EXISTENCE ANALYSIS OF A SINGLE-PHASE FLOW MIXTURE MODEL WITH VAN DER WAALS PRESSURE

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ABSTRACT. The transport of single-phase fluid mixtures in porous media is described by cross-diffusion equations for the mass densities. The equations are obtained in a thermo-dynamic consistent way from mass balance, Darcy's law, and the van der Waals equation of state for mixtures. The model consists of parabolic equations with cross diffusion with a hypocoercive diffusion operator. The global-in-time existence of weak solutions in a bounded domain with equilibrium boundary conditions is proved, extending the boundedness-by-entropy method. Based on the free energy inequality, the large-time convergence of the solution to the constant equilibrium mass density is shown. For the two-species model and specific diffusion matrices, an integral inequality is proved, which reveals a minimum principle for the mass fractions. Without mass diffusion, the two-dimensional pressure is shown to converge exponentially fast to a constant. Numerical examples in one space dimension illustrate this convergence.

1. INTRODUCTION

The transport of fluid mixtures in porous media has many important industrial applications like oil and gas extraction, dispersion of contaminants in underground water reservoirs, nuclear waste storage, and carbon sequestration. Although there are many papers on the modeling and numerical solution of such compositional models [1, 6, 7, 11, 17, 19], there are no results on their mathematical analysis. In this paper, we provide an existence analysis for a single-phase compositional model with van der Waals pressure in an isothermal setting. From a mathematical viewpoint, the model consists of strongly coupled degenerate parabolic equations for the mass densities. The cross-diffusion coupling and the hypocoercive diffusion operator constitute the main difficulty of the analysis.

Our analysis is a continuation of the program of the first and third author to develop a theory for cross-diffusion equations possessing an entropy (here: free energy) structure [13, 23]. The mathematical novelties are the complex structure of the equations and the observation that the solution of the binary model, for specific diffusion matrices, satisfies

an unexpected integral inequality giving rise to a minimum principle, which generally does not hold for strongly coupled diffusion systems.

Model equations. More specifically, we consider an isothermal fluid mixture of n mass densities $c_i(x,t)$ in a domain $\Omega \subset \mathbb{R}^d$ ($d \le 3$), whose evolution is governed by the transport equations

$$(1) \qquad \partial_t c_i = \mathrm{div}\left(c_i \nabla p + \varepsilon \sum_{j=1}^n D_{ij}(c) \nabla \mu_j \right), \quad x \in \Omega,\ t > 0,\ i = 1, \ldots, n,$$

where $c = (c_1, \ldots, c_n)$. The van der Waals pressure $p = p(c)$ and the chemical potentials $\mu_1 = \mu_1(c), \ldots, \mu_n = \mu_n(c)$ are given by

$$(2) \qquad p = \frac{c_{\mathrm{tot}}}{1 - \sum_{j=1}^n b_j c_j} - \sum_{i,j=1}^n a_{ij} c_i c_j,$$

$$(3) \qquad \mu_i = \log c_i - \log\left(1 - \sum_{j=1}^n b_j c_j\right) + \frac{b_i c_{\mathrm{tot}}}{1 - \sum_{j=1}^n b_j c_j} - 2\sum_{j=1}^n a_{ij} c_j.$$

These expressions are well defined if $(c_1(x,t), \ldots, c_n(x,t)) \in \mathscr{D}$ a.e., where

$$(4) \qquad \mathscr{D} = \left\{ (c_1, \ldots, c_n) \in \mathbb{R}^n : c_i > 0 \text{ for } i = 1, \ldots, n,\ \sum_{j=1}^n b_j c_j < 1 \right\}.$$

Here, $c_{\mathrm{tot}} = \sum_{i=1}^n c_i$ is the total mass density and $\varepsilon > 0$ is a (small) parameter. The parameter $a_{ij} = a_{ji} > 0$ measures the attraction between the ith and jth species, and $b_j > 0$ is a measure of the size of the molecules. The diffusion matrix $D(c) = (D_{ij}(c))$ is assumed to be symmetric and positive semidefinite. Moreover, we suppose that the following bound holds:

$$(5) \qquad D_0 |\Pi v|^2 \le \sum_{i,j=1}^n D_{ij}(c) v_i v_j \le D_1 |\Pi v|^2 \quad \text{for all } v \in \mathbb{R}^n,\ c \in \mathscr{D},$$

for some $D_0, D_1 > 0$, where $\Pi = I - \ell \otimes \ell$ is the projection on the subspace of $\mathbb{R}^n$ orthogonal to $\ell := (1, \ldots, 1)/\sqrt{n}$. A property like (5) is known in the literature as *hypocoercivity*, that is, coercivity on a subspace of the considered vector space. In our case, the matrix $D(c)$ in (5) is coercive on the orthogonal complement of the subspace generated by ℓ. Bound (5) is justified in the derivation of model (1)-(3), as the diffusion fluxes $J_i = -\varepsilon \sum_{j=1}^n D_{ij} \nabla \mu_j$ must sum up to zero (see Section 2).

Equation (2) is the van der Waals equation of state for mixtures, taking into account the finite size of the molecules. Equations (2)-(3) are derived from the Helmholtz free energy $\mathcal{F}(c)$ of the mixture; see (16) below. For details of the modeling and the underlying assumptions, we refer to Section 2.

We impose the boundary and initial conditions

$$(6) \qquad \mu_i = 0 \quad \text{on } \partial\Omega,\ t > 0, \quad c_i(\cdot, 0) = c_i^0 \quad \text{in } \Omega,\ i = 1, \ldots, n.$$

Note that we choose equilibrium boundary conditions. A physically more realistic choice would be to assume that the reservoir boundary is impermeable, leading to no-flux boundary conditions. However, conditions (6) are needed to obtain Sobolev estimates, together with the energy inequality (8) below. Numerical examples for homogeneous Neumann boundary conditions for the pressure in case $\varepsilon = 0$ are presented in Section 7.

Up to our knowledge, there are no analytical results for system (1)-(3) and (6). In the literature, Euler and Navier-Stokes models were considered with van der Waals pressure. For instance, the existence of global classical solutions to the corresponding Euler equations with small initial data was shown in [15]. The existence of traveling waves in one-dimensional Navier-Stokes with capillarity was studied in [21]. Furthermore, in [10] the existence and stability of shock fronts in the vanishing viscosity limit for Navier-Stokes equations with van der Waals type equations of state was established.

Main difficulties. A straightforward computation shows that the Gibbs-Duhem relation $\nabla p = \sum_{i=1}^{n} c_i \nabla \mu_i$ holds. Therefore, (1) can be written as

$$(7) \qquad \partial_t c_i = \operatorname{div} \sum_{j=1}^{n} \big((c_i c_j + \varepsilon D_{ij}(c)) \nabla \mu_j \big), \quad i = 1, \ldots, n,$$

which is a cross-diffusion system in the so-called entropy variables μ_i [13]. The matrix $(c_i c_j) \in \mathbb{R}^{n \times n}$ is of rank one with two eigenvalues, a positive one and the other one equal to zero (with algebraic multiplicity $n - 1$). Thus, if $\varepsilon = 0$, system (1) is not parabolic in the sense of Petrovski [2], and an existence theory for such diffusion systems is highly nontrivial, which is the *first difficulty*. The property on the eigenvalues is reflected in the energy estimate. Indeed, a formal computation, made rigorous below, shows that

$$(8) \qquad \frac{d}{dt} \int_\Omega \mathcal{F}(c) dx + \int_\Omega |\nabla p|^2 dx + \varepsilon \int_\Omega \nabla \mu : D(c) \nabla \mu \, dx \le 0.$$

In case $\varepsilon = 0$ we obtain only one gradient estimate for p which is not sufficient for the analysis. There exist some results for so-called strongly degenerate parabolic equations (for which the diffusion matrix vanishes in some subset of positive d-dimensional measure) [3]. However, the techniques cannot be applied to the present problem. Therefore, we need to assume that $\varepsilon > 0$. Then the gradient estimates for $\Pi\mu$ and p together with the boundary conditions (6) yield uniform H^1 bounds, which are the basis of the existence proof. The behavior of the solutions for $\varepsilon = 0$ are studied numerically in Section 7.

The *second difficulty* is the invertibility of the relation between c and μ, i.e. to define for given μ the mass density vector $c = \Phi^{-1}(\mu)$, where $\mu = (\mu_1, \ldots, \mu_n)$ and $\Phi : \mathscr{D} \to \mathbb{R}^n$ is defined by (3). A key ingredient for the proof is the positive definiteness of the Hessian $\mathcal{F}''$ of the free energy since $\partial \Phi_i / \partial c_j = \partial^2 \mathcal{F} / \partial c_i \partial c_j$. This is only possible under a smallness condition on the eigenvalues of (a_{ij}); see Lemma 6. This condition is not surprising since it just means that phase separation is prohibited. The analysis of multiphase flows requires completely different mathematical techniques; see, e.g., [25] for phase transitions in Euler equations with van der Waals pressure.

The *third difficulty* is the proof of $c(x,t) \in \mathscr{D}$ a.e. This property is needed to define p and μ_i through (2)-(3), but generally a maximum principle cannot be applied to the strongly coupled system (1). The idea is to employ the boundedness-by-entropy method as in [13, 23], i.e. to work with the entropy variables $\mu = \Phi(c)$. We show first the existence of weak solutions $\mu = (\mu_1, \ldots, \mu_n)$ to a regularized version of (7), define $c = \Phi^{-1}(\mu)$ and perform the de-regularization limit to obtain the existence of a weak solution c to (1). Since $c(x,t) = \Phi^{-1}(\mu(x,t)) \in \mathscr{D}$ a.e. by definition of Φ, $c_i(x,t)$ turns out to be bounded. This idea avoids the maximum principle and is the core of the boundedness-by-entropy method. Let us now detail our main results.

Global existence of solutions. Using the boundedness-by-entropy method and the energy inequality (8), we are able to prove the global existence of bounded weak solutions. We set $c_{\text{tot}}^0 = \sum_{i=1}^n c_i^0$ and $c_{\text{tot}}^\Gamma = \sum_{i=1}^n c_i^\Gamma$.

Theorem 1 (Existence and large-time asymptotics). *Let $c_i^0 : \Omega \to \mathscr{D}$, $i = 1, \ldots, n$, be Lebesgue measurable and let $c^\Gamma = \Phi^{-1}(0) \in \mathscr{D}$ such that $\log c_{\text{tot}}^\Gamma \in L^1(\Omega)$, where $\Phi : \mathscr{D} \to \mathbb{R}^n$, $\Phi(c) = \mu$, is defined by (3). Furthermore, let the matrices (D_{ij}) and (a_{ij}) be symmetric and satisfy (5) as well as*

$$(9) \qquad \kappa := \frac{1}{16} \frac{\min_{i=1,\ldots,n} b_i}{\max_{i=1,\ldots,n} b_i} - \frac{\lambda^*}{\min_{i=1,\ldots,n} b_i} > 0, \quad K := 1 - \max_{1 \le i,j \le n} b_i^{-1} a_{ij} > 0,$$

respectively, where λ^* is the maximal eigenvalue of (a_{ij}). Then:

(i) *There exists a weak solution $c = (c_1, \ldots, c_n) : \Omega \times (0, \infty) \to \mathscr{D}$ to (1)-(6) satisfying the free energy inequality (8) and*

$$c_i - c_i^\Gamma \in L^2(0, \infty; H_0^1(\Omega)) \cap H^1(0, \infty; H^{-1}(\Omega)), \quad i = 1, \ldots, n,$$
$$|\nabla p| \in L^2(0, \infty; L^2(\Omega)), \quad \log c_{\text{tot}} \in L^\infty(0, \infty; L^2(\Omega)).$$

(ii) *There exists a constant $C > 0$, depending on κ and $\mathcal{F}^*(c^0) = \mathcal{F}(c^0) - \mathcal{F}(c^\Gamma)$ such that*

$$\sum_{i=1}^n \|c_i(t) - c_i^\Gamma\|_{L^2(\Omega)}^2 \le \frac{C}{1+t} \quad \text{for } t > 0.$$

The idea of the large-time asymptotics of $c_i(t) := c_i(\cdot, t)$ is to exploit the energy inequality (8). Since it is difficult to relate the free energy $\mathcal{F}$ and its energy dissipation $-d\mathcal{F}/dt$, we cannot prove an exponential decay rate although numerical experiments in [16] and Section 7 indicate that this is the case even when $\varepsilon = 0$. Instead, we show for the relative energy $\mathcal{F}^*(c) = \mathcal{F}(c) - \mathcal{F}(c^\Gamma) \ge 0$ that, for some constant $C > 0$ and some nonnegative function $\Psi \in L^1(0, \infty)$,

$$\frac{d}{dt} \int_\Omega \mathcal{F}^*(c) dx \le -\frac{C}{1+\Psi(t)} \left(\int_\Omega \mathcal{F}^*(c) dx \right)^2,$$

from which we deduce that the convergence is of order $1/t$ as $t \to \infty$. Since the free energy is strictly convex, by Lemma 6 below, we obtain convergence in the L^2 norm.

An integral inequality. If $\varepsilon = 0$, we obtain only a gradient estimate for p. This lack of parabolicity is compensated by the following – surprising – integral identity,

$$(10) \qquad \int_\Omega c_{\mathrm{tot}}(t) f\left(\frac{c_1(t)}{c_{\mathrm{tot}}(t)}, \ldots, \frac{c_{n-1}(t)}{c_{\mathrm{tot}}(t)}\right) dx = \int_\Omega c_{\mathrm{tot}}^0 f\left(\frac{c_1^0}{c_{\mathrm{tot}}^0}, \ldots, \frac{c_{n-1}^0}{c_{\mathrm{tot}}^0}\right) dx, \quad t > 0,$$

for arbitrary functions $f : (0,1)^{n-1} \to \mathbb{R}$; see the Appendix for a formal proof. This means that there exists a family of conserved quantities depending on a function of $n-1$ variables. It is unclear whether this identity is sufficient to perform the limit $\varepsilon \to 0$ and to prove the existence of a solution to (1) with $\varepsilon = 0$.

If $\varepsilon > 0$, the integral identity (10) does not hold in general. However, for specific diffusion matrices $D(c)$, the following inequality holds in place of (10):

$$(11) \qquad \int_\Omega c_{\mathrm{tot}}(t) f\left(\frac{c_1(t)}{c_{\mathrm{tot}}(t)}, \ldots, \frac{c_{n-1}(t)}{c_{\mathrm{tot}}(t)}\right) dx \leq \int_\Omega c_{\mathrm{tot}}^0 f\left(\frac{c_1^0}{c_{\mathrm{tot}}^0}, \ldots, \frac{c_{n-1}^0}{c_{\mathrm{tot}}^0}\right) dx, \quad t > 0,$$

for functions f specified in Theorem 3 below. Interestingly, this implies a minimum principle for $c_1/c_{\mathrm{tot}}, \ldots, c_{n-1}/c_{\mathrm{tot}}$. A choice of the diffusion matrix ensuring the validity of (11) is, for given $\alpha, \beta \in C^0(\overline{\mathscr{D}})$ with $\beta \geq 0$, $\alpha > 0$ in $\mathscr{D}$,

$$(12) \qquad D(c) = \alpha(c)(\mathcal{F}'')^{-1} + \beta(c)c \otimes c,$$

where $\mathcal{F}''$ is the Hessian of the free energy $\mathcal{F}$. Clearly, $D(c)$ is bounded and positive definite (although not strictly) for $c \in \mathscr{D}$. In particular, the constraint $\sum_{i=1}^n D_{ij}(c) = 0$ does not hold, and so the assumptions of Theorem 1 are not satisfied. However, with this choice of $D(c)$, equation (1) becomes

$$(13) \qquad \partial_t c_i = \mathrm{div}\left((1 + \varepsilon\beta(c))c_i \nabla p + \varepsilon\alpha(c)\nabla c_i\right) \quad i = 1, \ldots, n,$$

and the existence proof for (13) is simpler than in the case where $D(c)$ satisfies (5).

Corollary 2 (to Theorem 1). *Let $c_i^0 : \Omega \to \mathscr{D}$, $i = 1, \ldots, n$, be Lebesgue measurable and let $c^\Gamma = \Phi^{-1}(0) \in \mathscr{D}$, where $\Phi : \mathscr{D} \to \mathbb{R}^n$, $\Phi(c) = \mu$, is defined by (3). Furthermore, let the matrices (D_{ij}) and (a_{ij}) be symmetric and satisfy (9), (12). Then there exists a weak solution $c = (c_1, \ldots, c_n) : \Omega \times (0, \infty) \to \mathscr{D}$ to (1)-(3), (6), satisfying the free energy inequality (8) and, for $i = 1, \ldots, n$,*

$$c_i - c_i^\Gamma \in L^2(0, \infty; H_0^1(\Omega)) \cap H^1(0, \infty; H^{-1}(\Omega)),$$

$$\nabla\sqrt{c_i}, \ \nabla p, \ \nabla \log c_i \in L^2(0, \infty; L^2(\Omega)),$$

$$\log c_i \in L^\infty(0, \infty; L^1(\Omega)).$$

Our second main result reads as follows.

Theorem 3 (Integral inequality and minimum principle). *Let $c_i^0 = c_i^\gamma$ for $i = 1, \ldots, n$ on $\partial\Omega$. Under the assumptions of Corollary 2, the solution c to (1)-(3), (6) constructed in Corollary 2 satisfies (11) for all functions $f \in C^2([0,1]^{n-1})$ such that its Hessian f'' is positive semidefinite in $[0,1]^{n-1}$ and*

$$(14) \qquad f\left(\frac{c_1^\Gamma}{c_{\mathrm{tot}}^\Gamma}, \ldots, \frac{c_{n-1}^\Gamma}{c_{\mathrm{tot}}^\Gamma}\right) = 0, \quad \left|f'\left(\frac{c_1^\Gamma}{c_{\mathrm{tot}}^\Gamma}, \ldots, \frac{c_{n-1}^\Gamma}{c_{\mathrm{tot}}^\Gamma}\right)\right| = 0.$$

Moreover, for any $i = 1, \ldots, n$,

$$\inf_{\Omega \times (0,\infty)} \frac{c_i}{c_{\mathrm{tot}}} \geq \min \left\{ \inf_{\Omega} \frac{c_i^0}{c_{\mathrm{tot}}^0}, \ \frac{c_i^\Gamma}{c_{\mathrm{tot}}^\Gamma} \right\}.$$

Exponential convergence of the pressure. In the degenerate situation $\varepsilon = 0$, we are able to show an exponential decay rate for the pressure p, at least for sufficiently smooth solutions whose existence is assumed. The key idea of the proof is to analyze the parabolic equation satisfied by p,

$$\partial_t p = \widetilde{D} \Delta p + |\nabla p|^2, \quad \text{where } \widetilde{D} = \sum_{i,j=1}^n c_i c_j \frac{\partial^2 \mathcal{F}}{\partial c_i \partial c_j}.$$

Because of the quadratic gradient term, we need a smallness assumption on ∇p at time $t = 0$. Thus, the exponential convergence result holds sufficiently close to equilibrium.

Theorem 4 (Exponential decay of the pressure). *Let $\varepsilon = 0$, $d = 2$, and let $c = (c_1, \ldots, c_n)$ be a solution to (1)-(2) with isobaric boundary conditions $p = p^\Gamma$ on $\partial\Omega$, $t > 0$, for some constant $p^\Gamma \in \mathbb{R}$. Let $m := \min\{\inf_\Omega p(c^0), p^\Gamma\} > 0$. We assume that*

$$\nabla c_i \in L^4_{\mathrm{loc}}(0,\infty); L^2(\Omega)), \quad \nabla p \in C^0([0,\infty); L^2(\Omega)) \cap L^2(0,T; H^1(\Omega)),$$

and $\sup_{\Omega \times (0,T)} \sum_{i=1}^n b_i c_i < 1$ for any $T > 0$. Then there exists $K_0 > 0$, which depends on Ω and d, such that if $\|\nabla p(c^0)\|_{L^2(\Omega)} \leq K_0 m$, then, for some $\lambda > 0$,

$$\|\nabla p(c(t))\|_{L^2(\Omega)} \leq \|\nabla p(c^0)\|_{L^2(\Omega)} e^{-\lambda t}, \quad t > 0.$$

The paper is organized as follows. Details on the modeling of the fluid mixture are presented in Section 2. Auxiliary results on the Hessian of the free energy, the relation between c and μ, and the diffusion matrix (12) are shown in Section 3. In Section 4, we prove Theorem 1 and Corollary 2, while the proofs of Theorems 3 and 4 are presented in Section 5 and 6, respectively. The evolution of the one-dimensional mass densities and the pressure are illustrated numerically in Section 7 for the case $\varepsilon = 0$. Finally, identity (10) is verified in the Appendix.

2. Modeling and energy equation

We consider the isothermal flow of n chemical components in a porous domain $\Omega \subset \mathbb{R}^d$ with porosity φ. The transport of the partial mass densities c_i is governed by the balance equations for the mass,

$$\partial_t(\varphi c_i) + \mathrm{div}(c_i v_i) = 0, \quad i = 1, \ldots, n,$$

where v_i is the partial velocity of the ith species. In order to derive equations for the mass densities only, we impose some simplifying assumptions. To shorten the presentation, we set all physical constants equal to one. Moreover, we set $\varphi \equiv 1$ to simplify the mathematical analysis. Our results will be also valid for (smooth) space-dependent porosities. Introducing the diffusion fluxes by $J_i = c_i(v_i - v)$, where $v = \sum_{i=1}^n c_i v_i / c_{\mathrm{tot}}$

is the barycentric velocity and $c_{\text{tot}} = \sum_{i=1}^{n} c_i$ denotes the total mass density, the balance equations become

$$(15) \qquad \partial_t c_i + \text{div}(c_i v + J_i) = 0, \quad i = 1, \ldots, n.$$

We suppose that the barycentric velocity is given by Darcy's law $v = -\nabla p$, where p is the fluid pressure. We refer to [22] for a justification of this law. The second assumption is that the diffusion fluxes are driven by the gradients of the chemical potentials μ_i, i.e. $J_i = -\varepsilon \sum_{j=1}^{n} D_{ij} \nabla \mu_i$ for $i = 1, \ldots, n$; see, e.g., [14, Section 4.3]. Here, $\varepsilon > 0$ is some number and D_{ij} are diffusion coefficients depending on $c = (c_1, \ldots, c_n)$. According to Onsager's principle of thermodynamics, the diffusion matrix (D_{ij}) has to be symmetric and positive semidefinite; moreover, for consistency with the definition $J_i = c_i(v_i - v)$, it must hold that $\sum_{i=1}^{n} D_{ij} = 0$ for $j = 1, \ldots, n$.

The equations are closed by specifying the Helmholtz free energy density

$$(16) \qquad \mathcal{F}(c) = \sum_{i=1}^{n} c_i(\log c_i - 1) - c_{\text{tot}} \log \left(1 - \sum_{j=1}^{n} b_j c_j \right) - \sum_{i,j=1}^{n} a_{ij} c_i c_j,$$

where b_j and a_{ij} are positive numbers, and (a_{ij}) is symmetric. The first term in the free energy is the internal energy and the remaining two terms are the energy contributions of the van der Waals gas [12, Formula (4.3)].

The third assumption is that the fluid is in a single state, i.e., no phase-splitting occurs. Mathematically, this means that the free energy must be convex. This is the case if the maximal eigenvalue of (a_{ij}) is sufficiently small; see Lemma 6. The single-state assumption is restrictive from a physical viewpoint. It may be overcome by considering the transport equations for each phase separately and imposing suitable boundary conditions at the interface [14, Section 1]. However, this leads to free-boundary cross-diffusion problems which we are not able to treat mathematically. Another approach would be to consider a two-phase (or even multi-phase) compositional model with overlapping of different phases, like in [19]. In such a situation, a new formulation of the thermodynamic equilibrium based upon the minimization of the Helmholtz free energy is employed to describe the splitting of components among different phases.

The chemical potentials are defined in terms of the free energy by

$$\mu_i = \frac{\partial \mathcal{F}}{\partial c_i} = \log c_i - \log \left(1 - \sum_{j=1}^{n} b_j c_j \right) + \frac{b_i c_{\text{tot}}}{1 - \sum_{j=1}^{n} b_j c_j} - 2 \sum_{j=1}^{n} a_{ij} c_j,$$

and the pressure is determined by the Gibbs-Duhem equation [4, Formula (64)]

$$(17) \qquad p = \sum_{i=1}^{n} c_i \mu_i - \mathcal{F}(c) = \frac{c_{\text{tot}}}{1 - \sum_{j=1}^{n} b_j c_j} - \sum_{i,j=1}^{n} a_{ij} c_i c_j.$$

This describes the van der Waals equation of state for mixtures, where the parameter a_{ij} is a measure of the attractive force between the molecules of the ith and jth species, and the parameter b_j is a measure of the size of the molecules. The pressure stays finite if $\sum_{j=1} b_j c_j < 1$, which means that the mass densities are bounded. In the literature,

many modifications of the attractive term have been proposed. Examples are the so-called Peng-Robinson and Soave-Redlich-Kwong equations; see [20].

Taking the gradient of (17) and observing that $\partial\mathcal{F}/\partial c_i = \mu_i$, (17) can be written as

$$(18) \qquad\qquad \nabla p = \sum_{i=1}^{n} c_i \nabla \mu_i.$$

Therefore, we can formulate (15) as the cross-diffusion equations

$$\partial_t c_i = \operatorname{div}\left(\sum_{j=1}^{n} (c_i c_j + \varepsilon D_{ij}) \nabla \mu_j \right), \quad i = 1, \dots, n.$$

Multiplying this equation by μ_i, summing over $i = 1, \dots, n$, observing again that $\mu_i = \partial\mathcal{F}/\partial c_i$, and integrating by parts, we arrive at the energy equation

$$\frac{d}{dt}\int_\Omega \mathcal{F}(c)dx = \int_\Omega \sum_{i=1}^{n} \mu_i \partial_t c_i dx = -\int_\Omega \left| \sum_{i=1}^{n} c_i \nabla \mu_i \right|^2 dx - \varepsilon \int_\Omega \sum_{i,j=1}^{n} D_{ij} \nabla \mu_i \cdot \nabla \mu_j dx.$$

Since (D_{ij}) is assumed to be positive definite on $\operatorname{span}\{\ell\}^\perp$, where $\ell = (1, \dots, 1)/\sqrt{n}$, and $c \cdot \ell = c_{\text{tot}}/\sqrt{n}$, this gives, thanks to Lemma 5, L^2 estimates for $c_{\text{tot}}\nabla \mu_i$ and, thanks to the equilibrium boundary condition and Poincaré's inequality, H^1 estimates for c_i.

3. Auxiliary results

First we show a result estimating the norms of two vectors from below.

Lemma 5. *Let α, $\beta \in \mathbb{R}^n$ be such that $|\alpha| = |\beta| = 1$. Then, for any $v \in \mathbb{R}^n$,*

$$|\alpha \cdot v|^2 + |v - (\beta \cdot v)\beta|^2 \geq \frac{1}{4}(\alpha \cdot \beta)^2 |v|^2.$$

The constant $1/4$ is not optimal. For instance, if $\alpha = \beta$, we have the theorem of Pythagoras, $|\alpha \cdot v|^2 + |v - (\beta \cdot v)\beta|^2 = |v|^2$.

Proof. Let $w = (\beta \cdot v)\beta$ be the projection of v on β and $w^\perp = v - (\beta \cdot v)\beta$ be the orthogonal part. Then, clearly, $|v|^2 = |w|^2 + |w^\perp|^2$. By Young's inequality with $\delta = 3/4$ and $|\alpha| = 1$, we have

$$\begin{aligned}
|\alpha \cdot v|^2 + |v - (\beta \cdot v)\beta|^2 &= |\alpha \cdot (w + w^\perp)|^2 + |w^\perp|^2 \\
&= (\alpha \cdot w)^2 + (\alpha \cdot w^\perp)^2 + 2(\alpha \cdot w)(\alpha \cdot w^\perp) + |w^\perp|^2 \\
&\geq (1-\delta)(\alpha \cdot w)^2 + (1-\delta^{-1})(\alpha \cdot w^\perp)^2 + |w^\perp|^2 \\
&= \frac{1}{4}(\alpha \cdot w)^2 - \frac{1}{3}(\alpha \cdot w^\perp)^2 + |w^\perp|^2 \\
&\geq \frac{1}{4}(\beta \cdot v)^2 (\alpha \cdot \beta)^2 - \frac{1}{3}|w^\perp|^2 + |w^\perp|^2.
\end{aligned}$$

We deduce from $|\alpha| = |\beta| = 1$ that $(\alpha \cdot \beta)^2 \leq 1$, and thus,

$$|\alpha \cdot v|^2 + |v - (\beta \cdot v)\beta|^2 \geq \frac{1}{4}(\alpha \cdot \beta)^2 |w|^2 + \frac{2}{3}(\alpha \cdot \beta)^2 |w^\perp|^2$$

$$\geq \frac{1}{4}(\alpha \cdot \beta)^2 \big(|w|^2 + |w^\perp|^2\big) = \frac{1}{4}(\alpha \cdot \beta)^2 |v|^2,$$

finishing the proof. □

Lemma 6 (Positive definiteness of $\mathcal{F}''$). *Let $A = (a_{ij})$, defined in the pressure relation (2), be a symmetric matrix whose maximal eigenvalue $\lambda^* \in \mathbb{R}$ satisfies (9). Then the Hessian $\mathcal{F}''$ of the free energy $\mathcal{F}$ is positive definite, i.e.*

$$v \cdot \mathcal{F}''(c)v \geq \kappa \sum_{i=1}^n \frac{v_i^2}{c_i} \quad \text{for all } c \in \mathscr{D}, \ v \in \mathbb{R}^n,$$

where $\kappa > 0$ is given by (9). In particular, $c_{\text{tot}}\mathcal{F}''$ is uniformly positive definite.

Proof. A straightforward computation shows that $(\mathcal{F}'')_{ij} = B_{ij} - a_{ij}$, where

$$B_{ij} = (b_i + b_j)\sigma + b_i b_j c_{\text{tot}}\sigma^2 + \frac{\delta_{ij}}{c_i}, \quad \sigma = \frac{1}{1 - \sum_{j=1}^n b_j c_j} \geq 1.$$

Let $v \in \mathbb{R}^n$. It holds that

$$\sum_{i,j=1}^n B_{ij}v_i v_j = 2\sigma\left(\sum_{i=1}^n v_i\right)\left(\sum_{j=1}^n b_j v_j\right) + \sigma^2 c_{\text{tot}}\left(\sum_{i=1}^n b_j v_j\right)^2 + \sum_{i=1}^n \frac{v_i^2}{c_i}$$

$$= \left(\sigma\sqrt{c_{\text{tot}}}\sum_{j=1}^n b_j v_j + \frac{1}{\sqrt{c_{\text{tot}}}}\sum_{i=1}^n v_i\right)^2 + \sum_{i=1}^n \frac{v_i^2}{c_i} - \frac{1}{c_{\text{tot}}}\left(\sum_{i=1}^n v_i\right)^2.$$

Defining $w_i = v_i/\sqrt{c_i}$, $\widehat{\alpha}_i = \sigma\sqrt{c_{\text{tot}}c_i}b_i + \sqrt{c_i/c_{\text{tot}}}$, and $\beta_i = \sqrt{c_i/c_{\text{tot}}}$ for $i = 1, \ldots, n$, the quadratic form can be rewritten as

$$\sum_{i,j=1}^n B_{ij}v_i v_j = (\widehat{\alpha} \cdot w)^2 + |w - (\beta \cdot w)\beta|^2.$$

Since $|\widehat{\alpha}|^2 = \sum_{i=1}^n \sigma^2(c_{\text{tot}}b_i^2 c_i + 2\sigma b_i c_i) + 1 \geq 1$, we may define $\alpha = \widehat{\alpha}/|\widehat{\alpha}|$, which yields

$$(19) \qquad \sum_{i,j=1}^n B_{ij}v_i v_j \geq (\alpha \cdot w)^2 + |w - (\beta \cdot w)\beta|^2.$$

The norm of $\widehat{\alpha}$ can be estimated from above:

$$|\widehat{\alpha}|^2 \leq \sigma^2 c_{\text{tot}} \max_{j=1,\ldots,n} b_j \sum_{i=1}^n b_i c_i + 2\sigma \sum_{i=1}^n b_i c_i + 1.$$

Since $\sum_{i=1}^n b_i c_i < 1$, we have $\min_{j=1,\ldots,n} b_j c_{\text{tot}} < 1$ or $c_{\text{tot}} < 1/\min_{j=1,\ldots,n} b_j$, and $\sum_{i=1}^n b_i c_i < 1 \leq \sigma$. Therefore,

$$|\widehat{\alpha}|^2 \leq \sigma^2 \frac{\max_{j=1,\ldots,n} b_j}{\min_{j=1,\ldots,n} b_j} + 2\sigma^2 + \sigma^2 = \left(3 + \frac{\max_{j=1,\ldots,n} b_j}{\min_{j=1,\ldots,n} b_j}\right)\sigma^2.$$

We infer that $\alpha \cdot \beta$ is strictly positive:

$$(\alpha \cdot \beta)^2 = |\widehat{\alpha}|^{-2}\left(1 + \sigma \sum_{i=1}^n b_i c_i\right)^2 \geq \frac{(\sigma^{-1} + \sum_{i=1}^n b_i c_i)^2}{3 + \frac{\max_{j=1,\ldots,n} b_j}{\min_{j=1,\ldots,n} b_j}} = \frac{1}{3 + \frac{\max_{j=1,\ldots,n} b_j}{\min_{j=1,\ldots,n} b_j}}.$$

We apply Lemma 5 to (19) to obtain

$$4\sum_{i,j=1}^n B_{ij} v_i v_j \geq (\alpha \cdot \beta)^2 |w|^2 \geq \frac{|w|^2}{3 + \frac{\max_{j=1,\ldots,n} b_j}{\min_{j=1,\ldots,n} b_j}},$$

which, since $w_i = v_i/\sqrt{c_i}$, implies that

$$(20)\qquad 4\sum_{i,j=1}^n B_{ij} v_i v_j \geq \frac{\min_{j=1,\ldots,n} b_j}{3\min_{j=1,\ldots,n} b_j + \max_{j=1,\ldots,n} b_j}\sum_{i=1}^n \frac{v_i^2}{c_i} \geq \frac{\min_{j=1,\ldots,n} b_j}{4\max_{j=1,\ldots,n} b_j}\sum_{i=1}^n \frac{v_i^2}{c_i}.$$

The relation $c_{\text{tot}} < 1/\min_{j=1,\ldots,n} b_j$ and the definition of λ^* allow us to write

$$\sum_{i,j=1}^n a_{ij} v_i v_j \leq c_{\text{tot}} \sum_{i,j=1}^n a_{ij} \frac{v_i}{\sqrt{c_i}} \frac{v_j}{\sqrt{c_j}} \leq \frac{\lambda^*}{\min_{j=1,\ldots,n} b_j}\sum_{i=1}^n \frac{v_i^2}{c_i}.$$

This, together with (20), yields the desired lower bound for $\mathcal{F}''$. $\qquad\square$

Lemma 7 (Invertibility of $c \mapsto \mu$). *The mapping $\Phi : \mathscr{D} \to \mathbb{R}^n$, $\Phi(c) = \mu := (\mu_1, \ldots, \mu_n)$ is invertible.*

Proof. Since $\mathcal{F}'' = \partial\mu/\partial c$ is positive definite in $\mathscr{D}$, it follows that Φ is one-to-one and the image $\Phi(\mathscr{D})$ is open. We claim that $\Phi(\mathscr{D})$ is also closed. Then $\Phi(\mathscr{D}) = \mathbb{R}^2$, and the proof is complete.

Let $\mu^{(m)} = \Phi(c^{(m)})$, $m \in \mathbb{N}$, define a sequence in $\Phi(\mathscr{D})$ such that $\mu^{(m)} \to \overline{\mu}$ as $m \to \infty$. The claim follows if we prove that there exists $\overline{c} \in \mathscr{D}$ such that $\overline{\mu} = \Phi(\overline{c})$. Since $c^{(m)} = (c_1^{(m)}, \ldots, c_n^{(m)}) \in \mathscr{D}$ varies in a bounded subset of $\mathbb{R}^n$, the theorem of Bolzano-Weierstraß implies the existence of a subsequence, which is not relabeled, such that $c_i^{(m)}$ converges to some $\overline{c}_i$ as $m \to \infty$, where $\overline{c}_i \in \overline{\mathscr{D}}$, $i = 1, \ldots, n$. We assume, by contradiction, that $\overline{c} = (\overline{c}_1, \ldots, \overline{c}_n) \in \partial\mathscr{D}$. Let us distinguish two cases.

Case 1: There exists $j \in \{1, \ldots, n\}$ such that $\overline{c}_j = 0$. If $\sum_{i=1}^n b_i \overline{c}_i < 1$, then (3) implies that $\mu_j^{(m)} \to -\infty$, which contradicts the fact that $\mu^{(m)}$ is convergent. Thus it holds that $\sum_{i=1}^n b_i \overline{c}_i = 1$. This means that $\overline{c}_k > 0$ for some $k \in \{1, \ldots, n\}$. However, choosing $i = k$ in (3) and exploiting the relation $\sum_{i=1}^n b_i \overline{c}_i = 1$ leads to $\overline{\mu}_i = +\infty$, contradiction.

Case 2: For all $i \in \{1, \ldots, n\}$, it holds that $\overline{c}_i > 0$ and $\sum_{i=1}^n b_i \overline{c}_i = 1$. Arguing as in case 1, it follows that $\overline{\mu}_i = +\infty$ for all $i = 1, \ldots, n$, which is absurd.

We conclude that $\overline{c} \in \mathscr{D}$, which finishes the proof. $\qquad\square$

Lemma 8. *Let $B(c) = c \otimes c + \varepsilon D(c)$, $\widehat{B}(c) = \widehat{c} \otimes \widehat{c} + \varepsilon D(c)$ for $c \in \mathscr{D}$, where $\widehat{c} = c/|c|$ and $D(c)$ satisfies (5). Then for all $v \in \mathbb{R}^n$ and $c \in \mathscr{D}$,*

$$v \cdot Bv \geq k_B \left(c_{\text{tot}}^2 |v|^2 + |\Pi v|^2\right), \quad v \cdot \widehat{B}v \geq k_B' |v|^2,$$

where $k_B > 0$, $k_B' > 0$ only depend on εD_0 (the constant in (5)) and $b_1, \ldots, b_n$.

Proof. From (5), $|c|^2 \geq c_{\text{tot}}^2/n$, and $c_{\text{tot}} \leq 1/\min\{b_1, \ldots, b_n\}$ it follows that

$$v \cdot Bv \geq (c \cdot v)^2 + \varepsilon D_0 |\Pi v|^2$$

$$\geq c_{\text{tot}}^2 \left(\frac{1}{n} (\widehat{c} \cdot v)^2 + \frac{\varepsilon}{2} D_0 \min\{b_1, \ldots, b_n\}^2 |(I - \ell \otimes \ell)v|^2 \right) + \frac{\varepsilon}{2} D_0 |(I - \ell \otimes \ell)v|^2,$$

Applying Lemma 5 with $\alpha = \widehat{c}$ and $\beta = \ell$ to the expression in the brackets yields

$$v \cdot Bv \geq \frac{1}{4} \min \left\{ \frac{1}{n}, \frac{\varepsilon}{2} D_0 \min\{b_1, \ldots, b_n\}^2 \right\} c_{\text{tot}}^2 (\widehat{c} \cdot \ell)^2 |v|^2 + \frac{1}{2} \varepsilon D_0 |(I - \ell \otimes \ell)v|^2.$$

Since $|\widehat{c} \cdot \ell| = c_{\text{tot}}/|c| \geq 1$, this finishes the proof of the first inequality. The second one is proved in an analogous way. $\square$

4. PROOF OF THEOREM 1

We consider the following time-discretized and regularized problem in Ω:

$$(21) \qquad \frac{c_i^k - c_i^{k-1}}{\tau} = \text{div} \left(\sum_{j=1}^n B_{ij}^k \nabla \mu_j^k \right)$$

$$+ \tau \, \text{div} \left(|\widehat{c}^k \cdot \nabla \mu^k|^2 (\widehat{c}^k \cdot \nabla \mu^k) \widehat{c}_i^k + (\nabla \mu^k : D^k \nabla \mu^k) \sum_{j=1}^n D_{ij}^k \nabla \mu_j^k \right),$$

with homogenous Dirichlet boundary conditions

$$(22) \qquad\qquad\qquad \mu_i^k = 0 \quad \text{on } \partial\Omega, \; i = 1, \ldots, n,$$

where $c_i^{k-1} \in L^\infty(\Omega)$ is given, $\tau > 0$, $c^k = \Phi^{-1}(\mu^k)$, $\widehat{c}^k = c^k/|c^k|$, $D^k = D(c^k)$, and

$$B_{ij}^k = c_i^k c_j^k + \varepsilon D_{ij}(c^k).$$

We write $\nabla \mu^k : D^k \nabla \mu^k = \sum_{i,j=1}^n D_{ij}^k(c) \nabla \mu_i^k \cdot \nabla \mu_j^k$. Note that $B^k = (B_{ij}^k)$ is positive definite by Lemma 8.

4.1. **Existence for the time-discretized problem.** We reformulate (21)-(22) as a fixed-point problem for a suitable operator. Let $F : L^\infty(\Omega; \mathbb{R}^n) \times [0, 1] \to L^\infty(\Omega; \mathbb{R}^n)$, $F(\mu^*, \sigma) = \mu$, where $\mu = (\mu_1, \ldots, \mu_n)$ solves

$$(23) \qquad \frac{\sigma}{\tau} (c_i^* - c_i^{k-1}) = \text{div} \left(\sum_{j=1}^n B_{ij}^* \nabla \mu_j \right)$$

$$+ \tau \, \text{div} \left(|\widehat{c}^* \cdot \nabla \mu|^2 (\widehat{c}^* \cdot \nabla \mu) \widehat{c}_i^* + (\nabla \mu : D^* \nabla \mu) \sum_{j=1}^n D_{ij}^* \nabla \mu_j \right),$$

where

$$B_{ij}^* = c_i^* c_j^* + \varepsilon D_{ij}^*, \quad D^* = D(c^*), \quad c^* = \Phi^{-1}(\mu^*).$$

In order to solve (23), we show that the operator $\mathcal{A} : X \to X'$ defined by

$$\langle \mathcal{A}(u), v \rangle = \int_\Omega \left(\nabla v : B^* \nabla u + \tau (\widehat{c}^* \cdot \nabla v) \cdot (\widehat{c}^* \cdot \nabla u) |\widehat{c}^* \cdot \nabla u|^2 \right.$$

$$+ \tau (\nabla u : D^* \nabla u)(\nabla v : D^* \nabla u)\big) dx$$

with $X = W_0^{1,4}(\Omega; \mathbb{R}^n)$ satisfies the assumptions of Theorem 26A in [24]. Since $\mu^* \in L^\infty(\Omega; \mathbb{R}^n)$, we have $B^*, D^* \in L^\infty(\Omega; \mathbb{R}^{n \times n})$, and $\mathcal{A}$ is well defined.

Strict monotonicity: Let $u, v \in X$. Then

$$\langle \mathcal{A}(u) - \mathcal{A}(v), u - v \rangle = \int_\Omega \nabla(u - v) : B^* \nabla(u - v) dx$$

$$+ \tau \int_\Omega (\widehat{c}^* \cdot \nabla(u - v)) \cdot \big((\widehat{c}^* \cdot \nabla u)|\widehat{c}^* \cdot \nabla u|^2 - (\widehat{c}^* \cdot \nabla v)|\widehat{c}^* \cdot \nabla v|^2\big) dx$$

$$+ \tau \int_\Omega \nabla(u - v) : \big((\nabla u : D^* \nabla u) D^* \nabla u - (\nabla v : D^* \nabla v) D^* \nabla v\big) dx =: I_1 + I_2 + I_3.$$

The positive definiteness of B^* implies that $I_1 \geq 0$. We claim that also $I_2 \geq 0$. Indeed, by decomposing $\nabla u = \frac{1}{2}\nabla(u + v) + \frac{1}{2}\nabla(u - v)$ and $\nabla v = \frac{1}{2}\nabla(u + v) - \frac{1}{2}\nabla(u - v)$, we obtain

$$(\widehat{c}^* \cdot \nabla u)|\widehat{c}^* \cdot \nabla u|^2 - (\widehat{c}^* \cdot \nabla v)|\widehat{c}^* \cdot \nabla v|^2$$

$$= \frac{1}{2}\big(\widehat{c}^* \cdot \nabla(u + v)\big)\big(|\widehat{c}^* \cdot \nabla u|^2 - |\widehat{c}^* \cdot \nabla v|^2\big)$$

$$+ \frac{1}{2}\big(\widehat{c}^* \cdot \nabla(u - v)\big)\big(|\widehat{c}^* \cdot \nabla u|^2 + |\widehat{c}^* \cdot \nabla v|^2\big),$$

and since $(\widehat{c}^* \cdot \nabla(u - v)) \cdot (\widehat{c}^* \cdot \nabla(u + v)) = |\widehat{c}^* \cdot \nabla u|^2 - |\widehat{c}^* \cdot \nabla v|^2$, we deduce that

$$I_2 = \frac{\tau}{2} \int_\Omega \big((|\widehat{c}^* \cdot \nabla u|^2 - |\widehat{c}^* \cdot \nabla v|^2)^2 + |\widehat{c}^* \cdot \nabla(u - v)|^2(|\widehat{c}^* \cdot \nabla u|^2 + |\widehat{c}^* \cdot \nabla v|^2)\big) dx,$$

which means that $I_2 \geq 0$. With the same technique one can prove that also $I_3 \geq 0$. We conclude that $\mathcal{A}$ is monotone. If $\langle \mathcal{A}(u) - \mathcal{A}(v), u - v \rangle = 0$, then in particular $I_1 = 0$, which, thanks to the positive definiteness of B^*, implies that $\nabla u = \nabla v$ and $u = v$ in X. Therefore, $\mathcal{A}$ is strictly monotone.

Coercivity: Let $u \in X$. Since B^* is positive definite, we find that

$$\langle \mathcal{A}(u), u \rangle \geq \tau \int_\Omega \big(|\widehat{c}^* \cdot \nabla u|^4 + (\nabla u : D^* \nabla u)^2\big) dx$$

$$\geq \frac{\tau}{2} \int_\Omega \big(|\widehat{c}^* \cdot \nabla u|^2 + \nabla u : D^* \nabla u\big)^2 dx.$$

Lemma 8 implies that $|\widehat{c}^* \cdot \nabla u|^2 + \nabla u : D^* \nabla u \geq k_B'|\nabla u|^2$, so we infer from Poincaré's inequality (with constant $C_P > 0$) that

$$\frac{\langle \mathcal{A}(u), u \rangle}{\|u\|_X} \geq \frac{\tau(k_B')^2}{2\|u\|_X} \int_\Omega |\nabla u|^4 dx \geq \frac{\tau}{2}(k_B')^2 C_P \|u\|_X^3 \to \infty$$

as $\|u\|_X \to \infty$. Thus, $\mathcal{A}$ is coercive.

Hemicontinuity: Let $u, v, w \in X$. The function $t \mapsto \langle \mathcal{A}(u + tv), w \rangle$ is a polynomial and is, in particular, continuous. It follows that $\mathcal{A}$ is hemicontinuous.

The assumptions of Theorem 26A in [24] are fulfilled, and we infer the existence of a unique solution $\mu \in X$ to (23). This shows that the operator F is well defined. If $\sigma = 0$,

we have $F(\cdot, 0) = 0$ thanks to the uniqueness of the solution to (23). A uniform bound for all fixed points to (23) and $\sigma \in [0, 1]$ follows from the above coercivity estimate for $\mathcal{A}$.

Let us show that F is continuous. Then, because of the compact embedding $W^{1,4}(\Omega) \hookrightarrow L^\infty(\Omega)$ for $d \leq 3$, F is also compact. Let $(\mu^*)^{(m)} \in L^\infty(\Omega; \mathbb{R}^n)$, $n \in \mathbb{N}$, define a sequence converging to $\overline{\mu}^*$ in $L^\infty(\Omega)$ and let $\sigma^{(m)} \subset [0, 1]$ be such that $\sigma^{(m)} \to \overline{\sigma}$ as $m \to \infty$. Set $\mu^{(m)} := F((\mu^*)^{(m)}, \sigma^{(m)})$ and $\overline{\mu} := F(\overline{\mu}^*, \overline{\sigma})$. The claim follows if we show that $\mu^{(m)} \to \overline{\mu}$ in $L^\infty(\Omega)$. We formulate (23) compactly as $\mathcal{A}[\mu^*](\mu) = f(\mu^*, \sigma)$, where $f(\mu^*, \sigma) = \sigma\tau^{-1}(c^* - c^{k-1})$, putting in evidence the dependence on μ^*. By definition, $\mathcal{A}[(\mu^*)^{(m)}](\mu^{(m)}) = f((\mu^*)^{(m)}, \sigma^{(m)})$ and $\mathcal{A}[\overline{\mu}^*](\overline{\mu}) = f(\overline{\mu}^*, \overline{\sigma})$. It follows that

$$\left\langle \mathcal{A}[(\mu^*)^{(m)}](\mu^{(m)}) - \mathcal{A}[(\mu^*)^{(m)}](\overline{\mu}), \mu^{(m)} - \overline{\mu} \right\rangle + \left\langle \mathcal{A}[(\mu^*)^{(m)}](\overline{\mu}) - \mathcal{A}[\overline{\mu}^*](\overline{\mu}), \mu^{(m)} - \overline{\mu} \right\rangle$$

$$(24) \quad = \left\langle f((\mu^*)^{(m)}, \sigma^{(m)}) - f(\overline{\mu}^*, \overline{\sigma}), \mu^{(m)} - \overline{\mu} \right\rangle.$$

Clearly, $(\mu^{(m)})$ is bounded in $W^{1,4}(\Omega)$ and, by the compact embedding, also in $L^\infty(\Omega)$. This fact, together with the convergences $(\mu^*)^{(m)} \to \overline{\mu}^*$ in $L^\infty(\Omega)$ and $\sigma^{(m)} \to \sigma$, implies that

$$\left\langle \mathcal{A}[(\mu^*)^{(m)}](\overline{\mu}) - \mathcal{A}[\overline{\mu}^*](\overline{\mu}), \mu^{(m)} - \overline{\mu} \right\rangle \to 0,$$
$$\left\langle f((\mu^*)^{(m)}, \sigma^{(m)}) - f(\overline{\mu}^*, \overline{\sigma}), \mu^{(m)} - \overline{\mu} \right\rangle \to 0.$$

Consequently, by (24),

$$\left\langle \mathcal{A}[(\mu^*)^{(m)}](\mu^{(m)}) - \mathcal{A}[(\mu^*)^{(m)}](\overline{\mu}), \mu^{(m)} - \overline{\mu} \right\rangle \to 0.$$

The previous monotonicity estimate for $\mathcal{A}$ shows that

$$\left\langle \mathcal{A}[(\mu^*)^{(m)}](\mu^{(m)}) - \mathcal{A}[(\mu^*)^{(m)}](\overline{\mu}), \mu^{(m)} - \overline{\mu} \right\rangle \geq \int_\Omega \nabla(\mu^{(m)} - \overline{\mu})^\top (B^*)^{(m)} \nabla(\mu^{(m)} - \overline{\mu}) dx.$$

Then we deduce from the strict positivity of $(B^*)^{(m)}$ and the Poincaré inequality that $\mu^{(m)} \to \overline{\mu}$ strongly in $H^1(\Omega)$. The uniform bound for $(\mu^{(m)})$ in $W^{1,4}(\Omega)$ implies that $\mu^{(m)} \to \overline{\mu}$ strongly in $W^{1,q}(\Omega)$ for any $1 < q < 4$. Take $q \in (3, 4)$. Then the embedding $W^{1,q}(\Omega) \hookrightarrow L^\infty(\Omega)$ is compact, and, possibly for a subsequence, $\mu^{(m)} \to \overline{\mu}$ strongly in $L^\infty(\Omega)$. By the uniqueness of the limit, the convergence holds for the whole sequence. This shows the continuity of F.

We can now apply the fixed-point theorem of Leray-Schauder to conclude the existence of a weak solution to (21).

4.2. **Uniform estimates.** Let $\mu^k \in X$ be a solution to (21). Employing μ_i^k as a test function and summing over $i = 1, \ldots, n$ gives

$$\frac{1}{\tau} \sum_{i=1}^n (c_i^k - c_i^{k-1})\mu_i^k dx + \int_\Omega \left(\nabla\mu^k : B^k \nabla\mu^k + \tau|\hat{c}^k \cdot \nabla\mu^k|^4 + \tau(\nabla\mu^k : D^k \nabla\mu^k)^2 \right) dx = 0,$$

where $c^k = \Phi^{-1}(\mu^k)$. Since $\mu_i^k = \partial \mathcal{F}(c^k)/\partial c_i$ and $\mathcal{F}(c^k)$ is convex, it follows that $\sum_{i=1}^n (c_i^k - c_i^{k-1})\mu_i^k \geq \mathcal{F}(c^k) - \mathcal{F}(c^{k-1})$ and therefore,

$$(25) \qquad \int_\Omega \mathcal{F}(c^k)dx + \int_\Omega \left(\nabla(\mu^k : B^k \nabla \mu^k + \tau |\widehat{c}^k \cdot \nabla \mu^k|^4 + \tau(\nabla \mu^k : D^k \nabla \mu^k)^2 \right) dx$$
$$\leq \int_\Omega \mathcal{F}(c^{k-1})dx.$$

Lemma 8 shows that

$$(26) \qquad \nabla(\mu^k)^\top B^k \nabla \mu^k \geq k_B \left((c_{\text{tot}}^k)^2 |\nabla \mu^k|^2 + |\nabla(\Pi\mu^k)|^2 \right),$$

$$(27) \qquad |\widehat{c}^k \cdot \nabla \mu^k|^4 + (\nabla \mu^k \cdot D^k \nabla \mu^k)^2 \geq \frac{1}{2}(k_B')^2 |\nabla \mu^k|^4.$$

Let $T > 0$, $\tau = T/N$ for some $N \in \mathbb{N}$. We introduce the piecewise constant functions in time $\mu^{(\tau)}(x,t) = \mu^k(x)$ for $x \in \Omega$ and $t \in ((k-1)\tau, k\tau]$, $k = 1, \ldots, N$. The functions $c^{(\tau)}$ and $B^{(\tau)}$ are defined in a similar way. Furthermore, we introduce the shift operator $\sigma_\tau \mu^{(\tau)}(x,t) = \mu^{k-1}(x)$ for $x \in \Omega$ and $t \in ((k-1)\tau, k\tau]$. Then (21) can be formulated as

$$(28) \qquad \frac{c^{(\tau)} - \sigma_\tau c^{(\tau)}}{\tau} = \text{div}\left(B^{(\tau)}\nabla \mu^{(\tau)} \right)$$
$$+ \tau \, \text{div}\left(|\widehat{c}^{(\tau)} \cdot \nabla \mu^{(\tau)}|^2 (\widehat{c}^{(\tau)} \cdot \nabla \mu^{(\tau)}) \cdot \widehat{c}^{(\tau)} + (\nabla \mu^{(\tau)} : D^{(\tau)}\nabla \mu^{(\tau)})D^{(\tau)}\nabla \mu^{(\tau)} \right).$$

Now, we sum (25) over $k = 1, \ldots, N$ and employ (26) and (27) to obtain

$$(29) \qquad \int_\Omega \mathcal{F}(c^{(\tau)}(x,T))dx + k_B \int_0^T \int_\Omega \left((c_{\text{tot}}^{(\tau)})^2 |\nabla \mu^{(\tau)}|^2 + |\nabla \Pi \mu^{(\tau)}|^2 \right)dxdt$$
$$+ \frac{\tau(k_B')^2}{2} \int_0^T \int_\Omega |\nabla \mu^{(\tau)}|^4 dxdt \leq \int_\Omega \mathcal{F}(c_i^0)dx.$$

In the following, $C > 0$ denotes a generic constant independent of τ and T, while $C_T > 0$ denotes a constant depending on T but not on τ. We deduce from (29) and Poincarè's Lemma that

$$(30) \qquad \|p^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|\Pi\mu^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} \leq C,$$

$$(31) \qquad \tau^{1/4}\|\mu^{(\tau)}\|_{L^4(0,T;W^{1,4}(\Omega))} \leq C.$$

By Lemma 6, the matrix $c_{\text{tot}}^{(\tau)}\mathcal{F}''(c^{(\tau)})$ is uniformly positive definite. Thus, the uniform bound for $c_{\text{tot}}\nabla \mu_i$ in L^2 provided by (29) implies a uniform bound for

$$\frac{\partial c^{(\tau)}}{\partial x_j} = (c_{\text{tot}}^{(\tau)}\mathcal{F}'')^{-1} c_{\text{tot}}^{(\tau)} \frac{\partial \mu^{(\tau)}}{\partial x_j}$$

for all $j = 1, \ldots, n$ in $L^2(Q_T)$, where $Q_T = \Omega \times (0,T)$. Therefore, since $\mathscr{D}$ is bounded and $c^{(\tau)}(x,t) \in \mathscr{D}$,

$$(32) \qquad \|c_i^{(\tau)}\|_{L^\infty(Q_T)} + \|c_i^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} \leq C, \quad i = 1, \ldots, n.$$

In particular, $B^{(\tau)}$ is uniformly bounded in $L^\infty(Q_T)$. Using these estimates in (28) shows that

$$(33) \qquad \tau^{-1}\|c_i^{(\tau)} - \sigma_\tau c_i^{(\tau)}\|_{L^{4/3}(0,T;W^{1,4}(\Omega)')} \leq C\big(\|\nabla p\|_{L^{4/3}(Q_T)} + \|\nabla\Pi\mu\|_{L^{4/3}(Q_T)}$$
$$+ \tau\|\nabla\mu\|_{L^4(Q_T)}^3\big) \leq C.$$

4.3. **The limit $\tau \to 0$.** In view of estimates (32) and (33), we can apply the Aubin-Lions lemma in the version of [8], ensuring the existence of a subsequence, which is not relabeled, such that, as $\tau \to 0$,

$$c_i^{(\tau)} \to c_i \quad \text{strongly in } L^4(Q_T), \ i = 1, \ldots, n.$$

In fact, in view of the $L^\infty(Q_T)$ bound (32), this convergence holds in $L^q(Q_T)$ for any $q < \infty$. Furthermore, we have

$$\tau^{-1}(c_i^{(\tau)} - \sigma_\tau c_i^{(\tau)}) \rightharpoonup \partial_t c_i \quad \text{weakly in } L^{4/3}(0,T;W^{1,4}(\Omega)'), \ i = 1, \ldots, n.$$

It holds that $c(x,t) \in \overline{\mathscr{D}}$ for a.e. $(x,t) \in Q_T$. Let $\mu := \Phi(c), p = p(c) \in (\mathbb{R} \cup \{\pm\infty\})^n$. By (30), (32), and Fatou's lemma, we infer that, for a subsequence,

$$\|p\|_{L^2(Q_T)} \leq \liminf_{\tau \to 0} \|p^{(\tau)}\|_{L^2(Q_T)} \leq C,$$
$$(34) \qquad \|\Pi\mu\|_{L^2(Q_T)} \leq \liminf_{\tau \to 0} \|\Pi\mu^{(\tau)}\|_{L^2(Q_T)} \leq C,$$

which implies that $|p|, |\Pi\mu| < \infty$ a.e. in Q_T. The fact that $p < \infty$ a.e. in Q_T implies that $\sum_{i=1}^n b_i c_i < 1$ a.e. in Q_T. This property and the relation $|\Pi\mu| < \infty$ a.e. in Q_T imply that

$$\gamma_i^{(\tau)} := \log c_i^{(\tau)} - \frac{1}{n}\sum_{j=1}^n \log c_j^{(\tau)}$$

is a.e. convergent as $\tau \to 0$ for $i = 1, \ldots, n$. Let $(x,t) \in Q_T$ be such that $\gamma_i^{(\tau)}(x,t)$ is convergent for $i = 1, \ldots, n$ and let

$$J = \Big\{i \in \{1, \ldots, n\} : \lim_{\tau \to 0} c_i^{(\tau)}(x,t) = 0\Big\}.$$

We want to show that either $J = \emptyset$ or $J = \{1, \ldots, n\}$. Let us assume by contradition that $0 < |J| < n$ (here $|J|$ is the number of elements in J). It follows that

$$\sum_{i \in J} \gamma_i^{(\tau)}(x,t) = \Big(1 - \frac{|J|}{n}\Big)\sum_{i \in J} \log c_i^{(\tau)}(x,t) - \frac{|J|}{n}\sum_{i \notin J} \log c_i^{(\tau)}(x,t).$$

Since $0 < |J| < n$, the first sum on the right-hand side diverges to $-\infty$, while the second sum is convergent. So the right-hand side of the above equality is divergent, while the left-hand side is convergent, by assumption. This is a contradiction. Thus either the set J is empty or it equals $\{1, \ldots, n\}$, i.e. for a.e. $(x,t) \in Q_T$, either $c_i(x,t) > 0$ for $i = 1, \ldots, n$, or $c_{\text{tot}}(x,t) = 0$. Summarizing up, $c \in \mathscr{D} \cup \{0\}$.

It follows from (30)–(33) that $\xi \in L^2(Q_T)^n$ exists such that

$$\nabla(\Pi\mu^{(\tau)}) \rightharpoonup \xi \quad \text{weakly in } L^2(Q_T),$$

$$\nabla p^{(\tau)} \rightharpoonup \nabla p \quad \text{weakly in } L^2(Q_T),$$

$$\tau |\nabla \mu^{(\tau)}|^3 \to 0 \quad \text{strongly in } L^{4/3}(Q_T),$$

$$D(c^{(\tau)}) \to D(c) \quad \text{strongly in } L^q(Q_T; \mathbb{R}^{n \times n}), \ q < \infty.$$

Moreover, since $c \in \mathscr{D} \cup \{0\}$, we infer that $\xi = \nabla(\Pi\mu)$ on $\{c_{\text{tot}} > 0\}$. These convergences allow us to perform the limit $\tau \to 0$ in (28), obtaining

(35) $$\partial_t c = \text{div}(c\nabla p + D(c)\xi) \qquad \text{in } Q_T.$$

We will now show that $c_{\text{tot}} > 0$ a.e. in Q_T. Then this implies that $\xi = \nabla(\Pi\mu)$ a.e. in Q_T and so $D(c)\xi = D(c)\nabla\mu$, since $D(c)\ell = 0$. To this end, summing up the components in (35) yields (remember that $\sum_{i=1}^n D_{ij} = 0$ in $\mathscr{D}$)

(36) $$\partial_t c_{\text{tot}} = \text{div}(c_{\text{tot}}\nabla p) \quad \text{in } \Omega.$$

Let $\delta > 0$. We employ the test function $1/(\delta + c_{\text{tot}}^\Gamma) - 1/(\delta + c_{\text{tot}})$ in (36) giving

$$\frac{d}{dt} \int_\Omega \left(\frac{c_{\text{tot}}}{\delta + c_{\text{tot}}^\Gamma} + \log \frac{1}{\delta + c_{\text{tot}}} \right) dx = -\int_\Omega \frac{c_{\text{tot}}}{(\delta + c_{\text{tot}})^2} \nabla c_{\text{tot}} \cdot \nabla p \, dx.$$

An integration in time in the interval $[0, t]$ (for some $t \in [0, T]$) yields

$$\int_\Omega \log \frac{\delta + c_{\text{tot}}^0(x)}{\delta + c_{\text{tot}}(x, t)} dx + \int_\Omega \frac{c_{\text{tot}}(x, t) - c_{\text{tot}}(x, 0)}{\delta + c_{\text{tot}}^\Gamma} dx$$

$$= -\int_0^t \int_\Omega \frac{c_{\text{tot}}}{(\delta + c_{\text{tot}})^2} \nabla c_{\text{tot}} \cdot \nabla p \, dx \, ds.$$

Since the function inside the integral on the right-hand side vanishes in the region $c_{\text{tot}} = 0$, we can rewrite the above equation as

(37) $$\int_\Omega \log \frac{\delta + c_{\text{tot}}^0(x)}{\delta + c_{\text{tot}}(x, t)} dx + \int_\Omega \frac{c_{\text{tot}}(x, t) - c_{\text{tot}}(x, 0)}{\delta + c_{\text{tot}}^\Gamma} dx$$

$$= -\int_0^t \int_{\{c_{\text{tot}} > 0\}} \frac{c_{\text{tot}}^2}{(\delta + c_{\text{tot}})^2} \nabla \log c_{\text{tot}} \cdot \nabla p \, dx \, ds.$$

We want to show that the integral on the right-hand side is bounded from above by a constant that depends on T but not on δ. We show first that $\nabla \log(p/c_{\text{tot}}) \in L^2(0, \infty; L^2(\Omega))$. First, we observe that, because of (9),

$$p \geq c_{\text{tot}} \left(1 - \sum_{i,j=1}^n b_i^{-1} a_{ij} b_i c_i \frac{c_j}{c_{\text{tot}}} \right) = c_{\text{tot}} \left(1 - \max_{i,j=1,\dots,n} (b_i^{-1} a_{ij}) \sum_{k=1}^n b_k c_k \sum_{\ell=1}^n \frac{c_\ell}{c_{\text{tot}}} \right)$$

$$\geq c_{\text{tot}} \left(1 - \max_{i,j=1,\dots,n} (b_i^{-1} a_{ij}) \right) = c_{\text{tot}} K.$$

This implies that $c_{\text{tot}} \nabla \log(p/c_{\text{tot}}) = (c_{\text{tot}}/p)\nabla p - \nabla c_{\text{tot}} \in L^2(0, \infty; L^2(\Omega))$. Let $\eta = 1/(2 \max_{1 \leq i \leq n} b_i)$. We decompose

$$|\nabla \log(p/c_{\text{tot}})| = |\nabla \log(p/c_{\text{tot}})|\chi_{\{c_{\text{tot}} > \eta\}} + |\nabla \log(p/c_{\text{tot}})|\chi_{\{c_{\text{tot}} \leq \eta\}}.$$

The first term on the right-hand side is bounded in $L^2(0, \infty; L^2(\Omega))$. The same holds true for the second term since $1 - b \cdot c \geq 1/2$ for $c_{\text{tot}} \leq \eta$ and $\partial(p/c_{\text{tot}})/\partial c_i$ is uniformly bounded in $\{c_{\text{tot}} \leq \eta\}$. We infer that $\nabla \log(p/c_{\text{tot}}) \in L^2(0, \infty; L^2(\Omega))$, showing the claim.

The right-hand side of (37) becomes

$$
-\int_0^t \int_{\{c_{\text{tot}}>0\}} \frac{c_{\text{tot}}^2}{(\delta + c_{\text{tot}})^2} \nabla \log c_{\text{tot}} \cdot \nabla p \, dxds
$$

$$
= -\int_0^t \int_{\{c_{\text{tot}}>0\}} \frac{c_{\text{tot}}^2}{(\delta + c_{\text{tot}})^2} \left(\nabla \log p - \nabla \log \frac{p}{c_{\text{tot}}} \right) \cdot \nabla p \, dxds
$$

$$
= -4\int_0^t \int_{\{c_{\text{tot}}>0\}} \frac{c_{\text{tot}}^2 |\nabla \sqrt{p}|^2}{(\delta + c_{\text{tot}})^2} dxds + \int_0^t \int_{\{c_{\text{tot}}>0\}} \frac{c_{\text{tot}}^2}{(\delta + c_{\text{tot}})^2} \nabla \log \frac{p}{c_{\text{tot}}} \cdot \nabla p \, dxds
$$

$$
\leq C.
$$

Identity (37), the bound for c_{tot}, and the above estimate imply that

$$
\int_\Omega \log \frac{\delta + c_{\text{tot}}(x, 0)}{\delta + c_{\text{tot}}(x, t)} dx + \int_0^t \int_{\{c_{\text{tot}}>0\}} \frac{4c_{\text{tot}}^2}{(\delta + c_{\text{tot}})^2} |\nabla \sqrt{p}|^2 dxds \leq C \quad \text{for } \delta > 0, \ t > 0.
$$

Taking the limit inferior $\delta \to 0$ on both sides and applying Fatou's lemma, we obtain

$$
\int_\Omega \log \frac{c_{\text{tot}}^0}{c_{\text{tot}}(x, t)} dx + 4 \int_0^t \int_{\{c_{\text{tot}}>0\}} |\nabla \sqrt{p}|^2 dxds \leq C, \quad t > 0,
$$

which implies that $c_{\text{tot}}(x, t) > 0$ for a.e. $x \in \Omega$, $t > 0$, and $\nabla \sqrt{p} \in L^2(0, \infty; L^2(\Omega))$.

As a consequence, c is a weak solution to (1)-(6). Actually, equation (1) is satisfied for test functions in $L^4(0, T; W^{1,4}(\Omega))$ but a density argument shows that the equation holds in $L^2(0, T; H^1(\Omega))$.

Next, we show that $\mathcal{F}(c^{(\tau)}) \to \mathcal{F}(c)$ strongly in $L^q(Q_T)$ for any $q < 2$. Since $c^{(\tau)} \to c$ a.e. in Q_T and $c^{(\tau)}$ is uniformly bounded, it suffices to show that the term $c_{\text{tot}}^{(\tau)} \log(1 - \sum_{i=1}^n b_i c_i^{(\tau)})$ is strongly convergent (see (16)). This is a consequence of the fact that both

$$
c_{\text{tot}}^{(\tau)} \left| \log \left(1 - \sum_{i=1}^n b_i c_i^{(\tau)} \right) \right| \leq \frac{c_{\text{tot}}^{(\tau)}}{1 - \sum_{i=1}^n b_i c_i^{(\tau)}} = p^{(\tau)} + \sum_{i,j=1}^n a_{ij} c_i^{(\tau)} c_j^{(\tau)}
$$

and $p^{(\tau)}$ are uniformly bounded in $L^2(Q_T)$. The convergence of $(\mathcal{F}(c^{(\tau)}))$, together with Fatou's lemma, then allows us to take the limit $\tau \to 0$ in (25) and to obtain (8).

We point out that, since all the constants C appearing in the previous estimates are independent of the final time T, all the bounds that have been found hold true in the time interval $(0, \infty)$.

We conclude the existence proof by showing that $\log c_{\text{tot}} \in L^\infty(0, \infty; L^2(\Omega))$. We use the test function $\Theta_\delta(c_{\text{tot}}) - \Theta_\delta(c_{\text{tot}}^\Gamma)$ in (36), where

$$
\Theta_\delta(u) := \frac{1}{u + \delta} \log \left(\frac{u + \delta}{M + \delta} \right), \quad M = \frac{1}{\min_{1 \leq i \leq n} b_i}.
$$

Notice that $c_{tot} \leq M$ a.e. in Ω, $t > 0$. It follows that

$$\frac{1}{2} \int_\Omega \left| \log \left(\frac{c_{tot}(x,t) + \delta}{M + \delta} \right) \right|^2 dx - \frac{1}{2} \int_\Omega \left| \log \left(\frac{c_{tot}(x,0) + \delta}{M + \delta} \right) \right|^2 dx$$

$$- \Theta_\delta(c_{tot}^\Gamma) \int_\Omega (c_{tot}(x,t) - c_{tot}(x,0)) dx$$

$$= - \int_0^t \int_\Omega \frac{c_{tot}}{c_{tot} + \delta} \left(1 - \log \left(\frac{c_{tot} + \delta}{M + \delta} \right) \right) \nabla p \cdot \nabla \log c_{tot} dx ds.$$

Inserting $\nabla \log c_{tot} = \nabla \log p - \nabla \log(p/c_{tot})$ on the right-hand side, the first term is non-positive (because of $c_{tot} \leq M$, we have $1 - \log((c_{tot} + \delta)/(M + \delta)) \geq 0$) and we end up with

$$\frac{1}{2} \int_\Omega \left| \log \left(\frac{c_{tot}(x,t) + \delta}{M + \delta} \right) \right|^2 dx - \frac{1}{2} \int_\Omega \left| \log \left(\frac{c_{tot}^0(x) + \delta}{M + \delta} \right) \right|^2 dx$$

$$\leq C + \int_0^t \int_\Omega \frac{c_{tot}}{c_{tot} + \delta} \left(1 - \log \left(\frac{c_{tot} + \delta}{M + \delta} \right) \right) \nabla p \cdot \nabla \log \frac{p}{c_{tot}} dx ds = C + I_1 + I_2,$$

where the constant $C > 0$ estimates the term proportional to $\Theta_\delta(c_{tot}^\Gamma)$ and

$$I_1 := \int_0^t \int_{\{c_{tot} \leq \eta\}} \frac{2c_{tot}\sqrt{p}}{c_{tot} + \delta} \left(1 - \log \left(\frac{c_{tot} + \delta}{M + \delta} \right) \right) \nabla \sqrt{p} \cdot \nabla \log \frac{p}{c_{tot}} dx ds,$$

$$I_2 := \int_0^t \int_{\{c_{tot} > \eta\}} \frac{c_{tot}}{c_{tot} + \delta} \left(1 - \log \left(\frac{c_{tot} + \delta}{M + \delta} \right) \right) \nabla p \cdot \nabla \log \frac{p}{c_{tot}} dx ds,$$

and $\eta = 1/(2 \min_{1 \leq i \leq n} b_i)$.

It is straightforward to see that $\sqrt{p} \log((c_{tot} + \delta)/(M + \delta))$ is uniformly bounded with respect to δ in the region $\{c_{tot} \leq \eta\}$. Since $\nabla \sqrt{p} \in L^2(0, \infty; L^2(\Omega))$, we deduce that I_1 is uniformly bounded with respect to δ. Furthermore, the regularity $\nabla p \in L^2(0, \infty; L^2(\Omega))$ implies that I_2 is uniformly bounded with respect to δ. As a consequence,

$$\int_\Omega \left| \log \left(\frac{c_{tot} + \delta}{M + \delta} \right) \right|^2 dx \leq C, \quad t > 0.$$

Taking the limit inferior $\delta \to 0$ on both sides of the above inequality and applying Fatou's Lemma, we conclude that $\log c_{tot} \in L^\infty(0, \infty; L^2(\Omega))$. This finishes the proof of part (i).

4.4. **Large-time asymptotics.** We first show that, for some generic constant $C > 0$,

(38) $$|(c_{tot}\mathcal{F}'')^{-1}\mu| \leq C \left(1 + p + |\log c_{tot}| \right).$$

Let $w := (c_{tot}\mathcal{F}'')^{-1}\mu$, i.e. $c_{tot}\mathcal{F}''w = \mu$. It follows from Lemma 6 that

$$c_{tot} \sum_{i=1}^n \frac{w_i^2}{c_i} \leq \frac{1}{\kappa} w \cdot (c_{tot}\mathcal{F}'')w = \frac{1}{\kappa}\mu \cdot w = \frac{1}{\kappa} \sum_{i=1}^n \frac{\sqrt{c_i}}{\sqrt{c_{tot}}} \mu_i \frac{\sqrt{c_{tot}}}{\sqrt{c_i}} w_i$$

$$\leq \frac{1}{\kappa}\left(\sum_{j=1}^{n}\frac{\sqrt{c_j}}{\sqrt{c_{\text{tot}}}}|\mu_j|\right)\left(c_{\text{tot}}\sum_{i=1}^{n}\frac{w_i^2}{c_i}\right)^{1/2}.$$

This gives

$$(39) \qquad |w| \leq \left(c_{\text{tot}}\sum_{i=1}^{n}\frac{w_i^2}{c_i}\right)^{1/2} \leq \frac{1}{\kappa}\sum_{j=1}^{n}\frac{\sqrt{c_j}}{\sqrt{c_{\text{tot}}}}|\mu_j|.$$

It remains to estimate the right-hand side. We claim that $0 \leq -\log(1-b\cdot c) \leq C(1+p)$. Indeed, with $\eta = 1/(2\max_{i=1,\dots,n}b_i)$, we have

$$-\log(1-b\cdot c) \leq \chi_{\{c_{\text{tot}}\leq\eta\}}\log\frac{1}{1-b\cdot c} + \frac{c_{\text{tot}}}{\eta}\chi_{\{c_{\text{tot}}>\eta\}}\log\frac{1}{1-b\cdot c}.$$

The first term on the right-hand side is bounded since $c_{\text{tot}} \leq \eta$ implies that $1-b\cdot c \geq 1/2$. Then, since $\log(1/z) \leq 1/z$ for $z > 0$,

$$0 \leq -\log(1-b\cdot c) \leq C + 2\max_{i=1,\dots,n}b_i\frac{c_{\text{tot}}}{1-b\cdot c} \leq C(1+p).$$

Hence, by definition (3) of μ_i,

$$\frac{\sqrt{c_i}}{\sqrt{c_{\text{tot}}}}|\mu_i| \leq C(1+p) + \frac{\sqrt{c_i}}{\sqrt{c_{\text{tot}}}}|\log c_i|$$

$$\leq C(1+p) + 2\frac{\sqrt{c_i}}{\sqrt{c_{\text{tot}}}}\left|\log\frac{\sqrt{c_i}}{\sqrt{c_{\text{tot}}}}\right| + \frac{\sqrt{c_i}}{\sqrt{c_{\text{tot}}}}|\log c_{\text{tot}}|,$$

and therefore,

$$(40) \qquad \frac{\sqrt{c_i}}{\sqrt{c_{\text{tot}}}}|\mu_i| \leq C(1+p+|\log c_{\text{tot}}|).$$

Putting together (39) and (40) yields (38).

A computation shows that $\mathcal{F}(c) = -p(c) + \sum_{i=1}^{n}c_i\mu_i$ (in fact, this is the Gibbs-Duhem relation, see (17)) and $\nabla\mathcal{F}(c) = c\cdot\nabla\mu$ (this follows from (18)). Since $c^\Gamma = \Phi^{-1}(\mu)|_{\mu=0}$, we have $\mathcal{F}(c^\Gamma) = -p(c^\Gamma)$. We use the fact that c_i varies in a bounded domain and employ the Poincaré inequality with constant C_P and the identity $\nabla\mu = \mathcal{F}''(c)\nabla c$ to find that

$$\int_\Omega \mathcal{F}^*(c)dx \leq C_P\int_\Omega |\nabla\mathcal{F}(c)|dx = C_P\int_\Omega |\mu\cdot\nabla c|dx$$

$$= C_P\int_\Omega \sum_{i,j=1}^{n}\left|c_{\text{tot}}((\mathcal{F}'')^{-1})_{ij}\mu_i c_{\text{tot}}\nabla\mu_j\right|dx$$

$$\leq C_P\|(c_{\text{tot}}\mathcal{F}'')^{-1}\mu\|_{L^2(\Omega)}\|c_{\text{tot}}\nabla\mu\|_{L^2(\Omega)},$$

which, thanks to (38), leads to

$$\left(\int_\Omega \mathcal{F}^*(c)dx\right)^2 \leq C\left(1 + \|p\|_{L^2(\Omega)}^2 + \|\log c_{\text{tot}}\|_{L^2(\Omega)}^2\right)\|c_{\text{tot}}\nabla\mu\|_{L^2(\Omega)}^2.$$

Taking into account (8) and Lemma 8, we obtain

$$\|c_{\text{tot}}\nabla\mu\|_{L^2(\Omega)}^2 \le C\int_\Omega \nabla\mu : B(c)\nabla\mu dx = C\left(-\frac{d}{dt}\int_\Omega \mathcal{F}^*(c)dx\right).$$

We deduce from the above inequalities and the facts that $p \in L^2(0,T;L^2(\Omega))$ and $\log c_{\text{tot}} \in L^\infty(0,T;L^2(\Omega))$,

$$\left(\int_\Omega \mathcal{F}^*(c)dx\right)^2 \le C(\Psi(t)+1)\left(-\frac{d}{dt}\int_\Omega \mathcal{F}^*(c)dx\right),$$

where $\Psi = \|p\|_{L^2(\Omega)}^2 \in L^1(0,\infty)$. A nonlinear Gronwall inequality shows that

$$(41) \qquad \int_\Omega \mathcal{F}^*(c)dx \le \frac{S_0}{1+CS_0\psi(t)}, \quad t > 0,$$

where $S_0 := \int_\Omega \mathcal{F}^*(c^0)dx$ and $\psi(t) := \int_0^t (1+\Psi(\tau))^{-1}d\tau$.

We define now $f : (0,1] \to \mathbb{R}$, $f(x) = 1/x - 1$. Clearly, f is decreasing and convex. Jensen's inequality and the fact that $\Phi \in L^1(0,\infty)$ yield

$$f\left(\frac{\psi(t)}{t}\right) \le \frac{1}{t}\int_0^t f\left((1+\Psi(\tau))^{-1}\right)d\tau = \frac{1}{t}\int_0^t \Psi(\tau)d\tau \le \frac{C}{t}.$$

Since f (and also its inverse f^{-1}) is decreasing, it follows that

$$\frac{\psi(t)}{t} \ge f^{-1}\left(\frac{C}{t}\right) = \frac{1}{1+Ct^{-1}} \ge \frac{1}{2} \qquad \text{for } t \ge C.$$

We conclude from this fact and (41) that

$$(42) \qquad \int_\Omega \mathcal{F}^*(c)dx \le \frac{C}{1+t}, \quad t > 0.$$

By Lemma 6, the Hessian $\mathcal{F}''$ is positive definite. Moreover, $\mathcal{F}'(c^\Gamma) = \mu|_{c=c^\Gamma} = 0$. Thus, a Taylor expansion shows that

$$\int_\Omega F^*(c)dx = \int_\Omega \left(\mathcal{F}'(c^\Gamma)\cdot(c-c^\Gamma) + \frac{1}{2}(c-c^\Gamma):\mathcal{F}''(\xi)(c-c^\Gamma)\right)dx \ge \frac{\kappa}{2}\int_\Omega |c-c^\Gamma|^2 dx,$$

where $\kappa > 0$ is specified in (9). This finishes the proof of Theorem 1.

4.5. **Proof of Corollary 2.** The existence proof is similar to that one of Theorem 1. The main difference is that we lose the information on the chemical potentials $\mu_1,\ldots,\mu_n$ due to the possible degeneracy of D (since $\mathcal{F}''$ is unbounded). However, thanks to the simple structure of (13), we do not need uniform estimates on $\mu_1,\ldots,\mu_n$ in order to be able to pass to the deregularization limit.

Compared to (21), we employ a slightly different time discretization to overcome the difficulty that D is not strictly positive definite:

$$(43) \qquad \frac{c_i^k - c_i^{k-1}}{\tau} = \text{div}\left(\sum_{j=1}^n B_{ij}^k\nabla\mu_j^k\right) + \tau\,\text{div}\left(|\nabla\mu_i^k|^2\nabla\mu_i^k\right) \quad \text{in } \Omega,\ i = 1,\ldots,n.$$

The uniform estimates for p^k, c^k provided by (30), (32), repsectively, still hold. Lemma 6 allows us to infer that $\nabla \mu^k \cdot \nabla c^k = \nabla c^k \cdot (\mathcal{F}^k)'' \nabla c^k \geq \kappa |\nabla \sqrt{c^k}|^2$. The limit mass densities $c_1, \ldots, c_n$ satisfy $c \in \overline{\mathscr{D}}$. The proof that $c \in \mathscr{D}$ is slightly different than in the proof of Theorem 1. Indeed, the $L^\infty(0, \infty; L^1(\Omega))$ bound for $\mathcal{F}$ implies that $\sum_{i=1}^n b_i c_i < 1$ a.e. in Ω, $t > 0$. This fact and the previous bounds allow us to take the limit $\tau \to 0$ in (43) and to obtain (13) together with the properties

$$c_i - c_i^\Gamma \in L^2(0, \infty; H^1(\Omega)) \cap H^1(0, \infty; H^1(\Omega)'), \quad \nabla \sqrt{c_i}, \ \nabla p \in L^2(0, \infty; L^2(\Omega)).$$

In order to prove that $c_i > 0$ a.e. in Ω, $t > 0$, for $i = 1, \ldots, n$, we choose $\delta > 0$, employ the test function $(\delta + c_i^\Gamma)^{-1} - (\delta + c_i)^{-1}$ in (13), and sum over $i = 1, \ldots, n$:

$$\frac{d}{dt} \int_\Omega \sum_{i=1}^n \left(\frac{c_i}{\delta + c_i^\Gamma} - \log(\delta + c_i) \right) dx$$

$$= - \sum_i \int_\Omega \left(\frac{(1 + \varepsilon\beta)c_i}{c_i + \delta} \nabla p \cdot \nabla \log(c_i + \delta) + \alpha |\nabla \log(c_i + \delta)|^2 \right) dx.$$

Since α is strictly positive, β is bounded, and $\nabla p \in L^2(0, \infty; L^2(\Omega))$, by applying Young's inequality and integrating in time, we conclude that

$$\| \log(\delta + c_i) \|_{L^\infty(0, \infty; L^1(\Omega))} + \| \nabla \log(\delta + c_i) \|_{L^2(0, \infty; L^2(\Omega))} \leq C, \quad i = 1, \ldots, n.$$

Fatou's Lemma allows us to conclude that $\log c_i \in L^\infty(0, \infty; L^1(\Omega))$ and $\nabla \log(\delta + c_i) \in L^2(0, \infty; L^2(\Omega))$ for $i = 1, \ldots, n$; in particular $c_i > 0$ a.e. in Ω, $t > 0$. The free energy inequality (8) follows with the same argument as in the proof of Theorem 1. This finishes the proof of Corollary 2.

5. Proof of Theorem 3

5.1. **Integral inequality.** Let $\delta > 0$ be arbitrary, and let $z = (z_1, \ldots, z_{n-1})$, $z_i = c_i/c_{\text{tot}}$, $z^\delta = (z_1^\delta, \ldots, z_{n-1}^\delta)$, $z_i^\delta = (\delta + c_i)/(\delta + c_{\text{tot}})$ for $i = 1, \ldots, n-1$. Moreover, let $\psi_\delta(c) = (c_{\text{tot}} + \delta) f(z^\delta)$ for $c \in \mathscr{D}$, where $f : [0, 1]^{n-1} \to \mathbb{R}$ satisfies the assumptions of Theorem 3. A simple computation yields

$$\frac{\partial z_k^\delta}{\partial c_i} = \frac{\delta_{ik}}{c_{\text{tot}} + \delta} - \frac{c_k + \delta}{(c_{\text{tot}} + \delta)^2},$$

$$\frac{\partial^2 \psi_\delta(c)}{\partial c_i \partial c_j} = (c_{\text{tot}} + \delta) \sum_{k,s=1}^{n-1} \frac{\partial^2 f}{\partial z_k \partial z_s} \frac{\partial z_k^\delta}{\partial c_i} \frac{\partial z_s^\delta}{\partial c_j}, \quad i, j = 1, \ldots, n.$$

Employing $\partial \psi_\delta(c)/\partial c_i - \partial \psi_\delta(c^\Gamma)/\partial c_i$ as a test function in (13) leads to

$$(44) \quad \int_\Omega \left(\psi_\delta(c(x, t)) - \psi_\delta(c(x, 0)) \right) dx - \sum_{i=1}^n \frac{\partial \psi_\delta}{\partial c_i}(c^\Gamma) \int_\Omega (c_i(x, t) - c_i(x, 0)) dx = -J_1 - J_2,$$

where

$$J_1 = \sum_{i,j=1}^{n} \int_0^t \int_\Omega (1 + \varepsilon\beta(c))\nabla c_j \cdot \nabla p(c_{\mathrm{tot}} + \delta) \sum_{k,s=1}^{n-1} \frac{\partial^2 f}{\partial z_k \partial z_s} \frac{\partial z_k^\delta}{\partial c_i} \frac{\partial z_s^\delta}{\partial c_j} c_i dx ds,$$

$$J_2 = \varepsilon \sum_{i,j=1}^{n} \int_0^t \int_\Omega \alpha(c)\nabla c_j \cdot \nabla c_i (c_{\mathrm{tot}} + \delta) \sum_{k,s=1}^{n-1} \frac{\partial^2 f}{\partial z_k \partial z_s} \frac{\partial z_k^\delta}{\partial c_i} \frac{\partial z_s^\delta}{\partial c_j} dx ds.$$

It holds that

$$J_2 = \varepsilon \int_0^t \int_\Omega \alpha(c)(c_{\mathrm{tot}} + \delta) \sum_{k,s=1}^{n-1} \frac{\partial^2 f}{\partial z_k \partial z_s} \nabla z_k^\delta \cdot \nabla z_s^\delta \; dx ds,$$

and so $J_2 \geq 0$, since f is convex. We show now that $|J_1| \to 0$ as $\delta \to 0$. We compute

$$\sum_{i=1}^{n} \frac{\partial z_k^\delta}{\partial c_i} c_i = \frac{\delta(c_k - c_{\mathrm{tot}})}{(c_{\mathrm{tot}} + \delta)^2} \to 0 \quad \text{a.e. in } \Omega \times (0,\infty) \text{ as } \delta \to 0,$$

$$(c_{\mathrm{tot}} + \delta) \left| \frac{\partial z_k^\delta}{\partial c_j} \right| + \left| \sum_{i=1}^{n} \frac{\partial z_k^\delta}{\partial c_i} c_i \right| \leq C \quad \text{a.e. in } \Omega \times (0,\infty), \; j = 1, \ldots, n.$$

The above relations, together with the boundedness of β and f'', allow us to apply the dominated convergence theorem and deduce that $|J_1| \to 0$ as $\delta \to 0$. Moreover, (14) implies that $\partial\psi_\delta(c^\Gamma)/\partial c_i \to 0$ as $\delta \to 0$, $i = 1, \ldots, n$. The continuity and boundedness of f imply that $\psi_\delta(c(\cdot,0)) \to c_{\mathrm{tot}}^0 f(c_1^0/c_{\mathrm{tot}}^0, \ldots, c_{n-1}^0, c_{\mathrm{tot}}^0)$ in $L^1(\Omega)$ as $\delta \to 0$. Taking the limit inferior $\delta \to 0$ on both sides of (44) and exploiting all the convergence relations as well as the nonnegativity of J_2 yield

$$\liminf_{\delta \to 0} \int_\Omega \psi_\delta(c(x,t)) dx \leq \int_\Omega c_{\mathrm{tot}}^0 f\left(\frac{c_1^0}{c_{\mathrm{tot}}^0}, \ldots, \frac{c_{n-1}^0}{c_{\mathrm{tot}}^0} \right) dx.$$

Finally, by Fatou's Lemma, we conclude that (11) holds.

5.2. **Maximum principle.** The final statement of Theorem 3 is a consequence of the following lemma.

Lemma 9. *Let c_i, $c_i^0 \in L^\infty(\Omega)$ for $i = 1, \ldots, n$ be positive functions such that $c_i = c_i^0 = c_i^\Gamma$ on $\partial\Omega$ for some constant $c_i^\Gamma > 0$, $i = 1, \ldots, n$. Let a constant $m \in (0, c_1^\Gamma/c_{\mathrm{tot}}^\Gamma)$ exist such that $c_1^0/c_{\mathrm{tot}}^0 \geq m$ in Ω. Finally, assume that (11) holds for any $f \in C^2(0,1)$ satisfying (14). Then $c_1/c_{\mathrm{tot}} \geq m$ in Ω.*

Proof. Let $f(x) = (m - x)_+^3$ for $0 \leq x \leq 1$. Clearly $f \in C^2(0,1)$ satisfies (14). Taking into account the assumptions of the lemma, we deduce that (11) holds for the above choice of f. Since $c_1^0/c_{\mathrm{tot}}^0 \geq m$, the right-hand side vanishes. Because of the nonnegativity of f and the positivity of c_i, we infer that $0 = f(c_1/c_{\mathrm{tot}}) = (m - c_1/c_{\mathrm{tot}})_+^3$ in Ω and $c_1/c_{\mathrm{tot}} \geq m$ in Ω, concluding the proof. $\square$

6. Proof of Theorem 4

6.1. Derivation of the evolution equation for p.

We multiply (1) by $\partial p/\partial c_i$, sum over $i = 1, \ldots, n$, and compute in the sense of distributions:

$$(45) \qquad \partial_t p = \sum_{i=1}^n \frac{\partial p}{\partial c_i} \operatorname{div}(c_i \nabla p) = \sum_{i=1}^n \frac{\partial p}{\partial c_i}(\nabla c_i \cdot \nabla p + c_i \Delta p) = |\nabla p|^2 + \widetilde{D}\Delta p,$$

where $\widetilde{D} = \sum_{i=1}^n (\partial p/\partial c_i)c_i$. Because of the Gibbs-Duhem relation (17), it follows that $\partial p/\partial c_i = \sum_{j=1}^n c_j \partial^2 \mathcal{F}/\partial c_i \partial c_j$, and consequently,

$$\widetilde{D} = \sum_{i,j=1}^n c_i c_j \frac{\partial^2 \mathcal{F}}{\partial c_i \partial c_j}.$$

We claim that $\widetilde{D} \geq p$. Indeed, definition (16) leads to

$$\frac{\partial^2 \mathcal{F}}{\partial c_i \partial c_j} = (b_i + b_j)\sigma + b_i b_j c_{\text{tot}}\sigma^2 + \frac{\delta_{ij}}{c_i} - a_{ij}, \quad \sigma = \frac{1}{1 - \sum_{i=1}^n b_i c_i} \geq 1.$$

Then

$$\widetilde{D} = 2c_{\text{tot}}\sigma \sum_{i=1}^n b_i c_i + c_{\text{tot}}\sigma^2 \left(\sum_{i=1}^n b_i c_i\right)^2 + c_{\text{tot}} - \sum_{i,j=1}^n a_{ij} c_i c_j$$

$$= c_{\text{tot}}\left(1 + \sigma \sum_{i=1}^n b_i c_i\right)^2 - \sum_{i,j=1}^n a_{ij} c_i c_j = \frac{c_{\text{tot}}}{(1 - \sum_{i=1}^n b_i c_i)^2} - \sum_{i,j=1}^n a_{ij} c_i c_j \geq p.$$

6.2. Lower bound for the pressure.

We show that $p \geq m$ in Ω, $t > 0$, where $m = \min\{\min_\Omega p(c^0), p^\Gamma\} > 0$. Then equation (45) is uniformly parabolic. Using $(p - m)_- = \min\{0, p - m\}$ as a test function in (45) and integrating by parts gives

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (p - m)_-^2 dx = -\int_\Omega \left(\widetilde{D} - (p - m)_-\right)|\nabla(p - m)_|^2 dx$$

$$- \int_\Omega (p - m)_- \nabla \widetilde{D} \cdot \nabla(p - m)_- dx.$$

Since $\widetilde{D} \geq p$, it follows that $\widetilde{D} - (p - m)_- \geq D - (p - m) \geq m$. Thus, together with Young's inequality, we find that

$$(46) \qquad \frac{1}{2}\frac{d}{dt}\int_\Omega (p - m)_-^2 dx \leq -\frac{m}{2}\int_\Omega |\nabla(p - m)_-|^2 + \frac{1}{2m}\int_\Omega |\nabla \widetilde{D}|^2 (p - m)_-^2 dx.$$

The second term on the right-hand side can be bounded by means of the Cauchy-Schwarz, Gagliardo-Nirenberg (with constant $C_{GN} > 0$, using $d = 2$), and Young inequalities:

$$\int_\Omega |\nabla \widetilde{D}|^2 (p - m)_-^2 dx \leq \|\nabla \widetilde{D}\|_{L^4(\Omega)}^2 \|(p - m)_-\|_{L^4(\Omega)}^2$$

$$\leq C_{GN}\|\nabla \widetilde{D}\|_{L^4(\Omega)}^2 \|(p - m)_-\|_{L^2(\Omega)}\|(p - m)_-\|_{H^1(\Omega)}$$

$$\leq \frac{m^2}{2} \int_\Omega |\nabla(p-m)_-|^2 dx + \left(\frac{C_{GN}^2}{2m^2}\|\nabla\widetilde{D}\|_{L^4(\Omega)}^4 + \frac{m^2}{2}\right) \int_\Omega (p-m)_-^2 dx.$$

So (46) implies that

$$\frac{d}{dt} \int_\Omega (p-m)_-^2 dx \leq -\frac{m}{2} \int_\Omega |\nabla(p-m)_-|^2 + \left(\frac{C_{GN}^2}{2m^3}\|\nabla\widetilde{D}\|_{L^4(\Omega)}^4 + \frac{m}{2}\right) \int_\Omega (p-m)_-^2 dx.$$

In view of our regularity assumptions on ∇c_i, we have $\nabla\widetilde{D}\|_{L^4(\Omega)}^4 \in L^1_{\text{loc}}(0,\infty)$, and we conclude with Gronwall's lemma that $(p-m)_- = 0$, i.e. $p \geq m$ in Ω, $t > 0$.

6.3. Gradient estimate for the pressure.
We multiply (45) with Δp and use the lower bound $\widetilde{D} \geq p \geq m$ and the Gagliardo-Nirenberg inequality with $d = 2$:

$$\frac{1}{2}\frac{d}{dt} \int_\Omega |\nabla p|^2 dx + m\|\Delta p\|_{L^2(\Omega)}^2 \leq \int_\Omega |\nabla p|^2 \Delta p\, dx \leq \|\nabla p\|_{L^4(\Omega)}^2 \|\Delta p\|_{L^2(\Omega)}$$

$$\leq C_{GN}^2 \|\nabla p\|_{H^1(\Omega)}^{1/2} \|\nabla p\|_{L^2(\Omega)}^{1/2} \|\Delta p\|_{L^2(\Omega)}$$

$$(47) \qquad = C_{GN}^2 \left(\|\nabla^2 p\|_{L^2(\Omega)}^2 + \|\nabla p\|_{L^2(\Omega)}^2\right)^{1/2} \|\nabla p\|_{L^2(\Omega)} \|\Delta p\|_{L^2(\Omega)}.$$

We claim that $\|\nabla p\|_{L^2(\Omega)} \leq C_0\|\Delta p\|_{L^2(\Omega)}$ for some constant $C_0 > 0$ which only depends on Ω and d. Because of $p = p^\Gamma = \text{const.}$ on $\partial\Omega$, we have $\int_\Omega \nabla p\, dx = \int_{\partial\Omega} p\nu\, ds = p^\Gamma \int_{\partial\Omega} \nu\, dx = 0$, which implies that

$$\|\nabla p\|_{L^2(\Omega)} = \left\|\nabla p - \frac{1}{\text{meas}(\Omega)} \int_\Omega \nabla p\, dx\right\|_{L^2(\Omega)} \leq C_P\|\nabla^2 p\|_{L^2(\Omega)},$$

where $C_P > 0$ is the Poincaré constant. The function $v := p - p^\Gamma$ satisfies $\Delta v = f := \Delta p$ in Ω and $v = 0$ on $\partial\Omega$. By elliptic regularity,

$$(48) \qquad \|\nabla^2 p\|_{L^2(\Omega)} \leq \|v\|_{H^2(\Omega)} \leq C_E\|f\|_{L^2(\Omega)} = C_E\|\Delta p\|_{L^2(\Omega)}$$

for some constant $C_E > 0$, and therefore,

$$(49) \qquad \|\nabla p\|_{L^2(\Omega)} \leq C_P C_E\|\Delta p\|_{L^2(\Omega)}.$$

We infer from (48) and (49) that (47) becomes

$$\frac{1}{2}\frac{d}{dt} \int_\Omega |\nabla p|^2 dx + m\|\Delta p\|_{L^2(\Omega)}^2 \leq C_{GN}^2 C_E(1+C_P^2)^{1/2}\|\Delta p\|_{L^2(\Omega)}\|\nabla p\|_{L^2(\Omega)}\|\Delta p\|_{L^2(\Omega)},$$

and hence,

$$(50) \qquad \frac{d}{dt} \int_\Omega |\nabla p|^2 dx + 2\big(m - C_1\|\nabla p\|_{L^2(\Omega)}\big)\|\Delta p\|_{L^2(\Omega)}^2 \leq 0,$$

where $C_1 = C_{GN}^2 C_E(1 + C_P)^{1/2}$. Let $0 < K_0 < 1/C_1$. Then, by assumption, $\lambda := m - C_1\|\nabla p(c^0)\|_{L^2(\Omega)} > 0$. Since $|\nabla p| \in C^0([0,\infty); L^2(\Omega))$, the coefficient remains positive in a small time interval $[0, t^*)$. As a consequence, $t \mapsto \|\nabla p(c(t))\|_{L^2(\Omega)}^2$ is nonincreasing in

$[0, t^*)$. A standard prolongation argument then implies that $m - C_1\|\nabla p(c(t))\|_{L^2(\Omega)} > 0$ and $t \mapsto \|\nabla p(c(t))\|_{L^2(\Omega)}^2$ is nonincreasing for all $t > 0$. In particular,

$$m - C_1\|\nabla p(c(t))\|_{L^2(\Omega)} \geq \lambda.$$

From this fact and estimates (50) and (49), we deduce that

$$\frac{d}{dt}\int_\Omega |\nabla p|^2 dx \leq -2\lambda\|\Delta p\|_{L^2(\Omega)}^2 \leq -2\lambda(C_P C_E)^{-2}\|\nabla p\|_{L^2(\Omega)}^2,$$

and Gronwall's lemma allows us to conclude.

7. NUMERICAL EXPERIMENTS

We solve system (1)-(2) numerically in one space dimension for the case $\varepsilon = 0$ and $n = 2$, imposing Dirichlet and homogeneous Neumann boundary conditions for p. Let $\{t_k : k \geq 0\}$ with $t_0 = 0$ be a discretization of the time interval $[0, \infty)$ and $\{x_j : 0 \leq j \leq N\}$ with $N \in \mathbb{N}$, $x_j = jh$, and $h = 1/N$, be a uniform discretization of the space interval $\Omega = (0, 1)$. We set $\tau_k = t_k - t_{k-1}$ for $k \geq 1$. For the discretization of (1), we distinguish between the two boundary conditions.

7.1. Homogeneous Neumann boundary conditions.
We employ the staggered grid $y_j = x_{j-1/2} = (x_j + x_{j-1})/2$ and denote by $c_{i,j}^k$ and p_j^k the approximations of $c_i(y_j, t_k)$ and $p(y_j, t_k)$, respectively. The values at the interior points are the unknowns of the problem, while the values at the boundary points are determined according to

$$c_{i,0}^k = c_{i,1}^k, \quad c_{i,N+1}^k = c_{i,N}^k, \quad k \geq 0, \ i = 1, 2.$$

The initial condition is discretized by

$$c_{i,j}^0 = \frac{1}{2}\big(c_i^0(x_j) + c_i^0(x_{j-1})\big), \quad j = 1, \ldots, N, \ i = 1, 2.$$

Approximating the time derivative by the implicit Euler scheme and the diffusion flux $J_i := -c_i \partial_x p$ at $(y_{j+1/2}, t_k)$ by the implicit upwind scheme

$$(51) \qquad J_{i,j+1/2}^k = c_{i,j}^k \max\{v_{j+1/2}^k, 0\} + c_{i,j+1}^k \min\{v_{j+1/2}^k, 0\}, \quad v_{j+1/2}^k = -\frac{p_{j+1} - p_j}{h},$$

the finite-difference scheme for (1) becomes

$$(52) \qquad \frac{1}{\tau_k}\big(c_{i,j}^k - c_{i,j}^{k-1}\big) + \frac{1}{h}\big(J_{i,j+1/2}^k - J_{i,j-1/2}^k\big) = 0,$$

where $1 \leq j \leq N$, $k \geq 1$, $i = 1, 2$. To be consistent with the boundary conditions, we define $p_0^k = p_1^k$ and $p_{N+1}^k = p_N^k$, $k \geq 0$.

7.2. Dirichlet boundary conditions.
Here, we do not need to employ the staggered grid, so we use the original grid $\{x_j : 0 \leq j \leq N\}$. The implicit scheme (51)-(52) works also in this situation, with the only difference that the boundary conditions are simply given by $c_{i,0}^k = c_i(0, t_k)$, $c_{i,N}^k = c_i(1, t_k)$, and the initial condition is defined by $c_{i,j}^0 = c_i^0(x_j)$.

7.3. **Iteration procedure.** The nonlinear equations are solved by using the MATLAB function `fsolve`, with $c_{i,j}^{k-1}$ as the initial guess. The time step τ_k is chosen in an adaptive way. At each time iteration, once the new iterate $c_{i,j}^k$ is computed, the relative difference between two consecutive iterates,

$$\rho^k = \sqrt{\frac{\sum_{i=1}^2 \sum_{j=1}^N |c_{i,j}^k - c_{i,j}^{k-1}|^2}{\sum_{i=1}^2 \sum_{j=1}^N |c_{i,j}^{k-1}|^2}},$$

is evaluated and compared to the maximal tolerance $\mathrm{tol_M}$. If $\rho^k \geq \mathrm{tol_M}$, the iterate is rejected, the time step τ_k is halved, and the step is repeated. Otherwise, the iterate is accepted. Before the next iterate is computed, ρ^k is compared to the minimal tolerance $\mathrm{tol_m}$ (with $\mathrm{tol_m} < \mathrm{tol_M}$). If $\rho^k < \mathrm{tol_m}$, the time step is increased by a factor $5/4$. Otherwise, τ_k is kept unchanged. In the simulations, we have chosen the values $\mathrm{tol_m} = 4 \cdot 10^{-4}$, $\mathrm{tol_M} = 6 \cdot 10^{-4}$, and $N = 201$.

7.4. **Numerical results.** We present the results of four numerical simulations, referring to the different boundary conditions and different choices of the parameters, namely

$$b_1 = 1, \quad b_2 = \frac{1}{2}, \quad a_{11} = \eta, \quad a_{12} = \eta, \quad a_{22} = \frac{3}{2}\eta,$$

where $\eta = \eta_m := 10^{-3}$ and $\eta = \eta_M := 1.185186593672589$, which corresponds to a lower bound on the Hessian of the free energy (16) approximately equal to 10^{-6}. In all cases, the initial data have the form

$$c_1^{in}(x) = c_{1,A} + (c_{1,B} - c_{1,A})x^{10}, \quad c_2^{in}(x) = c_{2,A} + (c_{2,B} - c_{2,A})x^{1/10},$$

which describes an accumulation of c_1, c_2 close to $x = 1$, $x = 0$, respectively. The parameters $c_{i,A}$, $c_{i,B}$, $i = 1, 2$, are chosen in such a way that $p(c_{1,A}, c_{2,A}) = p(c_{1,B}, c_{2,B}) = 1$, which is necessary in order to have convergence to a steady state in the case of Dirichlet boundary conditions, since any steady state is characterized by the pressure assuming a constant value.

For homogeneous Neumann boundary conditions and $\eta = \eta_m$ (Case I), Figure 1 shows the evolution of the mass densities c_1, c_2 and the pressure p at the time instants $t = 0, 5 \cdot 10^{-3}, 50 \cdot 10^{-3}, 1$ (the solution at $t = 1$ represents the steady state) as well as the relative free energy $\mathcal{F}(c(t)) - \mathcal{F}(c^0)$. As expected, the pressure converges to a constant function for "large" times. The stationary mass densities are nonconstant. The Neumann boundary condition is numerically satisfied, but we observe a boundary layer at $x = 0$, originating from the "constraint" of constant pressure. The relative free energy decays exponential fast. After $t \approx 0.7$, the stationary state is almost reached and the values of the free energy are of the order to the numerical precision.

In Figure 2, we present the results for $\eta = \eta_M$ (Case II), still with homogeneous Neumann boundary conditions. We observe that the relative free energy decay is slightly slower than in Case I but still exponential fast.

For the case of Dirichlet boundary conditions, an additional term has to be added to the free energy in order to have free energy decay, due to the presence of additional boundary
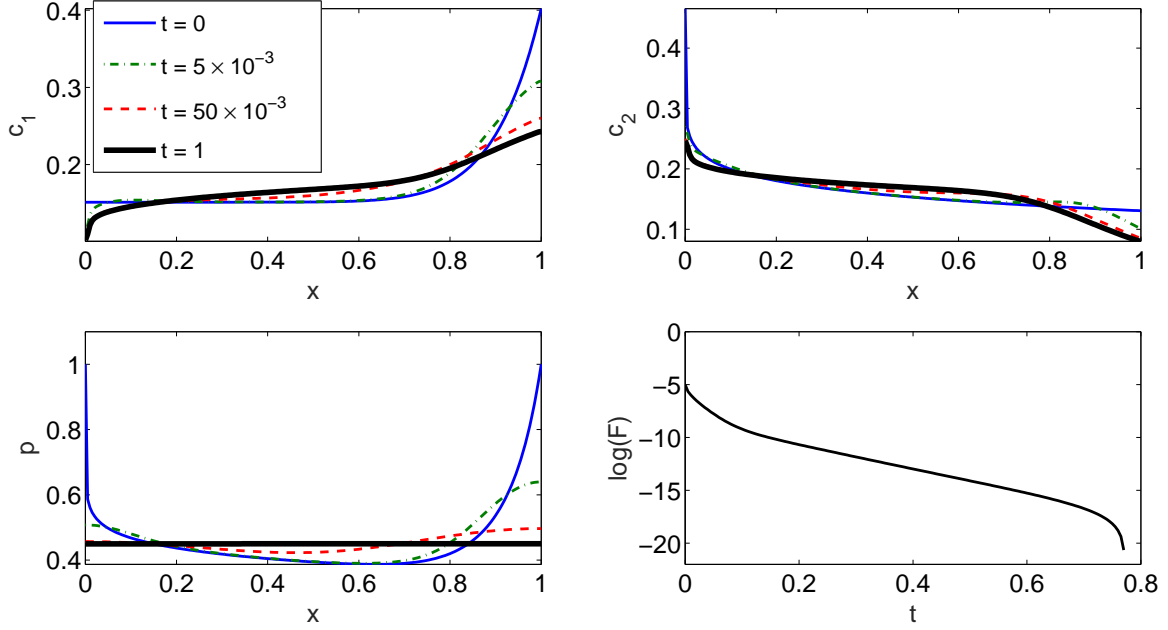
FIGURE 1. Case I (Neumann conditions, $\eta = \eta_m$): evolution of the mass densities c_1, c_2, pressure p, and logarithm of the relative free energy $\mathcal{F}(c(t)) - \mathcal{F}(c^0)$.

contributions in the free energy balance equation. More precisely, we choose the modified free energy $\widetilde{\mathcal{F}}(c) := \mathcal{F}(c) - (\alpha_1 c_1 + \alpha_2 c_2)$, where α_1, $\alpha_2 \in \mathbb{R}$ are such that the boundary term in

$$\frac{d}{dt} \int_\Omega \widetilde{\mathcal{F}}(c) dx = \int_\Omega \sum_{i=1}^2 \frac{\partial \mathcal{F}}{\partial c_i} \operatorname{div}(c_i \nabla p) dx - \int_\Omega \sum_{j=1}^2 \alpha_j \operatorname{div}(c_j \nabla p) dx$$

$$= -\int_\Omega |\nabla p|^2 dx + \int_{\partial\Omega} \left(\sum_{i=1}^2 c_i \mu_i - \sum_{j=1}^2 \alpha_j c_j \right) \nabla p \cdot \nu ds$$

vanishes. Here, we have used the relations $\partial \mathcal{F}/\partial c_i = \mu_i$ and $\sum_{i=1}^2 c_i \nabla \mu_i = \nabla p$ (see (18)). The boundary term vanishes if (α_1, α_2) solves the linear system

$$\begin{pmatrix} c_1^L & c_2^L \\ c_1^R & c_2^R \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} c_1^L \mu_1^L + c_2^L \mu_2^L \\ c_1^R \mu_1^R + c_2^R \mu_2^R \end{pmatrix},$$

where c_i^L, c_i^R are the values of c_i at $x = 0$, $x = 1$, respectively, and $\mu_i^{L/R} = \mu_i(c_1^{L/R}, c_2^{L/R})$ for $i = 1, 2$. If $c_1^L/c_2^L \neq c_1^R/c_2^R$, the above linear system is uniquely solvable. We remark that the modified free energy $\widetilde{\mathcal{F}}$ does not change the energy dissipation $\int_\Omega |\nabla p|^2 dx$ but it is nontrivial, as $\int_\Omega (\alpha_1 c_1 + \alpha_2 c_2) dx$ is nonconstant in time.
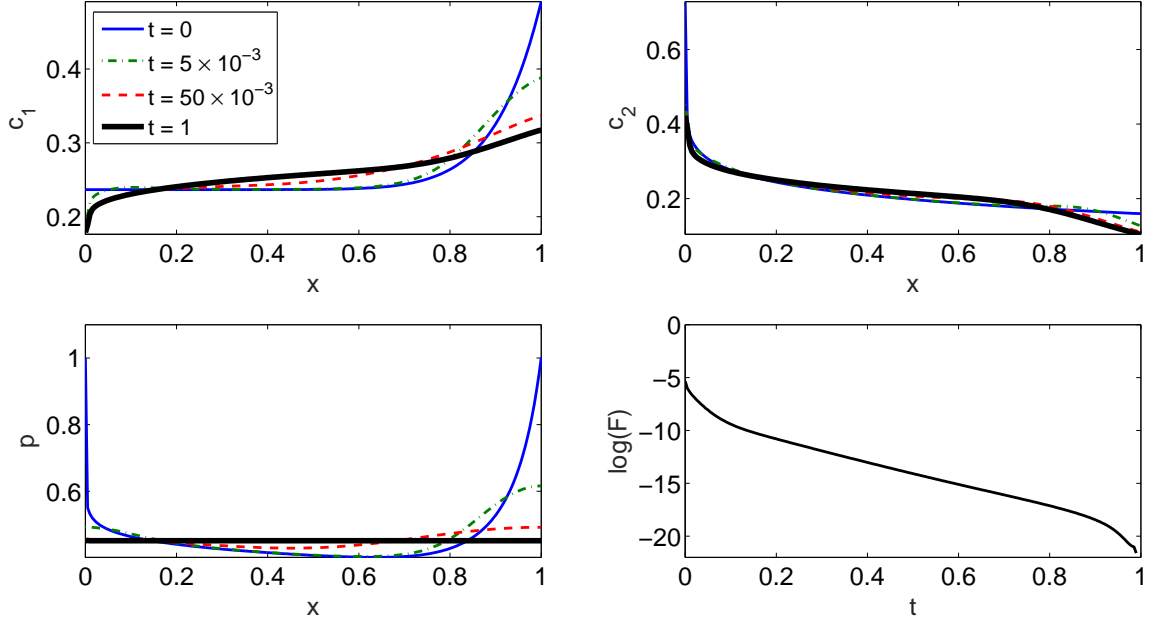
FIGURE 2. Case II (Neumann conditions, $\eta = \eta_M$): evolution of the mass densities c_1, c_2, pressure p, and logarithm of the relative free energy $\mathcal{F}(c(t)) - \mathcal{F}(c^0)$.

Figures 3 and 4 illustrate the evolution of c_1, c_2, p, and of the modified relative free energy $\widetilde{\mathcal{F}}(c(t)) - \widetilde{\mathcal{F}}(c^0)$. Again, the mass densities at $t = 1$ (they are basically stationary) are nonconstant, and the modified relative free energy converges exponentially fast. The decay rate is faster for $\eta = \eta_M$, contrarily to what happens in the case of Neumann boundary conditions.

APPENDIX A. FORMAL PROOF OF (10)

We prove the integral identity (10) in a formal setting. We proceed as in the proof of Theorem 3. Let $\psi(c) = c_{\text{tot}} f(c_1/c_{\text{tot}}, \ldots, c_{n-1}/c_{\text{tot}})$ for $c \in \mathscr{D}$, and let $z_i = c_i/c_{\text{tot}}$. Since $\varepsilon = 0$, the statement follows if $\sum_{j=1}^n c_j \partial^2 \psi / \partial c_i \partial c_j = 0$ for $i = 1, \ldots, n$. A straightforward computation gives

$$\frac{\partial^2 \psi}{\partial c_i \partial c_j} = \sum_{k=1}^{n-1} \frac{\partial f}{\partial z_k} \left(\frac{\partial z_k}{\partial c_i} + \frac{\partial z_k}{\partial c_j} + c_{\text{tot}} \frac{\partial^2 z_k}{\partial c_i \partial c_j} \right) + c_{\text{tot}} \sum_{k,s=1}^{n-1} \frac{\partial^2 f}{\partial z_k \partial z_s} \frac{\partial z_k}{\partial c_i} \frac{\partial z_s}{\partial c_j}.$$

Since $\partial z_k / \partial c_i = \delta_{ik}/c_{\text{tot}} - c_k/c_{\text{tot}}^2$, it follows that

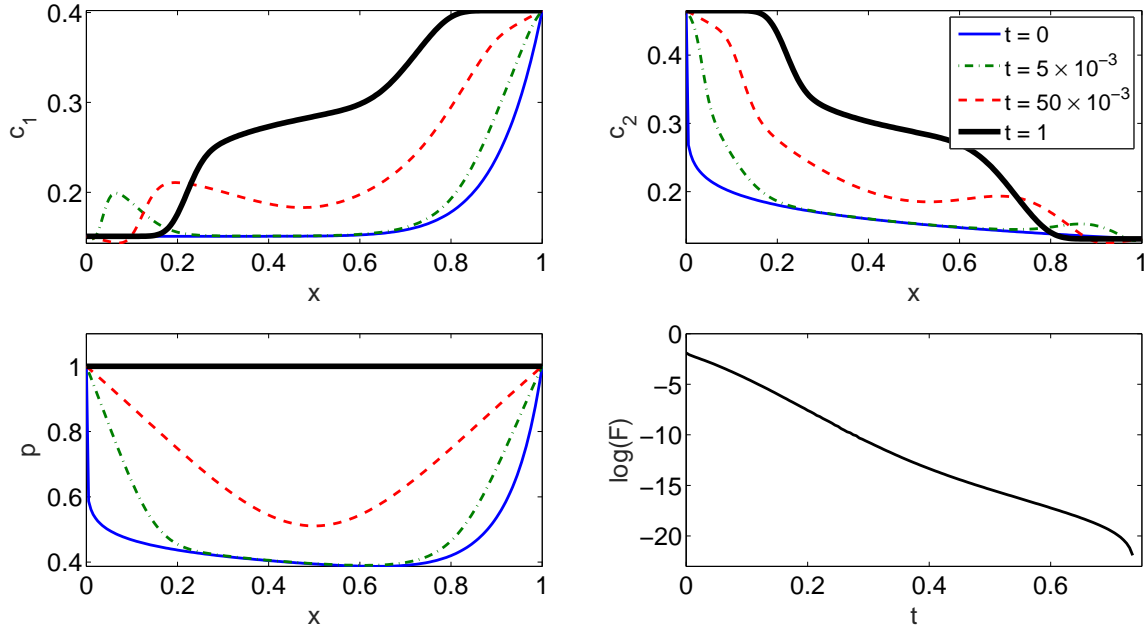$$\sum_{i=1}^n c_i \frac{\partial z_k}{\partial c_i} = 0, \quad k = 1, \ldots, n-1.$$

FIGURE 3. Case III (Dirichlet conditions, $\eta = \eta_m$): evolution of the mass densities c_1, c_2, pressure p, and logarithm of the relative modified free energy $\widetilde{\mathcal{F}}(c(t)) - \widetilde{\mathcal{F}}(c^0)$.

Moreover,

$$\frac{\partial z_k}{\partial c_i} + \frac{\partial z_k}{\partial c_j} + c_{\mathrm{tot}}\frac{\partial^2 z_k}{\partial c_i \partial c_j} = 0, \quad k = 1, \ldots, n-1, \ i, j = 1, \ldots, n.$$

Putting these three identities together yields $\sum_{j=1}^{n} c_j \partial^2 \psi / \partial c_i \partial c_j = 0$ for $i = 1, \ldots, n$.

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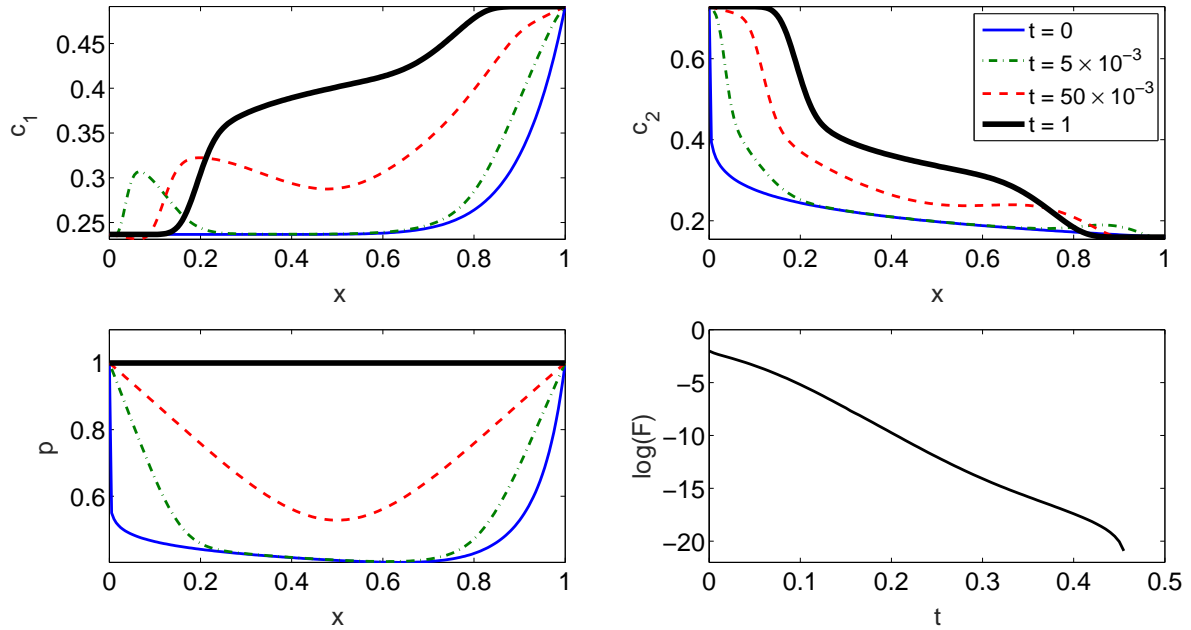
FIGURE 4. Case IV (Dirichlet conditions, $\eta = \eta_M$): evolution of the mass densities c_1, c_2, pressure p, and logarithm of the relative modified free energy $\widetilde{\mathcal{F}}(c(t)) - \widetilde{\mathcal{F}}(c^0)$.

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