

Existence and weak–strong uniqueness for Maxwell–Stefan–Cahn–Hilliard systems

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Abstract. A Maxwell–Stefan system for fluid mixtures with driving forces depending on Cahn–Hilliard-type chemical potentials is analyzed. The corresponding parabolic cross-diffusion equations contain fourth-order derivatives and are considered in a bounded domain with no-flux boundary conditions. The nonconvex part of the energy is assumed to have a bounded Hessian. The main difficulty of the analysis is the degeneracy of the diffusion matrix, which is overcome by proving the positive-definiteness of the matrix on a subspace and using the Bott–Duffin matrix inverse. The global existence of weak solutions and a weak–strong uniqueness property are shown by a careful combination of (relative) energy and entropy estimates, yielding $H^2(\Omega)$ bounds for the densities, which cannot be obtained from the energy or entropy inequalities alone.

1. Introduction

The evolution of fluid mixtures is important in many scientific fields, like biology and nanotechnology, to understand the diffusion-driven transport of species. The transport can be modeled by the Maxwell–Stefan equations [29, 31], which consist of mass balance equations and relations between the driving forces and the fluxes. The driving forces involve chemical potentials of the species, which in turn are determined by the (free) energy. When the fluid is immiscible, the energy can be assumed to consist of thermodynamic entropy and phase separation energy, given by a density gradient [5]. The gradient energetically penalizes the formation of an interface and restrains the segregation. This leads to a system of cross-diffusion equations with fourth-order derivatives. The aim of this paper is to provide a global existence and weak–strong uniqueness analysis for multicomponent systems of Maxwell–Stefan–Cahn–Hilliard type.

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1.1. Model equations and state of the art

The equations for the partial densities c_i and partial velocities u_i are

$$\partial_t c_i + \operatorname{div}(c_i u_i) = 0, \quad i = 1, \dots, n, \tag{1}$$

$$c_i \nabla \mu_i - \frac{c_i}{\sum_{k=1}^n c_k} \sum_{j=1}^n c_j \nabla \mu_j = - \sum_{j=1}^n K_{ij}(\mathbf{c}) c_j u_j, \tag{2}$$

$$\sum_{j=1}^n c_j u_j = 0, \tag{3}$$

supplemented by the initial and boundary conditions

$$\mathbf{c}(\cdot, 0) = \mathbf{c}^0 \text{ in } \Omega, \quad c_i u_i \cdot \nu = \nabla c_i \cdot \nu = 0 \text{ on } \partial\Omega, t > 0, i = 1, \dots, n, \tag{4}$$

where $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) is a bounded domain, ν is the exterior unit normal vector on the boundary $\partial\Omega$, $\mathbf{c} = (c_1, \dots, c_n)$ is the density vector, and $K_{ij}(\mathbf{c})$ are the friction coefficients. The left-hand side of (2) can be interpreted as the driving forces of the thermodynamic system, and the right-hand side is the sum of the friction forces. The chemical potentials

$$\mu_i = \frac{\delta \mathcal{E}}{\delta c_i} = \log c_i - \Delta c_i, \quad i = 1, \dots, n, \tag{5}$$

are the variational derivatives of the (free) energy

$$\mathcal{E}(\mathbf{c}) = \mathcal{H}(\mathbf{c}) + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla c_i|^2 dx, \quad \mathcal{H}(\mathbf{c}) = \sum_{i=1}^n \int_{\Omega} (c_i (\log c_i - 1) + 1) dx, \tag{6}$$

and $\mathcal{H}(\mathbf{c})$ is the thermodynamic entropy. Note that this energy is convex; we show in Section 5 that our results still hold if the energy contains a nonconvex part with bounded Hessian (like the potential in [11]). We assume that $\sum_{i=1}^n K_{ij}(\mathbf{c}) = 0$ for $j = 1, \dots, n$, meaning that the linear system in $\nabla \mu_j$ is invertible only on a subspace, and that $\sum_{i=1}^n c_i^0 = 1$ in Ω , which implies that $\sum_{i=1}^n c_i(t) = 1$ in Ω for all time $t > 0$. This means that the mixture is saturated and c_i can be interpreted as a volume fraction. For simplicity, we have normalized all physical constants.

Model (1)–(5) has been derived rigorously in [21] in the high-friction limit from a multicomponent Euler–Korteweg system for a general convex energy functional depending on \mathbf{c} and $\nabla \mathbf{c}$. A thermodynamics-based derivation can be found in [30]. When the energy equals $\mathcal{E}(\mathbf{c}) = \mathcal{H}(\mathbf{c})$, the model reduces to the classical Maxwell–Stefan equations, analyzed first in [3, 18, 19] for local-in-time smooth solutions and later in [26] for global-in-time weak solutions. In the single-species case, model (1)–(5) becomes a fourth-order Cahn–Hilliard-type equation with convex potential $\phi(c) = c(\log c - 1)$. Such a model, additionally including a nonconvex potential, was analyzed in, e.g., [11, 32]. Convergence from the Euler–Korteweg in the high-friction limit to the Cahn–Hilliard equation

with nonconvex potential is provided in [17]. Only a few works are concerned with the multispecies situation, and all of them require additional conditions. The mobility matrix in [4, 28] is assumed to be diagonal and that in [27] has constant entries, while [10, 12] suppose a particular (but nondiagonal) structure of the mobility matrix. We also mention [1, 2] on related models with free energies of type \mathcal{H} .

The proof of the uniqueness of solutions to cross-diffusion or fourth-order systems is quite delicate due to the lack of a maximum principle and regularity of the solutions. The uniqueness of strong solutions to Maxwell–Stefan systems has been shown in [19, 23], and uniqueness results for weak solutions in a very special case can be found in [7]. A weak–strong uniqueness result was proved for reaction–diffusion systems in [15] and for Maxwell–Stefan systems in [22]. Concerning uniqueness results for fourth-order equations, we refer to [8] for single-species Cahn–Hilliard equations, [24] for single-species thin-film equations, and [14] for the quantum drift-diffusion equations. To our knowledge, there are no uniqueness results for multicomponent Cahn–Hilliard-type systems. In this paper, we analyze these equations in a general setting for the first time.

1.2. Key ideas of the analysis

Before stating the main results, we explain the mathematical ideas needed to analyze model (1)–(5). First, we rewrite (2) by introducing the matrix $D(\mathbf{c}) \in \mathbb{R}^{n \times n}$ with entries

$$D_{ij}(\mathbf{c}) = \frac{1}{\sqrt{c_i}} K_{ij}(\mathbf{c}) \sqrt{c_j}$$

in the unknowns $(\sqrt{c_1}u_1, \dots, \sqrt{c_n}u_n)$:

$$\begin{aligned} \sqrt{c_i} \nabla \mu_i - \frac{\sqrt{c_i}}{\sum_{k=1}^n c_k} \sum_{j=1}^n c_j \nabla \mu_j &= - \sum_{j=1}^n D_{ij}(\mathbf{c}) \sqrt{c_j} u_j, \\ \sum_{i=1}^n \sqrt{c_i} (\sqrt{c_i} u_i) &= 0. \end{aligned} \tag{7}$$

We show in Lemma 3 that this linear system has a unique solution in the space $L(\mathbf{c}) := \{\mathbf{z} \in \mathbb{R}^n : \sum_{i=1}^n \sqrt{c_i} z_i = 0\}$, and the solution reads

$$\sqrt{c_i} u_i = - \sum_{j=1}^n D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j} \nabla \mu_j,$$

where $D^{\text{BD}}(\mathbf{c})$ is the so-called Bott–Duffin matrix inverse; see Lemmas 3 and 4 for the definition and some properties. Then, defining the matrix $B(\mathbf{c}) \in \mathbb{R}^{n \times n}$ with elements

$$B_{ij}(\mathbf{c}) = \sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j}, \quad i, j = 1, \dots, n, \tag{8}$$

system (1)–(2) can be formulated as (see Section 2.1 for details)

$$\partial_t c_i = \operatorname{div} \sum_{j=1}^n B_{ij}(\mathbf{c}) \nabla \mu_j, \quad i = 1, \dots, n.$$

The matrix $B(\mathbf{c})$ is often called the Onsager or mobility matrix in the literature. The major difficulty of the analysis comes from the fact that the matrix $B(\mathbf{c})$ is singular and degenerates when $c_i \rightarrow 0$ for some $i \in \{1, \dots, n\}$. Formally computing the energy identity

$$\frac{d\mathcal{E}}{dt}(\mathbf{c}) + \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \mu_i \cdot \nabla \mu_j \, dx = 0,$$

the degeneracy at $c_i = 0$ prevents uniform estimates for $\nabla \mu_i$ in $L^2(\Omega)$. In some works, this issue has been compensated for. For instance, there exists an entropy equality for the model of [12] yielding an $L^2(\Omega)$ bound for Δc_i , and the decoupled mobilities in [6, 28] allow for decoupled entropy estimates. In our model, the energy identity does not provide a gradient estimate for the full vector $(\nabla \mu_1, \dots, \nabla \mu_n)$ but only for a projection:

$$\frac{d\mathcal{E}}{dt}(\mathbf{c}) + C_1 \sum_{i=1}^n \int_{\Omega} \left| \sum_{j=1}^n (\delta_{ij} - \sqrt{c_i c_j}) \sqrt{c_j} \nabla \mu_j \right|^2 \, dx \leq 0,$$

where δ_{ij} is the Kronecker delta; see Lemma 5. (The constant $C_1 > 0$ and all constants that follow do not depend on \mathbf{c} .) To address the degeneracy issue, we compute the time derivative of the entropy:

$$\frac{d\mathcal{H}}{dt}(\mathbf{c}) + \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \log c_i \cdot \nabla \mu_j \, dx = 0.$$

This does not provide a uniform estimate for Δc_i , but we show (see Lemma 5) that

$$\begin{aligned} \frac{d\mathcal{H}}{dt}(\mathbf{c}) + C_2 \sum_{i=1}^n \int_{\Omega} (\Delta c_i)^2 \, dx \\ \leq C_3 \sum_{i=1}^n \int_{\Omega} \left| \sum_{j=1}^n (\delta_{ij} - \sqrt{c_i c_j}) \sqrt{c_j} \nabla \mu_j \right|^2 \, dx. \end{aligned}$$

Combining the energy and entropy inequalities in a suitable way, the last integral cancels:

$$\frac{d}{dt} \left(\mathcal{H}(\mathbf{c}) + \frac{C_3}{C_1} \mathcal{E}(\mathbf{c}) \right) + C_2 \sum_{i=1}^n \int_{\Omega} (\Delta c_i)^2 \, dx \leq 0. \tag{9}$$

This provides the desired $H^2(\Omega)$ bound for c_i . Note that the energy or entropy inequality alone does not give estimates for c_i . The combined energy–entropy inequality is the key idea of the paper for both the existence and weak–strong uniqueness analysis. Observe that the term $\mathcal{H}(\mathbf{c}) + (C_3/C_1)\mathcal{E}(\mathbf{c})$ can also be written as

$$(1 + C_3/C_1)\mathcal{H}(\mathbf{c}) + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla c_i|^2 \, dx.$$

1.3. Main results

We make the following assumptions:

- (A1) Domain: $\Omega \subset \mathbb{R}^d$ with $d \leq 3$ is a bounded domain. We set $Q_T = \Omega \times (0, T)$ for $T > 0$.
- (A2) Initial data: $c_i^0 \in H^1(\Omega)$ satisfies $c_i^0 \geq 0$ in Ω , $i = 1, \dots, n$, and $\sum_{i=1}^n c_i^0 = 1$ in Ω .

The assumption $d \leq 3$ is made for convenience, it can be relaxed for higher space dimensions by choosing another regularization in the existence proof; see (83). The constraint $\sum_{i=1}^n c_i^0 = 1$ expresses the saturation of the mixture and it propagates to the solution. We introduce the matrix $D_{ij}(\mathbf{c}) = (1/\sqrt{c_i})K_{ij}(\mathbf{c})\sqrt{c_j}$ for $i, j = 1, \dots, n$ and set

$$L(\mathbf{c}) = \{\mathbf{x} \in \mathbb{R}^n : \sqrt{\mathbf{c}} \cdot \mathbf{x} = 0\}, \quad L^\perp(\mathbf{c}) = \text{span}\{\sqrt{\mathbf{c}}\}, \tag{10}$$

where $\sqrt{\mathbf{c}} = (\sqrt{c_1}, \dots, \sqrt{c_n})$. The projections $P_L(\mathbf{c}), P_{L^\perp}(\mathbf{c}) \in \mathbb{R}^{n \times n}$ on $L(\mathbf{c}), L(\mathbf{c})^\perp$, respectively, are given by

$$P_L(\mathbf{c})_{ij} = \delta_{ij} - \sqrt{c_i c_j}, \quad P_{L^\perp}(\mathbf{c})_{ij} = \sqrt{c_i c_j}, \quad \text{for } i, j = 1, \dots, n. \tag{11}$$

We impose for any given $\mathbf{c} \in [0, 1]^n$ the following assumptions on $D(\mathbf{c}) = (D_{ij}(\mathbf{c})) \in \mathbb{R}^{n \times n}$:

- (B1) $D(\mathbf{c})$ is symmetric and $\text{ran } D(\mathbf{c}) = L(\mathbf{c}), \text{ker}(D(\mathbf{c})P_L(\mathbf{c})) = L^\perp(\mathbf{c})$.
- (B2) For all $i, j = 1, \dots, n, D_{ij} \in C^1([0, 1]^n)$ is bounded.
- (B3) The matrix $D(\mathbf{c})$ is positive semidefinite, and there exists $\rho > 0$ such that all eigenvalues $\lambda \neq 0$ of $D(\mathbf{c})$ satisfy $\lambda \geq \rho$.
- (B4) For all $i, j = 1, \dots, n, K_{ij}(\mathbf{c}) = \sqrt{c_i}D_{ij}(\mathbf{c})/\sqrt{c_j}$ is bounded in $[0, 1]^n$.

Examples of matrices $D(\mathbf{c})$ satisfying these assumptions are presented in Section 6. Our first main result is the global existence of weak solutions.

Theorem 1 (Global existence). *Let Assumptions (A1)–(A2) and (B1)–(B4) hold. Then there exists a weak solution \mathbf{c} to (1)–(5) satisfying $0 \leq c_i \leq 1, \sum_{i=1}^n c_i = 1$ in $\Omega \times (0, \infty)$,*

$$c_i \in L_{\text{loc}}^\infty(0, \infty; H^1(\Omega)) \cap L_{\text{loc}}^2(0, \infty; H^2(\Omega)), \quad \partial_t c_i \in L_{\text{loc}}^2(0, \infty; H^1(\Omega)'),$$

the initial condition in (4) is satisfied in the sense of $H^1(\Omega)'$, and for all $\phi_i \in C_0^\infty(\Omega \times (0, \infty))$,

$$\begin{aligned} 0 = & - \int_0^\infty \int_\Omega c_i \partial_t \phi_i \, dx \, dt + \sum_{j=1}^n \int_0^\infty \int_\Omega B_{ij}(\mathbf{c}) \nabla \log c_i \cdot \nabla \phi_i \, dx \, dt \\ & + \sum_{j=1}^n \int_0^\infty \int_\Omega \text{div}(B_{ij}(\mathbf{c}) \nabla \phi_i) \Delta c_j \, dx \, dt, \end{aligned} \tag{12}$$

where $B_{ij}(\mathbf{c})$ is defined in (8). Furthermore,

$$\begin{aligned} & \mathcal{H}(\mathbf{c}(\cdot, T)) + C_1 \mathcal{E}(\mathbf{c}(\cdot, T)) + C_2 \int_0^T \int_{\Omega} (|\nabla \sqrt{\mathbf{c}}|^2 + |\Delta \mathbf{c}|^2) dx dt \\ & + C_2 \int_0^T \int_{\Omega} |\xi|^2 dx dt \leq \mathcal{H}(\mathbf{c}^0) + C_1 \mathcal{E}(\mathbf{c}^0), \end{aligned} \tag{13}$$

where $C_1 > 0$ depends on $\rho, n, \|D(\mathbf{c})\|_F$ and $C_2 > 0$ depends on $n, \|D(\mathbf{c})\|_F$ (where $\|\cdot\|_F$ is the Frobenius matrix norm and ρ is introduced in Assumption (B3)). Moreover, ξ is the weak $L^2(\Omega)$ limit of an approximating sequence of $\sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \mu_j$.

Some comments are in order. First, by Assumption (B2), the elements of the matrix $D(\mathbf{c})$ are bounded for any $\mathbf{c} \in [0, 1]^n$ and therefore, the quantity $\|D(\mathbf{c})\|_F$ is bounded uniformly in \mathbf{c} . Second, the weak formulation (12) makes sense since $B_{ij}(\mathbf{c}) \nabla \log c_i \in L^2(Q_T)$. Indeed, by the definition of $B(\mathbf{c})$, we have

$$B_{ij}(\mathbf{c}) \nabla \log c_j = \sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c}) \frac{1}{\sqrt{c_j}} \nabla c_j,$$

and the matrix $\sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c}) / \sqrt{c_j}$ is bounded for all $\mathbf{c} \in [0, 1]^n$; see Lemma 4 (iii) below. However, note that the expression $\sum_{j=1}^n B_{ij}(\mathbf{c}) \nabla \mu_j$ is generally not an element of $L^2(Q_T)$. In particular, we cannot expect that $\nabla \Delta c_i \in L^2(Q_T)$. Third, we have not been able to identify the weak limit ξ because of low regularity. However, if

$$\sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \mu_j \in L^2_{\text{loc}}(0, \infty; L^2(\Omega))$$

holds for all $i = 1, \dots, n$, then we can identify $\xi_i = \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \mu_j$; see Lemma 9.

To prove Theorem 1, we first introduce a truncation with parameter $\delta \in (0, 1)$ as in [12] to avoid the degeneracy. Then we reduce the cross-diffusion system to $n - 1$ equations by replacing c_n by $1 - \sum_{i=1}^{n-1} c_i$. The advantage is that the diffusion matrix of the reduced system is positive definite (with a lower bound depending on δ). The existence of solutions c_i^δ to the truncated, reduced system is proved by an approximation as in [25] and the Leray–Schauder fixed-point theorem; see Section 3.1. An approximate version of the free energy estimate (13) (proved in Lemma 8 in Section 3.2) provides suitable uniform bounds that allow us to perform the limit $\delta \rightarrow 0$. The approximate densities c_i^δ may be negative but, by exploiting the entropy bound for c_i^δ , its limit c_i turns out to be nonnegative. The limit $\delta \rightarrow 0$ is then performed in Section 3.3, using the uniform estimates and compactness arguments.

Our second main result is concerned with the weak–strong uniqueness. For this, we define the relative entropy and free energy in the spirit of [16] by, respectively,

$$\begin{aligned} \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) & := \mathcal{H}(\mathbf{c}) - \mathcal{H}(\bar{\mathbf{c}}) - \frac{\partial \mathcal{H}}{\partial \mathbf{c}}(\bar{\mathbf{c}}) \cdot (\mathbf{c} - \bar{\mathbf{c}}) \\ & = \sum_{i=1}^n \int_{\Omega} \left(c_i \log \frac{c_i}{\bar{c}_i} - (c_i - \bar{c}_i) \right) dx, \end{aligned} \tag{14}$$

$$\begin{aligned} \mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}) &:= \mathcal{E}(\mathbf{c}) - \mathcal{E}(\bar{\mathbf{c}}) - \frac{\partial \mathcal{E}}{\partial \mathbf{c}}(\bar{\mathbf{c}}) \cdot (\mathbf{c} - \bar{\mathbf{c}}) \\ &= \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla(c_i - \bar{c}_i)|^2 dx. \end{aligned} \tag{15}$$

Theorem 2 (Weak–strong uniqueness). *Let Assumptions (A1)–(A2), (B1)–(B4) hold, let \mathbf{c} be a weak solution to (1)–(5) with initial datum \mathbf{c}^0 , and let $\bar{\mathbf{c}}$ be a strong solution to (1)–(5) with initial datum $\bar{\mathbf{c}}^0$. We assume that the weak solution \mathbf{c} satisfies*

$$\sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \mu_j \in L^2_{\text{loc}}(0, \infty; L^2(\Omega)) \quad \text{for } i, j = 1, \dots, n \tag{16}$$

(see (11) for the definition of $P_L(\mathbf{c})$) and for all $T > 0$ the energy and entropy inequalities

$$\mathcal{E}(\mathbf{c}(T)) + \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \mu_i \cdot \nabla \mu_j dx dt \leq \mathcal{E}(\mathbf{c}^0), \tag{17}$$

$$\mathcal{H}(\mathbf{c}(T)) + \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \log c_i \cdot \nabla \mu_j dx dt \leq \mathcal{H}(\mathbf{c}^0). \tag{18}$$

The strong solution $\bar{\mathbf{c}}$ is supposed to be strictly positive, i.e., there exists $m > 0$ such that $\bar{c}_i \geq m$ in $\Omega, t > 0$, and satisfies the regularity

$$\bar{c}_i \in L^\infty_{\text{loc}}(0, \infty; W^{3,\infty}(\Omega)), \quad \nabla \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \in L^\infty_{\text{loc}}(0, \infty; L^\infty(\Omega))$$

for $i = 1, \dots, n$, as well as for any $T > 0$ the energy and entropy conservation identities

$$\mathcal{E}(\bar{\mathbf{c}}(T)) + \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_i \cdot \nabla \bar{\mu}_j dx dt = \mathcal{E}(\bar{\mathbf{c}}^0), \tag{19}$$

$$\mathcal{H}(\bar{\mathbf{c}}(T)) + \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\bar{\mathbf{c}}) \nabla \log \bar{c}_i \cdot \nabla \bar{\mu}_j dx dt = \mathcal{H}(\bar{\mathbf{c}}^0), \tag{20}$$

where $\mu_i = \log c_i - \Delta c_i$ and $\bar{\mu}_i = \log \bar{c}_i - \Delta \bar{c}_i$. Then, for any $T > 0$, there exist constants C_1 , only depending on $\|D(\mathbf{c})\|_F, n, \rho$, and $C_2(T) > 0$, only depending on $T, \operatorname{meas}(\Omega), n, \rho$, such that

$$\mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + C_1 \mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) \leq C_2(T) (\mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + C_1 \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0)). \tag{21}$$

In particular, if $\mathbf{c}^0 = \bar{\mathbf{c}}^0$ then the weak and strong solutions coincide.

Observe that we need stronger assumptions on the weak solutions than those obtained in Theorem 1. Assumption (16) guarantees that the flux $\sum_{j=1}^n B_{ij}(\mathbf{c}) \nabla \mu_j$ lies in $L^2(Q_T)$.

Indeed, we prove in Lemma 4 (i) in Section 2 that $D_{ij}^{\text{BD}}(\mathbf{c})$ is bounded for $\mathbf{c} \in [0, 1]^n$. Therefore, since $D^{\text{BD}}(\mathbf{c}) = D^{\text{BD}}(\mathbf{c})P_L(\mathbf{c})$, assumption (16) and $c_i \in L^\infty(Q_T)$ imply that

$$\sum_{j=1}^n B_{ij}(\mathbf{c})\nabla\mu_j = \sqrt{c_i} \sum_{j,k=1}^n D_{ik}^{\text{BD}}(\mathbf{c})P_L(\mathbf{c})_{kj} \sqrt{c_j}\nabla\mu_j \in L^2(Q_T). \tag{22}$$

By the way, it follows from $\sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla \log c_j = 2\nabla \sqrt{c_i} \in L^2(Q_T)$ that

$$\sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla \Delta c_j = \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla (\log c_j - \mu_j) \in L^2(Q_T). \tag{23}$$

Since $\nabla \Delta c_i$ may not be in $L^2(Q_T)$, we interpret (23) in the sense of distributions, i.e., for all $\Phi \in C_0^\infty(\Omega; \mathbb{R}^d)$,

$$\begin{aligned} & \left\langle \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla \Delta c_j, \Phi \right\rangle \\ &= - \sum_{j=1}^n \int_{\Omega} (\nabla(P_L(\mathbf{c})_{ij} \sqrt{c_j}) \cdot \Phi + P_L(\mathbf{c})_{ij} \sqrt{c_j} \operatorname{div} \Phi) \Delta c_j \, dx. \end{aligned}$$

For the proof of Theorem 2, we estimate first the time derivative of the relative entropy (14):

$$\begin{aligned} & \frac{d\mathcal{H}}{dt}(\mathbf{c}|\bar{\mathbf{c}}) + C_1 \sum_{i=1}^n \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx + C_1 \sum_{i=1}^n \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx \\ & \leq C_2 \sum_{i=1}^n \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla (\mu_j - \bar{\mu}_j) \right|^2 dx + C_3 \int_{\Omega} \mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}) \, dx, \end{aligned}$$

where $C_i > 0$ are some constants depending only on the data. The first term on the right-hand side can be handled by estimating the time derivative of the relative energy (15):

$$\begin{aligned} & \frac{d\mathcal{E}}{dt}(\mathbf{c}|\bar{\mathbf{c}}) + C_4 \sum_{i=1}^n \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla (\mu_j - \bar{\mu}_j) \right|^2 dx \\ & \leq \theta \sum_{i=1}^n \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j}\nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx + \theta \sum_{i=1}^n \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx \\ & \quad + C_5(\theta) \int_{\Omega} \mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}) \, dx, \end{aligned}$$

where $\theta > 0$ can be arbitrarily small. Choosing $\theta = C_1 C_4 / C_2$, we can combine both estimates leading to

$$\frac{d}{dt} \left(\mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{C_2}{C_4} \mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}) \right) \leq \left(C_3 + \frac{C_2 C_5}{C_4} \right) \mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}),$$

and the theorem follows after applying Grönwall’s lemma. As the computations are quite involved, we compute first in Section 4.1 the time derivative of the relative entropy and energy for *smooth* solutions. The rigorous proof of the combined relative entropy–energy inequality for weak solutions \mathbf{c} and strong solutions $\bar{\mathbf{c}}$ is then performed in Section 4.2.

The paper is organized as follows. The Bott–Duffin matrix inverse is introduced in Section 2, some properties of the mobility matrix $B(\mathbf{c})$ are proved, and the combined energy–entropy inequality (9) is derived for smooth solutions. The global existence of solutions (Theorem 1) is shown in Section 3, while Section 4 is concerned with the proof of the weak–strong uniqueness property (Theorem 2). The case of nonconvex energies is investigated in Section 5, showing that Theorems 1 and 2 still hold if the convex part of the energy equals the Boltzmann entropy (see (6)) and the Hessian of the nonconvex part is bounded. Finally, we present some examples verifying Assumptions (B1)–(B4) in Section 6.

Notation

Elements of the matrix $A \in \mathbb{R}^{n \times n}$ are denoted by A_{ij} , $i, j = 1, \dots, n$, and elements of a vector $\mathbf{c} \in \mathbb{R}^n$ are c_1, \dots, c_n . We use the notation $f(\mathbf{c}) = (f(c_1), \dots, f(c_n))$ for $\mathbf{c} \in \mathbb{R}^n$ and a function $f: \mathbb{R} \rightarrow \mathbb{R}$. The expression $|\nabla f(\mathbf{c})|^2$ is defined by $\sum_{i=1}^n |\nabla f(c_i)|^2$ and $|\cdot|$ is the usual Euclidean norm. The matrix $R(\mathbf{c}) \in \mathbb{R}^{n \times n}$ is the diagonal matrix with elements $\sqrt{c_1}, \dots, \sqrt{c_n}$, i.e., $R_{ij}(\mathbf{c}) = \sqrt{c_i} \delta_{ij}$ for $i, j = 1, \dots, n$, where δ_{ij} denotes the Kronecker delta. We understand by $\nabla \boldsymbol{\mu}$ the matrix with entries $\partial_{x_i} \mu_j$. Furthermore, $C > 0$, $C_i > 0$ are generic constants with values changing from line to line.

2. Properties of the mobility matrix and a priori estimates

We wish to express the fluxes $c_i u_i$ as a linear combination of the gradients of the chemical potentials. Since $K(\mathbf{c})$ has a nontrivial kernel, we need to use a generalized matrix inverse, the Bott–Duffin inverse. This inverse and its properties are studied in Section 2.1. The properties allow us to derive in Section 2.2 some a priori estimates for the Maxwell–Stefan–Cahn–Hilliard system.

2.1. The Bott–Duffin inverse

We wish to invert (2) or, equivalently, (7). We recall definition (11) of the projection matrices $P_L(\mathbf{c}) \in \mathbb{R}^{n \times n}$ on $L(\mathbf{c})$ and $P_{L^\perp}(\mathbf{c}) \in \mathbb{R}^{n \times n}$ on $L^\perp(\mathbf{c})$, where $L(\mathbf{c})$ and $L^\perp(\mathbf{c})$ are defined in (10). Then (7) is equivalent to the following problem:

$$\text{Solve } D(\mathbf{c})\mathbf{z} = -P_L(\mathbf{c})R(\mathbf{c})\nabla \boldsymbol{\mu} \text{ in the space } \mathbf{z} \in L(\mathbf{c}), \tag{24}$$

where $z_i = \sqrt{c_i} u_i$, recalling that $R(\mathbf{c}) = \text{diag}(\sqrt{\mathbf{c}})$.

Lemma 3 (Solution of (24)). *Suppose that $D(\mathbf{c})$ satisfies Assumption (B1). The Bott–Duffin inverse*

$$D^{\text{BD}}(\mathbf{c}) = P_L(\mathbf{c})(D(\mathbf{c})P_L(\mathbf{c}) + P_{L^\perp}(\mathbf{c}))^{-1}$$

is well defined, symmetric, and satisfies $\ker D^{\text{BD}}(\mathbf{c}) = L^\perp(\mathbf{c})$. Furthermore, for any $\mathbf{y} \in L(\mathbf{c})$, the linear problem $D(\mathbf{c})\mathbf{z} = \mathbf{y}$ for $\mathbf{z} \in L(\mathbf{c})$ has a unique solution given by $\mathbf{z} = D^{\text{BD}}(\mathbf{c})\mathbf{y}$.

We refer to [22, Lemma 17] for the proof. The property for the kernel follows from $\ker D^{\text{BD}}(\mathbf{c}) = \ker P_L(\mathbf{c}) = L^\perp(\mathbf{c})$. Since $P_L(\mathbf{c})R(\mathbf{c})\nabla\boldsymbol{\mu} \in L(\mathbf{c})$ (this follows from the definition of $P_L(\mathbf{c})$ and $\sum_{i=1}^n c_i = 1$), we infer from Lemma 3 that (24) has the unique solution $\mathbf{z} = -D^{\text{BD}}(\mathbf{c})P_L(\mathbf{c})R(\mathbf{c})\nabla\boldsymbol{\mu} \in L(\mathbf{c})$ or, componentwise,

$$c_i u_i = \sqrt{c_i} z_i = - \sum_{j=1}^n \sqrt{c_i} (D^{\text{BD}}(\mathbf{c})P_L(\mathbf{c}))_{ij} \sqrt{c_j} \nabla\mu_j = - \sum_{j=1}^n \sqrt{c_i} D^{\text{BD}}(\mathbf{c})_{ij} \sqrt{c_j} \nabla\mu_j$$

for $i = 1, \dots, n$, where the last equality follows from $D^{\text{BD}}(\mathbf{c})P_L(\mathbf{c}) = D^{\text{BD}}(\mathbf{c})$; see [22, (81)]. Then we can formulate equation (1) as

$$\partial_t c_i = \operatorname{div} \sum_{j=1}^n B_{ij}(\mathbf{c}) \nabla\mu_j, \quad \text{where } B_{ij}(\mathbf{c}) = \sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j}, \quad i, j = 1, \dots, n. \quad (25)$$

The boundary conditions $c_i u_i \cdot \nu = 0$ on $\partial\Omega$ yield

$$\sum_{j=1}^n B_{ij}(\mathbf{c}) \nabla\mu_j \cdot \nu = 0 \quad \text{on } \partial\Omega, t > 0, i = 1, \dots, n. \quad (26)$$

We recall some properties of the Bott–Duffin inverse.

Lemma 4 (Properties of $D^{\text{BD}}(\mathbf{c})$). *Suppose that $D(\mathbf{c}) \in \mathbb{R}^{n \times n}$ satisfies Assumptions (B1)–(B4). Then we have the following properties:*

- (i) *The coefficients $D_{ij}^{\text{BD}} \in C^1([0, 1]^n)$ are bounded for $i, j = 1, \dots, n$.*
- (ii) *Let $\lambda(\mathbf{c})$ be an eigenvalue of $(D(\mathbf{c})P_L(\mathbf{c}) + P_{L^\perp}(\mathbf{c}))^{-1}$. Then $\lambda_m \leq \lambda(\mathbf{c}) \leq \lambda_M$, where*

$$\lambda_m = (1 + n\|D(\mathbf{c})\|_F)^{-1}, \quad \lambda_M = \max\{1, \rho^{-1}\},$$

$\|\cdot\|_F$ is the Frobenius matrix norm, and $\rho > 0$ is a lower bound for the eigenvalues of $D(\mathbf{c})$; see Assumption (B3).

- (iii) *The functions $\mathbf{c} \mapsto \sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c}) / \sqrt{c_j}$ are bounded in $[0, 1]^n$ for $i, j = 1, \dots, n$.*

A consequence of (ii) are the inequalities

$$\lambda_m |P_L(\mathbf{c})\mathbf{z}|^2 \leq \mathbf{z}^\top D^{\text{BD}}(\mathbf{c})\mathbf{z} \leq \lambda_M |P_L(\mathbf{c})\mathbf{z}|^2 \quad \text{for } \mathbf{z} \in \mathbb{R}^n. \quad (27)$$

Note that the Frobenius norm of $D(\mathbf{c})$ is bounded uniformly in $\mathbf{c} \in [0, 1]^n$, since D_{ij} is bounded by Assumption (B1).

Proof of Lemma 4. Points (i) and (ii) are proved in [22, Lemma 11] in an interval $[m, 1]^n$ for some $m > 0$. In fact, we can conclude (i)–(ii) in the full interval $[0, 1]^n$, since our Assumptions (B2)–(B3) are stronger than those in [22].

For the proof of (iii), dropping the argument \mathbf{c} and observing that $RDR^{-1} = K$, we obtain

$$\begin{aligned} RD^{\text{BD}}R^{-1} &= RP_L(DP_L + P_{L^\perp})^{-1}R^{-1} = RP_L(R^{-1}R)(DP_L + P_{L^\perp})^{-1}R^{-1} \\ &= RP_LR^{-1}(R(DP_L + P_{L^\perp})R^{-1})^{-1} \\ &= RP_LR^{-1}(RDR^{-1}RP_LR^{-1} + RP_{L^\perp}R^{-1})^{-1} \\ &= RP_LR^{-1}(KRP_LR^{-1} + RP_{L^\perp}R^{-1})^{-1}. \end{aligned}$$

The determinant of the expression in the brackets equals

$$\det(R(DP_L + P_{L^\perp})R^{-1}) = \det(DP_L + P_{L^\perp}).$$

Therefore, denoting by “adj” the adjugate matrix, it follows that

$$RD^{\text{BD}}R^{-1} = \frac{RP_LR^{-1} \text{adj}(KRP_LR^{-1} + RP_{L^\perp}R^{-1})}{\det(DP_L + P_{L^\perp})}. \tag{28}$$

By Assumption (B3), the eigenvalues of D are not smaller than $\rho > 0$. The proof of [22, Lemma 11] shows that the eigenvalues of $DP_L + P_{L^\perp}$ are not smaller than $\rho > 0$, too. This implies that $\det(DP_L + P_{L^\perp}) \geq \rho^{n-1} > 0$. The coefficients

$$(RP_LR^{-1})_{ij} = \delta_{ij} - c_i, \quad (RP_{L^\perp}R^{-1})_{ij} = c_i$$

are bounded for $\mathbf{c} \in [0, 1]^n$ and, by Assumption (B4), the coefficients of K are also bounded. Therefore, all elements of $\text{adj}(KRP_LR^{-1} + RP_{L^\perp}R^{-1})$ are bounded. We conclude from (28) that the entries of $RD^{\text{BD}}R^{-1}$ are bounded in $[0, 1]^n$, i.e., point (iii) holds. ■

The most important property is the positive-definiteness of $D^{\text{BD}}(\mathbf{c})$ on $L(\mathbf{c})$; see (27). This property implies the a priori estimates proved in the following subsection.

2.2. A priori estimates

We show an energy inequality for smooth solutions.

Lemma 5 (Free energy inequality). *Let $\mathbf{c} \in C^\infty(\Omega \times (0, \infty); \mathbb{R}^n)$ be a positive, bounded, smooth solution to (1)–(5). Then, for any $0 < \lambda < \lambda_m$,*

$$\begin{aligned} \frac{d}{dt} \left(\mathcal{H}(\mathbf{c}) + \frac{(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}) \right) &+ 2\lambda \int_\Omega |\nabla \sqrt{\mathbf{c}}|^2 dx + \lambda \int_\Omega |\Delta \mathbf{c}|^2 dx \\ &+ \frac{(\lambda_M - \lambda)^2}{2\lambda} \int_\Omega |P_L(\mathbf{c})R(\mathbf{c})\nabla \boldsymbol{\mu}|^2 dx \leq 0, \end{aligned}$$

where the entropy $\mathcal{H}(\mathbf{c})$ and the free energy $\mathcal{E}(\mathbf{c})$ are given by (6) and λ_m, λ_M are defined in Lemma 4.

Proof. We derive first the energy inequality. To this end, we multiply equation (25) for c_i by $\mu_i = (\partial\mathcal{E}/\partial c_i)(\mathbf{c})$, integrate over Ω , integrate by parts (using the boundary conditions (26)), and take into account the lower bound (27) for $D^{\text{BD}}(\mathbf{c})$:

$$\begin{aligned} \frac{d\mathcal{E}}{dt}(\mathbf{c}) &= \sum_{i=1}^n \int_{\Omega} \frac{\partial\mathcal{E}}{\partial c_i}(\mathbf{c}) \partial_t c_i \, dx = - \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \mu_i \cdot \nabla \mu_j \, dx \\ &= - \sum_{i,j=1}^n D_{ij}^{\text{BD}}(\mathbf{c}) (\sqrt{c_i} \nabla \mu_i) \cdot (\sqrt{c_j} \nabla \mu_j) \, dx \\ &\leq -\lambda_m \int_{\Omega} |P_L(\mathbf{c})R(\mathbf{c})\nabla\boldsymbol{\mu}|^2 \, dx. \end{aligned} \tag{29}$$

The entropy inequality is derived by multiplying (25) by $\log c_i$, integrating over Ω , and integrating by parts (using the boundary conditions (26)):

$$\frac{d\mathcal{H}}{dt}(\mathbf{c}) = \sum_{i=1}^n \int_{\Omega} (\log c_i) \partial_t c_i \, dx = - \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \log c_i \cdot \nabla \mu_j \, dx.$$

To estimate the right-hand side, we set $G = RP_L R$ (omitting the argument \mathbf{c}) and $M := B - \lambda G$ for $\lambda \in (0, \lambda_m)$. Then

$$\begin{aligned} \frac{d\mathcal{H}}{dt}(\mathbf{c}) &= - \sum_{i,j=1}^n \int_{\Omega} M_{ij} \nabla \log c_i \cdot \nabla \mu_j \, dx - \lambda \sum_{i,j=1}^n \int_{\Omega} G_{ij} \nabla \log c_i \cdot \nabla \mu_j \, dx \\ &=: I_1 + I_2. \end{aligned} \tag{30}$$

Before estimating the integrals I_1 and I_2 , we start with some preparation. We use Lemma 4 (ii) and $P_L^\top P_L = P_L$ to obtain

$$\mathbf{z}^\top B \mathbf{z} = (R\mathbf{z})^\top D^{\text{BD}} R \mathbf{z} \geq \lambda_m |P_L R \mathbf{z}|^2 = \lambda_m (P_L R \mathbf{z})^\top (P_L R \mathbf{z}) = \lambda_m \mathbf{z}^\top G \mathbf{z} \quad \text{for } \mathbf{z} \in \mathbb{R}^n.$$

The matrix M is positive semidefinite since for any $\mathbf{z} \in \mathbb{R}^n$,

$$\mathbf{z}^\top M \mathbf{z} = \mathbf{z}^\top B \mathbf{z} - \lambda \mathbf{z}^\top G \mathbf{z} \geq (\lambda_m - \lambda) \mathbf{z}^\top G \mathbf{z} = (\lambda_m - \lambda) |P_L R \mathbf{z}|^2. \tag{31}$$

Furthermore, by Lemma 4 (ii) again, we have the upper bound

$$\mathbf{z}^\top M \mathbf{z} = \mathbf{z}^\top (B - \lambda G) \mathbf{z} \leq (\lambda_M - \lambda) \mathbf{z}^\top G \mathbf{z} = (\lambda_M - \lambda) |P_L R \mathbf{z}|^2. \tag{32}$$

We are now in the position to estimate the integral I_1 , using Young’s inequality for any $\theta > 0$:

$$\begin{aligned} I_1 &\leq \frac{\theta}{2} \sum_{i,j=1}^n \int_{\Omega} M_{ij} \nabla \log c_i \cdot \nabla \log c_j \, dx + \frac{1}{2\theta} \sum_{i,j=1}^n \int_{\Omega} M_{ij} \nabla \mu_i \cdot \nabla \mu_j \, dx \\ &\leq \frac{\theta}{2} (\lambda_M - \lambda) \int_{\Omega} |P_L R \nabla \log \mathbf{c}|^2 \, dx + \frac{\lambda_M - \lambda}{2\theta} \int_{\Omega} |P_L R \nabla \boldsymbol{\mu}|^2 \, dx \\ &= 2\theta (\lambda_M - \lambda) \int_{\Omega} |\nabla \sqrt{\mathbf{c}}|^2 \, dx + \frac{\lambda_M - \lambda}{2\theta} \int_{\Omega} |P_L R \nabla \boldsymbol{\mu}|^2 \, dx, \end{aligned}$$

where the last step follows from $\sum_{j=1}^n (P_L)_{ij} R_j \nabla \log c_j = 2 \nabla \sqrt{c_i}$, which is a consequence of $\sum_{j=1}^n \nabla c_j = 0$. For the integral I_2 , we use the definitions $G_{ij} = c_i \delta_{ij} - c_i c_j$ and $\mu_j = \log c_j - \Delta c_j$:

$$\begin{aligned} I_2 &= -\lambda \sum_{i,j=1}^n \int_{\Omega} (c_i \delta_{ij} - c_i c_j) \frac{\nabla c_i}{c_i} \cdot \nabla (\log c_j - \Delta c_j) \, dx \\ &= -\lambda \sum_{i=1}^n \int_{\Omega} \nabla c_i \cdot \nabla (\log c_i - \Delta c_i) \, dx + \lambda \int_{\Omega} \sum_{i=1}^n \nabla c_i \cdot \sum_{j=1}^n c_j \nabla (\log c_j - \Delta c_j) \, dx \\ &= -\lambda \sum_{i=1}^n \int_{\Omega} \nabla c_i \cdot \nabla (\log c_i - \Delta c_i) \, dx = -\lambda \int_{\Omega} (4|\nabla \sqrt{c}|^2 + |\Delta c|^2) \, dx, \end{aligned}$$

where we integrated by parts in the last step.

Inserting the estimates for I_1 and I_2 into (30) yields

$$\begin{aligned} \frac{d\mathcal{H}}{dt}(c) + 4\lambda \int_{\Omega} |\nabla \sqrt{c}|^2 \, dx + \lambda \int_{\Omega} |\Delta c|^2 \, dx \\ \leq 2\theta(\lambda_M - \lambda) \int_{\Omega} |\nabla \sqrt{c}|^2 \, dx + \frac{\lambda_M - \lambda}{2\theta} \int_{\Omega} |P_L R \nabla \mu|^2 \, dx. \end{aligned}$$

We set $\theta = \lambda/(\lambda_M - \lambda)$ to conclude that

$$\frac{d\mathcal{H}}{dt}(c) + 2\lambda \int_{\Omega} |\nabla \sqrt{c}|^2 \, dx + \lambda \int_{\Omega} |\Delta c|^2 \, dx \leq \frac{(\lambda_M - \lambda)^2}{2\lambda} \int_{\Omega} |P_L R \nabla \mu|^2 \, dx. \tag{33}$$

The right-hand side can be absorbed by the corresponding term in (29). Indeed, adding the previous inequality to (29) times $(\lambda_M - \lambda)^2/(\lambda_m \lambda)$ finishes the proof. ■

Note that the energy inequality (29) or the entropy inequality (33) alone are not sufficient to control the derivatives of c but only a suitable linear combination. We will prove these inequalities rigorously in the following section for weak solutions; see Lemma 8.

3. Proof of Theorem 1

We prove the existence of global weak solutions to (1)–(4). For this, we construct an approximate system depending on a parameter $\delta > 0$, similarly to [12], and then pass to the limit $\delta \rightarrow 0$.

3.1. An approximate system

In order to deal with the degeneracy of the matrix $B(c)$ when a component of c vanishes, we introduce the cutoff function $\chi_{\delta}: \mathbb{R}^n \rightarrow \mathbb{R}^n$, with

$$(\chi_{\delta} c)_i := \begin{cases} \delta & \text{for } c_i < \delta, \\ c_i & \text{for } \delta \leq c_i \leq 1 - \delta, \\ 1 - \delta & \text{for } c_i > 1 - \delta, \end{cases}$$

and define the approximate matrix

$$B^\delta(\mathbf{c}) := R(\chi_\delta \mathbf{c}) D^{\text{BD}}(\chi_\delta \mathbf{c}) R(\chi_\delta \mathbf{c}), \tag{34}$$

recalling that $R(\chi_\delta \mathbf{c}) = \text{diag}(\sqrt{\chi_\delta \mathbf{c}})$. We wish to solve the approximate problem

$$\partial_t c_i^\delta = \text{div} \sum_{j=1}^n B_{ij}^\delta(\mathbf{c}^\delta) \nabla \mu_j^\delta, \quad \mu_j^\delta = \frac{\partial \mathcal{E}^\delta}{\partial c_j}(\mathbf{c}^\delta) \text{ in } \Omega, \quad t > 0, \tag{35}$$

$$c_i^\delta(\cdot, 0) = c_i^0 \text{ in } \Omega, \quad \sum_{j=1}^n B_{ij}^\delta(\mathbf{c}^\delta) \nabla \mu_j^\delta \cdot \nu = 0, \quad \nabla c_i^\delta \cdot \nu = 0 \text{ on } \partial\Omega, \tag{36}$$

where $i = 1, \dots, n$, $\sum_{i=1}^n c_i^0 = 1$, and the approximate energy is defined by

$$\begin{aligned} \mathcal{E}^\delta(\mathbf{c}) &:= \mathcal{H}^\delta(\mathbf{c}) + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla c_i|^2 dx, \quad \mathcal{H}^\delta(\mathbf{c}) := \sum_{i=1}^n \int_{\Omega} h_i^\delta(c_i) dx, \\ h_i^\delta(r) &= \begin{cases} r \log \delta - \delta/2 + r^2/(2\delta) & \text{for } r < \delta, \\ r \log r & \text{for } \delta \leq r \leq 1 - \delta, \\ r \log(1 - \delta) - (1 - \delta)/2 + r^2/(2(1 - \delta)) & \text{for } r > 1 - \delta. \end{cases} \end{aligned} \tag{37}$$

Observe that the solutions c_i^δ may be negative. We will show below that c_i^δ converges to a nonnegative function as $\delta \rightarrow 0$. The approximate entropy density is chosen in such a way that $h_i^\delta \in C^2(\mathbb{R})$. Indeed, we obtain

$$(h_i^\delta)'(c_i) = \begin{cases} \log \delta + c_i/\delta & \text{for } c_i < \delta, \\ \log c_i + 1 & \text{for } \delta < c_i < 1 - \delta, \\ \log(1 - \delta) + c_i/(1 - \delta) & \text{for } c_i > 1 - \delta, \end{cases} \quad (h_i^\delta)''(c_i) = \frac{1}{(\chi_\delta \mathbf{c})_i}.$$

With these definitions, we obtain $\mu_i^\delta = (h_i^\delta)'(c_i^\delta) - \Delta c_i^\delta$ for $i = 1, \dots, n$.

Theorem 6 (Existence for the approximate system). *Let Assumptions (A1)–(A2) and (B1)–(B4) hold and let $\delta > 0$. Then there exists a weak solution $(\mathbf{c}^\delta, \boldsymbol{\mu}^\delta)$ to (35)–(36) satisfying $\sum_{i=1}^n c_i^\delta(t) = 1$ in Ω , $t > 0$,*

$$\begin{aligned} c_i^\delta &\in L^\infty_{\text{loc}}(0, \infty; H^1(\Omega)) \cap L^2_{\text{loc}}(0, \infty; H^2(\Omega)), \\ \partial_t c_i &\in L^2_{\text{loc}}(0, \infty; H^2(\Omega)'), \quad \mu_i^\delta \in L^2_{\text{loc}}(0, \infty; H^1(\Omega)), \quad i = 1, \dots, n, \end{aligned}$$

and the first equation in (35) as well as the initial condition in (36) are satisfied in the sense of $L^2_{\text{loc}}(0, \infty; H^2(\Omega)')$.

The proof of this theorem is deferred to Appendix A, since it is technical and involves well-established techniques. We show some properties of the matrix $B^\delta(\mathbf{c})$. We introduce the matrices $P_L(\chi_\delta \mathbf{c}), P_{L^\perp}(\chi_\delta \mathbf{c}) \in \mathbb{R}^{n \times n}$ with entries

$$P_L(\chi_\delta \mathbf{c})_{ij} = \delta_{ij} - \frac{\sqrt{(\chi_\delta \mathbf{c})_i (\chi_\delta \mathbf{c})_j}}{\sum_{k=1}^n (\chi_\delta \mathbf{c})_k}, \quad P_{L^\perp}(\chi_\delta \mathbf{c})_{ij} = \frac{\sqrt{(\chi_\delta \mathbf{c})_i (\chi_\delta \mathbf{c})_j}}{\sum_{k=1}^n (\chi_\delta \mathbf{c})_k}, \quad i, j = 1, \dots, n.$$

Lemma 7 (Properties of $B^\delta(\mathbf{c})$). *Suppose that $D(\mathbf{c})$ satisfies Assumptions (B1)–(B4). Then Lemmas 3 and 4 hold with $P_L(\mathbf{c})$, $P_{L^\perp}(\mathbf{c})$, and $D^{\text{BD}}(\mathbf{c})$ replaced by $P_L(\chi_\delta \mathbf{c})$, $P_{L^\perp}(\chi_\delta \mathbf{c})$, and $D^{\text{BD}}(\chi_\delta \mathbf{c})$. As a consequence, the matrix $B^\delta(\mathbf{c})$, defined in (34), satisfies*

$$\mathbf{z}^\top B^\delta(\mathbf{c}) \mathbf{z} \geq \lambda_m |P_L(\chi_\delta \mathbf{c}) R(\chi_\delta \mathbf{c}) \mathbf{z}|^2 \quad \text{for any } \mathbf{z}, \mathbf{c} \in \mathbb{R}^n, \quad (38)$$

and the first $(n-1) \times (n-1)$ submatrix $\tilde{B}^\delta(\mathbf{c})$ of $B^\delta(\mathbf{c})$ is positive definite and satisfies for $\eta(\delta) = \lambda_m \delta^2/n$,

$$\tilde{\mathbf{z}}^\top \tilde{B}^\delta(\mathbf{c}) \tilde{\mathbf{z}} \geq \eta(\delta) |\tilde{\mathbf{z}}|^2 \quad \text{for any } \tilde{\mathbf{z}} \in \mathbb{R}^{n-1}. \quad (39)$$

Proof. It can be verified that Assumptions (B1)–(B2) hold for $D(\chi_\delta \mathbf{c})$, so Lemmas 3 and 4 still hold for the matrix $D(\chi_\delta \mathbf{c})$. Inequality (38) is a direct consequence of Lemma 4 (ii). It remains to prove (39). We define for given $\tilde{\mathbf{z}} \in \mathbb{R}^{n-1}$ the vector $\mathbf{z} \in \mathbb{R}^n$ with $z_i = \tilde{z}_i$ for $i = 1, \dots, n-1$ and $z_n = 0$. Then (38) becomes

$$\tilde{\mathbf{z}}^\top \tilde{B}^\delta(\mathbf{c}) \tilde{\mathbf{z}} \geq \lambda_m |\tilde{P}_L(\chi_\delta \mathbf{c}) \tilde{R}(\chi_\delta \mathbf{c}) \tilde{\mathbf{z}}|^2 = \lambda_m (\tilde{R}(\chi_\delta \mathbf{c}) \tilde{\mathbf{z}})^\top \tilde{P}_L(\chi_\delta \mathbf{c}) (\tilde{R}(\chi_\delta \mathbf{c}) \tilde{\mathbf{z}}), \quad (40)$$

where \tilde{A} denotes the first $(n-1) \times (n-1)$ submatrix of a given matrix $A \in \mathbb{R}^{n \times n}$. It follows from the Cauchy–Schwarz inequality that for any $\zeta \in \mathbb{R}^{n-1}$,

$$\begin{aligned} \zeta^\top \tilde{P}_L(\chi_\delta \mathbf{c}) \zeta &= \sum_{i=1}^{n-1} \zeta_i^2 - \left(\sum_{j=1}^{n-1} \sqrt{\frac{(\chi_\delta \mathbf{c})_j}{\sum_{k=1}^n (\chi_\delta \mathbf{c})_k}} \zeta_j \right)^2 \geq |\zeta|^2 - \sum_{j=1}^{n-1} \frac{(\chi_\delta \mathbf{c})_j}{\sum_{k=1}^n (\chi_\delta \mathbf{c})_k} |\zeta|^2 \\ &= \frac{(\chi_\delta \mathbf{c})_n}{\sum_{k=1}^n (\chi_\delta \mathbf{c})_k} |\zeta|^2 \geq \frac{\delta}{n} |\zeta|^2. \end{aligned}$$

Therefore, (40) becomes

$$\tilde{\mathbf{z}}^\top \tilde{B}^\delta(\mathbf{c}) \tilde{\mathbf{z}} \geq \frac{\lambda_m \delta}{n} \sum_{i=1}^{n-1} |\sqrt{(\chi_\delta \mathbf{c})_i} \tilde{z}_i|^2 = \frac{\lambda_m \delta}{n} \sum_{i=1}^{n-1} (\chi_\delta \mathbf{c})_i |\tilde{z}_i|^2 \geq \frac{\lambda_m \delta^2}{n} |\tilde{\mathbf{z}}|^2,$$

which proves (39). ■

3.2. Uniform estimates

We derive energy and entropy estimates for the solutions to (35), which are uniform in δ .

Lemma 8 (Energy and entropy inequalities). *Let \mathbf{c}^δ be a weak solution to (35)–(36), constructed in Theorem 6. Then the following inequalities hold for any $T > 0$:*

$$\mathcal{E}^\delta(\mathbf{c}^\delta(\cdot, T)) + \sum_{i,j=1}^n \int_0^T \int_\Omega B_{ij}^\delta(\mathbf{c}^\delta) \nabla \mu_i^\delta \cdot \nabla \mu_j^\delta dx dt \leq \mathcal{E}^\delta(\mathbf{c}^0), \quad (41)$$

$$\mathcal{H}^\delta(\mathbf{c}^\delta(\cdot, T)) + \sum_{i,j=1}^n \int_0^T \int_\Omega B_{ij}^\delta(\mathbf{c}^\delta) \nabla (h_i^\delta)'(c_i^\delta) \cdot \nabla \mu_j^\delta dx dt \leq \mathcal{H}^\delta(\mathbf{c}^0), \quad (42)$$

$$\begin{aligned}
 \mathcal{H}^\delta(\mathbf{c}^\delta(\cdot, T)) &+ \frac{(\lambda_M - \lambda)^2}{2\lambda_m\lambda} \mathcal{E}^\delta(\mathbf{c}^\delta(\cdot, T)) + \lambda \sum_{i=1}^n \int_0^T \int_\Omega \frac{|\nabla c_i^\delta|^2}{(\chi_\delta \mathbf{c}^\delta)_i} dx dt \\
 &+ \lambda \sum_{i=1}^n \int_0^T \int_\Omega (\Delta c_i^\delta)^2 dx dt \\
 &+ \frac{(\lambda_M - \lambda)^2}{2\lambda} \int_0^T \int_\Omega |P_L(\chi_\delta \mathbf{c}^\delta) R(\chi_\delta \mathbf{c}^\delta) \nabla \mu^\delta|^2 dx dt \\
 &\leq \mathcal{H}^\delta(\mathbf{c}^0) + \frac{(\lambda_M - \lambda)^2}{2\lambda_m\lambda} \mathcal{E}^\delta(\mathbf{c}^0), \tag{43}
 \end{aligned}$$

where λ satisfies $0 < \lambda < \lambda_m$, λ_m, λ_M are introduced in Lemma 4, and $R(\chi_\delta \mathbf{c}^\delta) = \text{diag}(\sqrt{\chi_\delta \mathbf{c}^\delta})$.

Proof. Summing (89) with $\sigma = 1$ over $k = 1, \dots, N$, we find that

$$\begin{aligned}
 \tilde{\mathcal{E}}^\delta(\tilde{\mathbf{c}}(\tau)(\cdot, T)) &+ \sum_{i,j=1}^{n-1} \int_0^T \int_\Omega \tilde{B}_{ij}^\delta(\tilde{\mathbf{c}}(\tau)) \nabla w_i^{(\tau)} \cdot \nabla w_j^{(\tau)} dx dt \\
 &+ \varepsilon \sum_{i=1}^n \int_0^T \int_\Omega ((\Delta w_i^{(\tau)})^2 + (w_i^{(\tau)})^2) dx dt \leq \tilde{\mathcal{E}}^\delta(\tilde{\mathbf{c}}^0).
 \end{aligned}$$

We know from (92) and the construction of χ_δ that $(\mathbf{w}^{(\tau)})$ is bounded in $L^2(0, T; H^1(\Omega))$ and $(\tilde{B}_{ij}^\delta(\tilde{\mathbf{c}}))$ is bounded in $L^\infty(Q_T)$ with respect to (ε, τ) . Therefore, we can pass to the limit $(\varepsilon, \tau) \rightarrow 0$ in the previous inequality, and weak lower semicontinuity of the integral functionals leads to (41).

To show (42), we use $(h_i^\delta)'(c_i^\delta) - (h_i^\delta)'(c_n^\delta)$ as a test function in the weak formulation of (82) and sum over $i = 1, \dots, n - 1$:

$$\mathcal{H}^\delta(\mathbf{c}(\cdot, T)) + \sum_{i,j=1}^{n-1} \int_0^T \int_\Omega \tilde{B}_{ij}^\delta(\tilde{\mathbf{c}}^\delta) \nabla((h_i^\delta)'(c_i^\delta) - (h_i^\delta)'(c_n^\delta)) \cdot \nabla w_j^\delta dx dt \leq \mathcal{H}^\delta(\mathbf{c}^0).$$

This inequality can be rewritten as (42) using $w_i^\delta = \mu_i^\delta - \mu_n^\delta$. Finally, we derive (43) by combining (42) and (41) and proceeding as in the proof of Lemma 5. ■

3.3. Proof of Theorem 1

We perform the limit $\delta \rightarrow 0$ to finish the proof of Theorem 1. It follows from [13, Lemma 2.1] that for sufficiently small $\delta > 0$, there exists $C > 0$ (independent of δ) such that for all $r_1, \dots, r_n \in \mathbb{R}$ satisfying $\sum_{i=1}^n r_i = 1$,

$$\sum_{i=1}^n h_i^\delta(r_i) \geq -C. \tag{44}$$

Therefore, estimate (43) implies that

$$\begin{aligned} & \sum_{i=1}^n \int_{\Omega} |\nabla c_i^\delta(\cdot, T)|^2 dx + \sum_{i=1}^n \int_0^T \int_{\Omega} \frac{|\nabla c_i^\delta|^2}{(\chi_\delta c^\delta)_i} dx dt + \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta c_i^\delta)^2 dx dt \\ & + \int_0^T \int_{\Omega} |P_L(\chi_\delta c^\delta) R(\chi_\delta c^\delta) \nabla \mu^\delta|^2 dx dt \leq C, \end{aligned} \tag{45}$$

and the constant $C > 0$ depends on λ_m, λ_M , and c^0 . Mass conservation (or using the test function $\phi_i = 1$ in the weak formulation of (35)) shows that $\int_{\Omega} c_i^\delta(\cdot, T) dx = \int_{\Omega} c_0^\delta dx$ for any $T > 0$, i.e., $\|c^\delta\|_{L^\infty(0,T;L^1(\Omega))} \leq C$. We conclude from the Poincaré–Wirtinger inequality that

$$\|c^\delta\|_{L^\infty(0,T;H^1(\Omega))} + \|c^\delta\|_{L^2(0,T;H^2(\Omega))} \leq C. \tag{46}$$

Next, we estimate $\partial_t c_i^\delta$. Lemma 7 implies that the entries of

$$(D(\chi_\delta c^\delta) P_L(\chi_\delta c^\delta) + P_{L^\perp}(\chi_\delta c^\delta))^{-1}$$

are uniformly bounded. Thus, by the definition of $D^{\text{BD}}(\chi_\delta c^\delta)$ and (27),

$$\int_0^T \int_{\Omega} \left| \sum_{j=1}^n B_{ij}^\delta(c^\delta) \nabla \mu_j^\delta \right|^2 dx dt \leq \lambda_M \int_0^T \int_{\Omega} |P_L(\chi_\delta c^\delta) R(\chi_\delta c^\delta) \nabla \mu^\delta|^2 dx dt,$$

and the right-hand side is bounded by (45). Setting $J_i^\delta := \sum_{j=1}^n B_{ij}^\delta(c^\delta) \nabla \mu_j^\delta$, this means that (J_i^δ) is bounded in $L^2(Q_T)$. Therefore, there exists a subsequence that is not relabeled such that, as $\delta \rightarrow 0$,

$$J_i^\delta \rightharpoonup J_i \text{ weakly in } L^2(Q_T).$$

This implies that

$$\|\partial_t c_i^\delta\|_{L^2(0,T;H^1(\Omega)')} \leq C. \tag{47}$$

We conclude from (46) and (47), using the Aubin–Lions lemma, that, for a subsequence (if necessary),

$$\begin{aligned} c_i^\delta &\rightarrow c_i && \text{strongly in } L^2(0, T; H^1(\Omega)), \\ c_i^\delta &\overset{*}{\rightharpoonup} c_i && \text{weakly-}\star \text{ in } L^\infty(0, T; H^1(\Omega)), \\ c_i^\delta &\rightharpoonup c_i && \text{weakly in } L^2(0, T; H^2(\Omega)), \\ \partial_t c_i^\delta &\rightharpoonup \partial_t c_i && \text{weakly in } L^2(0, T; H^1(\Omega)'). \end{aligned} \tag{48}$$

Performing the limit $\delta \rightarrow 0$ in (35), we see that $\partial_t c_i = \text{div } J_i$ holds in the sense of $L^2(0, T; H^1(\Omega)')$.

We prove that $c_i \geq 0$ in Q_T , $i = 1, \dots, n$, following [13]. By definition (37) and the lower bound (44), we have for $0 < \delta < 1$,

$$\begin{aligned} C &\geq \int_{\Omega} h_i^\delta(c_i^\delta) dx \\ &\geq -C + \int_{\{c_i^\delta < \delta\}} \left(c_i^\delta \log \delta - \frac{\delta}{2} + \frac{(c_i^\delta)^2}{2\delta} \right) dx \\ &\geq -C + \int_{\{c_i^\delta < 0\}} c_i^\delta \log \delta dx + \int_{\{0 < c_i^\delta < \delta\}} c_i^\delta \log \delta dx - C\delta \\ &\geq -C + \log \delta \int_{\{c_i^\delta < 0\}} c_i^\delta dx + C\delta \log \delta - C\delta. \end{aligned}$$

Hence, we obtain

$$\int_{\Omega} \max\{0, -c_i^\delta\} dx = \int_{\{c_i^\delta < 0\}} |c_i^\delta| dx \leq \frac{C}{|\log \delta|}.$$

The limit $\delta \rightarrow 0$ leads to

$$\int_{\Omega} \max\{0, -c_i\} dx \leq 0,$$

implying that $c_i \geq 0$ in Q_T . The limit $\delta \rightarrow 0$ in $\sum_{i=1}^n c_i^\delta = 1$ gives $\sum_{i=1}^n c_i = 1$, hence $c_i \leq 1$ holds in Q_T .

Next, we identify J_i by showing that $J_i = \sum_{j=1}^n B_{ij}(c) \nabla(\log c_j - \Delta c_j)$ in the sense of distributions. Inserting the definition of μ_i^δ and choosing a test function $\phi_i \in L^\infty(0, T; W^{2,\infty}(\Omega))$ satisfying $\nabla \phi_i \cdot \nu = 0$ on $\partial\Omega$, we find that

$$\begin{aligned} &\int_0^T \int_{\Omega} J_i^\delta \cdot \nabla \phi_i dx dt \\ &= \sum_{j=1}^n \int_0^T \int_{\Omega} B_{ij}^\delta(c^\delta) \nabla \phi_i \cdot \nabla((h_j^\delta)'(c_j^\delta) - \Delta c_j^\delta) dx dt \\ &= \sum_{j=1}^n \int_0^T \int_{\Omega} B_{ij}^\delta(c^\delta) \nabla \phi_i \cdot \nabla(h_j^\delta)'(c_j^\delta) dx dt \\ &\quad + \sum_{j=1}^n \int_0^T \int_{\Omega} \Delta c_j^\delta \operatorname{div}(B_{ij}^\delta(c^\delta) \nabla \phi_i) dx dt \\ &=: I_5 + I_6. \end{aligned} \tag{49}$$

By definition (34) of $B_{ij}^\delta(c^\delta)$, we have

$$I_5 = \sum_{j=1}^n \int_0^T \int_{\Omega} \sqrt{(\chi_\delta c^\delta)_i} D_{ij}^{\text{BD}}(\chi_\delta c^\delta) \nabla \phi_i \cdot \frac{\nabla c_j^\delta}{\sqrt{(\chi_\delta c^\delta)_j}} dx dt.$$

Lemma 4 shows that $\sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c})/\sqrt{c_j}$ is bounded in $[0, 1]^n$ and in particular when $c_k = 0$ for some index k . The strong convergence $\mathbf{c}^\delta \rightarrow \mathbf{c}$ implies that $\chi_\delta \mathbf{c}^\delta \rightarrow \mathbf{c}$ in $L^q(0, T; L^q(\Omega))$ for any $q < \infty$ such that

$$\begin{aligned} I_5 &\rightarrow \sum_{j=1}^n \int_0^T \int_\Omega \sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c}) \frac{1}{\sqrt{c_j}} \nabla \phi_i \cdot \nabla c_j \, dx \, dt \\ &= \sum_{j=1}^n \int_0^T \int_\Omega B_{ij}(\mathbf{c}) \nabla \phi_i \cdot \nabla \log c_j \, dx \, dt. \end{aligned}$$

The limit in I_6 is more involved. We decompose $I_6 = I_{61} + I_{62}$, where

$$\begin{aligned} I_{61} &= \sum_{j=1}^n \int_0^T \int_\Omega \Delta c_j^\delta B_{ij}^\delta(\mathbf{c}^\delta) \Delta \phi_i \, dx \, dt, \\ I_{62} &= \sum_{j=1}^n \int_0^T \int_\Omega \Delta c_j^\delta \nabla B_{ij}^\delta(\mathbf{c}^\delta) \cdot \nabla \phi_i \, dx \, dt. \end{aligned}$$

We deduce from the strong convergence of \mathbf{c}^δ and the weak convergence of Δc_j^δ that

$$I_{61} \rightarrow \sum_{j=1}^n \int_0^T \int_\Omega \Delta c_j B_{ij}(\mathbf{c}) \Delta \phi_i \, dx \, dt.$$

To show the convergence of I_{62} , we consider

$$\begin{aligned} &\int_0^T \int_\Omega |\nabla(B_{ij}^\delta(\mathbf{c}^\delta) - B_{ij}(\mathbf{c}))|^2 \, dx \, dt \\ &= \int_0^T \int_\Omega \left| \sum_{k=1}^n \left\{ \left(\frac{\partial B_{ij}^\delta}{\partial c_k}(\mathbf{c}^\delta) - \frac{\partial B_{ij}}{\partial c_k}(\mathbf{c}) \right) \nabla c_k + \frac{\partial B_{ij}^\delta}{\partial c_k}(\mathbf{c}^\delta) \nabla (c_k^\delta - c_k) \right\} \right|^2 \, dx \, dt. \end{aligned}$$

By Lemma 4(i), $\partial D_{ij}^{\text{BD}}/\partial c_k$ exists and is bounded in $[0, 1]^n$. Then, by the definition of $B_{ij}(\mathbf{c})$, we have $(\partial B_{ij}^\delta/\partial c_k)(\mathbf{c}^\delta) \rightarrow (\partial B_{ij}/\partial c_k)(\mathbf{c})$ strongly in $L^2(Q_T)$. It follows from $\nabla c_k^\delta \rightarrow \nabla c_k$ strongly in $L^2(Q_T)$ that the right-hand side of the previous identity converges to zero. We infer that

$$I_{62} \rightarrow \sum_{j=1}^n \int_0^T \int_\Omega \Delta c_j \nabla B_{ij}(\mathbf{c}) \cdot \nabla \phi_i \, dx \, dt.$$

Consequently, we have

$$\begin{aligned} I_6 &\rightarrow \sum_{j=1}^n \int_0^T \int_\Omega \Delta c_j (B_{ij}(\mathbf{c}) \Delta \phi_i + \nabla B_{ij}(\mathbf{c}) \cdot \nabla \phi_i) \, dx \, dt \\ &= \sum_{j=1}^n \int_0^T \int_\Omega \Delta c_j \operatorname{div}(B_{ij}(\mathbf{c}) \nabla \phi_i) \, dx \, dt. \end{aligned}$$

We have shown that (49) becomes in the limit $\delta \rightarrow 0$

$$\begin{aligned} & \int_0^T \int_{\Omega} J_i \cdot \nabla \phi \, dx \, dt \\ &= \sum_{j=1}^n \int_0^T \int_{\Omega} (B_{ij}(\mathbf{c}) \nabla \phi_i \cdot \nabla \log c_j + \Delta c_j \operatorname{div}(B_{ij}(\mathbf{c}) \nabla \phi_i)) \, dx \, dt \end{aligned}$$

and hence, in the sense of distributions,

$$J_i = \sum_{j=1}^n B_{ij}(\mathbf{c}) \nabla (\log c_j - \Delta c_j), \quad i = 1, \dots, n.$$

Step 2: Energy and entropy inequalities. The limit $c_i^\delta \rightharpoonup c_i$ weakly- \star in $L^\infty(0, T; H^1(\Omega))$ (see (48)) and the weak lower semicontinuity of the energy and entropy show that

$$\begin{aligned} \mathcal{H}(\mathbf{c}(\cdot, T)) &\leq \liminf_{\delta \rightarrow 0} \mathcal{H}^\delta(\mathbf{c}^\delta(\cdot, T)), \\ \mathcal{E}(\mathbf{c}(\cdot, T)) &\leq \liminf_{\delta \rightarrow 0} \mathcal{E}^\delta(\mathbf{c}^\delta(\cdot, T)). \end{aligned}$$

Moreover, because of the weak convergence of Δc_i^δ in $L^2(Q_T)$ from (48),

$$\sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta c_i)^2 \, dx \, dt \leq \liminf_{\delta \rightarrow 0} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta c_i^\delta)^2 \, dx \, dt.$$

The combined energy–entropy inequality (43) and the property $|\nabla(\chi_\delta \mathbf{c}^\delta)_i| \leq |\nabla c_i^\delta|$ give

$$\|\nabla \sqrt{(\chi_\delta \mathbf{c}^\delta)_i}\|_{L^2(Q_T)} = \frac{1}{2} \left\| \frac{\nabla c_i^\delta}{\sqrt{(\chi_\delta \mathbf{c}^\delta)_i}} \right\|_{L^2(Q_T)} \leq C,$$

which, together with $(\chi_\delta \mathbf{c}^\delta)_i \rightarrow c_i$ strongly in $L^2(Q_T)$, leads to

$$\nabla \sqrt{(\chi_\delta \mathbf{c}^\delta)_i} \rightharpoonup \nabla \sqrt{c_i} \quad \text{weakly in } L^2(Q_T). \tag{50}$$

We conclude that

$$\|\nabla \sqrt{c_i}\|_{L^2(Q_T)} \leq \liminf_{\delta \rightarrow 0} \|\nabla \sqrt{(\chi_\delta \mathbf{c}^\delta)_i}\|_{L^2(Q_T)}.$$

Finally, by (43), we observe that $P_L(\chi_\delta \mathbf{c}^\delta)R(\chi_\delta \mathbf{c}^\delta)\nabla \mu^\delta$ is uniformly bounded in $L^2(Q_T)$ such that, up to a subsequence,

$$P_L(\chi_\delta \mathbf{c}^\delta)R(\chi_\delta \mathbf{c}^\delta)\nabla \mu^\delta \rightharpoonup \xi \quad \text{weakly in } L^2(Q_T).$$

Hence, again by weak lower semicontinuity of the norm,

$$\|\xi\|_{L^2(0,T;L^2(\Omega))} \leq \liminf_{\delta \rightarrow 0} \|P_L(\chi_\delta \mathbf{c}^\delta)R(\chi_\delta \mathbf{c}^\delta)\nabla \mu^\delta\|_{L^2(0,T;L^2(\Omega))}.$$

It remains to take the limit inferior $\delta \rightarrow 0$ in (43) to conclude that the combined energy–entropy inequality (13) holds.

Lemma 9 (Identification of ξ). *Let the regularity condition (16) hold and let ξ be the weak $L^2(Q_T)$ limit of $P_L(\chi_\delta \mathbf{c}^\delta)R(\chi_\delta \mathbf{c}^\delta)\nabla\mu^\delta$. Then $\xi = P_L(\mathbf{c})R(\mathbf{c})\nabla\mu$.*

Proof. Let $\phi_i \in C_0^\infty(Q_T)$ be a test function. Then, inserting the definition $\mu_j^\delta = (h_j^\delta)'(c_j^\delta) - \Delta c_j^\delta$ and integrating by parts,

$$\begin{aligned} & \sum_{j=1}^n \int_0^T \int_\Omega (P_L(\chi_\delta \mathbf{c}^\delta)_{ij} \sqrt{(\chi_\delta \mathbf{c}^\delta)_j} \nabla \mu_j^\delta - P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \mu_j) \cdot \nabla \phi_i \, dx \, dt \\ &= \sum_{j=1}^n \int_0^T \int_\Omega (P_L(\chi_\delta \mathbf{c}^\delta)_{ij} \sqrt{(\chi_\delta \mathbf{c}^\delta)_j} \nabla (h_j^\delta)'(c_j^\delta) - P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log c_j) \cdot \nabla \phi_i \, dx \, dt \\ &+ \sum_{j=1}^n \int_0^T \int_\Omega \operatorname{div} \{ (P_L(\chi_\delta \mathbf{c}^\delta)_{ij} \sqrt{(\chi_\delta \mathbf{c}^\delta)_j} - P_L(\mathbf{c})_{ij} \sqrt{c_j}) \nabla \phi_i \} \Delta c_j^\delta \, dx \, dt \\ &+ \sum_{j=1}^n \int_0^T \int_\Omega \operatorname{div} (P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \phi_i) \Delta (c_j^\delta - c_j) \, dx \, dt. \end{aligned} \quad (51)$$

The bracket in the first integral on the right-hand side can be written as

$$\begin{aligned} & P_L(\chi_\delta \mathbf{c}^\delta)_{ij} \sqrt{(\chi_\delta \mathbf{c}^\delta)_j} \nabla (h_j^\delta)'(c_j^\delta) - P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log c_j \\ &= P_L(\chi_\delta \mathbf{c}^\delta)_{ij} \frac{\nabla c_j^\delta}{\sqrt{(\chi_\delta \mathbf{c}^\delta)_j}} - P_L(\mathbf{c})_{ij} \frac{\nabla c_j}{\sqrt{c_j}}. \end{aligned}$$

Thanks to the convergences (48) and (50), we can pass to the limit $\delta \rightarrow 0$ in (51):

$$\lim_{\delta \rightarrow 0} \sum_{j=1}^n \int_0^T \int_\Omega (P_L(\chi_\delta \mathbf{c}^\delta)_{ij} \sqrt{(\chi_\delta \mathbf{c}^\delta)_j} \nabla \mu_j^\delta - P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \mu_j) \cdot \nabla \phi_i \, dx \, dt = 0.$$

By the uniqueness of the limit, the claim $\xi = P_L(\mathbf{c})R(\mathbf{c})\nabla\mu$ follows. \blacksquare

4. Proof of Theorem 2

In this section, we prove the weak–strong uniqueness property. First, we compute a combined *relative energy–entropy inequality*. Then we use this inequality to derive a stability estimate, which leads to the desired weak–strong uniqueness result.

4.1. Evolution of the relative energy and entropy

We start by calculating the time evolution of the relative entropy (14) and the relative energy (15) for *smooth* solutions \mathbf{c} and $\bar{\mathbf{c}}$. Inserting (25) and integrating by parts leads to

$$\begin{aligned} \frac{d\mathcal{H}}{dt}(\mathbf{c}|\bar{\mathbf{c}}) &= \sum_{i=1}^n \int_{\Omega} \left(\log \frac{c_i}{\bar{c}_i} \partial_t c_i - \left(\frac{c_i}{\bar{c}_i} - 1 \right) \partial_t \bar{c}_i \right) dx \\ &= - \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \mu_j dx \\ &\quad + \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\bar{\mathbf{c}}) \nabla \left(\frac{c_i}{\bar{c}_i} \right) \cdot \nabla \bar{\mu}_j dx \\ &= - \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla (\mu_j - \bar{\mu}_j) dx \\ &\quad - \sum_{i,j=1}^n \int_{\Omega} \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \bar{\mu}_j dx. \end{aligned}$$

Next, we compute

$$\begin{aligned} \frac{d\mathcal{E}}{dt}(\mathbf{c}|\bar{\mathbf{c}}) &= \sum_{i=1}^n \int_{\Omega} \left(\log \frac{c_i}{\bar{c}_i} \partial_t c_i - \left(\frac{c_i}{\bar{c}_i} - 1 \right) \partial_t \bar{c}_i \right) dx \\ &\quad + \sum_{i=1}^n \int_{\Omega} \nabla (c_i - \bar{c}_i) \cdot \nabla \partial_t (c_i - \bar{c}_i) dx \\ &= \sum_{i=1}^n \int_{\Omega} \left\{ \left(\log \frac{c_i}{\bar{c}_i} - \Delta (c_i - \bar{c}_i) \right) \partial_t c_i - \left(\frac{c_i}{\bar{c}_i} - 1 - \Delta (c_i - \bar{c}_i) \right) \partial_t \bar{c}_i \right\} dx \\ &= - \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla (\mu_i - \bar{\mu}_i) \cdot \nabla \mu_j dx \\ &\quad + \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\bar{\mathbf{c}}) \nabla \left(\frac{c_i}{\bar{c}_i} - 1 - \Delta (c_i - \bar{c}_i) \right) \cdot \nabla \bar{\mu}_j dx. \tag{52} \end{aligned}$$

We add and subtract the expression $\sum_{i=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla (\mu_i - \bar{\mu}_i) \cdot \nabla \bar{\mu}_j dx$:

$$\begin{aligned} \frac{d\mathcal{E}}{dt}(\mathbf{c}|\bar{\mathbf{c}}) &= - \sum_{i=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla (\mu_i - \bar{\mu}_i) \cdot \nabla (\mu_j - \bar{\mu}_j) dx \\ &\quad + \sum_{i,j=1}^n \int_{\Omega} \left\{ B_{ij}(\bar{\mathbf{c}}) \left(\frac{c_i}{\bar{c}_i} \nabla \log \frac{c_i}{\bar{c}_i} - \nabla \Delta (c_i - \bar{c}_i) \right) \right. \\ &\quad \left. - B_{ij}(\mathbf{c}) \nabla (\mu_i - \bar{\mu}_i) \right\} \cdot \nabla \bar{\mu}_j dx \end{aligned}$$

$$\begin{aligned}
 &= - \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla(\mu_j - \bar{\mu}_j) \, dx \\
 &\quad - \sum_{i,j=1}^n \int_{\Omega} \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \bar{\mu}_j \, dx \\
 &\quad + \sum_{i,j=1}^n \int_{\Omega} B_{ij}(\bar{\mathbf{c}}) \left(\frac{c_i}{\bar{c}_i} - 1 \right) \nabla \Delta(c_i - \bar{c}_i) \cdot \nabla \bar{\mu}_j \, dx. \tag{53}
 \end{aligned}$$

We want to reformulate the expression $\bar{c}_i^{-1}(c_i - \bar{c}_i) \nabla \Delta(c_i - \bar{c}_i)$ in the last integral. For this, we observe that for any smooth function f , it holds that

$$\begin{aligned}
 f \nabla \Delta f &= \nabla(f \Delta f) - \nabla f \Delta f \\
 &= \nabla(\operatorname{div}(f \nabla f) - |\nabla f|^2) - \operatorname{div}(\nabla f \otimes \nabla f) + \frac{1}{2} \nabla |\nabla f|^2 \\
 &= \nabla \operatorname{div}(f \nabla f) - \frac{1}{2} \nabla |\nabla f|^2 - \operatorname{div}(\nabla f \otimes \nabla f).
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 (c_i - \bar{c}_i) \nabla \Delta(c_i - \bar{c}_i) &= \nabla \operatorname{div}((c_i - \bar{c}_i) \nabla(c_i - \bar{c}_i)) - \frac{1}{2} \nabla |\nabla(c_i - \bar{c}_i)|^2 \\
 &\quad - \operatorname{div}(\nabla(c_i - \bar{c}_i) \otimes \nabla(c_i - \bar{c}_i)).
 \end{aligned}$$

Inserting this expression into the last term of (53) and integrating by parts, we find that

$$\begin{aligned}
 \frac{d\mathcal{E}}{dt}(\mathbf{c}|\bar{\mathbf{c}}) &= - \sum_{i=1}^n \int_{\Omega} B_{ij}(\mathbf{c}) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla(\mu_j - \bar{\mu}_j) \, dx \\
 &\quad - \sum_{i,j=1}^n \int_{\Omega} \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \bar{\mu}_j \, dx \\
 &\quad + \sum_{i,j=1}^n \int_{\Omega} (c_i - \bar{c}_i) \nabla(c_i - \bar{c}_i) \cdot \nabla \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx \\
 &\quad + \frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} |\nabla(c_i - \bar{c}_i)|^2 \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx \\
 &\quad + \sum_{i,j=1}^n \int_{\Omega} \nabla(c_i - \bar{c}_i) \otimes \nabla(c_i - \bar{c}_i) : \nabla \otimes \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx,
 \end{aligned}$$

where $\nabla \otimes (\bar{c}_i^{-1} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j)$ is a matrix with entries $\partial_{x_k} (\bar{c}_i^{-1} B_{ij}(\bar{\mathbf{c}}) \partial_{x_\ell} \bar{\mu}_j)$ for $k, \ell = 1, \dots, n$ and “:” denotes the Frobenius matrix product.

The following lemma states the rigorous result. Since we suppose that the weak solution satisfies energy and entropy *inequalities* instead of *equalities*, we obtain also inequalities for the relative energy and entropy.

Lemma 10 (Relative energy and entropy). *Let \mathbf{c} and $\bar{\mathbf{c}}$ be a weak and strong solution to (1)–(5) with initial data \mathbf{c}^0 and $\bar{\mathbf{c}}^0$, respectively. Assume that \mathbf{c} satisfies the regularity (16) and the energy and entropy inequalities (17)–(18). Furthermore, we suppose that $\bar{\mathbf{c}}$ is strictly positive and satisfies the regularity*

$$\begin{aligned} \bar{\mu}_i &= \log \bar{c}_i - \Delta \bar{c}_i \in L^2_{\text{loc}}(0, \infty; H^2(\Omega)), \\ \bar{c}_i &\in L^\infty_{\text{loc}}(0, \infty; W^{3,\infty}(\Omega)), \quad i = 1, \dots, n. \end{aligned}$$

Then the following relative energy and entropy inequalities hold for any $T > 0$:

$$\begin{aligned} &\mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \sum_{i=1}^n \int_0^T \int_\Omega B_{ij}(\mathbf{c}) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla(\mu_j - \bar{\mu}_j) \, dx \, dt \\ &\leq \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) - \sum_{i,j=1}^n \int_0^T \int_\Omega \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \bar{\mu}_j \, dx \, dt \\ &\quad + \sum_{i,j=1}^n \int_0^T \int_\Omega (c_i - \bar{c}_i) \nabla(c_i - \bar{c}_i) \cdot \nabla \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx \, dt \\ &\quad + \frac{1}{2} \sum_{i,j=1}^n \int_0^T \int_\Omega |\nabla(c_i - \bar{c}_i)|^2 \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx \, dt \\ &\quad + \sum_{i,j=1}^n \int_0^T \int_\Omega \nabla(c_i - \bar{c}_i) \otimes \nabla(c_i - \bar{c}_i) : \nabla \otimes \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx \, dt, \quad (54) \end{aligned}$$

$$\begin{aligned} \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) &\leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ &\quad - \sum_{i,j=1}^n \int_0^T \int_\Omega B_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla(\mu_j - \bar{\mu}_j) \, dx \, dt \\ &\quad - \sum_{i,j=1}^n \int_0^T \int_\Omega \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \bar{\mu}_j \, dx \, dt. \quad (55) \end{aligned}$$

The integrals in (54) and (55) are well defined because of the regularity properties for weak solutions \mathbf{c} and the regularity assumptions on the strong solution $\bar{\mathbf{c}}$. Indeed, we have $B_{ij}(\mathbf{c}) \nabla \mu_j \in L^2(Q_T)$ (see (22)), $B_{ij}(\mathbf{c}) \nabla \log c_i = 2D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{\bar{c}_j} \nabla \sqrt{c_i} \in L^2(Q_T)$ (see (13)), and using definition (8), assumption (16), and Lemma 4 (i), we have

$$\begin{aligned} &B_{ij}(\mathbf{c}) \nabla \mu_i \cdot \nabla \mu_j \\ &= D_{ij}^{\text{BD}}(\mathbf{c}) (2\nabla \sqrt{c_i} - \sqrt{c_i} \nabla \Delta c_i) \cdot (2\nabla \sqrt{c_j} - \sqrt{c_j} \nabla \Delta c_j) \in L^1(Q_T). \end{aligned}$$

Proof of Lemma 10. The relative energy and entropy inequalities are proved from the weak formulation of (1) by choosing suitable test functions. For this, we observe that, by (12), $c_i - \bar{c}_i$ satisfies

$$\begin{aligned}
 0 &= \int_0^\infty \int_\Omega (c_i - \bar{c}_i) \partial_t \phi_i \, dx \, dt \\
 &\quad + \int_\Omega (c_i^0(x) - \bar{c}_i^0(x)) \phi_i(x, 0) \, dx \\
 &\quad - \sum_{j=1}^n \int_0^\infty \int_\Omega (B_{ij}(\mathbf{c}) \nabla \log c_j - B_{ij}(\bar{\mathbf{c}}) \nabla \log \bar{c}_j) \cdot \nabla \phi_i \, dx \, dt \\
 &\quad - \sum_{j=1}^n \int_0^\infty \int_\Omega (\operatorname{div}(B_{ij}(\mathbf{c}) \nabla \phi_i) \Delta c_j - \operatorname{div}(B_{ij}(\bar{\mathbf{c}}) \nabla \phi_i) \Delta \bar{c}_j) \, dx \, dt. \tag{56}
 \end{aligned}$$

By density, this formulation also holds for $\phi_i = \bar{\mu}_i \theta_\varepsilon(t)$, where

$$\theta_\varepsilon(t) = \begin{cases} 1 & \text{for } 0 \leq t \leq T, \\ \frac{(T-t)}{\varepsilon} + 1 & \text{for } T < t < T + \varepsilon, \\ 0 & \text{for } t \geq T + \varepsilon. \end{cases}$$

Then, passing to the limit $\varepsilon \rightarrow 0$ and summing over $i = 1, \dots, n$, we arrive at

$$\begin{aligned}
 &\sum_{i=1}^n \int_\Omega (c_i - \bar{c}_i) \bar{\mu}_i \, dx \Big|_0^T \\
 &= \sum_{i=1}^n \int_0^T \langle \partial_t \bar{\mu}_i, c_i - \bar{c}_i \rangle \, dt \\
 &\quad - \sum_{i,j=1}^n \int_0^T \int_\Omega (B_{ij}(\mathbf{c}) \nabla \log c_j \cdot \nabla \bar{\mu}_i + \operatorname{div}(B_{ij}(\mathbf{c}) \nabla \bar{\mu}_i) \Delta c_j) \, dx \, dt \\
 &\quad + \sum_{i,j=1}^n \int_0^T \int_\Omega (B_{ij}(\bar{\mathbf{c}}) \nabla \log \bar{c}_j \cdot \nabla \bar{\mu}_i + \operatorname{div}(B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_i) \Delta \bar{c}_j) \, dx \, dt \\
 &=: I_7 + I_8 + I_9,
 \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the duality bracket between $H^1(\Omega)'$ and $H^1(\Omega)$. This product is well defined, since it holds in the sense of $H^1(\Omega)'$ that

$$\partial_t \bar{\mu}_i = \partial_t (\log \bar{c}_i - \Delta \bar{c}_i) = \sum_{j=1}^n \frac{1}{\bar{c}_i} \operatorname{div}(B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j) - \sum_{j=1}^n \Delta \operatorname{div}(B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j).$$

Inserting this expression into I_7 , the dual product can be written as an integral:

$$\begin{aligned}
 I_7 &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(\bar{c}) \nabla \left(\frac{c_i}{\bar{c}_i} - 1 \right) \cdot \nabla \bar{\mu}_j + \Delta(c_i - \bar{c}_i) \operatorname{div}(B_{ij}(\bar{c}) \nabla \bar{\mu}_j) \right) dx dt \\
 &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\bar{c}) \nabla \left(\frac{c_i}{\bar{c}_i} - 1 \right) \cdot \nabla \bar{\mu}_j dx dt \\
 &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \bar{c}_i \Delta(c_i - \bar{c}_i) \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{c}) \nabla \bar{\mu}_j \right) dx dt \\
 &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \frac{1}{\bar{c}_i} B_{ij}(\bar{c}) \Delta(c_i - \bar{c}_i) \nabla \bar{c}_i \cdot \nabla \bar{\mu}_j dx dt.
 \end{aligned}$$

Replacing Δc_j by $\log c_j - \mu_j$ in I_8 and integrating by parts in the term involving the divergence, some terms cancel and we find that

$$\begin{aligned}
 I_8 &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(c) \nabla \bar{\mu}_i \cdot \nabla \log c_j + \operatorname{div}(B_{ij}(c) \nabla \bar{\mu}_i) (\log c_j - \mu_j) \right) dx dt \\
 &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(c) \nabla \bar{\mu}_i \cdot \nabla \mu_j dx dt.
 \end{aligned}$$

Assumption (16) guarantees that the flux has the regularity

$$\sum_{j=1}^n B_{ij}(c) \nabla \mu_j \in L^2(Q_T)$$

such that the last integral is defined. The remaining term I_9 is reformulated in a similar way, leading to

$$I_9 = \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\bar{c}) \nabla \bar{\mu}_i \cdot \nabla \bar{\mu}_j dx dt.$$

It follows from the definition of the relative energy, inequality (17) for $\mathcal{E}(c)$, and identity (19) for $\mathcal{E}(\bar{c})$ that

$$\begin{aligned}
 &\mathcal{E}(c(T)|\bar{c}(T)) - \mathcal{E}(c^0|\bar{c}^0) \\
 &= (\mathcal{E}(c(T)) - \mathcal{E}(c^0)) - (\mathcal{E}(\bar{c}(T)) - \mathcal{E}(\bar{c}^0)) - \int_{\Omega} \bar{\mu} \cdot (c - \bar{c}) dx \Big|_0^T \\
 &\leq - \sum_{i,j=1}^n \int_0^T \int_{\Omega} (B_{ij}(c) \nabla \mu_i \cdot \nabla \mu_j - B_{ij}(\bar{c}) \nabla \bar{\mu}_i \cdot \nabla \bar{\mu}_j) dx dt \\
 &\quad - (I_7 + I_8 + I_9)
 \end{aligned}$$

$$\begin{aligned}
 &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\mathbf{c}) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \mu_j \, dx \, dt \\
 &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} B_{ij}(\bar{\mathbf{c}}) \nabla\left(\frac{c_i}{\bar{c}_i} - 1\right) \cdot \nabla \bar{\mu}_j \, dx \, dt \\
 &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \bar{c}_i \Delta(c_i - \bar{c}_i) \operatorname{div}\left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j\right) \, dx \, dt \\
 &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \Delta(c_i - \bar{c}_i) \nabla \bar{c}_i \cdot \nabla \bar{\mu}_j \, dx \, dt.
 \end{aligned}$$

This inequality is just a reformulation of (52), which leads, by proceeding as in (53) and the subsequent calculations, to (54).

Next, we verify the relative entropy inequality. Taking the test function $\phi_i = (\log \bar{c}_i) \theta_\varepsilon(t)$ in (56), passing to the limit $\varepsilon \rightarrow 0$, and summing over $i = 1, \dots, n$ leads to

$$\begin{aligned}
 \sum_{i=1}^n \int_{\Omega} (c_i - \bar{c}_i) \log \bar{c}_i \, dx \Big|_0^T &= \sum_{i=1}^n \int_0^T \int_{\Omega} (c_i - \bar{c}_i) \partial_t (\log \bar{c}_i) \, dx \, dt \\
 &\quad - \sum_{j=1}^n \int_0^\infty \int_{\Omega} (B_{ij}(\mathbf{c}) \nabla \log c_j - B_{ij}(\bar{\mathbf{c}}) \nabla \log \bar{c}_j) \cdot \nabla \log \bar{c}_i \, dx \, dt \\
 &\quad - \sum_{j=1}^n \int_0^\infty \int_{\Omega} (\operatorname{div}(B_{ij}(\mathbf{c}) \nabla \log \bar{c}_i) \Delta c_j - \operatorname{div}(B_{ij}(\bar{\mathbf{c}}) \nabla \log \bar{c}_i) \Delta \bar{c}_j) \, dx \, dt.
 \end{aligned}$$

This yields, together with (18), (20), an integration by parts, and regularity assumption (16), that

$$\begin{aligned}
 &\mathcal{H}(\mathbf{c}(T) | \bar{\mathbf{c}}(T)) - \mathcal{H}(\mathbf{c}^0 | \bar{\mathbf{c}}^0) \\
 &= (\mathcal{H}(\mathbf{c}(T)) - \mathcal{H}(\mathbf{c}^0)) - (\mathcal{H}(\bar{\mathbf{c}}(T)) - \mathcal{H}(\bar{\mathbf{c}}^0)) - \int_{\Omega} (\mathbf{c} - \bar{\mathbf{c}}) \cdot \log \bar{\mathbf{c}} \, dx \Big|_0^T \\
 &\leq - \sum_{i,j=1}^n \int_0^T \int_{\Omega} (B_{ij}(\mathbf{c}) \nabla \log c_i \cdot \nabla \mu_j - B_{ij}(\bar{\mathbf{c}}) \nabla \log \bar{c}_i \cdot \nabla \bar{\mu}_j) \, dx \, dt \\
 &\quad - \sum_{i=1}^n \int_0^T \int_{\Omega} (c_i - \bar{c}_i) \partial_t (\log \bar{c}_i) \, dx \, dt \\
 &\quad + \sum_{i,j=1}^n \int_0^\infty \int_{\Omega} (B_{ij}(\mathbf{c}) \nabla \mu_j \cdot \nabla \log \bar{c}_i - B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \cdot \nabla \log \bar{c}_i) \, dx \, dt \\
 &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(\mathbf{c}) \nabla \mu_j \cdot \nabla \left(\log \frac{c_i}{\bar{c}_i} \right) - \nabla \left(\frac{c_i}{\bar{c}_i} - 1 \right) \cdot B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) \, dx \, dt,
 \end{aligned}$$

which readily gives (55). ■

4.2. Proof of the weak–strong uniqueness property

We proceed with the proof of Theorem 2. First, we estimate the relative entropy inequality (55) and then the relative energy inequality (54). A combination of both estimates shows (21), which proves the weak–strong uniqueness property.

Step 1: Estimating the relative entropy. As in the proof of Lemma 5, we decompose the matrix $B(\mathbf{c})$ by setting $M(\mathbf{c}) := B(\mathbf{c}) - \lambda G(\mathbf{c})$ such that $B(\mathbf{c}) = M(\mathbf{c}) + \lambda G(\mathbf{c})$, where $G(\mathbf{c}) = R(\mathbf{c})P_L(\mathbf{c})R(\mathbf{c})$ has the entries $G_{ij}(\mathbf{c}) = c_i\delta_{ij} - c_i c_j$ and $0 < \lambda < \lambda_m$. In terms of these matrices, we can formulate (55) as

$$\begin{aligned} & \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) - \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ & \leq - \sum_{i,j=1}^n \int_0^T \int_{\Omega} M_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla (\mu_j - \bar{\mu}_j) \, dx \, dt \\ & \quad - \lambda \sum_{i,j=1}^n \int_0^T \int_{\Omega} G_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla (\mu_j - \bar{\mu}_j) \, dx \, dt \\ & \quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \bar{\mu}_j \, dx \, dt \\ & =: I_{10} + I_{11} + I_{12}. \end{aligned} \tag{57}$$

Step 1a: Estimate of I_{10} . We know from (31) and (32) that $M(\mathbf{c})$ is positive semidefinite and satisfies

$$\mathbf{z}^\top M(\mathbf{c}) \mathbf{z} \leq (\lambda_M - \lambda) |P_L(\mathbf{c})R(\mathbf{c})\mathbf{z}|^2$$

for all $\mathbf{z} \in \mathbb{R}^n$. Therefore, using Young’s inequality with $\theta > 0$,

$$\begin{aligned} I_{10} & \leq \frac{\theta}{4} \sum_{i,j=1}^n \int_0^T \int_{\Omega} M_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \log \frac{c_j}{\bar{c}_j} \, dx \, dt \\ & \quad + \frac{1}{\theta} \sum_{i,j=1}^n \int_0^T \int_{\Omega} M_{ij}(\mathbf{c}) \nabla (\mu_i - \bar{\mu}_i) \cdot \nabla (\mu_j - \bar{\mu}_j) \, dx \, dt \\ & \leq \frac{\theta}{4} (\lambda_M - \lambda) \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{\bar{c}_j} \nabla \log \frac{c_i}{\bar{c}_i} \right|^2 \, dx \, dt \\ & \quad + \frac{1}{\theta} (\lambda_M - \lambda) \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{\bar{c}_j} \nabla (\mu_j - \bar{\mu}_j) \right|^2 \, dx \, dt. \end{aligned} \tag{58}$$

Step 1b: Estimate of I_{11} . In the term I_{11} , we replace $\mu_j - \bar{\mu}_j$ by $\log(c_j/\bar{c}_j) - \Delta(c_j - \bar{c}_j)$ and compute both terms in the difference separately. Now, the definition $G_{ij}(\mathbf{c}) =$

$\sqrt{c_i} P_L(\mathbf{c})_{ij} \sqrt{c_j}$ and the property $P_L(\mathbf{c})^2 = P_L(\mathbf{c})$ lead to

$$\begin{aligned} & \sum_{i,j=1}^n \int_0^T \int_{\Omega} G_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \log \frac{c_j}{\bar{c}_j} dx dt \\ &= \sum_{i,j=1}^n \int_0^T \int_{\Omega} \sqrt{c_i} P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \log \frac{c_j}{\bar{c}_j} dx dt \\ &= \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt. \end{aligned} \tag{59}$$

Furthermore, we use $G_{ij}(\mathbf{c}) = c_i \delta_{ij} - c_i c_j$ and integration by parts to find that

$$\begin{aligned} & \sum_{i,j=1}^n \int_0^T \int_{\Omega} G_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \Delta(c_j - \bar{c}_j) dx dt \\ &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \operatorname{div} \left((c_i \delta_{ij} - c_i c_j) \nabla \log \frac{c_i}{\bar{c}_i} \right) \Delta(c_j - \bar{c}_j) dx dt \\ &= - \sum_{i=1}^n \int_0^T \int_{\Omega} \operatorname{div}(\nabla c_i - c_i \nabla \log \bar{c}_i) \Delta(c_i - \bar{c}_i) dx dt \\ &\quad + \sum_{i,j=1}^n \int_0^T \int_{\Omega} \operatorname{div}(c_j \nabla c_i - c_i c_j \nabla \log \bar{c}_i) \Delta(c_j - \bar{c}_j) dx dt \\ &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \operatorname{div}(\nabla c_i - c_i \nabla \log \bar{c}_i) \Delta(c_i - \bar{c}_i) dx dt \\ &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) \Delta(c_j - \bar{c}_j) dx dt, \end{aligned}$$

where we used $\sum_{i=1}^n c_j \nabla c_i = 0$ in the last step. We mention that $\sum_{j=1}^n G_{ij}(\mathbf{c}) \nabla \Delta c_j \in L^2(Q_T)$ because of (23), so the first integral in the previous computation is well defined. It follows from $\Delta c_i \Delta(c_i - \bar{c}_i) = (\Delta(c_i - \bar{c}_i))^2 + \Delta \bar{c}_i \Delta(c_i - \bar{c}_i)$ that

$$\begin{aligned} & \sum_{i,j=1}^n \int_0^T \int_{\Omega} G_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \Delta(c_i - \bar{c}_i) dx dt \\ &= - \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\ &\quad - \sum_{i=1}^n \int_0^T \int_{\Omega} \operatorname{div}(\nabla \bar{c}_i - c_i \nabla \log \bar{c}_i) \Delta(c_i - \bar{c}_i) dx dt \\ &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) \Delta(c_j - \bar{c}_j) dx dt. \end{aligned} \tag{60}$$

We multiply (59) by $-\lambda$ and (60) by λ and sum both expressions to find that

$$\begin{aligned}
 I_{11} &= -\lambda \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\
 &\quad - \lambda \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad - \lambda \sum_{i=1}^n \int_0^T \int_{\Omega} \operatorname{div}(\nabla \bar{c}_i - c_i \nabla \log \bar{c}_i) \Delta(c_i - \bar{c}_i) dx dt \\
 &\quad - \lambda \sum_{i,j=1}^n \int_0^T \int_{\Omega} \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) \Delta(c_j - \bar{c}_j) dx dt. \tag{61}
 \end{aligned}$$

We apply Young’s inequality to the last two terms. The third term in (61) becomes

$$\begin{aligned}
 &-\lambda \sum_{i=1}^n \int_0^T \int_{\Omega} \operatorname{div}(\nabla \bar{c}_i - c_i \nabla \log \bar{c}_i) \Delta(c_i - \bar{c}_i) dx dt \\
 &\leq \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad + \lambda \sum_{i=1}^n \int_0^T \int_{\Omega} |\operatorname{div}((c_i - \bar{c}_i) \nabla \log \bar{c}_i)|^2 dx dt \\
 &\leq \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad + \lambda \sum_{i=1}^n \|\nabla \log \bar{c}_i\|_{L^\infty(Q_T)} \int_0^T \int_{\Omega} |\nabla(c_i - \bar{c}_i)|^2 dx dt \\
 &\quad + \lambda \sum_{i=1}^n \|\Delta \log \bar{c}_i\|_{L^\infty(Q_T)} \int_0^T \int_{\Omega} (c_i - \bar{c}_i)^2 dx dt \\
 &\leq \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad + \lambda C \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt,
 \end{aligned}$$

where the constant $C > 0$ depends on the L^∞ norms of $\nabla \log \bar{c}$ and $\Delta \log \bar{c}$. Next, for the fourth term in (61),

$$\begin{aligned} & -\lambda \sum_{i,j=1}^n \int_0^T \int_\Omega \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) \Delta(c_j - \bar{c}_j) \, dx \, dt \\ & \leq \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_\Omega (\Delta(c_i - \bar{c}_i))^2 \, dx \, dt \\ & \quad + \lambda \sum_{j=1}^n \int_0^T \int_\Omega \left| \sum_{i=1}^n \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) \right|^2 \, dx \, dt. \end{aligned}$$

Taking into account that

$$\nabla \sum_{i=1}^n \bar{c}_i \nabla \log \bar{c}_i = \sum_{i=1}^n \nabla \bar{c}_i = 0,$$

we estimate the integrand of the last term:

$$\begin{aligned} \sum_{i=1}^n \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) &= \sum_{i=1}^n \operatorname{div}((c_i - \bar{c}_i) c_j \nabla \log \bar{c}_i) \\ &= \sum_{i=1}^n c_j \operatorname{div}((c_i - \bar{c}_i) \nabla \log \bar{c}_i) + \sum_{i=1}^n (c_i - \bar{c}_i) \nabla \log \bar{c}_i \cdot \nabla c_j \\ &= \sum_{i=1}^n c_j \operatorname{div}((c_i - \bar{c}_i) \nabla \log \bar{c}_i) + \sum_{i=1}^n c_i \nabla \log \bar{c}_i \cdot \nabla (c_j - \bar{c}_j) \\ & \quad + \sum_{i=1}^n (c_i - \bar{c}_i) \nabla \log \bar{c}_i \cdot \nabla \bar{c}_j \\ & \leq C \sum_{i=1}^n (|c_i - \bar{c}_i| + |\nabla(c_i - \bar{c}_i)|), \end{aligned}$$

where $C > 0$ depends on the L^∞ norms of $\nabla \log \bar{c}$ and $\Delta \log \bar{c}$. This yields

$$\begin{aligned} & -\lambda \sum_{i,j=1}^n \int_0^T \int_\Omega \operatorname{div}(c_i c_j \nabla \log \bar{c}_i) \Delta(c_j - \bar{c}_j) \, dx \, dt \\ & \leq \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_\Omega (\Delta(c_i - \bar{c}_i))^2 \, dx \, dt \\ & \quad + \lambda C \sum_{i=1}^n \int_0^T \int_\Omega ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) \, dx \, dt. \end{aligned}$$

Using these estimates in (61), we arrive at

$$\begin{aligned}
 I_{11} &\leq -\lambda \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\
 &\quad - \frac{\lambda}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad + \lambda C \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \tag{62}
 \end{aligned}$$

Step 1c: Estimate of I_{12} . By definition of $B_{ij}(\mathbf{c})$ and Young’s inequality with $\theta' > 0$,

$$\begin{aligned}
 I_{12} &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \sqrt{c_i} \left(D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j} - \sqrt{\frac{c_i}{\bar{c}_i}} D_{ij}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \right) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \bar{\mu}_j dx dt \\
 &\leq \frac{\theta'}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} c_i \left| \nabla \log \frac{c_i}{\bar{c}_i} \right|^2 dx dt \\
 &\quad + \frac{n}{\theta'} \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j} - \sqrt{\frac{c_i}{\bar{c}_i}} D_{ij}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \right)^2 |\nabla \bar{\mu}_j|^2 dx dt.
 \end{aligned}$$

The bracket of the second term can be estimated according to

$$\begin{aligned}
 &\left| D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j} - \sqrt{\frac{c_i}{\bar{c}_i}} D_{ij}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \right| \\
 &= \left| D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j} - D_{ij}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} - \frac{\sqrt{c_i} - \sqrt{\bar{c}_i}}{\sqrt{\bar{c}_i}} D_{ij}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \right| \\
 &\leq \frac{C}{\sqrt{m}} \sum_{i=1}^n (|c_i - \bar{c}_i| + |\sqrt{c_i} - \sqrt{\bar{c}_i}|) \\
 &\leq C(m) \sum_{i=1}^n |c_i - \bar{c}_i|, \tag{63}
 \end{aligned}$$

using the assumption $\bar{c}_i \geq m > 0$ and the boundedness of D_{ij}^{BD} (see Lemma 4 (i)). It follows that

$$\begin{aligned}
 I_{12} &\leq \frac{\theta'}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} c_i \left| \nabla \log \frac{c_i}{\bar{c}_i} \right|^2 dx dt \\
 &\quad + C(m, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} (c_i - \bar{c}_i)^2 dx dt. \tag{64}
 \end{aligned}$$

Step 1d: Combining the estimates. We deduce from (57), after inserting estimates (58), (62), and (64) for I_{10} , I_{11} , and I_{12} , respectively, that

$$\begin{aligned} \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) &\leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ &+ \left(\frac{\theta}{4}(\lambda_M - \lambda) - \lambda\right) \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ &+ \frac{\lambda_M - \lambda}{\theta} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla (\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ &- \frac{\lambda}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\ &+ \lambda C \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt \\ &+ \frac{\theta'}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} c_i \left| \nabla \log \frac{c_i}{\bar{c}_i} \right|^2 dx dt + C(m, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} (c_i - \bar{c}_i)^2 dx dt. \end{aligned} \tag{65}$$

The last but one term on the right-hand side still needs to be estimated. To this end, we decompose $I = P_L(\mathbf{c}) + P_{L^\perp}(\mathbf{c})$:

$$\begin{aligned} \sum_{i=1}^n c_i \left| \nabla \log \frac{c_i}{\bar{c}_i} \right|^2 &= \sum_{i=1}^n \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 \\ &+ \sum_{i=1}^n \left| \sum_{j=1}^n P_{L^\perp}(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2. \end{aligned}$$

The first term on the right-hand side can be absorbed for sufficiently small $\theta' > 0$ by the second term on the left-hand side of (65). For the other term, we use the definition $P_{L^\perp}(\mathbf{c})_{ij} = \sqrt{c_i c_j}$ and $\sum_{j=1}^n \nabla c_j = \sum_{j=1}^n \nabla \bar{c}_j = 0$:

$$\sum_{j=1}^n P_{L^\perp}(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} = \sqrt{c_i} \sum_{j=1}^n c_j \nabla \log \frac{c_j}{\bar{c}_j} = \sqrt{c_i} \sum_{j=1}^n (c_j - \bar{c}_j) \nabla \log \bar{c}_j.$$

This gives

$$\begin{aligned} &\sum_{i=1}^n \int_0^T \int_{\Omega} c_i \left| \nabla \log \frac{c_i}{\bar{c}_i} \right|^2 dx dt \\ &\leq \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ &\quad + \sum_{j=1}^n \|\nabla \log \bar{c}_j\|_{L^\infty(Q_T)} \int_0^T \int_{\Omega} (c_i - \bar{c}_i)^2 dx dt. \end{aligned} \tag{66}$$

Hence, choosing $\theta = \lambda/(\lambda_M - \lambda)$ and $\theta' = \lambda$, we conclude from (65) that

$$\begin{aligned} & \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \frac{\lambda}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ & \quad + \frac{\lambda}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\ & \leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ & \quad + \frac{(\lambda_M - \lambda)^2}{\lambda} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla (\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ & \quad + C \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned} \tag{67}$$

We show in the next step that the second term on the right-hand side can be estimated by the relative energy inequality.

Step 2: Estimating the relative energy. We start from the relative energy inequality (54). Observing that due to Lemma 4 (ii),

$$\begin{aligned} & \sum_{i,j=1}^n B_{ij}(\mathbf{c}) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla(\mu_j - \bar{\mu}_j) \\ & = \sum_{i,j=1}^n D_{ij}^{\text{BD}}(\mathbf{c}) (\sqrt{c_i} \nabla(\mu_i - \bar{\mu}_i)) \cdot (\sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j)) \\ & \geq \lambda_m \sum_{i=1}^n \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2, \end{aligned}$$

inequality (54) becomes

$$\begin{aligned} & \mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \lambda_m \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ & \leq \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + I_{13} + I_{14} + I_{15} + I_{16}, \end{aligned} \tag{68}$$

where

$$\begin{aligned} I_{13} & = - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \bar{\mu}_j dx dt, \\ I_{14} & = \sum_{i,j=1}^n \int_0^T \int_{\Omega} (c_i - \bar{c}_i) \nabla(c_i - \bar{c}_i) \cdot \nabla \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) dx dt, \end{aligned}$$

$$\begin{aligned}
 I_{15} &= \frac{1}{2} \sum_{i,j=1}^n \int_0^T \int_{\Omega} |\nabla(c_i - \bar{c}_i)|^2 \operatorname{div} \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) dx dt, \\
 I_{16} &= \sum_{i,j=1}^n \int_0^T \int_{\Omega} \nabla(c_i - \bar{c}_i) \otimes \nabla(c_i - \bar{c}_i) : \nabla \left(\frac{1}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j \right) dx dt.
 \end{aligned}$$

The terms I_{14} , I_{15} , and I_{16} can be estimated directly by using the regularity assumption $\nabla \operatorname{div}((1/\bar{c}_i) B_{ij}(\bar{\mathbf{c}}) \nabla \bar{\mu}_j) \in L^\infty(Q_T)$:

$$I_{14} + I_{15} + I_{16} \leq C \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \tag{69}$$

The estimate for I_{13} is more involved. First, we use the definition of $B(\mathbf{c})$ and decompose $I = P_L(\mathbf{c}) + P_{L^\perp}(\mathbf{c})$. Then

$$I_{13} = \sum_{i,j=1}^n \int_0^T \int_{\Omega} \sqrt{c_i} E_{ij}(\mathbf{c}, \bar{\mathbf{c}}) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \bar{\mu}_j dx dt =: I_{131} + I_{132},$$

where

$$\begin{aligned}
 E_{ij}(\mathbf{c}, \bar{\mathbf{c}}) &= D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{c_j} - \sqrt{\frac{c_i}{\bar{c}_i}} D_{ij}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j}, \\
 I_{131} &= \sum_{i,j,k,\ell=1}^n \int_0^T \int_{\Omega} P_L(\mathbf{c})_{i\ell} E_{\ell j}(\mathbf{c}, \bar{\mathbf{c}}) P_L(\mathbf{c})_{ik} \sqrt{c_k} \nabla(\mu_k - \bar{\mu}_k) \cdot \nabla \bar{\mu}_j dx dt, \\
 I_{132} &= \sum_{i,j,k,\ell=1}^n \int_0^T \int_{\Omega} P_{L^\perp}(\mathbf{c})_{i\ell} E_{\ell j}(\mathbf{c}, \bar{\mathbf{c}}) P_{L^\perp}(\mathbf{c})_{ik} \sqrt{c_k} \nabla(\mu_k - \bar{\mu}_k) \cdot \nabla \bar{\mu}_j dx dt.
 \end{aligned}$$

For I_{131} , it is sufficient to apply Young’s inequality and to use estimate (63) for $E_{ij}(\mathbf{c}, \bar{\mathbf{c}})$:

$$\begin{aligned}
 I_{131} &\leq \frac{\lambda_m}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\
 &\quad + \frac{n}{2\lambda_m} \sum_{i,j=1}^n \int_0^T \int_{\Omega} |E_{ij}(\mathbf{c}, \bar{\mathbf{c}})|^2 |\nabla \bar{\mu}_j|^2 dx dt \\
 &\leq \frac{\lambda_m}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\
 &\quad + C(m) \sum_{i=1}^n \int_0^T \int_{\Omega} (c_i - \bar{c}_i)^2 dx dt, \tag{70}
 \end{aligned}$$

where $C(m) > 0$ depends on m, n, λ_m , and the $L^\infty(Q_T)$ norm of $\nabla \bar{\mu}$.

For I_{132} , we observe that the property $\text{ran } D^{\text{BD}}(\mathbf{c}) = L(\mathbf{c})$, which follows from Lemma 3, implies that $P_{L^\perp}(\mathbf{c})D^{\text{BD}}(\mathbf{c})\mathbf{z} = \mathbf{0}$ for all $\mathbf{z} \in \mathbb{R}^n$. Hence,

$$\sum_{\ell=1}^n P_{L^\perp}(\mathbf{c})_{i\ell} E_{\ell j}(\mathbf{c}, \bar{\mathbf{c}}) = - \sum_{\ell=1}^n P_{L^\perp}(\mathbf{c})_{i\ell} \sqrt{\frac{c_\ell}{\bar{c}_\ell}} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j}.$$

We infer from the definitions $P_{L^\perp}(\mathbf{c})_{ik} = \sqrt{\bar{c}_i c_k}$ and $\mu_k - \bar{\mu}_k = \log(c_k/\bar{c}_k) - \Delta(c_k - \bar{c}_k)$ that

$$\begin{aligned} I_{132} &= - \sum_{i,j,k,\ell=1}^n \int_0^T \int_\Omega P_{L^\perp}(\mathbf{c})_{ik} \sqrt{c_k} P_{L^\perp}(\mathbf{c})_{i\ell} \sqrt{\frac{c_\ell}{\bar{c}_\ell}} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \nabla(\mu_k - \bar{\mu}_k) \\ &\quad \cdot \nabla \bar{\mu}_j \, dx \, dt \\ &= - \sum_{j,k,\ell=1}^n \int_0^T \int_\Omega \sum_{i=1}^n c_i c_k \frac{c_\ell}{\sqrt{\bar{c}_\ell}} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \nabla(\mu_k - \bar{\mu}_k) \cdot \nabla \bar{\mu}_j \, dx \, dt \\ &= - \sum_{j,k,\ell=1}^n \int_0^T \int_\Omega c_k \frac{c_\ell - \bar{c}_\ell}{\sqrt{\bar{c}_\ell}} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \nabla \log \frac{c_k}{\bar{c}_k} \cdot \nabla \bar{\mu}_j \, dx \, dt \\ &\quad - \sum_{j,k,\ell=1}^n \int_0^T \int_\Omega \text{div} \left(c_k \frac{c_\ell - \bar{c}_\ell}{\sqrt{\bar{c}_\ell}} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \nabla \bar{\mu}_j \right) \Delta(c_k - \bar{c}_k) \, dx \, dt \\ &=: J_1 + J_2, \end{aligned} \tag{71}$$

where we added the expression $-\sum_{\ell=1}^n \sqrt{\bar{c}_\ell} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) = 0$, which follows from $\ker D^{\text{BD}}(\bar{\mathbf{c}}) = L^\perp(\bar{\mathbf{c}}) = \text{span}\{\sqrt{\bar{\mathbf{c}}}\}$ (see Lemma 4) and the symmetry of $D^{\text{BD}}(\bar{\mathbf{c}})$ (see Lemma 3), and we integrated by parts in the last integral.

To estimate J_1 , we use Young’s inequality with $\theta > 0$, Lemma 4 (iii), and (66):

$$\begin{aligned} J_1 &\leq \frac{\theta}{4} \sum_{k=1}^n \int_0^T \int_\Omega c_k \left| \nabla \log \frac{c_k}{\bar{c}_k} \right|^2 \, dx \, dt \\ &\quad + \frac{n}{\theta} \sum_{j,k,\ell=1}^n \int_0^T \int_\Omega (c_\ell - \bar{c}_\ell)^2 \frac{c_k}{\bar{c}_\ell} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}})^2 \bar{c}_j |\nabla \bar{\mu}_j|^2 \, dx \, dt \\ &\leq \frac{\theta}{4} \sum_{i=1}^n \int_0^T \int_\Omega \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{\bar{c}_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 \, dx \, dt \\ &\quad + C\theta \sum_{i=1}^n \int_0^T \int_\Omega (c_i - \bar{c}_i)^2 \, dx \, dt \\ &\quad + \frac{C}{\theta} \sum_{\ell=1}^n \int_0^T \int_\Omega (c_\ell - \bar{c}_\ell)^2 \, dx \, dt, \end{aligned}$$

where $C > 0$ depends on the $L^\infty(Q_T)$ norms of $\nabla \bar{\mathbf{c}}$ and $\nabla \bar{\boldsymbol{\mu}}$.

Next, we use Young’s inequality again, with $\theta' > 0$:

$$\begin{aligned}
 J_2 &\leq \frac{\theta'}{4} \sum_{k=1}^n \int_{\Omega} (\Delta(c_k - \bar{c}_k))^2 dx dt \\
 &\quad + \frac{n}{\theta'} \sum_{k,\ell=1}^n \int_0^T \int_{\Omega} |\operatorname{div}(c_k(c_\ell - \bar{c}_\ell)Q_\ell(\bar{\mathbf{c}}))|^2 dx dt, \tag{72}
 \end{aligned}$$

where we defined

$$Q_\ell(\bar{\mathbf{c}}) := \sum_{j=1}^n \frac{1}{\sqrt{\bar{c}_\ell}} D_{\ell j}^{\text{BD}}(\bar{\mathbf{c}}) \sqrt{\bar{c}_j} \nabla \bar{\mu}_j.$$

Estimating

$$\begin{aligned}
 |\operatorname{div}(c_k(c_\ell - \bar{c}_\ell)Q_\ell(\bar{\mathbf{c}}))| &= |c_k(c_\ell - \bar{c}_\ell) \operatorname{div} Q_\ell(\bar{\mathbf{c}}) + c_k \nabla(c_\ell - \bar{c}_\ell) \cdot Q_\ell(\bar{\mathbf{c}}) \\
 &\quad + (c_\ell - \bar{c}_\ell) \nabla(c_k - \bar{c}_k) \cdot Q_\ell(\bar{\mathbf{c}}) + (c_\ell - \bar{c}_\ell) \nabla \bar{c}_k \cdot Q_\ell(\bar{\mathbf{c}})| \\
 &\leq C(|c_\ell - \bar{c}_\ell| + |\nabla(c_\ell - \bar{c}_\ell)| + |\nabla(c_k - \bar{c}_k)|),
 \end{aligned}$$

where $C > 0$ depends on the $L^\infty(Q_T)$ norm of $Q_\ell(\bar{\mathbf{c}})$, we deduce from (72) that

$$J_2 \leq \frac{\theta'}{4} \sum_{k=1}^n \int_{\Omega} (\Delta(c_k - \bar{c}_k))^2 dx dt + \frac{C}{\theta'} \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt.$$

Inserting the estimates for J_1 and J_2 into (71) leads to

$$\begin{aligned}
 I_{132} &\leq \frac{\theta}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\
 &\quad + \frac{\theta'}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad + C(\theta, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt.
 \end{aligned}$$

Then, together with (70), we find that

$$\begin{aligned}
 I_{13} &\leq \frac{\lambda_m}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla (\mu_j - \bar{\mu}_j) \right|^2 dx dt \\
 &\quad + \frac{\theta}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\
 &\quad + \frac{\theta'}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\
 &\quad + C(\theta, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \tag{73}
 \end{aligned}$$

Finally, we insert this estimate and estimate (69) for I_{14} , I_{15} , and I_{16} into (68), observing that the first term on the right-hand side of (73) is absorbed by the second term on the left-hand side of (68):

$$\begin{aligned} & \mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \frac{\lambda_m}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla (\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ & \leq \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{\theta}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ & \quad + \frac{\theta'}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\ & \quad + C(\theta, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned} \tag{74}$$

Step 3: Combining the relative energy and relative entropy inequalities. Next, multiply (74) by $4(\lambda_M - \lambda)^2/(\lambda_m \lambda)$, choose $\theta' = \lambda_m \lambda^2/(4(\lambda_M - \lambda)^2)$, and add this expression to (67) (which estimates $\mathcal{H}(\mathbf{c}|\bar{\mathbf{c}})$). Then some terms on the right-hand side can be absorbed by the corresponding expressions on the left-hand side, leading to

$$\begin{aligned} & \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \frac{4(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) \\ & \quad + \frac{(\lambda_M - \lambda)^2}{\lambda} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla (\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ & \quad + \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ & \quad + \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\ & \leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{4(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ & \quad + C(\theta, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned}$$

The last term can be bounded in terms of the free energy, since $c_i \log(c_i/\bar{c}_i) - (c_i - \bar{c}_i) \geq (c_i - \bar{c}_i)^2/2$ [22, Lemma 18]:

$$\begin{aligned} \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \frac{4(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) & \leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{4(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ & \quad + C \int_0^T \mathcal{E}(\mathbf{c}(t)|\bar{\mathbf{c}}(t)) dt. \end{aligned}$$

Then the theorem follows after applying Grönwall’s lemma.

5. Nonconvex potential energies

In this section, we consider the case of a possibly nonconvex potential energy $\psi(\mathbf{c})$. We work with the functionals

$$\begin{aligned} \mathcal{E}(\mathbf{c}) &= \mathcal{H}(\mathbf{c}) + \int_{\Omega} \psi(\mathbf{c}) \, dx + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla c_i|^2 \, dx, \\ \mathcal{H}(\mathbf{c}) &= \sum_{i=1}^n \int_{\Omega} (c_i(\log c_i - 1) + 1) \, dx. \end{aligned}$$

Then the chemical potential associated to $\mathcal{E}(\mathbf{c})$ is given by

$$\tilde{\mu}_i = \frac{\delta \mathcal{E}}{\delta c_i} = \frac{\partial \psi}{\partial c_i}(\mathbf{c}) + \log c_i - \Delta c_i = \frac{\partial \psi}{\partial c_i}(\mathbf{c}) + \mu_i,$$

where μ_i is defined by (5). The resulting model is system (1)–(3) with μ_i replaced by $\tilde{\mu}_i$. We assume that $\psi(\mathbf{c})$ is a general function satisfying

(P) $\psi \in C^3([0, 1]^n)$ satisfies $\|\psi\|_{C^3([0, 1]^n)} \leq C$ for some constant $C > 0$.

In the following, we show that our main results, Theorems 1 and 2, can be extended to this situation.

5.1. The energy inequality and existence of solutions

We show that Lemma 5 still holds true. We outline only the points where the proof needs to be modified. First, with $\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu} + D\psi(\mathbf{c})$, the energy inequality (29) becomes

$$\begin{aligned} \frac{d\mathcal{E}}{dt}(\mathbf{c}) &\leq -\lambda_m \int_{\Omega} |P_L(\mathbf{c})R(\mathbf{c})\nabla \tilde{\boldsymbol{\mu}}|^2 \, dx = -\lambda_m \int_{\Omega} |P_L(\mathbf{c})R(\mathbf{c})\nabla(\boldsymbol{\mu} + D\psi(\mathbf{c}))|^2 \, dx \\ &\leq -\frac{\lambda_m}{2} \int_{\Omega} |P_L(\mathbf{c})R(\mathbf{c})\nabla \boldsymbol{\mu}|^2 \, dx + \lambda_m \int_{\Omega} |P_L(\mathbf{c})R(\mathbf{c})D^2\psi(\mathbf{c})\nabla \mathbf{c}|^2 \, dx \\ &\leq -\frac{\lambda_m}{2} \int_{\Omega} |P_L(\mathbf{c})R(\mathbf{c})\nabla \boldsymbol{\mu}|^2 \, dx + C\lambda_m \int_{\Omega} |\nabla \mathbf{c}|^2 \, dx, \end{aligned} \tag{75}$$

where we used the definition $R_{ij}(\mathbf{c}) = \sqrt{c_i}\delta_{ij}$ and the boundedness of $D^2\psi(\mathbf{c})$. We compute the time derivative of $\mathcal{H}(\mathbf{c})$ along solutions to (1)–(3):

$$\begin{aligned} \frac{d\mathcal{H}}{dt}(\mathbf{c}) &= - \sum_{i,j=1}^n \int_{\Omega} M_{ij} \nabla \log c_i \cdot \nabla \tilde{\mu}_j \, dx - \lambda \sum_{i,j=1}^n \int_{\Omega} G_{ij} \nabla \log c_i \cdot \nabla \tilde{\mu}_j \, dx \\ &= - \sum_{i,j=1}^n \int_{\Omega} M_{ij} \nabla \log c_i \cdot \nabla \mu_j \, dx - \lambda \sum_{i,j=1}^n \int_{\Omega} G_{ij} \nabla \log c_i \cdot \nabla \mu_j \, dx \\ &\quad - \sum_{i,j=1}^n \int_{\Omega} M_{ij} \nabla \log c_i \cdot \nabla \frac{\partial \psi}{\partial c_j}(\mathbf{c}) \, dx - \lambda \sum_{i,j=1}^n \int_{\Omega} G_{ij} \nabla \log c_i \cdot \nabla \frac{\partial \psi}{\partial c_j}(\mathbf{c}) \, dx \\ &=: I_1 + I_2 + \tilde{I}_1 + \tilde{I}_2. \end{aligned}$$

The terms I_1 and I_2 were estimated in Section 2.2 so that it remains to bound the terms \tilde{I}_1 and \tilde{I}_2 coming from the nonconvex potential. To estimate \tilde{I}_1 , we recall property (iii) in Lemma 4, which implies that $B_{ij}/c_j = \sqrt{c_i} D_{ij}^{\text{BD}}(\mathbf{c})/\sqrt{c_j}$ is bounded (by the definition (25) of B_{ij}). Then the boundedness of $G_{ij}/c_j = \delta_{ij} - c_i$ implies that $M_{ij}/c_j = (B_{ij} - \lambda G_{ij})/c_j$ is bounded too. Thus, by Young’s inequality and assumption (P),

$$\begin{aligned} \tilde{I}_1 &= \sum_{i,j=1}^n \int_{\Omega} \frac{M_{ij}}{c_j} \nabla c_j \cdot \nabla \frac{\partial \psi}{\partial c_j}(\mathbf{c}) \, dx = \sum_{i,j,k=1}^n \int_{\Omega} \frac{M_{ij}}{c_j} \nabla c_j \cdot \left(\frac{\partial^2 \psi}{\partial c_j \partial c_k}(\mathbf{c}) \nabla c_k \right) \, dx \\ &\leq C \sum_{i,j=1}^n \int_{\Omega} \left| \frac{M_{ij}}{c_j} \right|^2 |\nabla c_j|^2 \, dx + \sum_{j,k=1}^n \int_{\Omega} \left| \frac{\partial^2 \psi}{\partial c_j \partial c_k} \nabla c_k \right|^2 \, dx \leq C \int_{\Omega} |\nabla \mathbf{c}|^2 \, dx. \end{aligned}$$

For the term \tilde{I}_2 , we use the definition of $G(\mathbf{c})$, $\sum_{i=1}^n \nabla c_i = 0$, and assumption (P):

$$\begin{aligned} \tilde{I}_2 &= -\lambda \sum_{i,j=1}^n \int_{\Omega} (c_i \delta_{ij} - c_i c_j) \frac{\nabla c_i}{c_i} \cdot \nabla \frac{\partial \psi}{\partial c_j}(\mathbf{c}) \, dx \\ &= -\lambda \sum_{i=1}^n \int_{\Omega} \nabla c_i \cdot \nabla \frac{\partial \psi}{\partial c_i}(\mathbf{c}) \, dx + \lambda \int_{\Omega} \sum_{i=1}^n \nabla c_i \cdot \sum_{j=1}^n c_j \nabla \frac{\partial \psi}{\partial c_j}(\mathbf{c}) \, dx \\ &= -\lambda \sum_{i,j=1}^n \int_{\Omega} \frac{\partial^2 \psi}{\partial c_i \partial c_j}(\mathbf{c}) \nabla c_i \cdot \nabla c_j \, dx \leq \lambda C \int_{\Omega} |\nabla \mathbf{c}|^2 \, dx. \end{aligned}$$

Collecting these estimates and I_1 and I_2 from (30), summarized in (33), we obtain

$$\begin{aligned} \frac{d\mathcal{H}}{dt}(\mathbf{c}) + 2\lambda \int_{\Omega} |\nabla \sqrt{c}|^2 \, dx + \lambda \int_{\Omega} |\Delta \mathbf{c}|^2 \, dx \\ \leq \frac{(\lambda_M - \lambda)^2}{2\lambda} \int_{\Omega} |P_L R \nabla \mu|^2 \, dx + C \int_{\Omega} |\nabla \mathbf{c}|^2 \, dx. \end{aligned}$$

Adding this inequality to (75), multiplied by $2(\lambda_M - \lambda)^2/(\lambda_m \lambda)$, leads to the free energy inequality

$$\begin{aligned} \frac{d}{dt} \left(\mathcal{H}(\mathbf{c}) + \frac{2(\lambda_M - \lambda)^2}{\lambda_m \lambda \ell} \mathcal{E}(\mathbf{c}) \right) + 2\lambda \int_{\Omega} |\nabla \sqrt{c}|^2 \, dx + \lambda \int_{\Omega} |\Delta \mathbf{c}|^2 \, dx \\ + \frac{(\lambda_M - \lambda)^2}{2\lambda} \int_{\Omega} |P_L(\mathbf{c}) R(\mathbf{c}) \nabla \mu|^2 \, dx \leq C \int_{\Omega} |\nabla \mathbf{c}|^2 \, dx \leq C \mathcal{E}(\mathbf{c}), \end{aligned}$$

and Grönwall’s inequality eventually gives

$$\begin{aligned} \mathcal{H}(\mathbf{c}(T)) + \frac{2(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}(T)) + 2\lambda \int_0^T \int_{\Omega} |\nabla \sqrt{c}|^2 \, dx \, dt + \lambda \int_0^T \int_{\Omega} |\Delta \mathbf{c}|^2 \, dx \, dt \\ + \frac{(\lambda_M - \lambda)^2}{2\lambda} \int_0^T \int_{\Omega} |P_L(\mathbf{c}) R(\mathbf{c}) \nabla \mu|^2 \, dx \, dt \\ \leq C(T) \left(\mathcal{H}(\mathbf{c}_0) + \frac{2(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}_0) \right). \end{aligned} \tag{76}$$

The estimated quantity in (76) equals (abbreviating $\alpha = 2(\lambda_M - \lambda)^2/\lambda_m\lambda$)

$$\begin{aligned} &\mathcal{H}(\mathbf{c}(T)) + \alpha \mathcal{E}(\mathbf{c}(T)) \\ &= \int_{\Omega} \left(\sum_{i=1}^n (c_i (\log c_i - 1) + 1) + \alpha \psi(\mathbf{c}) + \frac{\alpha}{2} \sum_{i=1}^n |\nabla c_i|^2 \right) dx. \end{aligned}$$

Since $c_i \in [0, 1]$, assumption (P) implies that $|\psi(\mathbf{c})| \leq C$, such that the term involving the nonconvex potential ψ can be absorbed by the right-hand side of (76).

The method of the proof of Theorem 1 in Section 3 still works, with the exception that we need to replace the estimates in Lemma 8 by the corresponding version of (76) for the approximate system.

5.2. The relative energy estimate and weak–strong uniqueness

For possibly nonconvex potentials satisfying assumption (P), the existence proof implies the same regularity of solutions as before and thus, Lemma 10 still holds. In order to prove the weak–strong uniqueness, we write $\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu} + D\psi(\mathbf{c})$ as in the previous subsection. The aim is to estimate the quantities

$$\mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) := \sum_{i=1}^n \int_{\Omega} \left(c_i \log \frac{c_i}{\bar{c}_i} - (c_i - \bar{c}_i) \right) dx, \tag{77}$$

$$\mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}) := \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla(c_i - \bar{c}_i)|^2 dx + \int_{\Omega} \psi(\mathbf{c}|\bar{\mathbf{c}}) dx, \tag{78}$$

where $\psi(\mathbf{c}|\bar{\mathbf{c}}) = \psi(\mathbf{c}) - \psi(\bar{\mathbf{c}}) - D\psi(\bar{\mathbf{c}}) \cdot (\mathbf{c} - \bar{\mathbf{c}})$, by following the lines of Section 4.2, but now accounting for the last term in (78) containing the nonconvex part.

First we consider the relative entropy $\mathcal{H}(\mathbf{c}|\bar{\mathbf{c}})$. Inequality (57) holds with $\mu_i, \bar{\mu}_i$ replaced by $\mu_i + D\psi(\mathbf{c}), \bar{\mu}_i + D\psi(\bar{\mathbf{c}})$:

$$\mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) - \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \leq I_{10} + I_{11} + I_{12} + \tilde{I}_{10} + \tilde{I}_{11} + \tilde{I}_{12}, \tag{79}$$

where

$$\tilde{I}_{10} = - \sum_{i,j=1}^n \int_0^T \int_{\Omega} M_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \left(\frac{\partial \psi}{\partial c_j}(\mathbf{c}) - \frac{\partial \psi}{\partial c_j}(\bar{\mathbf{c}}) \right) dx dt,$$

$$\tilde{I}_{11} = -\lambda \sum_{i,j=1}^n \int_0^T \int_{\Omega} G_{ij}(\mathbf{c}) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \left(\frac{\partial \psi}{\partial c_j}(\mathbf{c}) - \frac{\partial \psi}{\partial c_j}(\bar{\mathbf{c}}) \right) dx dt,$$

$$\tilde{I}_{12} = - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(\mathbf{c}) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{\mathbf{c}}) \right) \nabla \log \frac{c_i}{\bar{c}_i} \cdot \nabla \frac{\partial \psi}{\partial c_j}(\bar{\mathbf{c}}) dx dt,$$

and the terms I_{10} , I_{11} , I_{12} are defined in (57). The term \tilde{I}_{10} is estimated in a similar way to \tilde{I}_1 in the previous subsection:

$$\begin{aligned} \tilde{I}_{10} &= - \sum_{i,j,k=1}^n \int_0^T \int_{\Omega} \frac{M_{ij}}{c_i} (\nabla(c_i - \bar{c}_i) + (c_i - \bar{c}_i) \nabla \log \bar{c}_i) \\ &\quad \times \left(\frac{\partial^2 \psi}{\partial c_j \partial c_k}(\mathbf{c}) \nabla c_k - \frac{\partial^2 \psi}{\partial c_j \partial c_k}(\bar{\mathbf{c}}) \nabla \bar{c}_k \right) dx dt \\ &\leq C \int_0^T \int_{\Omega} (|\nabla(\mathbf{c} - \bar{\mathbf{c}})|^2 + |\mathbf{c} - \bar{\mathbf{c}}|^2) dx \\ &\quad + C \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left| \frac{\partial^2 \psi}{\partial c_j \partial c_k}(\mathbf{c}) \nabla(c_j - \bar{c}_j) \right|^2 dx dt \\ &\quad + C \int_0^T \int_{\Omega} \left| \left(\frac{\partial^2 \psi}{\partial c_j \partial c_k}(\mathbf{c}) - \frac{\partial^2 \psi}{\partial c_j \partial c_k}(\bar{\mathbf{c}}) \right) \nabla \bar{c}_j \right|^2 dx dt \\ &\leq C \int_0^T \int_{\Omega} (|\nabla(\mathbf{c} - \bar{\mathbf{c}})|^2 + |\mathbf{c} - \bar{\mathbf{c}}|^2) dx, \end{aligned}$$

where we used the Lipschitz continuity of the second derivative of ψ in the last step. For \tilde{I}_{11} , we take into account the property $\mathbf{y}^\top G \mathbf{z} = \mathbf{y}^\top R P_L R \mathbf{z} = (P_L R \mathbf{y})^\top (P_L R \mathbf{z})$ and apply Young's inequality:

$$\begin{aligned} \tilde{I}_{11} &\leq \frac{\lambda}{4} \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ &\quad + C \lambda \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \left(\frac{\partial \psi}{\partial c_i}(\mathbf{c}) - \frac{\partial \psi}{\partial c_i}(\bar{\mathbf{c}}) \right) \right|^2 dx dt \\ &\leq \frac{\lambda}{4} \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ &\quad + C \int_0^T \int_{\Omega} (|\mathbf{c} - \bar{\mathbf{c}}|^2 + |\nabla(\mathbf{c} - \bar{\mathbf{c}})|^2) dx dt. \end{aligned}$$

Because of the boundedness of $\|\nabla D\psi(\bar{\mathbf{c}})\|_{L^\infty}$, the term \tilde{I}_{12} can be estimated in the same way as (64) and consequently, it satisfies inequality (64). Inserting these estimates into (79) and using the estimate for I_{10} , I_{11} , and I_{12} from Section 4.2, we arrive at

$$\begin{aligned} \mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) &+ \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ &+ \frac{\lambda}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \end{aligned}$$

$$\begin{aligned} &\leq \mathcal{H}(c^0|\bar{c}^0) + \frac{(\lambda_M - \lambda)^2}{\lambda} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(c)_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ &\quad + C \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned} \tag{80}$$

This estimate equals (67) with the exception of the factor $\lambda/4$ instead of $\lambda/2$ in the second term on the left-hand side.

Next, we consider the estimate of the relative energy. Inequality (54) still holds true with $\mu_i, \bar{\mu}_i$ replaced by $\mu_i + (\partial\psi/\partial c_i)(c), \bar{\mu}_i + (\partial\psi/\partial c_i)(\bar{c})$. We can use the estimates for I_{14}, I_{15}, I_{16} in (68), but I_{13} needs to be estimated differently. This term reads here as

$$\begin{aligned} I'_{13} &= - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(c) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{c}) \right) \nabla(\mu_i - \bar{\mu}_i) \cdot \nabla \left(\bar{\mu}_j + \frac{\partial\psi}{\partial c_j}(\bar{c}) \right) dx dt \\ &\quad - \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(c) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{c}) \right) \nabla \left(\frac{\partial\psi}{\partial c_i}(c) - \frac{\partial\psi}{\partial c_i}(\bar{c}) \right) \\ &\quad \quad \cdot \nabla \left(\bar{\mu}_j + \frac{\partial\psi}{\partial c_j}(\bar{c}) \right) dx dt \\ &=: I'_{131} + I'_{132}. \end{aligned}$$

The term I'_{131} can be estimated in the same way as in (70)–(71), additionally taking into account the boundedness of $\partial^2\psi/\partial c_i\partial c_j$, and it satisfies (73), while I'_{132} is bounded by Young’s inequality according to

$$\begin{aligned} I'_{132} &\leq C \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left(B_{ij}(c) - \frac{c_i}{\bar{c}_i} B_{ij}(\bar{c}) \right)^2 dx dt \\ &\quad + C \sum_{i,j=1}^n \int_0^T \int_{\Omega} \left| \nabla \left(\frac{\partial\psi}{\partial c_i}(c) - \frac{\partial\psi}{\partial c_i}(\bar{c}) \right) \right|^2 \left| \nabla \left(\bar{\mu}_j + \frac{\partial\psi}{\partial c_j}(\bar{c}) \right) \right|^2 dx dt \\ &\leq C \int_0^T \int_{\Omega} |c - \bar{c}|^2 dx dt + \int_0^T \int_{\Omega} |\nabla(c - \bar{c})|^2 dx dt. \end{aligned}$$

Observe that this inequality does not alter the estimates of the relative energy (74), but the second term on the left-hand side contains the difference $\mu_j + (\partial\psi/\partial c_j)(c) - \bar{\mu}_j - (\partial\psi/\partial c_j)(\bar{c})$ instead of $\mu_j - \bar{\mu}_j$, which is bounded from below by

$$\begin{aligned} &\frac{\lambda_m}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(c)_{ij} \sqrt{c_j} \nabla \left(\mu_j + \frac{\partial\psi}{\partial c_i}(c) - \bar{\mu}_j - \frac{\partial\psi}{\partial c_i}(\bar{c}) \right) \right|^2 dx dt \\ &\geq \frac{\lambda_m}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(c)_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ &\quad - \frac{3\lambda_m}{2} \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(c)_{ij} \sqrt{c_j} \nabla \left(\frac{\partial\psi}{\partial c_j}(c) - \frac{\partial\psi}{\partial c_j}(\bar{c}) \right) \right|^2 dx dt \end{aligned}$$

$$\begin{aligned} &\geq \frac{\lambda_m}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ &\quad - C \lambda_m \int_0^T \int_{\Omega} (|\mathbf{c} - \bar{\mathbf{c}}|^2 + |\nabla(\mathbf{c} - \bar{\mathbf{c}})|^2) dx. \end{aligned}$$

Hence, combining (74) with (80), multiplied by $8(\lambda_M - \lambda)^2/(\lambda_m \lambda)$,

$$\begin{aligned} &\mathcal{H}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}(T)|\bar{\mathbf{c}}(T)) \\ &\quad + \frac{(\lambda_M - \lambda)^2}{\lambda} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla(\mu_j - \bar{\mu}_j) \right|^2 dx dt \\ &\quad + \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} \left| \sum_{j=1}^n P_L(\mathbf{c})_{ij} \sqrt{c_j} \nabla \log \frac{c_j}{\bar{c}_j} \right|^2 dx dt \\ &\quad + \frac{\lambda}{4} \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta(c_i - \bar{c}_i))^2 dx dt \\ &\leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ &\quad + C(\theta, \theta') \sum_{i=1}^n \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned} \tag{81}$$

This inequality corresponds to the estimate in Step 3 of Section 4.2. The convex part of the energy equals

$$\mathcal{E}_1(\mathbf{c}|\bar{\mathbf{c}}) := \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{1}{2} \int_{\Omega} |\nabla(\mathbf{c} - \bar{\mathbf{c}})|^2 dx.$$

Then the energy can be bounded from below as

$$\mathcal{E}(\mathbf{c}|\bar{\mathbf{c}}) = \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{1}{2} \int_{\Omega} |\nabla(\mathbf{c} - \bar{\mathbf{c}})|^2 dx + \int_{\Omega} \psi(\mathbf{c}|\bar{\mathbf{c}}) dx \geq \mathcal{E}_1(\mathbf{c}|\bar{\mathbf{c}}) - C_1 \int_{\Omega} |\mathbf{c} - \bar{\mathbf{c}}|^2 dx,$$

where the last integral comes from the nonconvex part. Thus, together with $\mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) \geq \frac{1}{2} \int_{\Omega} |\mathbf{c} - \bar{\mathbf{c}}|^2 dx$, we conclude from (81) that

$$\begin{aligned} &\frac{1}{2} \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{1}{4} \int_{\Omega} |\mathbf{c} - \bar{\mathbf{c}}|^2 dx + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}_1(\mathbf{c}|\bar{\mathbf{c}}) - \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} C_1 \int_{\Omega} |\mathbf{c} - \bar{\mathbf{c}}|^2 dx \\ &\leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ &\quad + C \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned}$$

We choose $\lambda = \lambda_M - \varepsilon$, where $\varepsilon^2 < \lambda_m \lambda_M / (64C_1)$ and $\varepsilon < \lambda_M / 2$. Then

$$\frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} C_1 = \frac{8\varepsilon^2 C_1}{\lambda_m (\lambda_M - \varepsilon)} < \frac{\lambda_m \lambda_M / 8}{\lambda_m \lambda_M / 2} = \frac{1}{4}.$$

Thus the $L^2(\Omega)$ norm of $\mathbf{c} - \bar{\mathbf{c}}$ cancels, and we find that

$$\begin{aligned} \frac{1}{2} \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}_1(\mathbf{c}|\bar{\mathbf{c}}) &\leq \mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \\ &\quad + C \int_0^T \int_{\Omega} ((c_i - \bar{c}_i)^2 + |\nabla(c_i - \bar{c}_i)|^2) dx dt. \end{aligned}$$

Arguing as in Step 3 of Section 4.2, we can apply Grönwall’s inequality to end up with

$$\frac{1}{2} \mathcal{H}(\mathbf{c}|\bar{\mathbf{c}}) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}_1(\mathbf{c}|\bar{\mathbf{c}}) \leq C \left(\mathcal{H}(\mathbf{c}^0|\bar{\mathbf{c}}^0) + \frac{8(\lambda_M - \lambda)^2}{\lambda_m \lambda} \mathcal{E}(\mathbf{c}^0|\bar{\mathbf{c}}^0) \right).$$

Thus, the weak–strong uniqueness result holds in the presence of the nonconvex part of the potential.

6. Examples

We present some models which satisfy Assumptions (B1)–(B4).

6.1. A Cahn–Hilliard model with degenerate mobility

Elliott and Garcke [12] studied equations (1)–(5), formulated in terms of the mobility matrix (8), where

$$B_{ij}(\mathbf{c}) = b_i(c_i) \left(\delta_{ij} - \frac{b_j(c_j)}{\sum_{k=1}^n b_k(c_k)} \right), \quad i, j = 1, \dots, n.$$

The functions $b_i \in C^1([0, 1])$ are nonnegative and satisfy $\beta_1 c_i \leq b_i(c_i) \leq \beta_2 c_i$ for $c_i \in [0, 1]$ and some constants $0 < \beta_1 \leq \beta_2$. The potential ψ is chosen as

$$\psi(\mathbf{c}) = \mathbf{c}^\top \hat{M} \mathbf{c},$$

where \hat{M} is a constant $n \times n$ matrix. This model describes phase transitions in multicomponent systems; in [33] it has been suggested that the dynamics of polymer mixtures are modeled with $b_i(c_i) = \beta_i c_i$ and $\beta_i > 0$. The subspace $L(\mathbf{c})$ becomes

$$L(\mathbf{c}) = \{ \mathbf{z} \in \mathbb{R}^n : \sum_{i=1}^n \sqrt{b_i(c_i)} z_i = 0 \},$$

and the matrix $D^{\text{BD}}(\mathbf{c})$ is determined directly from the mobility matrix:

$$D_{ij}^{\text{BD}}(\mathbf{c}) = \frac{B_{ij}(\mathbf{c})}{\sqrt{b_i(c_i) b_j(c_j)}} = \delta_{ij} - \frac{\sqrt{b_i(c_i) b_j(c_j)}}{\sum_{k=1}^n b_k(c_k)}.$$

Instead of checking Assumptions (B1)–(B4), it is more convenient to verify the statements of Lemma 4 directly. This has been done in [22, Section 2]. Moreover, condition (P) holds. While the global existence of weak solutions has been already proved in [12], we obtain the weak–strong uniqueness property as a new result.

As illustrated in [12], for $n = 2$, taking $\hat{M}_{ij} = \chi(1 - \delta_{ij})$ for $i, j = 1, 2$ with $\chi > 0$ in the previous example, the variable $u := c_1 - c_2$ satisfies the Cahn–Hilliard model with degenerate mobility matrix

$$\partial_t u = \operatorname{div}[(1 - u^2)\nabla((\log(1 + u) - \log(1 - u)) - \chi u - \Delta u)].$$

This corresponds to the energy

$$\mathcal{E} = \int_{\Omega} \left(\frac{1}{2}((1 + u) \log(1 + u) + (1 - u) \log(u)) - \frac{\chi}{2}u^2 \right) dx + \frac{1}{2} \int_{\Omega} |\nabla u|^2 dx,$$

which is expressed in terms of u rather than (c_1, c_2) .

6.2. The classical Maxwell–Stefan system

In the classical Maxwell–Stefan model, the matrix $K(\mathbf{c})$ has entries

$$K_{ij}(\mathbf{c}) = \delta_{ij} \sum_{\ell=1}^n k_{i\ell} c_{\ell} - k_{ij} c_i$$

for $i, j = 1, \dots, n$. The associated matrix $D^{\text{MS}}(\mathbf{c})$ is given by

$$D_{ij}^{\text{MS}}(\mathbf{c}) = \frac{1}{\sqrt{c_i}} K_{ij}(\mathbf{c}) \sqrt{c_j} = \delta_{ij} \sum_{\ell=1}^n k_{i\ell} c_{\ell} - k_{ij} \sqrt{c_i c_j}, \quad i, j = 1, \dots, n.$$

It is proved in [22, Section 5.4] that this matrix satisfies Assumptions (B1)–(B4). Thus, Theorems 1 and 2 hold for the model

$$\begin{aligned} \partial_t c_i + \operatorname{div}(c_i u_i) &= 0, \quad \sum_{i=1}^n c_i u_i = 0, \quad i = 1, \dots, n, \\ c_i \nabla \mu_i - \frac{c_i}{\sum_{k=1}^n c_k} \sum_{j=1}^n c_j \nabla \mu_j &= - \sum_{j=1}^n k_{ij} c_i c_j (u_i - u_j), \end{aligned}$$

where $\mu_i = \log c_i - \Delta c_i$. Compared to [22], the mobility does not only depend on c_i but also on Δc_i . This extends the existence and weak–strong uniqueness results to a more general case.

6.3. A physical vapor decomposition model for solar cells

Thin-film crystalline solar cells can be fabricated as thin coatings on a substrate by the physical vapor decomposition process. The dynamics of the volume fractions of the process components can be described by model (1)–(4) with the mobility matrix

$$B_{ij}(\mathbf{c}) = \delta_{ij} \sum_{\ell=1}^n k_{i\ell} c_i c_{\ell} - k_{ij} c_i c_j, \quad i, j = 1, \dots, n.$$

In this case, the Bott–Duffin matrix is given by $D_{ij}^{\text{BD}}(\mathbf{c}) = B_{ij}(\mathbf{c})/\sqrt{c_i c_j} = D_{ij}^{\text{MS}}(\mathbf{c})$, where $D^{\text{MS}}(\mathbf{c})$ is the Maxwell–Stefan matrix of the previous subsection. Thus, Assumptions (B1)–(B4) are verified for this matrix. With the energy

$$\begin{aligned} \mathcal{E}(\mathbf{c}) &= \sum_{i=1}^n \int_{\Omega} c_i (\log c_i - 1) \, dx + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} |\nabla c_i|^2 \, dx \\ &\quad + \beta \int_{\Omega} c_1 (1 - c_1) \, dx, \end{aligned}$$

the chemical potential becomes $\mu_i = \log c_i - \Delta c_i + \beta(1 - c_1)$, and the nonconvex part of the potential has a bounded second derivative. This energy is different from that used in [10], since here we consider the phase separation of all species, while the authors in [10] consider the case when only one species is separated from the others. We infer that Theorems 1 and 2 hold for the model

$$\begin{aligned} \partial_t c_i &= \operatorname{div} \sum_{j=1}^n k_{ij} c_i c_j \nabla (\mu_i - \mu_j), \\ \mu_i &= \log c_i - \Delta c_i + \beta(1 - 2c_1), \quad i = 1, \dots, n. \end{aligned}$$

When $\mu_i = \log c_i$ for all i , the global existence of weak solutions was proved in [1] and the weak–strong uniqueness of solutions was shown in [20]. A global existence result was obtained in [10] for $\mu_1 = \log c_1 - \Delta c_1 + \beta(1 - 2c_1)$ with $\beta > 0$ and $\mu_i = \log c_i$ for $i = 2, \dots, n$.

A. Proof of Theorem 6

The proof is divided into four steps. First, we reformulate (35) using the first $n - 1$ components. Second, a time-discretized regularized system, similarly to [25, Chapter 4], is constructed and the existence of weak solutions to this system is proved. Third, we derive some uniform estimates from the energy inequality. Finally, we perform the deregularization limit.

Step 1: Reformulation in $n - 1$ components. We reformulate the approximate system in terms of the $n - 1$ relative chemical potentials

$$w_i^\delta = \mu_i^\delta - \mu_n^\delta, \quad i = 1, \dots, n - 1.$$

It holds that

$$\sum_{j=1}^n (P_L(\chi_\delta \mathbf{c}) R(\chi_\delta \mathbf{c}))_{kj} = \sum_{j=1}^n \left(\delta_{kj} - \frac{\sqrt{(\chi_\delta \mathbf{c})_k (\chi_\delta \mathbf{c})_j}}{\sum_{\ell=1}^n (\chi_\delta \mathbf{c})_\ell} \right) \sqrt{(\chi_\delta \mathbf{c})_j} = 0.$$

Then, using $D^{\text{BD}}(\mathbf{c}) = D^{\text{BD}}(\mathbf{c})P_L(\mathbf{c})$ (which is a general property of the Bott–Duffin inverse; see [22, (81)]),

$$\begin{aligned} \sum_{j=1}^n B_{ij}^\delta(\mathbf{c}) &= \sum_{j=1}^n \sqrt{(\chi_\delta \mathbf{c})_i} D_{ij}^{\text{BD}}(\mathbf{c}) \sqrt{(\chi_\delta \mathbf{c})_j} \\ &= \sum_{j,k=1}^n \sqrt{(\chi_\delta \mathbf{c})_i} D_{ik}^{\text{BD}}(\mathbf{c}) (P_L(\chi_\delta \mathbf{c})R(\chi_\delta \mathbf{e}))_{kj} = 0. \end{aligned}$$

This shows that

$$\sum_{j=1}^n B_{ij}^\delta(\mathbf{c}) \nabla \mu_j^\delta = \sum_{j=1}^{n-1} B_{ij}^\delta(\mathbf{c}) \nabla \mu_j^\delta + B_{in}^\delta(\mathbf{c}) \nabla \mu_n^\delta = \sum_{j=1}^{n-1} B_{ij}^\delta(\mathbf{c}) \nabla (\mu_j^\delta - \mu_n^\delta).$$

Consequently, we can rewrite the first equation in (35) as

$$\partial_t c_i^\delta = \operatorname{div} \sum_{j=1}^{n-1} \tilde{B}_{ij}^\delta(\mathbf{c}^\delta) \nabla w_j^\delta, \quad i = 1, \dots, n-1, \quad c_n^\delta = 1 - \sum_{i=1}^{n-1} c_i^\delta, \quad (82)$$

recalling that \tilde{B}^δ is the first $(n-1) \times (n-1)$ submatrix of B^δ .

Step 2: Existence for a regularized system. We consider for given $\delta > 0, T > 0, N \in \mathbb{N}$, and $(c_1^{k-1}, \dots, c_{n-1}^{k-1})$ the regularized system

$$\frac{1}{\tau} (c_i^k - c_i^{k-1}) = \operatorname{div} \sum_{j=1}^{n-1} \tilde{B}_{ij}^\delta(\tilde{\mathbf{c}}^k) \nabla w_j^k - \varepsilon (\Delta^2 w_i^k + w_i^k) \quad \text{in } \Omega, \quad (83)$$

$$w_i^k = (h_i^\delta)'(c_i^k) - (h_n^\delta)'(c_n^k) - \Delta(c_i^k - c_n^k), \quad i = 1, \dots, n-1, \quad (84)$$

where $\tau = T/N$ and $c_n^k = 1 - \sum_{i=1}^{n-1} c_i^k$. Equation (83) is understood in the weak sense:

$$\begin{aligned} \frac{1}{\tau} \int_{\Omega} (c_i^k - c_i^{k-1}) \phi_i \, dx + \sum_{j=1}^{n-1} \int_{\Omega} \tilde{B}_{ij}^\delta(\mathbf{c}^k) \nabla \phi_i \cdot \nabla w_j^k \, dx \\ + \varepsilon \int_{\Omega} (\Delta w_i^k \Delta \phi_i + w_i^k \phi_i) \, dx = 0 \end{aligned}$$

for test functions $\phi_i \in H^2(\Omega)$.

The ε -regularization ensures that $w_i^k \in H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ since $d \leq 3$. In higher space dimensions, we can replace $\Delta^2 w_i^k$ by $(-\Delta)^m w_i^k$ with $m > d/2$, which gives $w_i^k \in H^m(\Omega) \hookrightarrow L^\infty(\Omega)$.

We prove the solvability of (83)–(84) in two steps.

Lemma 11 (Solvability of (84)). *Let $\mathbf{w} \in L^2(\Omega; \mathbb{R}^{n-1})$. Then there exists a unique strong solution $\tilde{\mathbf{c}} \in H^2(\Omega; \mathbb{R}^{n-1})$ to*

$$w_i = (h_i^\delta)'(c_i) - (h_n^\delta)'(c_n) - \Delta(c_i - c_n) \text{ in } \Omega, \quad \nabla c_i \cdot \nu = 0 \text{ on } \partial\Omega \quad (85)$$

for $i = 1, \dots, n - 1$, where $c_n = 1 - \sum_{i=1}^{n-1} c_i$. This defines the operator $\mathcal{L}: L^2(\Omega; \mathbb{R}^{n-1}) \rightarrow H^2(\Omega; \mathbb{R}^{n-1})$, $\mathcal{L}(\mathbf{w}) = \tilde{\mathbf{c}}$.

Proof. The system of equations can be written as

$$\operatorname{div}(M \nabla \tilde{\mathbf{c}})_i = (h_i^\delta)'(c_i) - (h_n^\delta)'(c_n) - w_i \quad \text{in } \Omega,$$

where the entries of the diffusion matrix M are $M_{ii} = 2$ and $M_{ij} = 1$ for all $i \neq j$. In particular, M is symmetric and positive definite. Thus, we can apply the theory for elliptic systems with sublinear growth function and conclude the existence of a unique weak solution $\tilde{\mathbf{c}} \in H^1(\Omega; \mathbb{R}^{n-1})$. It remains to verify that this solution lies in $H^2(\Omega; \mathbb{R}^{n-1})$. Summing (85) over $i = 1, \dots, n - 1$, we find that

$$\Delta c_n = - \sum_{i=1}^{n-1} \Delta c_i = \frac{1}{n} \sum_{i=1}^{n-1} (w_i - (h_i^\delta)'(c_i)) + \frac{n-1}{n} (h_n^\delta)'(c_n) \in L^2(\Omega)$$

with the boundary condition $\nabla c_n \cdot \nu = 0$ on $\partial\Omega$. We infer from elliptic regularity theory that $c_n \in H^2(\Omega)$. Consequently, $\Delta c_n \in L^2(\Omega)$ and elliptic regularity again implies that $c_i \in H^2(\Omega)$. ■

It follows from Lemma 11 that we can write (83) as

$$\begin{aligned} & \frac{1}{\tau} (\mathcal{L}(\mathbf{w}))_i - c_i^{k-1} \\ &= \operatorname{div} \sum_{j=1}^{n-1} \tilde{B}_{ij}^\delta(\tilde{\mathbf{c}}^k) \nabla w_j^k - \varepsilon (\Delta^2 w_i^k + w_i^k) \quad \text{in } \Omega, i = 1, \dots, n - 1. \end{aligned} \tag{86}$$

Lemma 12 (Solvability of (86)). *Let $\tilde{\mathbf{c}}^{k-1} \in H^2(\Omega; \mathbb{R}^{n-1})$. Then there exists a weak solution $\mathbf{w}^k \in H^2(\Omega; \mathbb{R}^{n-1})$ to (86) such that for all $\phi_i \in L^2(0, T; H^2(\Omega))$,*

$$\begin{aligned} & \frac{1}{\tau} \int_{\Omega} (\mathcal{L}(\mathbf{w}))_i - c_i^{k-1} \phi_i \, dx + \sum_{i,j=1}^{n-1} \int_{\Omega} \tilde{B}_{ij}^\delta(\mathcal{L}(\mathbf{w})) \nabla \phi_i \cdot \nabla w_j^k \, dx \\ &+ \varepsilon \sum_{i=1}^{n-1} \int_{\Omega} (\Delta w_i^k \Delta \phi_i + w_i^k \phi_i) \, dx = 0. \end{aligned}$$

Proof. Given $\bar{\mathbf{w}} \in L^\infty(\Omega; \mathbb{R}^{n-1})$ and $\sigma \in [0, 1]$, we wish to find a solution to the linear problem

$$\mathcal{A}(\mathbf{w}, \phi) = \mathcal{F}(\phi) \quad \text{for } \phi \in H^2(\Omega; \mathbb{R}^{n-1}), \tag{87}$$

where

$$\begin{aligned} \mathcal{A}(\mathbf{w}, \phi) &= \sum_{i,j=1}^{n-1} \int_{\Omega} \tilde{B}_{ij}^\delta(\mathcal{L}(\bar{\mathbf{w}})) \nabla \phi_i \cdot \nabla w_j \, dx + \varepsilon \sum_{i=1}^{n-1} \int_{\Omega} (\Delta w_i \Delta \phi_i + w_i \phi_i) \, dx, \\ \mathcal{F}(\phi) &= -\frac{\sigma}{\tau} \int_{\Omega} (\mathcal{L}(\bar{\mathbf{w}}) - \tilde{\mathbf{c}}^{k-1}) \cdot \phi \, dx. \end{aligned}$$

We infer from the boundedness of $\tilde{B}_{ij}^\delta(\mathcal{L}(\bar{w}))$ that the bilinear form \mathcal{A} is continuous on $H^2(\Omega; \mathbb{R}^{n-1})$. Furthermore, by the positive-definiteness of $\tilde{B}_{ij}^\delta(\mathcal{L}(\bar{w}))$, thanks to (39), \mathcal{A} is coercive. Moreover, \mathcal{F} is a continuous linear form on $H^2(\Omega; \mathbb{R}^{n-1})$. We conclude from the Lax–Milgram theorem that there exists a unique solution $\mathbf{w} \in H^2(\Omega; \mathbb{R}^{n-1})$ to (87). Since $d \leq 3$ by Assumption (A1), we have $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ and therefore $\mathbf{w} \in L^\infty(\Omega; \mathbb{R}^{n-1})$.

This defines the fixed-point operator $S: L^\infty(\Omega; \mathbb{R}^{n-1}) \times [0, 1] \rightarrow L^\infty(\Omega; \mathbb{R}^{n-1})$, $S(\bar{w}, \sigma) = \mathbf{w}$. The operator S is continuous, and it satisfies $S(\bar{w}, 0) = \mathbf{0}$ for all $\bar{w} \in L^\infty(\Omega; \mathbb{R}^{n-1})$. In view of the compact embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$, S is also compact. It remains to verify that all fixed points of $S(\cdot, \sigma)$ are uniformly bounded. To this end, let $\mathbf{w} \in L^\infty(\Omega; \mathbb{R}^{n-1})$ be such a fixed point. Then $\mathbf{w} \in H^2(\Omega; \mathbb{R}^{n-1})$ solves (87) with $\bar{w} = \mathbf{w}$. We choose the test function $\phi = \mathbf{w}$ in (87) to find that

$$\begin{aligned} \frac{\sigma}{\tau} \int_{\Omega} (\tilde{c} - \tilde{c}^{k-1}) \cdot \mathbf{w} \, dx + \sum_{i,j=1}^{n-1} \int_{\Omega} \tilde{B}_{ij}^\delta(\tilde{c}) \nabla w_i \cdot \nabla w_j \, dx \\ + \varepsilon \sum_{i=1}^{n-1} \int_{\Omega} ((\Delta w_i)^2 + w_i^2) \, dx = 0, \end{aligned} \tag{88}$$

where $\tilde{c} = \mathcal{L}(\mathbf{w}) = (c_1, \dots, c_{n-1})$ and c_i solves (84) with w_i^k replaced by w_i . Using the test function $c_i - c_i^{k-1}$ in the weak formulation of (84) leads to

$$\begin{aligned} \sum_{i=1}^{n-1} \int_{\Omega} (c_i - c_i^{k-1}) w_i \, dx = \sum_{i=1}^{n-1} \int_{\Omega} (\nabla(c_i - c_n) \cdot \nabla(c_i - c_i^{k-1}) \\ + ((h_i^\delta)'(c_i) - (h_i^\delta)'(c_n))(c_i - c_i^{k-1})) \, dx. \end{aligned}$$

The convexity of the function h_i^δ and $\sum_{i=1}^{n-1} c_i = 1 - c_n$ imply that

$$\begin{aligned} \sum_{i=1}^{n-1} (c_i - c_i^{k-1}) (h_i^\delta)'(c_i) &\geq \sum_{i=1}^{n-1} (h_i^\delta(c_i) - h_i^\delta(c_i^{k-1})), \\ - \sum_{i=1}^{n-1} (c_i - c_i^{k-1}) (h_n^\delta)'(c_n) &= (c_n - c_n^{k-1}) (h_n^\delta)'(c_n) \geq h_n^\delta(c_n) - h_n^\delta(c_n^{k-1}). \end{aligned}$$

Moreover, since $\sum_{i=1}^{n-1} \nabla c_i = -\nabla c_n$ and $\sum_{i=1}^{n-1} \nabla c_i^{k-1} = -\nabla c_n^{k-1}$,

$$\begin{aligned} \sum_{i=1}^{n-1} \nabla(c_i - c_n) \cdot \nabla(c_i - c_i^{k-1}) &= \sum_{i=1}^n |\nabla c_i|^2 - \sum_{i=1}^n \nabla c_i^{k-1} \cdot \nabla c_i \\ &\geq \frac{1}{2} \sum_{i=1}^n |\nabla c_i|^2 - \frac{1}{2} \sum_{i=1}^n |\nabla c_i^{k-1}|^2. \end{aligned}$$

This yields

$$\begin{aligned} & \sum_{i=1}^{n-1} \int_{\Omega} (c_i - c_i^{k-1}) w_i \, dx \\ & \geq \sum_{i=1}^n \int_{\Omega} (h_i^\delta(c_i) - h_i^\delta(c_i^{k-1})) \, dx + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} (|\nabla c_i|^2 - |\nabla c_i^{k-1}|^2) \, dx \\ & \geq \tilde{\mathcal{E}}^\delta(\tilde{c}) - \tilde{\mathcal{E}}^\delta(\tilde{c}^{k-1}), \end{aligned}$$

where

$$\tilde{\mathcal{E}}^\delta(\tilde{c}) := \tilde{\mathcal{H}}^\delta(\tilde{c}) + \sum_{i=1}^n \int_{\Omega} |\nabla c_i|^2 \, dx, \quad \tilde{\mathcal{H}}^\delta(\tilde{c}) := \mathcal{H}^\delta(c).$$

Inserting this inequality into (88) finally gives

$$\begin{aligned} & \sigma \tilde{\mathcal{E}}^\delta(\tilde{c}) + \tau \sum_{i,j=1}^{n-1} \int_{\Omega} \tilde{B}_{ij}^\delta(\tilde{c}) \nabla w_i \cdot \nabla w_j \, dx \\ & \quad + \varepsilon \tau \int_{\Omega} (|\Delta \mathbf{w}|^2 + |\mathbf{w}|^2) \, dx \leq \sigma \tilde{\mathcal{E}}^\delta(\tilde{c}^{k-1}). \end{aligned} \tag{89}$$

By the positive-definiteness of \tilde{B}^δ (positive-semidefiniteness is sufficient), this gives a uniform $H^2(\Omega)$ bound and consequently a uniform $L^\infty(\Omega)$ bound for \mathbf{w} . The Leray–Schauder fixed-point theorem now implies the existence of a solution to (83)–(84). ■

Step 3: Uniform estimates. We wish to derive estimates uniform in ε and τ . The starting point is the regularized energy estimate (89) and the positive-definiteness estimate (39). First, we introduce the piecewise constant in time functions $\mathbf{w}^{(\tau)}(x, t) = \mathbf{w}^k(x)$, $\tilde{c}^{(\tau)}(x, t) = \mathcal{L}(\mathbf{w}^k(x))$ for $x \in \Omega$ and $t \in ((k-1)\tau, k\tau]$, $k = 1, \dots, N$, and set $\mathbf{w}^{(\tau)}(x, 0) = (\partial \tilde{\mathcal{E}} / \partial \tilde{c})(\tilde{c}^0)$ and $\tilde{c}^{(\tau)}(x, 0) = \tilde{c}^0$. Then, introducing the shift operator $(\sigma_\tau \mathbf{w}^{(\tau)})(x, t) = \mathbf{w}^{(\tau)}(x, t - \tau)$ for $x \in \Omega$ and $t \geq \tau$, we can formulate (83)–(84) as

$$\frac{1}{\tau} (\tilde{c}^{(\tau)} - \sigma_\tau \tilde{c}^{(\tau)}) = \operatorname{div}(\tilde{B}^\delta(\tilde{c}) \nabla \mathbf{w}^{(\tau)}) - \varepsilon(\Delta^2 \mathbf{w}^{(\tau)} + \mathbf{w}^{(\tau)}), \tag{90}$$

$$w_i^{(\tau)} = (h_i^\delta)'(c_i^{(\tau)}) - (h_n^\delta)'(c_n^{(\tau)}) - \Delta(c_i^{(\tau)} - c_n^{(\tau)}), \quad i = 1, \dots, n-1, \tag{91}$$

recalling that $\tilde{c}^{(\tau)} = \mathcal{L}(\mathbf{w}^{(\tau)})$ is a function of $\mathbf{w}^{(\tau)}$. Then (89) can be written after summation over $k = 1, \dots, N$ as

$$\tilde{\mathcal{E}}^\delta(\tilde{c}^{(\tau)}(T)) + \eta(\delta) \int_0^T \int_{\Omega} |\nabla \mathbf{w}^{(\tau)}|^2 \, dx \, dt + \varepsilon C \int_0^T \|\mathbf{w}^{(\tau)}\|_{H^2(\Omega)}^2 \, dt \leq \tilde{\mathcal{E}}^\delta(\tilde{c}^0),$$

where we used (39) and the generalized Poincaré inequality with constant $C > 0$. This implies the estimates

$$C(\delta) \|\mathbf{w}^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \sqrt{\varepsilon} \|\mathbf{w}^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} \leq C, \tag{92}$$

where $C > 0$ denotes here and in the following a constant independent of ε and τ .

To derive a uniform estimate for $\tilde{\mathbf{c}}^{(\tau)}$, we multiply (91) by $-\Delta c_i^{(\tau)}$, integrate over $Q_T = \Omega \times (0, T)$, integrate by parts, and sum over $i = 1, \dots, n - 1$:

$$\begin{aligned} & \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} \nabla w_i^{(\tau)} \cdot \nabla c_i^{(\tau)} \, dx \, dt \\ &= \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} \nabla((h_i^\delta)'(c_i^{(\tau)}) - (h_n^\delta)'(c_n^{(\tau)})) \cdot \nabla c_i^{(\tau)} \, dx \, dt \\ & \quad + \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} ((\Delta c_i^{(\tau)})^2 - \Delta c_i^{(\tau)} \Delta c_n^{(\tau)}) \, dx \, dt =: I_3 + I_4. \end{aligned}$$

Since $\nabla(h_i^\delta)'(c_i^{(\tau)}) = (h_i^\delta)''(c_i^{(\tau)})\nabla c_i^{(\tau)} = \nabla c_i^{(\tau)} / (\chi_\delta \mathbf{c}^{(\tau)})_i$ and $\sum_{i=1}^{n-1} \nabla c_i^{(\tau)} = -\nabla c_n^{(\tau)}$, the term I_3 can be written as

$$I_3 = \sum_{i=1}^n \int_0^T \int_{\Omega} \frac{|\nabla c_i^{(\tau)}|^2}{(\chi_\delta \mathbf{c}^{(\tau)})_i} \, dx \, dt.$$

Using the property $\sum_{i=1}^{n-1} \Delta c_i^{(\tau)} = -\Delta c_n^{(\tau)}$, the remaining term I_4 becomes

$$I_4 = \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta c_i^{(\tau)})^2 \, dx \, dt.$$

Therefore, by Young’s inequality,

$$\begin{aligned} & \sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta c_i^{(\tau)})^2 \, dx \, dt + \sum_{i=1}^n \int_0^T \int_{\Omega} \frac{|\nabla c_i^{(\tau)}|^2}{(\chi_\delta \mathbf{c}^{(\tau)})_i} \, dx \, dt \\ &= \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} \nabla w_i^{(\tau)} \cdot \nabla c_i^{(\tau)} \, dx \, dt \\ &\leq \frac{1}{2} \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} \left(\frac{|\nabla c_i^{(\tau)}|^2}{(\chi_\delta \mathbf{c}^{(\tau)})_i} + (\chi_\delta \mathbf{c}^{(\tau)})_i |\nabla w_i^{(\tau)}|^2 \right) \, dx \, dt \\ &\leq \frac{1}{2} \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} \frac{|\nabla c_i^{(\tau)}|^2}{(\chi_\delta \mathbf{c}^{(\tau)})_i} \, dx \, dt + \frac{1}{2} \sum_{i=1}^{n-1} \int_0^T \int_{\Omega} |\nabla w_i^{(\tau)}|^2 \, dx \, dt. \end{aligned}$$

The first term on the right-hand side is absorbed by the left-hand side. Thus, we deduce from (92) that

$$\sum_{i=1}^n \int_0^T \int_{\Omega} (\Delta c_i^{(\tau)})^2 \, dx \, dt + \frac{1}{2} \sum_{i=1}^n \int_0^T \int_{\Omega} \frac{|\nabla c_i^{(\tau)}|^2}{(\chi_\delta \mathbf{c}^{(\tau)})_i} \, dx \, dt \leq \frac{1}{2} \|\nabla \mathbf{w}^{(\tau)}\|_{L^2(Q_T)}^2 \leq C.$$

Since $c_i^{(\tau)} \in L^\infty(Q_T)$, we infer from the previous estimate that

$$\|c_i^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} \leq C, \quad i = 1, \dots, n. \tag{93}$$

Finally, we derive an estimate for the discrete time derivative. It follows from (86) that

$$\begin{aligned} \frac{1}{\tau} \|c_i^{(\tau)} - \sigma_\tau c_i^{(\tau)}\|_{L^2(0,T;H^2(\Omega)')} &\leq \sum_{j=1}^{n-1} \|\tilde{B}_{ij}^\delta(\tilde{c}^{(\tau)})\|_{L^\infty(Q_T)} \|\nabla w_j^{(\tau)}\|_{L^2(Q_T)} \\ &\quad + \varepsilon \|w_i^{(\tau)}\|_{L^2(0,T;H^2(\Omega))}. \end{aligned}$$

The entries of $\tilde{B}^\delta(\tilde{c}^{(\tau)})$ are bounded since $\delta \leq (\chi_\delta c^{(\tau)})_i \leq 1 - \delta$. Thus, by (92),

$$\tau^{-1} \|c_i^{(\tau)} - \sigma_\tau c_i^{(\tau)}\|_{L^2(0,T;H^2(\Omega)')} \leq C, \quad i = 1, \dots, n - 1. \tag{94}$$

Step 4: Limit $(\varepsilon, \tau) \rightarrow 0$. In view of estimates (93) and (94), we can apply the version of the Aubin–Lions lemma in [9, Theorem 1] to conclude the existence of a subsequence, which is not relabeled, such that as $(\varepsilon, \tau) \rightarrow 0$,

$$c_i^{(\tau)} \rightarrow c_i \quad \text{strongly in } L^2(0, T; H^1(\Omega)), \quad i = 1, \dots, n - 1.$$

We deduce from (92)–(94) that, possibly for another subsequence,

$$\begin{aligned} c_i^{(\tau)} &\rightharpoonup c_i && \text{weakly in } L^2(0, T; H^2(\Omega)), \\ \tau^{-1}(c_i^{(\tau)} - \sigma_\tau c_i^{(\tau)}) &\rightharpoonup \partial_t c_i && \text{weakly in } L^2(0, T; H^2(\Omega)'), \\ w_i^{(\tau)} &\rightharpoonup w_i && \text{weakly in } L^2(0, T; H^1(\Omega)), \\ \varepsilon w_i^{(\tau)} &\rightarrow 0 && \text{strongly in } L^2(0, T; H^2(\Omega)), \quad i = 1, \dots, n - 1. \end{aligned}$$

We define $c_n := 1 - \sum_{i=1}^{n-1} c_i$. Then $c_n^{(\tau)} \rightarrow c_n$ strongly in $L^2(0, T; H^1(\Omega))$ and weakly in $L^2(0, T; H^2(\Omega))$. Furthermore, $(c_i^{(\tau)})$ converges, up to a subsequence, pointwise a.e., and its limit satisfies $\delta \leq (\chi_\delta c)_i \leq 1 - \delta, i = 1, \dots, n$. The matrix $\tilde{B}_{ij}^\delta(\tilde{c}^{(\tau)})$ is uniformly bounded and

$$\tilde{B}_{ij}^\delta(\tilde{c}^{(\tau)}) \rightarrow \tilde{B}_{ij}^\delta(\tilde{c}) \quad \text{strongly in } L^q(Q_T) \text{ for any } q < \infty, i, j = 1, \dots, n.$$

These convergence results allow us to pass to the limit $(\varepsilon, \tau) \rightarrow 0$ in the weak formulation of (90)–(91) to find that c solves

$$\partial_t c_i = \operatorname{div} \sum_{j=1}^{n-1} \tilde{B}_{ij}^\delta(\tilde{c}) \nabla w_j, \quad w_i = (h_i^\delta)'(c_i) - (h_n^\delta)'(c_n) - \Delta(c_i - c_n)$$

for $i = 1, \dots, n - 1$. Transforming back to the chemical potential μ via $w_i = \mu_i - \mu_n$ and $c_n = 1 - \sum_{i=1}^{n-1} c_i$, we see that $c^\delta := c$ solves system (35)–(36), where $\mu_i = (h_i^\delta)'(c_i) - \Delta c_i$.

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