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Analysis of a Poisson–Nernst–Planck–Fermi system for charge transport in ion channels ☆

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Abstract

A modified Poisson–Nernst–Planck system in a bounded domain with mixed Dirichlet–Neumann boundary conditions is analyzed. It describes the concentrations of ions immersed in a polar solvent and the correlated electric potential due to the ion–solvent interaction. The concentrations solve cross-diffusion equations, which are thermodynamically consistent. The considered mixture is saturated, meaning that the sum of the ion and solvent concentrations is constant. The correlated electric potential depends nonlocally on the electric potential and solves the fourth-order Poisson–Fermi equation. The existence of global bounded weak solutions is proved by using the boundedness-by-entropy method. The novelty of the paper is the proof of the weak–strong uniqueness property. In contrast to the existence proof, we include the solvent concentration in the cross-diffusion system, leading to a diffusion matrix with nontrivial kernel. Then the proof is based on the relative entropy method for the extended cross-diffusion system and the positive definiteness of a related diffusion matrix on a subspace.

MSC: 35J40; 35K51; 35Q92; 92C37

Keywords: Ion transport; Poisson–Nernst–Planck equations; Poisson–Fermi equation; Cross-diffusion systems; Existence of weak solutions

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1. Introduction

The modeling of the transport of ions through biological channels is of fundamental importance in cell biology. Several strategies have been developed in past decades, using molecular or Brownian dynamics or the Poisson–Nernst–Planck theory. This theory relies on the assumptions that the dynamics of ion transport is based on diffusion and electrostatic interaction only and that the solution is dilute. However, the presence of narrow channel pores requires a more sophisticated modeling. In particular, the ion size is not small compared to the biological channel diameter, and many-particle interactions due to the confined geometry need to be taken into account. In this paper, we analyze a modified Poisson–Nernst–Planck system modeling ion–water interactions and finite ion size constraints. We prove the existence of global weak solutions and, as the main novelty, the weak–strong uniqueness property using entropy methods.

1.1. The model setting

The evolution of n ionic species, immersed in a solvent (like water), is assumed to be given by the equations

$$\partial_t u_i + \operatorname{div} J_i = r_i(u), \quad J_i = -D_i(\nabla u_i - u_i \nabla \log u_0 + u_i z_i \nabla\Phi), \tag{1}$$

$$\lambda^2(\ell^2\Delta - 1)\Delta\Phi = \sum_{j=1}^n z_j u_j + f(x) \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n, \tag{2}$$

where $\Omega \subset \mathbb{R}^d$ ($d \ge 1$) is a bounded Lipschitz domain, $u = (u_1, \ldots, u_n)$ is the concentration vector, supplemented with initial and mixed Dirichlet–Neumann boundary conditions,

$$u_i(\cdot, 0) = u_i^0 \quad \text{in } \Omega, \quad i = 1, \ldots, n, \tag{3}$$

$$J_i \cdot \nu = 0 \text{ on } \Gamma_N, \quad u_i = u_i^D \text{ on } \Gamma_D,\ t>0, \tag{4}$$

$$\nabla\Phi \cdot \nu = \nabla\Delta\Phi \cdot \nu = 0 \text{ on } \Gamma_N, \quad \Phi = \Phi^D,\ \Delta\Phi = 0 \text{ on } \Gamma_D,\ t>0, \tag{5}$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$, and ν is the exterior unit normal vector to $\partial\Omega$.

The unknowns are the ion concentrations (or volume fractions) $u_i(x,t)$ of the ith ion species and the correlated electric potential $\Phi(x,t)$. The solvent concentration (or volume fraction) $u_0(x,t)$ is given by $u_0 = 1 - \sum_{i=1}^n u_i$, which means that the mixture is saturated. Equations (1) are cross-diffusion equations with the fluxes J_i and the reaction rates $r_i(u)$. The parameters are the diffusivities $D_i > 0$ and the valences $z_i \in \mathbb{Z}$. Equation (2) is the Poisson–Fermi equation with the scaled Debye length $\lambda > 0$, the correlation length $\ell > 0$, and the given background charge density $f(x)$. We assume that the domain is isolated on the Neumann boundary, while the concentrations and the electric potential are prescribed on the Dirichlet boundary. We refer to [24] for a derivation of (1)–(2) using an averaging procedure of a Langevin model.

In the following, we discuss definition (1) of the fluxes and equation (2) for the correlated electric potential. We recover the classical Poisson–Nernst–Planck equations if $u_0 = \text{const.}$ and $\ell = 0$. In this situation, we can write $J_i^{\text{id}} = -D_i u_i \nabla\mu_i^{\text{id}}$ with the electrochemical potential $\mu_i^{\text{id}} = \log u_i + z_i\Phi$ of an ideal dilute solution. In concentrated solutions, the finite size of the ions needs to be taken into account, expressed by the excess chemical potential μ_i^{ex}, so that the electrochemical potential becomes $\mu_i = \mu_i^{\rm id} + \mu_i^{\rm ex}$. Bikerman [4] suggested the choice $\mu_i^{\rm ex} = -\log(1 - \sum_{i=1}^n u_i) = -\log u_0$; also see [1, Sec. 3.1.2]. Then $J_i = -D_i u_i \nabla\mu_i$ coincides with the flux adopted in our model (1). Note that solving $\mu_i = \log(u_i/u_0) + z_i\Phi$ for the concentrations, we find that the ion profiles obey the Fermi–Dirac statistics

$$u_i = \frac{\exp(\mu_i - z_i\Phi)}{1 + \sum_{j=1}^n \exp(\mu_j - z_j\Phi)}, \quad i = 1, \ldots, n.$$

Then, given μ_i and Φ, the bounds $0 \le u_i \le 1$ are automatically satisfied. Other choices of the excess chemical potential were suggested in [3, Sec. 2.1].

In the literature, there exist also other approaches to define the fluxes J_i under finite size constraints. The diffusion limit of an on-lattice model, which takes into account that neighboring sites may be occupied (modeling size exclusion), was performed in [6], analyzed in [15], and numerically solved in [7], resulting to

$$J_i^{(1)} = -D_i(u_0\nabla u_i - u_i\nabla u_0 + u_0 u_i z_i \nabla\Phi), \quad i = 1, \ldots, n. \tag{6}$$

This model avoids the singular term $\nabla\log u_0$, which is delicate near $u_0 = 0$, but it introduces the diffusion term $u_0\nabla u_i$, which degenerates at $u_0 = 0$. Another flux definition was suggested in [16],

$$J_i^{(2)} = -D_i\left(\nabla u_i + u_i z_i\nabla\Phi - \sum_{j=1}^n z_j u_j \nabla\Phi\right), \quad i = 1, \ldots, n.$$

The additional term $-\sum_{j=1}^n z_j u_j \nabla\Phi$ comes from the force balance in the Euler momentum equation for zero fluid velocity. The ion–water interaction is described in [8] by

$$J_i^{(3)} = -D_i\left(\nabla u_i + u_i z_i\nabla\Phi - \frac{\partial\varepsilon_0}{\partial u_i}|\nabla\Phi|^2\right), \quad i = 1, \ldots, n,$$

where the dielectricity $\varepsilon_0 = \lambda^2$, instead of being constant, depends on u. This assumption is based on the experimental observation that the dielectric response of water decreases as ion concentrations increase [8]. Thus, $\partial\varepsilon_0/\partial u_i < 0$, showing that the ion–water interaction energy is always nonnegative. Finite ion size effects are modeled in [20] by including an approximation of the Lennard–Jones potential in the energy functional, leading to

$$J_i^{(4)} = -D_i\left(\nabla u_i + u_i\nabla\sum_{j=1}^n a_{ij}u_i + z_i\nabla\Phi\right), \quad i = 1, \ldots, n.$$

Assuming that (a_{ij}) is positive definite, the global existence of weak solutions for two species was proved in [18]. For the analysis of the stationary equations, see [14]. Finally, excluded volume effects can be included by considering nonlinear diffusivities $D_i(u_i) = 1 + \alpha u_i$, where $\alpha > 0$ is a measure of the volume exclusion interactions [5].

Our model has the advantage of being consistent with the thermodynamical model [11]

$$J_i = -\sum_{j=1}^n D_{ij}u_j\nabla(\mu_j - \mu_0), \quad \text{where } \mu_i = \log u_i + z_i\Phi, \quad \mu_0 = \log u_0 + z_0\Phi,$$

assuming that the diffusion matrix is diagonal, $D_{ij} = D_i\delta_{ij}$, and that the solvent is neutral, $z_0 = 0$.

The interaction of the ions with polar solvents like water is modeled by the potential in (2). Indeed, let ϕ be the electric potential of free ions, given by $-\lambda^2\Delta\phi = \rho$, where ρ is the total charge density. Then the correlated potential $\Phi = \ell^{-2}Y_\ell * \phi$ is the convolution between the Yukawa potential $Y_\ell(x) = (|x|/\ell)^{-1}\exp(-|x|/\ell)$ [22] and the electric potential, where $\ell > 0$ is the correlation length of the screening by ions and water [26]. As this potential satisfies $-\ell^2\Delta\Phi + \Phi = \phi$, we recover (2) with $\rho = \sum_{j=1}^n z_ju_j + f(x)$. Thus, the Poisson–Fermi equation (2) includes finite ion size effects and polarization correlations among water molecules. It generalizes the fourth-order differential permittivity operator of [23] and the nonlocal permittivity in ionic liquids of [2]. If there are no correlation and polarization effects ($\ell = 0$), we recover the standard Poisson equation for the electric potential. The expression $\varepsilon_0 = \lambda^2(\ell^2\Delta - 1)$ can be interpreted as a dielectric differential operator.

1.2. Entropy structure

System (1) can be written as a cross-diffusion system with a diffusion matrix which is neither symmetric nor positive definite. This issue is overcome by exploiting the entropy (or free energy) structure and using the boundedness-by-entropy method [19]. The free energy associated to (1)–(2) is given by [2,21]

$$H(u) = \int_\Omega h(u)dx, \quad \text{where} \tag{7}$$

$$h(u) = \sum_{i=0}^n \int_{u_i^D}^{u_i} \log\frac{s}{u_i^D}ds + \frac{\lambda^2}{2}|\nabla(\Phi - \Phi^D)|^2 + \frac{(\lambda\ell)^2}{2}|\Delta(\Phi - \Phi^D)|^2.$$

The energy density $h(u)$ consists of the internal, free-ion electric, and correlation electric energies. The free energy allows us to formulate equations (1) as a diffusion system with a positive semidefinite diffusion matrix. Indeed, we introduce the electrochemical potentials

$$\widetilde{\mu}_i = \frac{\partial h}{\partial u_i} = \log\frac{u_i}{u_0} - \log\frac{u_i^D}{u_0^D} + z_i(\Phi - \Phi^D), \quad i = 1, \ldots, n,$$

where $\partial h/\partial u_i$ denotes the variational derivative of h with respect to u_i (see [15, Lemma 7]) and $u_0^D = 1 - \sum_{i=1}^n u_i^D$. As in [15], we split the electrochemical potentials into the entropy variables w_i and the boundary contributions w_i^D by

$$w_i := \log\frac{u_i}{u_0} + z_i\Phi, \quad w_i^D := \log\frac{u_i^D}{u_0^D} + z_i\Phi^D. \tag{8}$$

Then equations (1) can be written as

$$\partial_t u_i - \operatorname{div} \sum_{j=1}^n B_{ij}(w, \Phi)\nabla w_j = r_i(u), \quad i = 1, \ldots, n, \tag{9}$$

where $B_{ij} = D_i u_i \delta_{ij}$ and $u_i = u_i(w, \Phi)$ is interpreted as a function of $w = (w_1, \ldots, w_n)$ and Φ according to

$$u_i(w, \Phi) = \frac{\exp(w_i - z_i\Phi)}{1 + \sum_{j=1}^n \exp(w_i - z_j\Phi)}. \tag{10}$$

The advantage of formulation (9) is that the new diffusion matrix $B = (B_{ij})$ is symmetric and positive semidefinite. Observe that system (9) is of degenerate type since $u_i = 0$ is possible, and $\det B = 0$ in this case. The formulation in terms of entropy variables has the further advantage that the ion concentrations u_i, defined by (10), are nonnegative and satisfy $\sum_{i=1}^n u_i \le 1$, thus fulfilling the saturation assumption.

1.3. Main results

We introduce the simplex $\mathcal{D} = \{u = (u_1, \ldots, u_n) \in (0,1)^n : \sum_{i=1}^n u_i < 1\}$ and set $\Omega_T = \Omega \times (0, T)$. The following hypotheses are imposed:

- (H1) Domain: $\Omega \subset \mathbb{R}^d$ $(1 \le d \le 3)$ is a bounded Lipschitz domain with $\partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$, Γ_N is open in $\partial\Omega$, and $\operatorname{meas}(\Gamma_D) > 0$.
- (H2) Data: $T > 0$, $D_i > 0$, $z_i \in \mathbb{R}$ for $i = 1, \ldots, n$, $f \in L^2(\Omega)$.
- (H3) Initial data: $u^0 = (u_1^0, \ldots, u_n^0) \in L^1(\Omega; \mathbb{R}^n)$ satisfies $u^0(x) \in \overline{\mathcal{D}}$ for a.e. $x \in \Omega$.
- (H4) Boundary data: $u^D = (u_1^D, \ldots, u_n^D) \in H^1(\Omega; \mathbb{R}^n)$ satisfies $u^D(x) \in \mathcal{D}$ for $x \in \Omega$, $\log u_0^D \in L^2(\Omega)$, and $\Phi^D \in H^2(\Omega)$ solves

$$\begin{aligned} &\lambda^2(\ell^2\Delta - 1)\Delta\Phi^D = f(x) \text{ in } \Omega, \\ &\nabla\Phi^D \cdot \nu = \nabla\Delta\Phi^D \cdot \nu = 0 \text{ on } \Gamma_N, \quad \Delta\Phi^D = 0 \text{ on } \Gamma_D. \end{aligned} \tag{11}$$

- (H5) Reaction rates: $r_i \in C^0([0,1]^n; \mathbb{R})$ for $i = 1, \ldots, n$, and there exists $C_r > 0$ such that for all $u \in L^\infty(\Omega_T; \mathcal{D})$ and Φ, given by (2) and (5),

$$\int_\Omega \sum_{i=1}^n r_i(u) \frac{\partial h}{\partial u_i} dx \le C_r(1 + H(u)). \tag{12}$$

The restriction to three space dimensions in Hypothesis (H1) is not needed. It can be removed by regularizing the Poisson–Fermi equation (2) to ensure that $\Phi \in L^\infty(\Omega)$; see Remark 3 below. In Hypothesis (H4), it is sufficient to define the boundary data on Γ_D. We have extended them to Ω with the special extension of Φ^D, fulfilling the fourth-order elliptic problem (11). This extension is needed to be consistent with the definition of the free energy and the entropy variables; see [15, Lemma 7]. The bound in Hypothesis (H5) is needed to derive gradient bounds on the concentrations from the free energy inequality; see (16) below. Since $\partial h/\partial u_i$ contains the logarithm, $r_i(u)$ needs to cancel the singularity in $\partial h/\partial u_i$ at $u_i=0$. It is sufficient to require Hypothesis (H5) for the logarithmic part of $\partial h/\partial u_i$. Indeed, since r_i is continuous, $r_i(u)$ is bounded for $u\in[0,1]^n$, and we infer from Poincaré's inequality that

$$\int_\Omega \sum_{i=1}^n r_i(u)(\Phi-\Phi^D)dx \le C\|\Phi-\Phi^D\|_{L^1(\Omega)} \le C + C\|\nabla(\Phi-\Phi^D)\|^2_{L^2(\Omega)} \le C(1+H(u)).$$

Therefore, we need the integrated version (12) instead of the pointwise inequality assumed in [19, Sec. 1.4].

We introduce the test spaces

$$H^1_D(\Omega)=\{v\in H^1(\Omega): v=0 \text{ on } \Gamma_D\},$$
$$H^2_{D,N}(\Omega)=\{v\in H^2(\Omega): v=0 \text{ on } \Gamma_D,\ \nabla v\cdot\nu=0 \text{ on } \Gamma_N\}.$$

Our first main result is as follows.

Theorem 1 *(Global existence of solutions). Let Hypotheses (H1)–(H5) hold and let $T>0$ be an arbitrary time end point. Then there exists a bounded weak solution $u_1,\ldots,u_n$ to (1)–(5) satisfying $u_i(x,t)\in\overline{\mathcal{D}}$ for a.e. $(x,t)\in\Omega_T$, $i=1,\ldots,n$,*

$$\sqrt{u_i}\in L^2(0,T;H^1(\Omega)), \quad u_i\in H^1(0,T;H^1_D(\Omega)')\cap C^0([0,T];L^2(\Omega)),$$
$$\Phi\in L^2(0,T;H^2(\Omega)), \quad \log u_0\in L^2(0,T;H^1(\Omega)),$$

the weak formulation

$$\int_0^T\langle\partial_t u_i,\phi_i\rangle dt - \int_0^T\int_\Omega J_i\cdot\nabla\phi_i dxdt = \int_0^T\int_\Omega r_i(u)\phi_i dxdt, \tag{13}$$

$$\lambda^2\int_0^T\int_\Omega(\ell^2\Delta\Phi\Delta\theta+\nabla\Phi\cdot\nabla\theta)dxdt = \int_0^T\int_\Omega\Big(\sum_{i=1}^n z_iu_i+f\Big)\theta dxdt \tag{14}$$

for all $\phi_i\in L^2(0,T;H^1_D(\Omega))$ and $\theta\in L^2(0,T;H^2_{D,N}(\Omega))$, where J_i is given by (1) and $\langle\cdot,\cdot\rangle$ is the dual product between $H^1_D(\Omega)'$ and $H^1_D(\Omega)$. The initial conditions (3) are satisfied a.e. in Ω, and the Dirichlet boundary conditions are fulfilled in the sense of traces in $L^2(\Gamma_D)$. Furthermore, if $r_i(u)=0$ for all $i=1,\ldots,n$ and the Dirichlet boundary conditions are in thermal equilibrium (e.g. $w_i^D:=\log(u_i^D/u_0^D)+z_i\Phi^D=$ const. in Ω), the solution satisfies for $0<s<t<T$ the free energy inequality

$$H(u(t))+\int_s^t\int_\Omega\sum_{i=1}^n D_iu_i\left|\nabla\Big(\log\frac{u_i}{u_0}+z_i\Phi\Big)\right|^2 dxd\sigma \le H(u(s)). \tag{15}$$

The energy dissipation is understood in the sense

$$u_i\left|\nabla\left(\log\frac{u_i}{u_0}+z_i\Phi\right)\right|^2=\left|2\nabla\sqrt{u_i}-\sqrt{u_i}\nabla\log u_0+\sqrt{u_i}z_i\nabla\Phi\right|^2.$$

We stress the fact that the solutions are nonnegative, have an upper bound, and conserve mass in the absence of reactions. More precisely, the solution of Theorem 1 satisfies:

- $u_0(x,t),u_1(x,t),\ldots,u_n(x,t)\in[0,1]$ and $\sum_{i=0}^n u_i(x,t)=1$ for a.e. $x\in\Omega$, $t>0$;
- the solvent concentration u_0 is positive a.e. in $\Omega\times(0,\infty)$;
- if $r_i(u)=0$ then $\int_\Omega u_i(x,t)dx=\int_\Omega u_i^0(x)dx$ for $t>0$, $i=1,\ldots,n$.

The second point is a consequence of the integrability of $\log u_0$ ensured in Theorem 1.

The assumption of thermal equilibrium at the Dirichlet boundary, also required in [15], is needed to avoid expressions involving ∇w_i^D in the free energy inequality. Thus, this condition, together with vanishing reactions, is natural to obtain the monotonicity of the free energy. The hypothesis of vanishing reactions is only required to derive the entropy inequality (15) and can be weakened. In fact, we may allow for nonnegative and quasipositive reaction terms; see Remark 17 for details. In Remark 16, we explain how the uniqueness of weak solutions can be proved under restrictive conditions on the parameters. Moreover, we refer to Remark 9 for the extension of the free energy inequality (15) to the case of nonzero reaction terms r_i.

The proof of Theorem 1 is, similarly as in [15], based on an approximation procedure, where we regularize (9) by an implicit Euler approximation and higher-order terms in the entropy variables. The uniform estimates that are needed to perform the de-regularization limit are derived from the free energy inequality, which (without regularization) reads as

$$\frac{dH}{dt}+\int_\Omega\sum_{i=1}^n D_iu_i|\nabla w_i|^2dx\le\int_\Omega\sum_{i=1}^n r_i(u)\cdot\frac{\partial h}{\partial u_i}dx\le C_r(1+H(u)),\tag{16}$$

recalling definition (8) of w_i, and we can conclude by Gronwall's lemma. The free energy dissipation term on the left-hand side can be estimated from above by (see Lemma 6)

$$\int_\Omega u_i|\nabla w_i|^2dx\ge\frac{1}{2}\int_\Omega\left(|\nabla\sqrt{u_i}|^2+|\nabla\log u_0|^2+|\nabla u_0|^2\right)dx-C\int_\Omega|\nabla\Phi|^2dx.$$

The last term is bounded by the electric energy part in $H(u)$, thus giving $H^1(\Omega)$ bounds for u_i for $i=0,\ldots,n$ and $\log u_0$. Compared to [15], we obtain gradient estimates for all the ion concentrations, but we have to deal with the singular term $\nabla\log u_0$ in (1). Moreover, compared to [13], where a similar Nernst–Planck system (with $\ell=0$) was investigated, we do not need any positivity condition on the initial solvent concentration.

While the existence proof relies on standard entropy methods, we need a new idea to prove the weak–strong uniqueness result. The uniqueness of *weak* solutions is an intricate problem. A uniqueness result for (1) with the fluxes (6) was shown in [15] for the case $D_i=D$ and $z_i=z$ for all i. In this simplified situation, the solvent concentration solves a Poisson–Nernst–Planck system for which the uniqueness of bounded weak solutions can be proved by a combination of $L^2(\Omega)$ estimates and Gajewski's entropy method. This strategy cannot be used for our system; see Remark 16 in Section 4. In fact, we need the $H^{-1}(\Omega)$ method and a strong regularity condition for $\nabla\Phi$, which restricts the geometry of the Dirichlet–Neumann boundary conditions. Therefore, we do not aim to prove the uniqueness of weak solutions but the weak–strong uniqueness property only, which has the advantage that we may allow for different coefficients D_i and z_i. The weak–strong uniqueness property means that any weak solution to system (1)–(5) coincides with a strong solution emanating from the same initial conditions as long as the latter exists. We say that $(\bar{u}, \bar{\Phi})$ is a *strong solution* to (1)–(5) if it is a weak solution and

$$\bar{u}_i \geq c > 0 \text{ in } \Omega_T, \quad \bar{u}_i,\ \Phi \in L^\infty(0,T;W^{1,\infty}(\Omega)) \quad \text{for all } i = 1,\ldots,n.$$

Our second main result is contained in the following theorem.

Theorem 2 *(Weak–strong uniqueness). Let the Dirichlet boundary data be in thermal equilibrium in the sense of Theorem 1 and let $r_i = 0$ for $i = 1,\ldots,n$. Let (u,Φ) be a weak solution and $(\bar{u},\bar{\Phi})$ be a strong solution to (1)–(5). Then $u(x,t) = \bar{u}(x,t)$, $\Phi(x,t) = \bar{\Phi}(x,t)$ for a.e. $x \in \Omega$ and $t \in (0,T)$.*

If the reaction rates are Lipschitz continuous and satisfy some sign conditions, Theorem 2 still holds. An exhaustive discussion on this point can be found in Remark 17. The condition that the Dirichlet boundary data are in thermal equilibrium is actually not needed, since in contrast to (15), the terms involving ∇w_i^D cancel out in the computations for the relative free energy

$$H(u,\Phi|\bar{u},\bar{\Phi}) = \int_\Omega \big(h_1(u|\bar{u}) + h_2(\Phi|\bar{\Phi})\big)dx, \quad \text{where}$$

$$h_1(u|\bar{u}) = \sum_{i=0}^n \left(u_i \log\frac{u_i}{\bar{u}_i} - (u_i - \bar{u}_i)\right),$$

$$h_2(\Phi|\bar{\Phi}) = \frac{\lambda^2}{2}\big(|\nabla(\Phi-\bar{\Phi})|^2 + \ell^2|\Delta(\Phi-\bar{\Phi})|^2\big),$$

which can be identified as the Bregman distance of the free energy. The key idea of the proof of Theorem 2 is to consider the solvent concentration u_0 as an independent variable and to formulate the parabolic equations for the extended concentration vector $U = (u_0, u_1, \ldots, u_n)$, leading to

$$\partial_t u_i = \operatorname{div}\sum_{j=0}^n \big(A_{ij}(U)\nabla\log u_j + Q_{ij}(U)\nabla\Phi\big), \quad i = 0,\ldots,n,$$

where $A_{ij}(U)$ and $Q_{ij}(U)$ depend linearly on U and

$$A = (A_{ij}) = \begin{pmatrix} \sum_{i=1}^n D_i u_i & -D_1 u_1 & \cdots & -D_n u_n \\ -D_1 u_1 & D_1 u_1 & & 0 \\ \vdots & 0 & \ddots & 0 \\ -D_n u_n & 0 & & D_n u_n \end{pmatrix},$$
$$Q = (Q_{ij}) = \begin{pmatrix} -\sum_{i=1}^n D_i z_i u_i & 0 & \cdots & 0 \\ 0 & D_1 z_1 u_1 & & 0 \\ \vdots & 0 & \ddots & 0 \\ 0 & 0 & & D_n z_n u_n \end{pmatrix}, \tag{17}$$

setting $z_0 := 0$. The matrix $(A_{ij}/\sqrt{u_i u_j}) \in \mathbb{R}^{(n+1)\times(n+1)}$ is positive definite only on the subspace $L = \{y \in \mathbb{R}^{n+1} : \sum_{i=0}^n \sqrt{u_i} y_i = 0\}$; see Lemma 10. This situation is similar to the Maxwell–Stefan system; see [17]. The time derivative of the relative free energy equals

$$\frac{dH}{dt}(u, \Phi|\bar{u}, \bar{\Phi}) = K_1 + K_2, \quad \text{where } K_1 = -\int_\Omega \sum_{j=0}^n A_{ij} \nabla \log \frac{u_i}{\bar{u}_i} \cdot \nabla \log \frac{u_j}{\bar{u}_j} dx,$$

and K_2 contains differences like $U_i - \bar{U}_i$ and $\Phi - \bar{\Phi}$. The properties of the matrices (A_{ij}) and (Q_{ij}) imply that

$$K_1 \le -\min_{i=1,\dots,n} D_i \int_\Omega \left(\frac{1}{u_0} |(P_L Y)_0|^2 + \sum_{i=1}^n |(P_L Y)_i|^2 \right) dx,$$

where P_L is the projection on L and $Y_i = \sqrt{u_i} \nabla \log(u_i/\bar{u}_i)$, as well as for any $\delta > 0$,

$$K_2 \le \delta \int_\Omega \left(\frac{1}{u_0} |(P_L Y)_0|^2 + \sum_{i=1}^n |(P_L Y)_i|^2 \right) dx$$
$$+ C(\delta) \left(\sum_{i=0}^n \|u_i - \bar{u}_i\|_{L^2(\Omega)}^2 + \|\nabla(\Phi - \bar{\Phi})\|_{L^2(\Omega)}^2 \right).$$

Consequently, choosing $\delta > 0$ sufficiently small,

$$\frac{dH}{dt}(u, \Phi|\bar{u}, \bar{\Phi}) \le C \left(\sum_{i=0}^n \|u_i - \bar{u}_i\|_{L^2(\Omega)}^2 + \|\nabla(\Phi - \bar{\Phi})\|_{L^2(\Omega)}^2 \right) \le C H(u, \Phi|\bar{u}, \bar{\Phi})$$

for some constant $C > 0$. Since the initial data of u and $\bar{u}$ coincide, we have $H((u, \Phi)(t)|(\bar{u}, \bar{\Phi})(t)) = 0$ and finally $u(t) = \bar{u}(t)$ and $\Phi(t) = \bar{\Phi}(t)$ for all $t > 0$. The idea to consider the parabolic system for the extended solution vector $U = (u_0, \dots, u_n)$ instead of $u = (u_1, \dots, u_n)$ is the main novelty of this paper. The Maxwell–Stefan equations can also be written as an extended system for U [17], but we are not aware of further volume-filling models with such a property. The understanding of volume-filling systems and mobility matrices with nontrivial kernels is a current field of research.

The article is organized as follows. The proof of Theorem 1 is presented in Section 2, while Section 3 contains the proof of Theorem 2. We make some remarks on the uniqueness of solutions in Section 4.

2. Proof of Theorem 1

We assume throughout this section that Hypotheses (H1)–(H5) hold.

2.1. Solution of an approximate system

We define the approximate problem by the implicit Euler scheme and using a higher-order regularization. Let $T > 0$, $N \in \mathbb{N}$, $\tau = T/N$, and $m \in \mathbb{N}$ with $m > d/2$. We assume that $u_i^D \geq \eta > 0$ for $i = 0, \ldots, n$. Then $w_i^D = \log(u_i^D/u_0^D) + z_i\Phi^D \in H^1(\Omega; \mathbb{R}^n) \cap L^\infty(\Omega; \mathbb{R}^n)$. Since the entropy variables are not needed in the weak formulation (13)–(14), we can pass to the limit $\eta \to 0$ at the end of the proof, thus requiring only $u_i^D > 0$. Let $k \geq 1$ and let $u^{k-1} - u^D \in H_D^1(\Omega; \mathbb{R}^n) \cap L^\infty(\Omega; \mathbb{R}^n)$ and $\Phi^{k-1} - \Phi^D \in H_{D,N}^2(\Omega)$ be given. If $k = 1$, $\Phi^0 \in H^2(\Omega)$ is the unique solution to (2) with u_j^0 instead of u_j on the right-hand side and satisfying the corresponding boundary conditions in (4)–(5). We wish to find a solution $v^k \in X := H^m(\Omega; \mathbb{R}^n) \cap H_D^1(\Omega; \mathbb{R}^n)$ and $\Phi^k - \Phi^D \in H_{D,N}^2(\Omega)$ to

$$\frac{1}{\tau}\int_\Omega (u^k - u^{k-1}) \cdot \phi dx + \int_\Omega \nabla\phi : B(v^k + w^D, \Phi^k)\nabla(v^k + w^D) dx \tag{18}$$

$$+ \varepsilon \int_\Omega \Big(\sum_{|\alpha|=m} D^\alpha v^k \cdot D^\alpha \phi + v^k \cdot \phi \Big) dx = \int_\Omega r(u^k) \cdot \phi dx,$$

$$\lambda^2 \int_\Omega \big(\ell^2 \Delta\Phi^k \Delta\theta + \nabla\Phi^k \cdot \nabla\theta\big) dx = \int_\Omega \Big(\sum_{i=1}^n z_i u_i^k + f \Big)\theta dx \tag{19}$$

for all $\phi \in X$ and $\theta \in H_{D,N}^2(\Omega)$. Here, we have set $u^k := u(v^k + w^D, \Phi^k)$, where $u(w, \Phi)$ is defined by (10), $B_{ij}(w, \Phi) = D_i u_i(w, \Phi)\delta_{ij}$, $r(u) = (r_1(u), \ldots, r_n(u))$, and $D^\alpha = \partial^{|\alpha|}/\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}$ is a partial derivative of order $|\alpha| = \alpha_1 + \cdots + \alpha_d$. Thanks to the higher-order regularization, we obtain approximate solutions $w^k := v^k + w^D \in H^m(\Omega; \mathbb{R}^n) \hookrightarrow L^\infty(\Omega; \mathbb{R}^n)$. Moreover, since $d \leq 3$, we have $\Phi^k \in H^2(\Omega) \hookrightarrow L^\infty(\Omega)$. Hence, $u_i(w^k, \Phi^k)$ is well defined and integrable.

Remark 3. Adding a higher-order regularization to the Poisson–Fermi equation (19), we may obtain $\Phi^k \in L^\infty(\Omega)$ by a Sobolev embedding similarly as for w^k. This allows us to remove the restriction $d \leq 3$ in Hypothesis (H1). □

Lemma 4. *There exists a unique solution $v^k \in H^m(\Omega; \mathbb{R}^n) \cap H_D^1(\Omega; \mathbb{R}^n)$ and $\Phi^k - \Phi^D \in H_{D,N}^2(\Omega)$ to (18)–(19).*

Proof. The proof is similar to that one of Lemma 5 in [15], therefore we give a sketch only. Let $y \in L^\infty(\Omega; \mathbb{R}^n)$ and $\sigma \in [0, 1]$. Let $\Phi^k \in H^2(\Omega)$ be the unique solution to

$$\lambda^2(\ell^2\Delta - 1)\Delta\Phi^k = \sum_{i=1}^n z_i u_i(y + w^D, \Phi^k) + f(x) \quad \text{in } \Omega$$

subject to the boundary conditions (5). This follows from the fact that the function $(x, \Phi) \mapsto u_i(w(x), \Phi)$ is bounded with values in $(0, 1)$ and Lipschitz continuous in Φ. By the Lax–Milgram lemma, there exists a unique solution $v \in X$ to the linear problem

$$\varepsilon \int_\Omega \Big(\sum_{|\alpha|=m} D^\alpha v \cdot D^\alpha \phi + v \cdot \phi \Big) ds + \int_\Omega \nabla\phi : B(y + w^D, \Phi^k)\nabla v dx \tag{20}$$
$$= \delta \int_\Omega r(u(y + w^D, \Phi^k)) \cdot \phi dx - \delta \int_\Omega \nabla\phi : B(y + w^D, \Phi^k)\nabla w^D dx$$
$$- \frac{\delta}{\tau} \int_\Omega \big(u(y + w^D, \Phi^k) - u^{k-1}\big) \cdot \phi dx.$$

Indeed, as B is positive semidefinite, the left-hand side is coercive in $H^m(\Omega; \mathbb{R}^n)$.

This defines the fixed-point operator $S : L^\infty(\Omega; \mathbb{R}^n) \times [0, 1] \to L^\infty(\Omega; \mathbb{R}^n)$, $S(y, \delta) = v$. Then $S(y, 0) = 0$, S is continuous and, because of the compact embedding $H^m(\Omega; \mathbb{R}^n) \hookrightarrow L^\infty(\Omega; \mathbb{R}^n)$, also compact. Using $\phi = v$ as a test function in (20), standard estimates lead to $\varepsilon\|v\|^2_{H^m(\Omega)} \le C(\tau)\|v\|_{H^m(\Omega)}$, giving a bound for v in $H^m(\Omega; \mathbb{R}^n)$ uniform in δ. Hence, all fixed points of $S(\cdot, \delta)$ are uniformly bounded in $L^\infty(\Omega; \mathbb{R}^n)$. We infer from the Leray–Schauder fixed-point theorem that there exists $v^k \in X$ such that $S(v^k, 1) = v^k$. Then (v^k, Φ^k) is a solution to (18)–(19). □

2.2. Uniform estimates

We deduce estimates uniform in (ε, τ) from the following free energy inequality.

Lemma 5 *(Discrete free energy inequality). Let (v^k, Φ^k) be a solution to (18)–(19) and set $w^k := v^k + w^D$ and $u^k := u(w^k, \Phi^k)$. Then*

$$H(u^k) - H(u^{k-1}) + \frac{\tau}{2} \int_\Omega \sum_{i=1}^n D_i u_i^k |\nabla w_i^k|^2 dx + \varepsilon\tau\|w^k - w^D\|^2_{H^m(\Omega)} \tag{21}$$
$$\le \tau C_r(1 + H(u^k)) + \frac{\tau}{2} \int_\Omega \sum_{i=1}^n D_i |\nabla w_i^D|^2 dx,$$

where H is defined in (7) and $C_r > 0$ is introduced in Hypothesis (H5).

Proof. We choose $\phi = \tau v^k = \tau(w^k - w^D) \in X$ as a test function in (18). Using the generalized Poincaré inequality to estimate the ε-regularization and Hypothesis (H5) to estimate the reaction rates, we find that

$$\int_\Omega (u^k - u^{k-1})\cdot(w^k - w^D)dx + \tau\int_\Omega \nabla(w^k - w^D) : B(w^k,\Phi^k)\nabla w^k dx$$
$$+ \varepsilon\tau C\|w^k - w^D\|^2_{H^m(\Omega)} \le \tau C_r(1 + H(u^k)).$$

It follows from the convexity of the function $g(u) = \sum_{i=0}^n \int_{u_i^D}^{u_i} \log(s/u_i^D)ds$ and the Poisson–Fermi equation (2) as in [15, Section 2] that

$$\begin{aligned}
\int_\Omega (u^k - u^{k-1})\cdot(w^k - w^D)dx &= \int_\Omega \sum_{i=1}^n (u_i^k - u_i^{k-1})\bigg(\log\frac{u_i^k}{u_0^k} - \log\frac{u_i^D}{u_0^D}\bigg)dx \\
&\quad + \int_\Omega \sum_{i=1}^n z_i(u_i^k - u_i^{k-1})(\Phi^k - \Phi^D)dx \\
&\ge \int_\Omega \big(g(u^k) - g(u^{k-1})\big)dx + \frac{\lambda^2}{2}\int_\Omega \big(\ell^2|\Delta(\Phi^k - \Phi^D)|^2 + |\nabla(\Phi^k - \Phi^D)|^2\big)dx \\
&\quad - \frac{\lambda^2}{2}\int_\Omega \big(\ell^2|\Delta(\Phi^{k-1} - \Phi^D)|^2 + |\nabla(\Phi^{k-1} - \Phi^D)|^2\big)dx = H(u^k) - H(u^{k-1}).
\end{aligned}$$

Inserting the definition $B_{ij}(w^k,\Phi^k) = D_i u_i^k \delta_{ij}$, we infer from Young's inequality that

$$\begin{aligned}
\nabla(w^k - w^D) : B(w^k,\Phi^k)\nabla w^k &= \sum_{i=1}^n D_i u_i^k \nabla(w_i^k - w_i^D)\cdot\nabla w_i^k \\
&\ge \frac{1}{2}\sum_{i=1}^n D_i u_i^k |\nabla w_i^k|^2 - \frac{1}{2}\sum_{i=1}^n D_i u_i^k |\nabla w_i^D|^2.
\end{aligned}$$

Collecting these estimates and observing that $u_i^k \le 1$ concludes the proof. □

We sum (21) over $k = 1,\ldots,j$,

$$\begin{aligned}
(1 - \tau C_r)H(u^j) &+ \frac{\tau}{2}\sum_{k=1}^j \int_\Omega \sum_{i=1}^n D_i u_i^k |\nabla w_i^k|^2 dx + \varepsilon\tau\sum_{k=1}^j \|w^k - w^D\|^2_{H^m(\Omega)} \\
&\le \tau C_r \sum_{k=1}^{j-1} H(u^k) + H(u^0) + j\tau C_r + \frac{\tau}{2}\sum_{k=1}^j \int_\Omega \sum_{i=1}^n D_i|\nabla w_i^D|^2 dx,
\end{aligned}$$

and, assuming $\tau < 1/C_r$, apply the discrete Gronwall inequality [9]:

$$H(u^j) + \frac{\tau}{2}\Big(\min_{i=1,\ldots,n} D_i\Big)\sum_{k=1}^j \int_\Omega \sum_{i=1}^n u_i^k |\nabla w_i^k|^2 dx + \varepsilon\tau\sum_{k=1}^j \|w^k - w^D\|^2_{H^m(\Omega)} \le C(T),$$

where $C(T) > 0$ does not depend on (ε, τ). We still need to bound the second term on the left-hand side from below.

Lemma 6. *It holds that*

$$\sum_{k=1}^N \tau \int_\Omega \sum_{i=1}^n u_i^k |\nabla w_i^k|^2 dx \geq \frac{1}{2} \sum_{k=1}^N \tau \int_\Omega \Big(\sum_{i=1}^n |\nabla (u_i^k)^{1/2}|^2 + |\nabla \log u_0^k|^2 + |\nabla u_0^k|^2 \Big) dx \\ - C \sum_{k=1}^N \tau \int_\Omega |\nabla \Phi^k|^2 dx,$$

where $C > 0$ depends on (D_i) and (z_i).

Proof. We infer from Young's inequality and the bound $u_i^k \leq 1$ that

$$u_i^k |\nabla w_i^k|^2 = u_i^k \left| \nabla \log \frac{u_i^k}{u_0^k} + z_i \nabla \Phi^k \right|^2 \geq \frac{1}{2} u_i^k \left| \nabla \log \frac{u_i^k}{u_0^k} \right|^2 - |z_i \nabla \Phi^k|^2.$$

The first term on the right-hand side is rewritten as

$$\begin{aligned} \frac{1}{2} u_i^k \left| \nabla \log \frac{u_i^k}{u_0^k} \right|^2 &= \frac{1}{2} \sum_{i=1}^n \frac{|\nabla u_i^k|^2}{u_i^k} + \frac{1}{2} \sum_{i=1}^n u_i^k |\nabla \log u_0^k|^2 - \sum_{i=1}^n \nabla u_i^k \cdot \nabla \log u_0^k \\ &= \frac{1}{2} \sum_{i=1}^n \frac{|\nabla u_i^k|^2}{u_i^k} + \frac{1}{2}(1 - u_0^k) |\nabla \log u_0^k|^2 - \nabla (1 - u_0^k) \cdot \nabla \log u_0^k \\ &= \frac{1}{2} \sum_{i=1}^n \frac{|\nabla u_i^k|^2}{u_i^k} + \frac{1}{2} |\nabla \log u_0^k|^2 + \frac{|\nabla u_0^k|^2}{2 u_0^k} \\ &\geq 2 \sum_{i=1}^n |\nabla (u_i^k)^{1/2}|^2 + \frac{1}{2} |\nabla \log u_0^k|^2 + \frac{1}{2} |\nabla u_0^k|^2, \end{aligned}$$

using $u_0^k \leq 1$ in the last step. □

Since the free energy is bounded from below, we conclude the following uniform bounds.

Lemma 7. *There exists $C > 0$ not depending on (ε, τ) such that for $i = 1, \ldots, n$,*

$$\sum_{k=1}^N \tau \big(\|(u_i^k)^{1/2}\|_{H^1(\Omega)}^2 + \|u_i^k\|_{H^1(\Omega)}^2 + \|u_0^k\|_{H^1(\Omega)}^2 + \|\log u_0^k\|_{H^1(\Omega)}^2 \big) \leq C, \\ \varepsilon \sum_{k=1}^N \tau \|w_i^k\|_{H^m(\Omega)}^2 + \sum_{k=1}^N \tau \|\Phi^k\|_{H^2(\Omega)}^2 \leq C.$$

Proof. The inequality

$$\|\nabla u_i^k\|_{L^2(\Omega)} \le 2\|(u_i^k)^{1/2}\|_{L^\infty(\Omega)}\|\nabla(u_i^k)^{1/2}\|_{L^2(\Omega)} \le 2\|\nabla(u_i^k)^{1/2}\|_{L^2(\Omega)}$$

shows that $\sum_{k=1}^N \tau\|\nabla u_i^k\|^2_{L^2(\Omega)} \le C$. The $H^2(\Omega)$ bound for Φ^k follows immediately from the Poisson–Fermi equation as its right-hand side is bounded in $L^2(\Omega)$. The $H^1(\Omega)$ bound for $\log u_0^k$ is a consequence of the $L^2(\Omega)$ bound for $\nabla \log u_0^k$ and the Poincaré inequality, using the fact that $\log u_0^D \in L^2(\Omega)$ by Hypothesis (H4). □

2.3. *Limit* $(\varepsilon, \tau) \to 0$

We introduce the piecewise constant in time functions $u_i^{(\tau)}(x,t) = u_i^k(x)$, $w_i^{(\tau)}(x,t) = w_i^k(x)$, and $\Phi^{(\tau)}(x,t) = \Phi^k(x)$ for $x \in \Omega$, $t \in ((k-1)\tau, k\tau]$. At time $t = 0$, we set $w^{(\tau)}(\cdot, 0) = h'(u^0)$ and $u_i^{(\tau)}(\cdot, 0) = u_i^0$. Furthermore, we introduce the shift operator $(\sigma_\tau u^{(\tau)})(\cdot, t) = u^{k-1}$ for $t \in ((k-1)\tau, k\tau]$. Then, summing (18)–(19) over $k = 1, \ldots, N$, we see that $(u^{(\tau)}, \Phi^{(\tau)})$ solves

$$\frac{1}{\tau}\int_0^T\int_\Omega (u^{(\tau)} - \sigma_\tau u^{(\tau)}) \cdot \phi\, dxdt + \int_0^T\int_\Omega \nabla\phi : B(w^{(\tau)}, \Phi^{(\tau)})\nabla w^{(\tau)} dxdt \tag{22}$$

$$+ \varepsilon\int_0^T\int_\Omega \Big(\sum_{|\alpha|=m} D^\alpha(w^{(\tau)} - w^D)\cdot D^\alpha\phi + (w^{(\tau)} - w^D)\cdot\phi\Big)dxdt$$

$$= \int_0^T\int_\Omega r(u^{(\tau)})\cdot\phi\, dxdt,$$

$$\lambda^2\int_0^T\int_\Omega \big(\ell^2\Delta\Phi^{(\tau)}\Delta\theta + \nabla\Phi^{(\tau)}\cdot\nabla\theta\big)dxdt = \int_0^T\int_\Omega \Big(\sum_{i=1}^n z_i u_i^{(\tau)} + f\Big)\theta\, dxdt \tag{23}$$

for piecewise constant in time functions $\phi : (0,T) \to X$ and $\theta : (0,T) \to H^2_{D,N}(\Omega)$, recalling that $X = H^m(\Omega;\mathbb{R}^n) \cap H^1_D(\Omega;\mathbb{R}^n)$. Lemma 7 and the $L^\infty(\Omega)$ estimate of u_i^k imply the uniform bounds

$$\|(u_i^{(\tau)})^{1/2}\|_{L^2(0,T;H^1(\Omega))} + \|u_i^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|u_i^{(\tau)}\|_{L^\infty(\Omega_T)} \le C, \tag{24}$$

$$\|u_0^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|u_0^{(\tau)}\|_{L^\infty(\Omega_T)} + \|\log u_0^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} \le C, \tag{25}$$

$$\sqrt{\varepsilon}\|w_i^{(\tau)}\|_{L^2(0,T;H^m(\Omega))} + \|\Phi^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} \le C, \tag{26}$$

where $i = 1, \ldots, n$. We also need a uniform bound for the discrete time derivative.

Lemma 8. *There exists a constant $C > 0$ independent of (ε, τ) such that for all $i = 1, \ldots, n$,*

$$\tau^{-1}\|u_i^{(\tau)} - \sigma_\tau u_i^{(\tau)}\|_{L^2(0,T;X')} + \tau^{-1}\|u_0^{(\tau)} - \sigma_\tau u_0^{(\tau)}\|_{L^2(0,T;X')} \le C.$$

Proof. Let $\phi : (0, T) \to X$ be piecewise constant. Since

$$\int_0^T \int_\Omega \nabla\phi : B(u^{(\tau)}, \Phi^{(\tau)})\nabla w^{(\tau)} dxdt$$

$$= \sum_{i=1}^n D_i \int_0^T \int_\Omega \big(\nabla u_i^{(\tau)} - u_i^{(\tau)}\nabla \log u_0^{(\tau)} + z_i u_i^{(\tau)}\nabla\Phi^{(\tau)}\big) \cdot \nabla\phi_i dxdt,$$

we find that

$$\begin{aligned}\frac{1}{\tau}\bigg|\int_0^T \int_\Omega (u_i^{(\tau)} - \sigma_\tau u_i^{(\tau)})\phi_i dxdt\bigg| &\le \varepsilon\|w_i^{(\tau)} - w_i^D\|_{L^2(0,T;H^m(\Omega))}\|\phi_i\|_{L^2(0,T;H^m(\Omega))} \\ &\quad + C\big(\|\nabla u_i^{(\tau)}\|_{L^2(\Omega_T)} + \|\nabla \log u_0^{(\tau)}\|_{L^2(\Omega_T)} + \|\nabla\Phi^{(\tau)}\|_{L^2(\Omega_T)}\big)\|\nabla\phi_i\|_{L^2(\Omega_T)} \\ &\quad + \|r_i(u^{(\tau)})\|_{L^2(\Omega_T)}\|\phi_i\|_{L^2(\Omega_T)} \\ &\le C\|\phi_i\|_{L^2(0,T;H^m(\Omega))}.\end{aligned}$$

By a density argument, this inequality holds for all $\phi_i \in L^2(0, T; X)$, showing the desired bound for the discrete time derivative of $u_i^{(\tau)}$. Summing the bounds over $i = 1, \dots, n$ yields the bound for $u_0^{(\tau)}$. □

Estimates (24)–(25) and Lemma 8 allow us to apply the Aubin–Lions lemma in the version of [10] to conclude the existence of a subsequence, which is not relabeled, such that for $i = 1, \dots, n$, as $(\varepsilon, \tau) \to 0$,

$$u_i^{(\tau)} \to u_i, \quad u_0^{(\tau)} \to u_0 \quad \text{strongly in } L^2(\Omega_T).$$

In view of the uniform $L^\infty(\Omega_T)$ bound for $u_i^{(\tau)}$ and $u_0^{(\tau)}$, these convergences hold in $L^p(\Omega_T)$ for all $p < \infty$. Moreover, by (26) and Lemma 8, up to a subsequence,

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

We claim that $\nabla \log u_0^{(\tau)} \rightharpoonup \nabla \log u_0$ weakly in $L^2(\Omega_T)$. It follows from (25) that (for a subsequence) $\nabla \log u_0^{(\tau)} \rightharpoonup v$ weakly in $L^2(\Omega_T)$. We need to identify $v = \nabla \log u_0$. We know that (again for a subsequence) $u_0^{(\tau)} \to u_0$ a.e. in Ω_T. Therefore $\log u_0^{(\tau)} \to \log u_0$ a.e. in Ω_T, since u_0 can vanish at most on a set of measure zero. The $L^2(\Omega_T)$ bound for $\log u_0^{(\tau)}$ shows that $\log u_0^{(\tau)} \to \log u_0$ strongly in $L^2(\Omega_T)$. Hence, we conclude that $v = \nabla \log u_0$, proving the claim.

These convergences are sufficient to pass to the limit $(\varepsilon, \tau) \to 0$ in (22)–(23) to find that (u, Φ) solves (13)–(14) for smooth test functions. By a density argument, we may choose test functions from $L^2(0,T;H^1_D(\Omega))$ and $L^2(0,T;H^2_{D,N}(\Omega))$, respectively. The validity of the initial and Dirichlet boundary conditions is shown as in [15]. Estimates similar as in the proof of Lemma 8 (with $\varepsilon=0$) show that $\partial_t u_i\in L^2(0,T;H^1_D(\Omega)')$ for $i=1,\ldots,n$. Then we conclude from $u_i\in L^2(0,T;H^1(\Omega))$ that $u_i\in C^0([0,T];L^2(\Omega))$. Thus, the initial datum is satisfied in the sense of $L^2(\Omega)$.

It remains to verify the free energy inequality (15) under the assumptions $r_i(u)=0$ and $\log(u_i^D/u_0^D)+z_i\Phi^D=c_i\in\mathbb{R}$ for $i=1,\ldots,n$. By definition of w_i^D, this implies that $\nabla w_i^D=0$. Then (21) becomes

$$H(u^k)-H(u^{k-1})+\tau\int_\Omega\sum_{i=1}^n D_iu_i^k\left|\nabla\left(\log\frac{u_i^k}{u_0^k}+z_i\Phi^k\right)\right|^2dx+\varepsilon\tau\|w^k-w^D\|^2_{H^m(\Omega)}\le 0.$$

A summation over $k=j,\ldots,J$ gives

$$H(u^{(\tau)}(t))-H(u^{(\tau)}(s))+\int_s^t\int_\Omega\sum_{i=1}^n D_iu_i^{(\tau)}\left|\nabla\left(\log\frac{u_i^{(\tau)}}{u_0^{(\tau)}}+z_i\Phi^{(\tau)}\right)\right|^2dxd\sigma \qquad (27)$$
$$+\varepsilon\int_s^t\|w^{(\tau)}-w^D\|^2_{H^m(\Omega)}d\sigma\le 0,$$

where $s\in((j-1)\tau,j\tau]$ and $t\in((J-1)\tau,J\tau]$. We wish to pass to the limit $(\varepsilon,\tau)\to 0$ in this inequality.

The a.e. convergence of $u_i^{(\tau)}$ implies that $H(u^{(\tau)}(t))\to H(u(t))$ for a.e. $t\in(0,T)$ and, since $u_i\in C^0([0,T];L^2(\Omega))$, this convergence holds in fact for all $t\in[0,T]$. Moreover, $\varepsilon(w^{(\tau)}-w^D)\to 0$ strongly $L^2(0,T;H^m(\Omega))$. It follows from the strong convergence of $u_i^{(\tau)}$ in $L^2(\Omega_T)$ that $(u_i^{(\tau)})^{1/2}\to\sqrt{u_i}$ strongly in $L^4(\Omega_T)$. Hence, together with the weak convergence of $\nabla\Phi^{(\tau)}$ in $L^2(\Omega_T)$, we have

$$(u_i^{(\tau)})^{1/2}\nabla\Phi^{(\tau)}\rightharpoonup\sqrt{u_i}\nabla\Phi\quad\text{weakly in }L^{4/3}(\Omega_T).$$

Furthermore, since $\nabla\log u_0^{(\tau)}\rightharpoonup\nabla\log u_0$ weakly in $L^2(\Omega_T)$,

$$(u_i^{(\tau)})^{1/2}\nabla\log\frac{u_i^{(\tau)}}{u_0^{(\tau)}}=2\nabla(u_i^{(\tau)})^{1/2}-(u_i^{(\tau)})^{1/2}\nabla\log u_0^{(\tau)} \qquad (28)$$
$$\rightharpoonup 2\nabla\sqrt{u_i}-\sqrt{u_i}\nabla\log u_0=:\sqrt{u_i}\nabla\log\frac{u_i}{u_0}\quad\text{weakly in }L^{4/3}(\Omega_T).$$

On the other hand, the sequences $\nabla(u_i^{(\tau)})^{1/2}$ and $(u_i^{(\tau)})^{1/2}\nabla\log u_0^{(\tau)}$ are uniformly bounded in $L^2(\Omega_T)$. Therefore, convergence (28) also holds in $L^2(\Omega_T)$. Consequently,

$$\int_\Omega u_i\left|\nabla\left(\log\frac{u_i}{u_0}+z_i\Phi\right)\right|^2dx=\int_\Omega\left|2\nabla\sqrt{u_i}-\sqrt{u_i}\nabla\log u_0+\sqrt{u_i}z_i\nabla\Phi\right|^2dx$$

$$\leq \liminf_{(\varepsilon,\tau)\to 0} \int_\Omega u_i^{(\tau)} \left| \nabla \left(\log \frac{u_i^{(\tau)}}{u_0^{(\tau)}} + z_i \Phi^{(\tau)} \right) \right|^2 dx.$$

Then (15) follows after passing to the limit inferior $(\varepsilon, \tau) \to 0$ in (27), completing the proof of Theorem 1.

Remark 9. Let the reaction rates $r_i : \overline{\mathcal{D}} \to \mathbb{R}$ be Lipschitz continuous and quasi-positive, i.e. $r_i(u) \geq 0$ for all $u \in \mathcal{D}$ with $u_i = 0$. We assume that the total reaction rate is nonnegative, i.e. $\sum_{i=1}^n r_i(u) \leq 0$ for all $u \in \mathcal{D}$, and that $r_i(u) \log u_i = 0$ if $u_i = 0$. This assumption is only needed to derive the free energy inequality. We claim that it becomes

$$H(u(t)) + \int_s^t \int_\Omega \sum_{i=1}^n D_i u_i |\nabla w_i|^2 dx d\sigma \leq H(u(s)) + \int_s^t \int_\Omega \sum_{i=1}^n r_i(u)(w_i - w_i^D) dx d\sigma. \quad (29)$$

This inequality follows from (27) after including the reaction rates and taking the limit (ε, τ) in

$$\int_s^t \int_\Omega \sum_{i=1}^n r_i(u^{(\tau)})(w_i^{(\tau)} - w_i^D) dx d\sigma$$
$$= \int_s^t \int_\Omega \sum_{i=1}^n r_i(u^{(\tau)}) \big(\log u_i^{(\tau)} - \log u_0^{(\tau)} + z_i \Phi^{(\tau)} - w_i^D \big) dx d\sigma.$$

Indeed, the strong limit $u_i^{(\tau)} \to u_i$ in $L^2(\Omega_T)$ shows that $r_i(u^{(\tau)}) w_i^D \to r_i(u) w_i^D$ strongly in $L^1(\Omega_T)$ as $(\varepsilon, \tau) \to 0$. Moreover, since $\log u_0^{(\tau)} \to \log u_0$ strongly in $L^2(\Omega)$, we have $r_i(u^{(\tau)}) \log u_0^{(\tau)} \to r_i(u) \log u_0$ strongly in $L^1(\Omega_T)$. It remains to show that $r_i(u^{(\tau)}) \log u_i^{(\tau)} \to r_i(u) \log u_i$ strongly in $L^1(\Omega_T)$. We have $r_i(u^{(\tau)}) \log u_i^{(\tau)} \to r_i(u) \log u_i$ a.e. in Ω_T if $u_i > 0$. If $u_i = 0$, by assumption, we have $r_i(u) \log u_i = 0$ and therefore $r_i(u^{(\tau)}) \log u_i^{(\tau)} \to r_i(u) \log u_i$ a.e. in Ω_T as well. Moreover, $r_i(u) \log u_i$ is bounded. Hence, by dominated convergence, $r_i(u^{(\tau)}) \log u_i^{(\tau)} \to r_i(u) \log u_i$ strongly in $L^1(\Omega_T)$, and the claim follows. □

3. Proof of Theorem 2

Let (u, Φ) be a weak solution and $(\bar{u}, \bar{\Phi})$ be a strong solution to (1)–(5). In this section, we interpret $H(u)$ and $H(\bar{u})$ as functionals depending on $u = (u_0, \ldots, u_n)$ and $\bar{u} = (\bar{u}_0, \ldots, \bar{u}_n)$. This notation is only needed to determine the variational derivative of H and will not lead to any confusion in the following computations. We split the lengthy proof in several steps.

Step 1: Calculation of the time derivative of $H(u, \Phi | \bar{u}, \bar{\Phi})$. In the following, we write

$$H(u, \Phi | \bar{u}, \bar{\Phi}) = H_1(u|\bar{u}) + H_2(\Phi|\bar{\Phi}), \quad \text{where}$$
$$H_1(u|\bar{u}) = H_1(u) - H_1(\bar{u}) - H_1'(\bar{u})(u - \bar{u}),$$
$$H_2(\Phi|\bar{\Phi}) = H_2(\Phi) - H_2(\bar{\Phi}) - H_2'(\bar{\Phi})(\Phi - \bar{\Phi}),$$

where $H_1(u)=\int_\Omega h_1(u)dx$ with $h_1(u)=\sum_{i=0}^n\int_{u_i^D}^{u_i}\log(s/u_i^D)ds$, $H_2(\Phi)=\frac{1}{2}\lambda^2\int_\Omega(\ell^2|\Delta(\Phi-\Phi^D)|^2+|\nabla(\Phi-\Phi^D)|^2)dx$, and $H_1'(\bar{u})(u-\bar{u})$ is the variational derivative of H_1 at $\bar{u}$ in the direction of $u-\bar{u}$ (similarly for $H_2'(\bar{\Phi})(\Phi-\bar{\Phi})$). We compute the time derivative of $H_1(u|\bar{u})$, split the sum over $i=0,\ldots,n$ into $i=0$ and the sum over $i=1,\ldots,n$, and insert $\partial_t u_0=-\sum_{i=1}^n\partial_t u_i$, $\partial_t\bar{u}_0=-\sum_{i=1}^n\partial_t\bar{u}_i$:

$$\begin{aligned}\frac{dH_1}{dt}(u|\bar{u})&=\frac{dH_1}{dt}(u)-\frac{dH_1}{dt}(\bar{u})-\frac{d}{dt}\int_\Omega\sum_{i=0}^n\frac{\partial h_1}{\partial u_i}(\bar{u})(u_i-\bar{u}_i)dx\\&=\frac{dH_1}{dt}(u)-\sum_{i=0}^n\bigg(\Big\langle\partial_t u_i,\frac{\partial h_1}{\partial u_i}(\bar{u})\Big\rangle+\Big\langle\partial_t\bar{u}_i,\frac{u_i}{\bar{u}_i}-1\Big\rangle\bigg)\\&=\frac{dH_1}{dt}(u)-\sum_{i=1}^n\bigg(\Big\langle\partial_t u_i,\frac{\partial h_1}{\partial u_i}(\bar{u})-\frac{\partial h_1}{\partial u_0}(\bar{u})\Big\rangle+\Big\langle\partial_t\bar{u}_i,\frac{u_i}{\bar{u}_i}-\frac{u_0}{\bar{u}_0}\Big\rangle\bigg).\end{aligned}$$

Next, we insert equation (1) for u_i and $\bar{u}_i$ and use $(\partial h_1/\partial u_i)(\bar{u})=\log(\bar{u}_i/u_i^D)$:

$$\begin{aligned}\frac{dH_1}{dt}(u|\bar{u})=\frac{dH_1}{dt}(u)&+\int_\Omega\sum_{i=1}^n D_iu_i\nabla w_i\cdot\nabla\bigg(\log\frac{\bar{u}_i}{\bar{u}_0}-\log\frac{u_i^D}{u_0^D}dx\bigg)dx\\&+\int_\Omega\sum_{i=1}^n D_i\bar{u}_i\nabla\bar{w}_i\cdot\bigg(\frac{u_i}{\bar{u}_i}\nabla\log\frac{u_i}{\bar{u}_i}-\frac{u_0}{\bar{u}_0}\nabla\log\frac{u_0}{\bar{u}_0}\bigg)dx.\end{aligned}$$

A similar computation for $H_2(\Phi|\bar{\Phi})$ leads to

$$\begin{aligned}\frac{dH_2}{dt}(\Phi|\bar{\Phi})&=\lambda^2\big\langle(\ell^2\Delta-1)\Delta\partial_t(\Phi-\bar{\Phi}),\Phi-\bar{\Phi}\big\rangle=\sum_{i=1}^n\langle z_i\partial_t(u_i-\bar{u}_i),\Phi-\bar{\Phi}\rangle\\&=-\int_\Omega\sum_{i=1}^n D_iz_i(u_i\nabla w_i-\bar{u}_i\nabla\bar{w}_i)\cdot\nabla(\Phi-\bar{\Phi})dx\\&=\frac{dH_2}{dt}(\Phi)+\int_\Omega\sum_{i=1}^n D_iz_i\big(u_i\nabla w_i\cdot\nabla\bar{\Phi}-u_i\nabla w_i\cdot\nabla\Phi^D+\bar{u}_i\nabla\bar{w}_i\cdot\nabla(\Phi-\bar{\Phi})\big)dx,\end{aligned}$$

where we abbreviated $\bar{w}_i=\log(\bar{u}_i/\bar{u}_0)+z_i\bar{\Phi}$. As u_i is only nonnegative, the expression $\nabla\log u_i$ may be not integrable. Therefore, we define $\nabla\log(u_i/u_0):=(2\nabla\sqrt{u_i}-\sqrt{u}_i\nabla\log u_0)/\sqrt{u_i}$ if $u_i>0$ and $\nabla\log(u_i/u_0):=0$ else. This expression may be still not integrable, but $\sqrt{u_i}\nabla\log(u_i/u_0)$ lies in $L^2(\Omega_T)$, since $\nabla\sqrt{u_i}$, $\nabla\log u_0\in L^2(\Omega_T)$. Thus, the expression $\sqrt{u_i}\nabla w_i=u_i\nabla\log(u_i/u_0)+u_iz_i\nabla\Phi\in L^2(\Omega_T)$ is well defined. In a similar way, we define $\nabla\log(u_i/\bar{u}_i)$, which is possible since $\bar{u}_i$ is strictly positive, and we have $\sqrt{u_i}\nabla\log(u_i/\bar{u}_i)\in L^2(\Omega_T)$.

We insert the free energy inequality (15), namely

$$\frac{dH_1}{dt}(u) + \frac{dH_2}{dt}(\Phi) \le -\int_\Omega \sum_{i=1}^n D_i u_i |\nabla w_i|^2 dx,$$

and rearrange the terms,

$$\begin{aligned}\frac{dH}{dt}(u,\Phi|\bar u,\bar\Phi) &= \frac{dH_1}{dt}(u|\bar u) + \frac{dH_2}{dt}(\Phi|\bar\Phi) \\ &\le -\int_\Omega \sum_{i=1}^n D_i u_i \nabla w_i \cdot \Big(\nabla \log\frac{u_i}{\bar u_i} - \nabla\log\frac{u_0}{\bar u_0} + z_i\nabla(\Phi-\bar\Phi)\Big)dx \\ &\quad + \int_\Omega \sum_{i=1}^n D_i \bar u_i \nabla \bar w_i \cdot \Big(\frac{u_i}{\bar u_i}\nabla\log\frac{u_i}{\bar u_i} - \frac{u_0}{\bar u_0}\nabla\log\frac{u_0}{\bar u_0} + z_i\nabla(\Phi-\bar\Phi)\Big)dx.\end{aligned} \tag{30}$$

At this point, we observe that the terms involving ∇w_i^D cancel even if ∇w_i^D does not vanish, since they also appear in the free energy inequality (15).

The terms involving the solvent concentrations u_0 and $\bar u_0$ can be integrated into the sum over i if we interpret system (1) as equations for $u_0, u_1, \ldots, u_n$. For this, we observe that u_0 solves

$$\partial_t u_0 = -\operatorname{div}\sum_{i=1}^n D_i u_i \nabla w_i = -\operatorname{div}\Big\{\sum_{i=1}^n D_i u_i \nabla\log\frac{u_i}{u_0} + \Big(\sum_{i=1}^n D_i z_i u_i\Big)\nabla\Phi\Big\}.$$

Then (1) reads as

$$\partial_t u_i = \operatorname{div}\sum_{j=0}^n (A_{ij}\nabla\log u_j + Q_{ij}\nabla\Phi), \quad i=0,\ldots,n, \tag{31}$$

where A_{ij} and Q_{ij} are defined in (17). Recall that $z_0 := 0$. We define in a similar way $\bar A$ and $\bar Q$. With this notation, (30) becomes

$$\begin{aligned}\frac{dH}{dt}(u,\Phi|\bar u,\bar\Phi) &\le -\int_\Omega \sum_{i,j=0}^n (A_{ij}\nabla\log u_j + Q_{ij}\nabla\Phi)\cdot\Big(\nabla\log\frac{u_i}{\bar u_i} + z_i\nabla(\Phi-\bar\Phi)\Big)dx \\ &\quad + \int_\Omega \sum_{i,j=0}^n (\bar A_{ij}\nabla\log\bar u_j + \bar Q_{ij}\nabla\bar\Phi)\cdot\Big(\frac{u_i}{\bar u_i}\nabla\log\frac{u_i}{\bar u_i} + z_i\nabla(\Phi-\bar\Phi)\Big)dx.\end{aligned}$$

We add and subtract the integral

$$\int_\Omega \sum_{i,j=0}^n (A_{ij}\nabla\log\bar u_j + Q_{ij}\nabla\bar\Phi)\cdot\Big(\nabla\log\frac{u_i}{\bar u_i} + z_i\nabla(\Phi-\bar\Phi)\Big)dx$$

and integrate over $(0,t)$:

$$H((u,\Phi)(t)|(\bar u,\bar\Phi)(t)) - H((u,\Phi)(0)|(\bar u,\bar\Phi)(0)) \le I_1 + I_2 + I_3, \quad \text{where} \tag{32}$$

$$I_1 = -\int_0^t\int_\Omega \sum_{i,j=0}^n \Big(A_{ij}\nabla\log\frac{u_j}{\bar u_j} + Q_{ij}\nabla(\Phi-\bar\Phi)\Big)\cdot\Big(\nabla\log\frac{u_i}{\bar u_i} + z_i\nabla(\Phi-\bar\Phi)\Big)dxds,$$

$$I_2 = -\int_0^t\int_\Omega \sum_{i,j=0}^n u_i\bigg\{\Big(\frac{A_{ij}}{u_i} - \frac{\bar A_{ij}}{\bar u_i}\Big)\nabla\log\bar u_j + \Big(\frac{Q_{ij}}{u_i} - \frac{\bar Q_{ij}}{\bar u_i}\Big)\nabla\bar\Phi\bigg\}\cdot\nabla\log\frac{u_i}{\bar u_i}dxds,$$

$$I_3 = -\int_0^t\int_\Omega \sum_{i,j=0}^n \big((A_{ij}-\bar A_{ij})\nabla\log\bar u_j + (Q_{ij}-\bar Q_{ij})\nabla\bar\Phi\big)\cdot z_i\nabla(\Phi-\bar\Phi)dxds.$$

Observe that $u(0)=\bar u(0)$, implying that $H((u,\Phi)(0)|(\bar u,\bar\Phi)(0))=0$.

Step 2: Estimation of I_3. By Young's inequality, we have

$$I_3 \le C\int_0^t \sum_{i=1}^n \big(\|u_i-\bar u_i\|_{L^2(\Omega)}^2 + \|\nabla(\Phi-\bar\Phi)\|_{L^2(\Omega)}^2\big)ds, \tag{33}$$

where $C>0$ depends on the $L^\infty(\Omega_T)$ norms of $\nabla\log\bar u_j$ and $\nabla\bar\Phi$.

The treatment of I_1 and I_2 is more delicate.

Step 3: Estimation of I_1. We write $I_1 = I_{11}+I_{12}+I_{13}$, where

$$I_{11} = -\int_0^t\int_\Omega \sum_{i,j=0}^n A_{ij}\nabla\log\frac{u_j}{\bar u_j}\cdot\nabla\log\frac{u_i}{\bar u_i}dxds,$$

$$I_{12} = -\int_0^t\int_\Omega \sum_{i,j=0}^n z_iQ_{ij}|\nabla(\Phi-\bar\Phi)|^2dxds,$$

$$I_{13} = -\int_0^t\int_\Omega \sum_{i,j=0}^n z_iA_{ij}\nabla\log\frac{u_j}{\bar u_j}\cdot\nabla(\Phi-\bar\Phi)dxds - \int_0^t\int_\Omega \sum_{i,j=0}^n Q_{ij}\nabla\log\frac{u_i}{\bar u_i}\cdot\nabla(\Phi-\bar\Phi)dxds.$$

It follows from $0\le u_i\le 1$ that $|Q_{ij}|\le C$ and consequently

$$I_{12} \le C\int_0^t \|\nabla(\Phi-\bar\Phi)\|_{L^2(\Omega)}^2ds.$$

The matrix A is not positive definite since $u_i = 0$ is possible. However, a modified matrix is positive definite on the subspace L, as shown in the following lemma.

Lemma 10. *The matrix G, defined by*

$$G_{ij} = \begin{cases} A_{ij}/\sqrt{u_i u_j} & \text{if } u_i u_j > 0, \\ 0 & \text{else}, \end{cases} \qquad i, j = 0, \dots, n, \tag{34}$$

is positive definite on the subspace $L = \{z \in \mathbb{R}^{n+1} : \sum_{i=0}^n \sqrt{u_i} z_i = 0\}$, namely

$$z^T G z \geq D_* \bigg(\frac{z_0^2}{u_0} + \sum_{i=1}^n z_i^2 \bigg) \quad \text{for every } z \in L, \tag{35}$$

where $D_* = \min_{i=1,\dots,n} D_i > 0$.

Proof. We start by considering the matrix

$$G_* = D_* \begin{pmatrix} u_0^{-1} \sum_{i=1}^n u_i & -\sqrt{u_1/u_0} & \cdots & -\sqrt{u_n/u_0} \\ -\sqrt{u_1/u_0} & 1 & & 0 \\ \vdots & 0 & \ddots & 0 \\ -\sqrt{u_n/u_0} & 0 & & 1 \end{pmatrix},$$

where $D_* = \min_{i=1,\dots,n} D_i > 0$. For every $\xi \in L$, we have $\sum_{i=1}^n \sqrt{u_i}\xi_i = -\sqrt{u_0}\xi_0$. Therefore, together with the size-exclusion constraint $\sum_{i=1}^n u_i = 1 - u_0$, we obtain

$$\begin{aligned} \xi^T G_* \xi &= D_* \frac{\xi_0^2}{u_0} \sum_{i=1}^n u_i - 2D_* \frac{\xi_0}{\sqrt{u_0}} \sum_{i=1}^n \sqrt{u_i}\xi_i + D_* \sum_{i=1}^n \xi_i^2 \\ &= D_* \frac{\xi_0^2}{u_0}(1 - u_0) + 2D_* \frac{\xi_0}{\sqrt{u_0}} \sqrt{u_0}\xi_0 + D_* \sum_{i=1}^n \xi_i^2 \\ &= D_* \bigg\{ \bigg(\frac{1}{u_0} + 1 \bigg) \xi_0^2 + \sum_{i=1}^n \xi_i^2 \bigg\} \geq D_* \bigg(\frac{\xi_0^2}{u_0} + \sum_{i=1}^n \xi_i^2 \bigg). \end{aligned}$$

This implies that

$$\begin{aligned} \xi^T (G - G_*) \xi &= \frac{\xi_0^2}{u_0} \sum_{i=1}^n (D_i - D_*) u_i - 2 \frac{\xi_0}{\sqrt{u_0}} \sum_{i=1}^n (D_i - D_*) \sqrt{u_i}\xi_i + \sum_{i=1}^n (D_i - D_*) \xi_i^2 \\ &= \sum_{i=1}^n (D_i - D_*) \bigg(\frac{\xi_0}{\sqrt{u_0}} \sqrt{u_i} - \xi_i \bigg)^2 \geq 0, \end{aligned}$$

and we infer that $\xi^T G z \geq \xi^T G_* \xi$, which ends the proof. □

Lemma 10 is crucial in the weak–strong uniqueness proof. The corresponding positive bound helps us to conclude a negative upper estimate for I_{11}, which is used to absorb the contributions from I_{13} and I_2. We introduce the projections

$$(P_L Y)_i = Y_i - \sqrt{u_i}\sum_{j=0}^n \sqrt{u_j}Y_j, \quad (P_{L^\perp} Y)_i = \sqrt{u_i}\sum_{j=0}^n \sqrt{u_j}Y_j,$$

for all $i = 0, \dots, n$ and $Y \in \mathbb{R}^{n+1}$.

Lemma 11. *Let $Y_i = \sqrt{u_i}\nabla\log(u_i/\bar{u}_i) \in L^2(\Omega_T)$ for $i = 0, \dots, n$. Then*

$$I_{11} \le -D_* \int_0^t \int_\Omega \left(\frac{|(P_L Y)_0|^2}{u_0} + \sum_{i=1}^n |(P_L Y)_i|^2 \right) dx ds,$$

where $D_* = \min_{i=1,\dots,n} D_i > 0$.

Proof. Recall that by definition, $\nabla\log(u_i/\bar{u}_i) = (2\nabla\sqrt{u_i} - \sqrt{u_i}\nabla\log\bar{u}_i)/\sqrt{u_i} = Y_i/\sqrt{u_i}$ if $u_i > 0$. In this case,

$$A_{ij}\nabla\log\frac{u_i}{\bar{u}_i}\cdot\nabla\log\frac{u_j}{\bar{u}_j} = G_{ij}Y_iY_j,$$

where the matrix G is defined in (34). If $u_i = 0$ or $u_j = 0$, either $Y_i = 0$ or $Y_j = 0$ and hence, the previous expression vanishes. Therefore, we rewrite I_{11} as

$$I_{11} = -\int_0^t \int_\Omega \sum_{i,j=0}^n G_{ij}Y_iY_j dx ds.$$

A straightforward computation shows that $\operatorname{ran} G = L$, implying that $\ker G = L^\perp$. Hence, for every $Y \in \mathbb{R}^{n+1}$,

$$Y^T G Y = (P_L Y)^T G (P_L Y),$$

where $(P_L Y)_i = Y_i - \sqrt{u_i}\sum_{j=0}^n \sqrt{u_j}Y_j$. Define $\xi_i := (P_L Y)_i = Y_i - \sqrt{u_i}\sum_{j=0}^n \sqrt{u_j}Y_j$ for $i = 0, \dots, n$. Then $\xi \in L$, since

$$\sum_{i=0}^n \sqrt{u_i}(P_L Y)_i = \sum_{i=0}^n \sqrt{u_i}Y_i - \left(\sum_{i=0}^n u_i\right)\sum_{j=0}^n \sqrt{u_j}Y_j = 0.$$

The inequality

$$(P_L Y)^T G (P_L Y) \ge \frac{|(P_L Y)_0|^2}{u_0} + \sum_{i=1}^n |(P_L Y)_i|^2, \tag{36}$$

follows directly from (35), applied to $\xi = P_L Y$. Recall that $u_0 > 0$ a.e. in Ω_T.

We choose now $Y_i = \sqrt{u_i}\nabla\log(u_i/\bar{u}_i)$. The expression

$$\frac{|(P_L Y)_0|^2}{u_0} = \left|\nabla\log\frac{u_0}{\bar{u}_0} - \sum_{j=0}^n \sqrt{u_j}Y_j\right|^2$$

is integrable in Ω_T since $\nabla\log u_0 \in L^2(\Omega_T)$, and $\sqrt{u_j}Y_j \in L^2(\Omega_T)$. Therefore, we can integrate inequality (36) to obtain

$$\begin{aligned} I_{11} &= -\int_0^t\int_\Omega Y^T GY dxds = -\int_0^t\int_\Omega (P_L Y)^T G(P_L Y)dxds \\ &\le -D_*\int_0^t\int_\Omega\left(\frac{|(P_L Y)_0|^2}{u_0} + \sum_{i=1}^n |(P_L Y)_i|^2\right)dxds, \end{aligned}$$

which finishes the proof. $\square$

Lemma 12. *Let $Y_i = \sqrt{u_i}\nabla\log(u_i/\bar{u}_i)$ for $i = 0, \ldots, n$. For any $\varepsilon > 0$, there exists $C(\varepsilon) > 0$ such that*

$$I_{13} \le \varepsilon\int_0^t\int_\Omega\left(\frac{|(P_L Y)_0|^2}{u_0} + \sum_{i=1}^n |(P_L Y)_i|^2\right)dxds + C(\varepsilon)\int_0^t \|\nabla(\Phi - \bar{\Phi})\|^2_{L^2(\Omega)}ds.$$

Proof. We take into account the structures of the matrices A and Q:

$$\begin{aligned} I_{13} = &-\int_0^t\int_\Omega\sum_{i=1}^n z_i\left(A_{i0}\nabla\log\frac{u_0}{\bar{u}_0} + A_{ii}\nabla\log\frac{u_i}{\bar{u}_i}\right)\cdot\nabla(\Phi - \bar{\Phi})dxds \\ &-\int_0^t\int_\Omega\left(Q_{00}\nabla\log\frac{u_0}{\bar{u}_0} + \sum_{i=1}^n Q_{ii}\nabla\log\frac{u_i}{\bar{u}_i}\right)\cdot\nabla(\Phi - \bar{\Phi})dxds. \end{aligned}$$

Since $Q_{00} = -\sum_{i=1}^n D_i z_i u_i$ and $Q_{ii} = D_i z_i u_i$, we have

$$Q_{00}\nabla\log\frac{u_0}{\bar{u}_0} + \sum_{i=1}^n Q_{ii}\nabla\log\frac{u_i}{\bar{u}_i} = -\sum_{i=1}^n D_i z_i u_i\nabla\left(\log\frac{u_0}{\bar{u}_0} - \log\frac{u_i}{\bar{u}_i}\right)dx.$$

Furthermore, because of $A_{i0} = -D_i u_i$ and $A_{ii} = D_i u_i$,

$$\sum_{i=1}^n z_i\left(A_{i0}\nabla\log\frac{u_0}{\bar{u}_0} + A_{ii}\nabla\log\frac{u_i}{\bar{u}_i}\right) = -\sum_{i=1}^n D_i z_i u_i\nabla\left(\log\frac{u_0}{\bar{u}_0} - \log\frac{u_i}{\bar{u}_i}\right)dx.$$

This gives

$$I_{13} = 2\int_0^t \int_\Omega \sum_{i=1}^n D_i z_i u_i \nabla\bigg(\log\frac{u_0}{\bar u_0} - \log\frac{u_i}{\bar u_i}\bigg)\cdot\nabla(\Phi-\bar\Phi)dxds$$
$$= 2\int_0^t \int_\Omega \sum_{i=1}^n D_i z_i \bigg(u_i\frac{Y_0}{\sqrt{u_0}} - \sqrt{u_i}Y_i\bigg)\cdot\nabla(\Phi-\bar\Phi)dxds.$$

Next, we calculate for $i=0,\ldots,n$,

$$(P_{L^\perp}Y)_i = \sqrt{u_i}\sum_{j=0}^n u_j\nabla\log\frac{u_j}{\bar u_j} = \sqrt{u_i}\sum_{j=0}^n(\nabla u_j - u_j\nabla\log\bar u_j) \tag{37}$$
$$= -\sqrt{u_i}\sum_{j=0}^n u_j\nabla\log\bar u_j = \sqrt{u_i}\sum_{j=0}^n(\bar u_j - u_j)\nabla\log\bar u_j,$$

where we used the constraint $\sum_{i=0}^n u_i = 1$ to cancel the term $\sum_{j=0}^n \nabla u_j$ in the third equality and we added $0=\sum_{j=0}^n\nabla\bar u_j = \sum_{j=0}^n \bar u_j\nabla\log\bar u_j$ in the last equality. Hence,

$$u_i\frac{(P_{L^\perp}Y)_0}{\sqrt{u_0}} - \sqrt{u_i}(P_{L^\perp}Y)_i = \frac{u_i}{\sqrt{u_0}}\bigg(\sqrt{u_0}\sum_{j=0}^n(\bar u_j-u_j)\nabla\log\bar u_j\bigg)$$
$$-\sqrt{u_i}\bigg(\sqrt{u_i}\sum_{j=0}^n(\bar u_j-u_j)\nabla\log\bar u_j\bigg) = 0.$$

We split $Y_i = (P_LY)_i + (P_{L^\perp}Y)_i$ in I_{13}, which leads to

$$I_{13} = 2\int_0^t \int_\Omega \sum_{i=1}^n D_i z_i \bigg(u_i\frac{(P_LY)_0}{\sqrt{u_0}} - \sqrt{u_i}(P_LY)_i\bigg)\cdot\nabla(\Phi-\bar\Phi)dxds.$$

An application of Young's lemma finishes the proof. □

The previous lemmas show that

$$I_1 \le (\varepsilon - D_*)\int_0^t\int_\Omega\bigg(\frac{|(P_LY)_0|^2}{u_0} + \sum_{i=1}^n|(P_LY)_i|^2\bigg)dxds + C(\varepsilon)\int_0^t\|\nabla(\Phi-\bar\Phi)\|^2_{L^2(\Omega)}ds. \tag{38}$$

Step 4: Estimation of I_2. We split $I_2 = I_{21} + I_{22}$, where

$$I_{21} = -\int_0^t\int_\Omega\sum_{i,j=0}^n u_i\bigg(\frac{A_{ij}}{u_i} - \frac{\bar A_{ij}}{\bar u_i}\bigg)\nabla\log\bar u_j\cdot\nabla\log\frac{u_i}{\bar u_i}dxds,$$

$$I_{22} = -\int_0^t \int_\Omega \sum_{i,j=0}^n u_i \left(\frac{Q_{ij}}{u_i} - \frac{\bar{Q}_{ij}}{\bar{u}_i} \right) \nabla \bar{\Phi} \cdot \nabla \log \frac{u_i}{\bar{u}_i} dx ds. \tag{39}$$

Lemma 13. *For any $\varepsilon > 0$, there exists $C(\varepsilon) > 0$ such that*

$$I_{21} \le \varepsilon \int_0^t \int_\Omega \frac{|(P_L Y)_0|^2}{u_0} dx ds + C(\varepsilon) \int_0^t \sum_{i=0}^n \|u_i - \bar{u}_i\|_{L^2(\Omega)}^2 ds.$$

Proof. Recalling that $Y_i = \sqrt{u_i} \nabla \log(u_i/\bar{u}_i)$, we reformulate I_{21} as

$$I_{21} = -\int_0^t \int_\Omega \sum_{i,j=0}^n u_i \left(\frac{A_{ij}}{u_i} - \frac{\bar{A}_{ij}}{\bar{u}_i} \right) \frac{Y_i}{\sqrt{u_i}} \cdot \nabla \log \bar{u}_j dx ds.$$

All rows of the matrix $(A_{ij}/u_i - \bar{A}_{ij}/\bar{u}_i)$ vanish except the first one,

$$\frac{A_{00}}{u_0} - \frac{\bar{A}_{00}}{\bar{u}_0} = \sum_{i=1}^n D_i \left(\frac{u_i}{u_0} - \frac{\bar{u}_i}{\bar{u}_0} \right), \quad \frac{A_{0j}}{u_0} - \frac{\bar{A}_{0j}}{\bar{u}_0} = -D_i \left(\frac{u_j}{u_0} - \frac{\bar{u}_j}{\bar{u}_0} \right) \text{ for } j = 1, \dots, n.$$

This shows that

$$\begin{aligned} I_{21} &= -\int_0^t \int_\Omega \sum_{j=0}^n u_0 \left(\frac{A_{0j}}{u_0} - \frac{\bar{A}_{0j}}{\bar{u}_0} \right) \frac{Y_0}{\sqrt{u_0}} \cdot \nabla \log \bar{u}_j dx ds \\ &= -\int_0^t \int_\Omega M \cdot \left(\frac{(P_L Y)_0}{\sqrt{u_0}} + \frac{(P_{L^\perp} Y)_0}{\sqrt{u_0}} \right) dx ds, \end{aligned} \tag{40}$$

where

$$\begin{aligned} M &= \sum_{j=0}^n \left(A_{0j} - \frac{u_0}{\bar{u}_0} \bar{A}_{0j} \right) \nabla \log \bar{u}_j \\ &= \sum_{i=1}^n D_i \left(u_i - \frac{u_0}{\bar{u}_0} \bar{u}_i \right) \nabla \log \bar{u}_0 - \sum_{i=1}^n D_i \left(u_i - \frac{u_0}{\bar{u}_0} \bar{u}_i \right) \nabla \log \bar{u}_i \\ &= \sum_{i=1}^n D_i (u_i - \bar{u}_i) \nabla \log \bar{u}_0 + \left(1 - \frac{u_0}{\bar{u}_0} \right) \sum_{i=1}^n D_i \bar{u}_i \nabla \log \bar{u}_0 \\ &\quad - \sum_{i=1}^n D_i (u_i - \bar{u}_i) \nabla \log \bar{u}_i - \left(1 - \frac{u_0}{\bar{u}_0} \right) \sum_{i=1}^n D_i \bar{u}_i \nabla \log \bar{u}_i \end{aligned}$$

$$= \sum_{i=1}^n D_i(u_i - \bar u_i)\nabla \log \frac{\bar u_0}{\bar u_i} + (u_0 - \bar u_0)\sum_{i=1}^n D_i \frac{\bar u_i}{\bar u_0}\nabla \log \frac{\bar u_0}{\bar u_i}.$$

Since $\nabla \log \bar u_i$ is bounded in $L^\infty(\Omega_T)$, we can bound the first term in I_{21}:

$$-\int_0^t\int_\Omega M\cdot \frac{(P_LY)_0}{\sqrt{u_0}}dxds \le C\int_0^t\int_\Omega \sum_{i=0}^n |u_i - \bar u_i|\frac{|(P_LY)_0|}{\sqrt{u_0}}dxds \tag{41}$$
$$\le \varepsilon\int_0^t\int_\Omega \frac{|(P_LY)_0|^2}{u_0}dxds + C(\varepsilon)\int_0^t\sum_{i=0}^n \|u_i - \bar u_i\|_{L^2(\Omega)}^2 ds,$$

where $\varepsilon > 0$ is arbitrary. To estimate the second term in I_{21}, we use (37) and the elementary inequality $(\sum_{i=0}^n |u_i - \bar u_i|)^2 \le (n+1)\sum_{i=0}^n |u_i - \bar u_i|^2$:

$$-\int_0^t\int_\Omega M\cdot \frac{(P_{L^\perp}Y)_0}{\sqrt{u_0}}dxds \le C\int_0^t\int_\Omega \sum_{i=0}^n |u_i - \bar u_i|\sum_{j=0}^n |\bar u_j - u_j|dxds \tag{42}$$
$$\le C(n+1)\int_0^t\int_\Omega \sum_{i=0}^n |u_i - \bar u_i|^2 dxds.$$

The lemma follows after inserting (41) and (42) into (40). □

Lemma 14. *For any $\varepsilon > 0$, there exists $C(\varepsilon) > 0$ such that*

$$I_{22} \le \varepsilon\int_0^t\int_\Omega \frac{|(P_LY)_0|^2}{u_0}dxds + C(\varepsilon)\int_0^t\sum_{i=0}^n \|u_i - \bar u_i\|_{L^2(\Omega)}^2,$$

recalling definition (39) of I_{22}.

Proof. All entries of the matrix $(Q_{ij}/u_i - \bar Q_{ij}/\bar u_i)$ vanish except the element $Q_{00}/u_0 - \bar Q_{00}/\bar u_0 = -\sum_{i=1}^n D_i z_i(u_i/u_0 - \bar u_i/\bar u_0)$. This leads to

$$I_{22} = \int_0^t\int_\Omega \sum_{i=1}^n D_i z_i u_0\Big(\frac{u_i}{u_0} - \frac{\bar u_i}{\bar u_0}\Big)\nabla\bar\Phi\cdot\nabla\log\frac{u_0}{\bar u_0}dxds$$
$$= \int_0^t\int_\Omega \sum_{i=1}^n D_i z_i\Big((u_i - \bar u_i) + \frac{\bar u_i}{\bar u_0}(\bar u_0 - u_0)\Big)\nabla\bar\Phi\cdot\frac{Y_0}{\sqrt{u_0}}dxds$$
$$= \int_0^t\int_\Omega \sum_{i=1}^n D_i z_i\Big((u_i - \bar u_i) + \frac{\bar u_i}{\bar u_0}(\bar u_0 - u_0)\Big)\Big(\frac{(P_LY)_0}{\sqrt{u_0}} + \frac{(P_{L^\perp}Y)_0}{\sqrt{u_0}}\Big)\cdot\nabla\bar\Phi dxds$$

$$\leq C\int_0^t\int_\Omega\sum_{j=0}^n|u_j-\bar u_j|\bigg(\frac{|(P_LY)_0|}{\sqrt{u_0}}+\frac{|(P_{L^\perp}Y)_0|}{\sqrt{u_0}}\bigg)|\nabla\bar\Phi|dsdx.$$

It follows from (37) that

$$\frac{|(P_{L^\perp}Y)_0|}{\sqrt{u_0}}=\bigg|\sum_{j=0}(\bar u_j-u_j)\nabla\log\bar u_j\bigg|\leq C\sum_{j=0}^n|\bar u_j-u_j|.$$

Hence, Young's inequality completes the proof. □

We conclude that

$$I_2\leq 2\varepsilon\int_0^t\int_\Omega\frac{|(P_LY)_0|^2}{u_0}dxds+C(\varepsilon)\int_0^t\sum_{i=0}^n\|u_i-\bar u_i\|^2_{L^2(\Omega)}ds. \tag{43}$$

Step 5: End of the proof. We collect (33), (38), and (43):

$$\begin{aligned}I_1+I_2+I_3\leq(3\varepsilon-D_*)\int_0^t\int_\Omega\bigg(\frac{|(P_LY)_0|^2}{u_0}+\sum_{i=1}^n|(P_LY)_i|^2\bigg)dxds\\+C(\varepsilon)\int_0^t\bigg(\sum_{i=0}^n\|u_i-\bar u_i\|^2_{L^2(\Omega)}+\|\nabla(\Phi-\bar\Phi)\|^2_{L^2(\Omega)}\bigg)ds.\end{aligned}$$

Thus, choosing $\varepsilon\leq D_*/3$, we conclude from (32) that

$$H((u,\Phi)(t)|(\bar u,\bar\Phi)(t))\leq C\int_0^t\bigg(\sum_{i=0}^n\|u_i-\bar u_i\|^2_{L^2(\Omega)}+\|\nabla(\Phi-\bar\Phi)\|^2_{L^2(\Omega)}\bigg)ds. \tag{44}$$

The first term on the right-hand side of (44) can be bounded by the relative entropy, as shown in the following lemma.

Lemma 15. *It holds for any $u,\bar u\in(0,1)$ that*

$$u\log\frac{u}{\bar u}\geq\frac{1}{2}(u-\bar u)^2.$$

Proof. The lemma has been proved in [17, Lemma 16]. For the convenience of the reader, we recall the short proof. Let $f(u)=u\log u$. Then, for $u,\bar u\in(0,1)$,

$$u\log\frac{u}{\bar u}-(u-\bar u)=f(u)-f(\bar u)-f'(\bar u)(u-\bar u)=f(\theta(u-\bar u)+\bar u)\big|_{\theta=0}^{1}-f'(\bar u)(u-\bar u)$$
$$=(u-\bar u)\int_0^t\big(f'(\theta(u-\bar u)+\bar u)-f'(\bar u)\big)d\theta=(u-\bar u)\int_0^1 f'(s(u-\bar u)+\bar u)\big|_{s=0}^{\theta}d\theta$$
$$=(u-\bar u)^2\int_0^1\int_0^\theta f''(s(u-\bar u)+\bar u)dsd\theta.$$

The result follows from the observation $f''(s(u-\bar u)+\bar u)=(s(u-\bar u)+\bar u)^{-1}\geq 1$. □

The previous lemma shows that

$$\sum_{i=0}^n\int_\Omega u_i\log\frac{u_i}{\bar u_i}dx\geq\frac{1}{2}\sum_{i=0}^n\int_\Omega(u_i-\bar u_i)^2dx \tag{45}$$

and hence,

$$2H(u,\Phi|\bar u,\bar\Phi)\geq\sum_{i=0}^n\|u_i-\bar u_i\|_{L^2(\Omega)}^2+\lambda^2\|\nabla(\Phi-\bar\Phi)\|_{L^2(\Omega)}^2.$$

Consequently, we obtain from (44):

$$H((u,\Phi)(t)|(\bar u,\bar\Phi)(t))\leq C\int_0^t H(u,\Phi|\bar u,\bar\Phi)ds,$$

and Gronwall's lemma finishes the proof.

4. Remarks on the uniqueness of solutions

Remark 16 *(Uniqueness of weak solutions).* The uniqueness of weak solutions for our model is more delicate than for the model of [15], even in the case $D_i=z_i=1$ for $i=1,\dots,n$. The reason is that we cannot use simple $L^2(\Omega)$ estimations. Instead, we use the $H^{-1}(\Omega)$ method under the (restrictive) condition that $\nabla\Phi\in L^\infty(\Omega_T)$. This regularity holds if the Dirichlet and Neumann boundaries do not intersect and if $\partial\Omega\in C^{1,1}$, $f\in L^p(\Omega)$, and $\Phi^D\in W^{2,p}(\Omega)$ for some $p>3$. Indeed, we conclude from elliptic regularity [25, Theorem 3.17] that $\Phi\in L^\infty(0,T;W^{2,p}(\Omega))\hookrightarrow L^\infty(0,T;W^{1,\infty}(\Omega))$. We also assume that $\sum_{i=1}^n r_i(u)=0$. Summing (1) over $i=1\dots,n$, the pair (u_0,Φ) solves

$$\partial_t u_0=\operatorname{div}(\nabla\log u_0-(1-u_0)\nabla\Phi),\quad \lambda^2(\ell^2\Delta-1)\Delta\Phi=1-u_0+f(x)\quad\text{in }\Omega, \tag{46}$$

together with the corresponding initial and boundary conditions (3)–(5). We claim that this system has at most one solution. Let (u_0,Φ) and (v_0,Ψ) be two weak solutions to this problem and let $\chi\in L^2(0,T;H^1(\Omega))$ be the unique solution to $-\Delta\chi=u_0-v_0$ in Ω, $\nabla\chi\cdot\nu=0$ on $\partial\Omega$.

This solution exists since $\int_\Omega (u_0 - v_0)dx = 0$ because of mass conservation. We use χ as a test function in the first equation of (46):

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla\chi|^2 dx + \int_\Omega (\log u_0 - \log v_0)(u_0 - v_0)dx$$
$$= \int_\Omega \big(- (u_0 - v_0)\nabla\Phi + (1 - v_0)\nabla(\Phi - \Psi)\big)\cdot \nabla\chi dx.$$

Using $(\log u_0 - \log v_0)(u_0 - v_0) \geq 4(\sqrt{u_0} - \sqrt{v_0})^2$ and $|u_0 - v_0| = |\sqrt{u_0} + \sqrt{v_0}||\sqrt{u_0} - \sqrt{v_0}| \leq 2|\sqrt{u_0} - \sqrt{v_0}|$, we find that

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla\chi|^2 dx + 4\int_\Omega (\sqrt{u_0} - \sqrt{v_0})^2 dx \leq C\|\sqrt{u_0} - \sqrt{v_0}\|_{L^2(\Omega_T)}\|\nabla\Phi\|_{L^\infty(\Omega_T)}\|\nabla\chi\|_{L^2(\Omega_T)}$$
$$+ C\|\nabla(\Phi - \Psi)\|_{L^2(\Omega_T)}\|\nabla\chi\|_{L^2(\Omega_T)}$$
$$\leq 2\|\sqrt{u_0} - \sqrt{v_0}\|^2_{L^2(\Omega_T)} + C\|\nabla\chi\|^2_{L^2(\Omega_T)},$$

where we used the elliptic estimate $\|\nabla(\Phi - \Psi)\|_{L^2(\Omega_T)} \leq C\|u_0 - v_0\|_{L^2(\Omega_T)}$ and the assumption $\|\nabla\Phi\|_{L^\infty(\Omega_T)} \leq C$. We conclude from Gronwall's lemma that $\nabla\chi(t) = 0$ and consequently $u_0(t) = v_0(t)$ and $\Phi(t) = \Psi(t)$ for $t > 0$. Now, the equation

$$\partial_t u_i = \operatorname{div}(\nabla u_i - u_i\nabla(\log u_0 - \Phi)) \tag{47}$$

can be interpreted as a drift-diffusion equation for u_i with given (u_0, Φ). The regularity $\nabla \log u_0 - \Phi \in L^2(\Omega_T)$ is sufficient for the application of Gajewski's entropy method; see [15, Sec. 3]. Thus, there exists at most one solution u_i to (47) with the corresponding initial and boundary conditions. □

Remark 17 *(Weak–strong uniqueness in the presence of reaction terms).* We claim that Theorem 2 holds for reaction rates $r_i : \overline{\mathcal{D}} \to \mathbb{R}$, which are Lipschitz continuous and quasi-positive (i.e. $r_i(u) \geq 0$ for all $u \in \mathcal{D}$ with $u_i = 0$) such that the total reaction rate is nonnegative, i.e. $\sum_{i=1}^n r_i(u) \leq 0$ for all $u \in \mathcal{D}$, and that $r_i(u)\log u_i = 0$ if $u_i = 0$. Proceeding as in Step 1 of the proof of Theorem 2 and taking into account Remark 9, we need to estimate additionally the expression

$$R = \int_\Omega \sum_{i=1}^n r_i(u)(w_i - \bar{w}_i)dx =: R_1 + R_2, \quad \text{where}$$
$$R_1 = \int_\Omega \sum_{i=1}^n \left\{ r_i(u)\left(\log\frac{u_i}{\bar{u}_i} - \log\frac{u_0}{\bar{u}_0}\right) - r_i(\bar{u})\left(\frac{u_i}{\bar{u}_i} - \frac{u_0}{\bar{u}_0}\right)\right\} dx,$$
$$R_2 = \int_\Omega \sum_{i=1}^n z_i(r_i(u) - r_i(\bar{u}))(\Phi - \bar{\Phi})dx.$$

The assumptions on r_i imply that $r_i(u)\log u_i$ is integrable. Therefore, following [12, p. 202f],

$$R_1 = \int_\Omega \sum_{i=1}^n \bigg\{ r_i(u)\bigg(\log\frac{u_i}{\bar u_i} - \frac{u_i}{\bar u_i} + 1\bigg) - (r_i(u) - r_i(\bar u))\bigg(\frac{u_i}{\bar u_i} - 1\bigg) \\ - r_i(u)\bigg(\log\frac{u_0}{\bar u_0} - \frac{u_0}{\bar u_0} + 1\bigg) + (r_i(\bar u) - r_i(\bar u))\bigg(\frac{u_0}{\bar u_0} - 1\bigg)\bigg\} dx.$$

We deduce from $0 \ge \log z - z + 1 \ge -|z-1|^2/\min\{1,z\}$ for $z > 0$ that

$$\begin{aligned} R_2 &\le \int_\Omega \sum_{i=1}^n \bigg\{ C_R u_i \frac{|u_i - \bar u_i|^2}{\bar u_i \min\{u_i, \bar u_i\}} + \frac{C}{\bar u_i}|r_i(u) - r_i(\bar u)||u_i - \bar u_i| \\ &\qquad - r_i(u)\bigg(\log\frac{u_0}{\bar u_0} - \frac{u_0}{\bar u_0} + 1\bigg) + \frac{C}{\bar u_0}|r_i(\bar u) - r_i(\bar u)||u_0 - \bar u_0|\bigg\} dx \\ &\le C\int_\Omega \sum_{i=1}^n |u_i - \bar u_i|^2 dx - \int_\Omega \sum_{i=1}^n r_i(u)\bigg(\log\frac{u_0}{\bar u_0} - \frac{u_0}{\bar u_0} + 1\bigg) dx \\ &\le C\int_\Omega \sum_{i=1}^n |u_i - \bar u_i|^2 dx, \end{aligned}$$

where we used in the last step the assumption $\sum_{i=1}^n r_i(u) \le 0$. Furthermore, by the Lipschitz continuity of r_i, the Poincaré inequality, and the elliptic estimate for the Poisson–Fermi equation,

$$R_2 \le C\sum_{i=1}^n \|u_i - \bar u_i\|_{L^2(\Omega)} \|\nabla(\Phi - \bar\Phi)\|_{L^2(\Omega)} \le C\sum_{i=1}^n \|u_i - \bar u_i\|_{L^2(\Omega)}^2.$$

Thus, estimate (44) is still valid with another constant, and Theorem 2 follows. □

Data availability

No data was used for the research described in the article.

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