|_2^2 + \|\nabla_h \tilde{\phi}_2^{k+1}\|_2^2) \\
& \leq \left(9\kappa^{(1)} + \kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \right) \Delta t \sum_{k=1}^n (\|\tilde{\phi}_1^k\|_{-1,h}^2 + \|\tilde{\phi}_2^k\|_{-1,h}^2) \\
& + \frac{5}{2} \left(\frac{1}{\mathcal{M}_1} \|\tilde{\phi}_1^1\|_{-1,h}^2 + \frac{1}{\mathcal{M}_2} \|\tilde{\phi}_2^1\|_{-1,h}^2 \right) + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2} \Delta t \sum_{k=1}^n (\|\tau_1^{k+1}\|_{-1,h}^2 + \|\tau_2^{k+1}\|_{-1,h}^2) \\
& + \left(A_1 \Delta t^2 \|\nabla_h \tilde{\phi}_1^1\|_2^2 + A_2 \Delta t^2 \|\nabla_h \tilde{\phi}_2^1\|_2^2 \right).
\end{aligned} \tag{5.67}$$

We need to analyze the error at the first time step separately, since the local truncation error is only second-order in time. Notice that $e_j^0 = 0$, by carefully calculation, we have the following error equation for the initial level:

$$e_1^1 = \Delta t \mathcal{M}_1 \Delta_h \tilde{\mu}_1^1 + \Delta t \tau_1^1, \tag{5.68}$$

$$\tilde{\mu}_1^1 = \frac{1}{2} \left(\delta_{\phi_1} G_{h,c}(\Phi_{1,N}^1, \Phi_{2,N}^1) - \delta_{\phi_1} G_{h,c}(\phi_1^1, \phi_2^1) \right) \tag{5.69}$$

$$e_2^1 = \Delta t \mathcal{M}_2 \Delta_h \tilde{\mu}_2^1 + \Delta t \tau_2^1, \tag{5.70}$$

$$\tilde{\mu}_2^1 = \frac{1}{2} \left(\delta_{\phi_2} G_{h,c}(\Phi_{1,N}^1, \Phi_{2,N}^1) - \delta_{\phi_2} G_{h,c}(\phi_1^1, \phi_2^1) \right), \tag{5.71}$$

where $\tau_j^1 \leq C(\Delta t^2 + h^2)$. Since $e_j^0 = 0$, we can omit the terms about the initial step $t = t_0$ in expressions above based on the intermediate value theorem. Taking the inner product with the error equation (5.68), (5.70) by $(-\Delta_h)^{-1} e_1^1$, $(-\Delta_h)^{-1} e_2^1$, respectively, and using summation-by-parts, we have

$$\begin{aligned}
& \frac{1}{\mathcal{M}_1} \|e_1^1\|_{-1,h}^2 + \frac{1}{\mathcal{M}_2} \|e_2^1\|_{-1,h}^2 + \Delta t (\langle e_1^1, \tilde{\mu}_1^1 \rangle + \langle e_2^1, \tilde{\mu}_2^1 \rangle) \\
& = \frac{\Delta t}{\mathcal{M}_1} \langle \tau_1^1, e_1^1 \rangle_{-1,h} + \frac{\Delta t}{\mathcal{M}_2} \langle \tau_2^1, e_2^1 \rangle_{-1,h}.
\end{aligned} \tag{5.72}$$

For the right side of (5.72), using the Cauchy-Schwartz inequality, we have

$$\begin{aligned}
& \frac{\Delta t}{\mathcal{M}_1} \langle \tau_1^1, e_1^1 \rangle_{-1,h} + \frac{\Delta t}{\mathcal{M}_2} \langle \tau_2^1, e_2^1 \rangle_{-1,h} \\
& \leq \frac{\Delta t^2}{2\mathcal{M}_1} \|\tau_1^1\|_{-1,h}^2 + \frac{\Delta t^2}{2\mathcal{M}_2} \|\tau_2^1\|_{-1,h}^2 + \frac{1}{2\mathcal{M}_1} \|e_1^1\|_{-1,h}^2 + \frac{1}{2\mathcal{M}_2} \|e_2^1\|_{-1,h}^2.
\end{aligned} \tag{5.73}$$

For the third term of the left hand side of (5.72), similar to $\langle \tilde{\phi}_1^{n+1}, \tilde{\mu}_1^{n+1} \rangle + \langle \tilde{\phi}_2^{n+1}, \tilde{\mu}_2^{n+1} \rangle$, we have

$$\begin{aligned} & \langle e_1^1, \tilde{\mu}_1^1 \rangle + \langle e_2^1, \tilde{\mu}_2^1 \rangle \\ & \geq \frac{\varepsilon_0^2}{144} (\|\nabla_h e_1^1\|_2^2 + \|\nabla_h e_2^1\|_2^2) - 2C(C^*)^4(\delta_0)^{-8}(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2)(\|e_1^1\|_{-1,h}^2 + \|e_2^1\|_{-1,h}^2). \end{aligned} \quad (5.74)$$

Combining (5.72)–(5.74) and (5.28), when the initial time step $\Delta t < \frac{(\delta_0)^8}{4\mathcal{M}_0 C(C^*)^4(\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2)}$, we have the following estimate

$$\|\tilde{\phi}_j^1\|_{-1,h}^2 + \frac{\varepsilon_0^2 \Delta t}{36} \|\nabla_h \tilde{\phi}_j^1\|_2^2 \leq \frac{C\Delta t^2}{2} (\|\tau_1^1\|_{-1,h}^2 + \|\tau_2^1\|_{-1,h}^2) \leq \hat{C}_2(\Delta t^3 + h^3)^2, \quad (5.75)$$

in which we have used the linear refinement $C_1 h \leq \Delta t \leq C_2 h$ in the second step.

Combining (5.75), taking $(\kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2}) \Delta t < \frac{1}{2\mathcal{M}_1}$, and $(\kappa^{(2)} + \frac{\mathcal{M}_1 + \mathcal{M}_2}{\mathcal{M}_1 \mathcal{M}_2}) \Delta t < \frac{1}{2\mathcal{M}_2}$ in (5.67), we get the following estimate by using the discrete Gronwall inequality

$$\|\tilde{\phi}_j^{n+1}\|_{-1,h} + \left(\frac{\varepsilon_0^2 \Delta t}{36} \sum_{k=1}^n \|\nabla_h \tilde{\phi}_j^{k+1}\|_2^2 \right)^{1/2} \leq \hat{C}_3(\Delta t^3 + h^3). \quad (5.76)$$

based on the truncation error accuracy $\|\tau_1^{n+1}\|_{-1,h}, \|\tau_2^{n+1}\|_{-1,h} \leq C(\Delta t^3 + h^4)$. This completes the refined error estimate.

Recovery of the a-priori assumption (5.35)

With the error estimate (5.76) at hand, we notice that the a-priori assumption in (5.35) is satisfied at the next time step t^{n+1} : we observe that the $L^2_{\Delta t}(0, T; H_h^1)$ error estimate in (5.67) implies that

$$\|\nabla_h \tilde{\phi}_j^{n+1}\|_2 \leq \frac{CC_3(\Delta t^3 + h^3)}{\Delta t^{\frac{1}{2}}} \leq CC_3(\Delta t^{\frac{5}{2}} + h^{\frac{5}{2}}),$$

in which we have used the linear refinement $C_1 h \leq \Delta t \leq C_2 h$ 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

$$\|\tilde{\phi}_j^{n+1}\|_2 \leq C\|\nabla_h \tilde{\phi}_j^{n+1}\|_2 \leq C^2 \hat{C}_3(\Delta t^{\frac{5}{2}} + h^{\frac{5}{2}}) \leq \Delta t^{\frac{7}{4}} + h^{\frac{7}{4}}, \quad j = 1, 2, \quad (5.77)$$

provided that Δt and h are sufficiently small. This completes the proof of Theorem 5.1.

Remark 5.4. The positivity-preserving and energy stability analyses, as stated in Theorems 3.1 and 4.1, are unconditional, and there is no requirement for the time step size in terms of the spatial mesh size. Meanwhile, in the statement of the convergence analysis and error estimate in Theorem 5.1, a linear refinement condition is required for the time step size, namely $C_1 h \leq \Delta t \leq C_2 h$, for certain technical reasons. In fact, this requirement is not the standard CFL condition, although it takes a similar form. In more details, such a linear refinement condition does not come from the stability requirement of the numerical scheme; instead, this condition comes from repeated applications of inverse inequality, as revealed in the rough error estimates (5.36), (5.43), etc. A careful calculation implies that, a combination of $\Delta t \leq C_2 h$ and $\Delta t \geq C_1 h$ enables us to derive the desired $\|\cdot\|_{\infty}$ rough error estimate (5.44), so that the phase separation property (5.45) becomes available for the numerical solution at the next time step, which will play an essential role in the refined error estimate.

Meanwhile, such a linear refinement condition (for the time step size) could be improved with the help of an even higher order consistency analysis via asymptotic expansion. In Section 5.1, we have performed an $O(\Delta t^3 + h^4)$ consistency estimate, and this consistency order is able to ensure the desired $\|\cdot\|_{\infty}$ rough error estimate (5.44), under the linear refinement condition. Instead, if we perform an $O(\Delta t^4 + h^4)$ consistency estimate, with the help of higher order asymptotic expansion, the desired $\|\cdot\|_{\infty}$ rough error estimate (5.44) could be derived with an improved time step constraint: $C_1 h^{\frac{3}{2}} \leq \Delta t \leq C_2 h^{\frac{3}{2}}$, and the a-priori assumption (5.35) could be rewritten as $\|\tilde{\phi}_j^k\|_2 \leq \Delta t^3 + h^3$, $k = n-1, n$, $j = 1, 2$. Of course, this constraint is much milder than the linear refinement requirement, and the time step size could be taken in the scale from $O(h^{\frac{3}{2}})$ to $O(h^{\frac{2}{3}})$.

In fact, under the assumption that the exact solution is sufficiently smooth, with higher and higher order consistency estimate via asymptotic expansion, such a time step constraint could be even improved to $C_1 h^{\beta_0} \leq \Delta t \leq C_2 h^{\alpha_0}$, for any $\beta_0 > 1$ and $0 < \alpha_0 < 1$. With a smaller value of scaling power index α_0 and a larger value of β_0 , there is more freedom in the choice of the time step size Δt . The technical details are skipped for the sake of brevity. In fact, the corresponding constraint for the time step size is only a technical issue in the theoretical justification of the convergence analysis.

Remark 5.5. The convergence estimate (5.7) (stated in Theorem 5.1) gives a second order convergence rate for the phase variables, in the $\ell^\infty(0, T; H_h^{-1})$ norm. Meanwhile, based on the higher order consistency estimate via the asymptotic expansion approach, we are able to derive the second order $\ell^\infty(0, T; \ell^2)$ convergence estimate. In particular, the higher order refined error estimate (5.76) leads to an ℓ^2 error estimate (5.77), with convergence order $O(\Delta t^{\frac{5}{2}} + h^{\frac{5}{2}})$. On the other hand, by the asymptotic expansion (5.8) for the constructed profile $\tilde{\phi}_j$, combined with the definition (5.27) for the higher order error functions, we immediately conclude that

$$\begin{aligned} \|e_j^{n+1}\|_2 &= \|\tilde{\phi}_j^{n+1} - \mathcal{P}_N(\Delta t^2 \Phi_{j,\Delta t} + h^2 \Phi_{j,h})\|_2 \\ &\leq \|\tilde{\phi}_j^{n+1}\|_2 + \Delta t^2 \|\mathcal{P}_N \Phi_{j,\Delta t}\|_2 + h^2 \|\mathcal{P}_N \Phi_{j,h}\|_2 \\ &\leq C^2 \hat{C}_2(\Delta t^{\frac{5}{2}} + h^{\frac{5}{2}}) + C(\Delta t^2 + h^2) \leq C(\Delta t^2 + h^2). \end{aligned} \quad (5.78)$$

Table 6.1

Errors and convergence rates. The ℓ^2 error, ℓ^∞ error and convergence rate for ϕ_1 and ϕ_2 when $T = 0.4$. The initial data are defined in (6.1). The refinement path is $\Delta t = 0.002$ h.

Grid sizes	$16^2 - 32^2$	$32^2 - 64^2$	$64^2 - 128^2$
ℓ^2 -error- ϕ_1	2.7223×10^{-2}	7.0546×10^{-3}	1.8240×10^{-3}
Rate	—	1.95	1.95
ℓ^2 -error- ϕ_2	2.6907×10^{-2}	6.8618×10^{-3}	1.7182×10^{-3}
Rate	—	1.97	2.00
ℓ^∞ -error- ϕ_1	8.2277×10^{-4}	2.1980×10^{-4}	5.7373×10^{-5}
Rate	—	1.90	1.94
ℓ^∞ -error- ϕ_2	8.1155×10^{-4}	2.1248×10^{-4}	5.4786×10^{-5}
Rate	—	1.93	1.96

As a result, a discrete L^2 error estimate has been theoretically established, with the second order accuracy in both time and space.

Of course, such a second order L^2 convergence estimate is under the linear refinement constraint condition, $C_1 h \leq \Delta t \leq C_2 h$. Under a milder constraint, $C_1 h^{\beta_0} \leq \Delta t \leq C_2 h^{\alpha_0}$, with $\beta_0 > 1$, $0 < \alpha_0 < 1$, a similar second order L^2 error estimate could be derived in a similar manner; the technical details are skipped for simplicity of presentation.

6. Numerical results

In this section, we present several numerical experiments using the proposed scheme. The nonlinear Full Approximation Scheme (FAS) multigrid method is used for solving the semi-implicit numerical scheme (2.4)–(2.7). The details are similar to earlier works [23,28,29,32–35], etc. We take the domain $\Omega = [0, 64]^2$, fixed space resolution $N = 256$ and choose the parameters in the model as $M_0 = 0.16$, $N_0 = 5.12$, $\chi_{12} = 4$, $\chi_{13} = 10$, $\chi_{23} = 1.6$ and $\mathcal{M}_1 = \mathcal{M}_2 = 1.0$. In addition, we set the artificial parameters as $A_1 = 1.25\chi_{13}^2 + 0.25(\chi_{12} - \chi_{13} - \chi_{23})^2$ and $A_2 = 2\chi_{23}^2 + 2(\chi_{12} - \chi_{13} - \chi_{23})^2$.

Example 6.1. The initial data is set as

$$\begin{aligned}\phi_1^0(x, y) &= 0.1 + 0.01 \cos(3\pi x/32) \cos(3\pi y/32), \\ \phi_2^0(x, y) &= 0.5 + 0.01 \cos(3\pi x/32) \cos(3\pi y/32).\end{aligned}\quad (6.1)$$

This example is designed to study the numerical accuracy in time. We use a linear refinement path, i.e., $\Delta t = Ch$. At the final time $T = 0.4$, we expect the global error to be $\mathcal{O}(\Delta t^2) + \mathcal{O}(h^2) = \mathcal{O}(h^2)$ under either the ℓ^2 or ℓ^∞ norm, as $h, \Delta t \rightarrow 0$. Since we do not have an exact solution, instead of calculating the error at the final time, we compute the Cauchy difference, which is defined as $\delta_\phi := \phi_{h_f} - I_c^f(\phi_{h_c})$, where I_c^f is a bilinear interpolation operator (We applied Nearest Neighbor Interpolation in Matlab, which is similar to the 2D case in [36]). This requires having a relatively coarse solution, parametrized by h_c , and a relatively fine solution, parametrized by h_f , where $h_c = 2h_f$, at the same final time. The ℓ^2 and ℓ^∞ errors for ϕ_1 and ϕ_2 are displayed in Table 6.1, respectively. The results confirm our expectation for the convergence order.

Example 6.2. A random initial perturbation is included in the initial data:

$$\begin{aligned}\phi_1^0(x, y) &= 0.1 + r_{i,j}, \\ \phi_2^0(x, y) &= 0.4 + r_{i,j},\end{aligned}\quad (6.2)$$

where the $r_{i,j}$ are uniformly distributed random numbers in $[-0.01, 0.01]$.

This example is designed to test the performance of the proposed scheme in preserving physical properties at discrete level. The energy evolution of the numerical solution with $\Delta t = 1.0 \times 10^{-4}$ is illustrated in Fig. 6.1, which indicates a clear energy decay. In Fig. 6.2, we also present the error evolutions of the total mass of ϕ_1 and ϕ_2 . In Fig. 6.3, the snapshot plots of ϕ_1 , ϕ_2 and ϕ_3 at a sequence of time instants are displayed, to make a comparison with the existing ternary MMC results. Moreover, the maximum values and minimum values of ϕ_1 , ϕ_2 and $\phi_1 + \phi_2$ are presented in Figs. 6.4 and 6.5. In summary, our numerical tests further confirm that the proposed numerical scheme respects mass conservation, energy dissipation, and positivity at discrete level.

7. Conclusions

A second order finite difference numerical scheme is proposed and analyzed for the ternary MMC system. The BDF temporal discrete and second-order Adams–Bashforth extrapolation formula has been used to construct the full discrete scheme. In the proposed numerical algorithmic, a unique solvability and positivity-preserving property turn to be available. Combined Douglas–Dupont regularization term, the energy stability property is estimated. Moreover, the second order convergence analysis are available in the theoretical level. To overcome a well-known difficulty associated with the highly nonlinear and singular nature of the surface

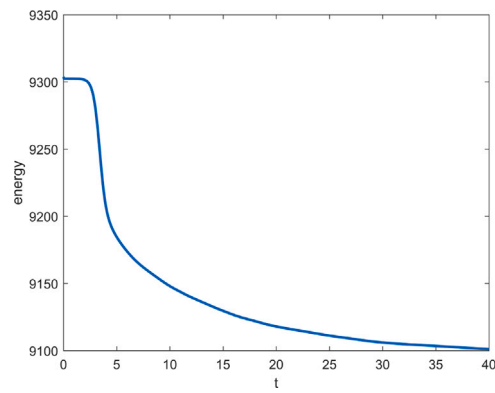


Fig. 6.1. Example 6.2: Evolution of the energy over time. The time step size is taken as $\Delta t = 1.0 \times 10^{-4}$.

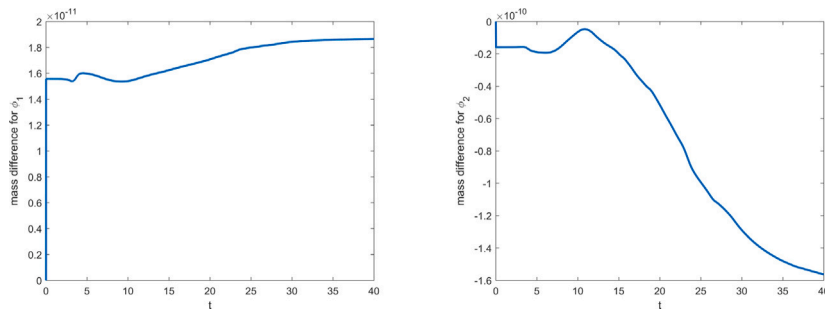


Fig. 6.2. Example 6.2: The error developments of the total mass for ϕ_1 and ϕ_2 , respectively.

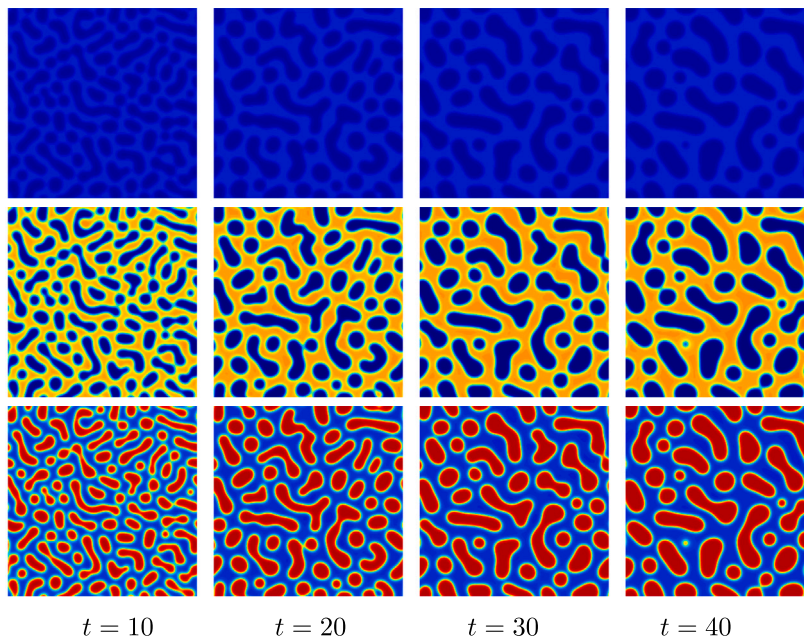


Fig. 6.3. Example 6.2: Evolution of three phase variables at $t = 10, 20, 30$ and 40 . The first line is for ϕ_1 , the second line is for ϕ_2 and the last line is for ϕ_3 . The time step size is taken as $\Delta t = 1.0 \times 10^{-4}$.

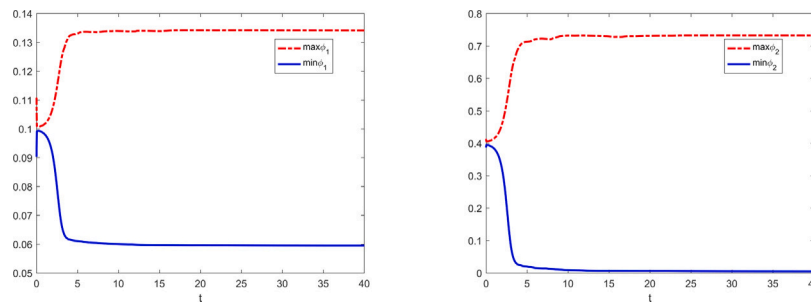


Fig. 6.4. Example 6.2: The time evolution of the maximum and minimum values for ϕ_1 and ϕ_2 , respectively.

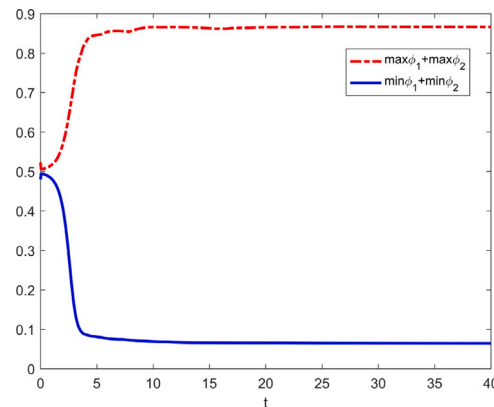


Fig. 6.5. Example 6.2: The time evolutions of the maximum and minimum values for $\phi_1 + \phi_2$, with $\Delta t = 1.0 \times 10^{-4}$.

diffusion coefficients, a rough error estimate has to be performed, so that the ℓ^∞ bound for ϕ_i could be derived. This ℓ^∞ estimate yields the upper and lower bounds of the three variables, and these bounds play a crucial role in the subsequent analysis. Finally, the refined error estimate is carried out to accomplish the desired convergence result. In addition, mass conservation, energy stability, bound of the numerical solution and the second order accurate are demonstrated in the numerical experiments.

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Data availability

Data will be made available on request.

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