

# ANALYSIS OF A POISSON–NERNST–PLANCK CROSS-DIFFUSION SYSTEM WITH STERIC EFFECTS

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**ABSTRACT.** A transient Poisson–Nernst–Planck system with steric effects is analyzed in a bounded domain with no-flux boundary conditions for the ion concentrations and mixed Dirichlet–Neumann boundary conditions for the electric potential. The steric repulsion of ions is modeled by a localized Lennard–Jones force, leading to cross-diffusion terms. The existence of global weak solutions, a weak–strong uniqueness property, and, in case of pure Neumann conditions, the exponential decay towards the thermal equilibrium state is proved. The main difficulties are the cross-diffusion terms and the different boundary conditions satisfied by the unknowns. These issues are overcome by exploiting the entropy structure of the equations and carefully taking into account the electric potential term. A numerical experiment illustrates the long-time behavior of the solutions when the potential satisfies mixed boundary conditions.

## 1. INTRODUCTION

The transport of ions is often modeled by the Nernst–Planck equations for the ion concentrations, self-consistently coupled with the Poisson equation for the electric potential [31, 32]. The Nernst–Planck theory is valid for dilute solutions only. In confined environments, the ions become crowded and steric repulsion may appear due to finite ion sizes. In such a situation, the Nernst–Planck equations need to be modified. The mutual repulsive force can be described by the nonlocal Lennard–Jones force term [21]. The localization limit leads to easier local interatomic forces. Then the free energy of the system consists of the local Lennard–Jones energy, the thermodynamic (Boltzmann) entropy, and the electric energy [30]. In this paper, we analyze the associated Euler–Lagrange equations in a bounded domain with biologically motivated boundary conditions. We show the existence of global weak solutions, prove a weak–strong uniqueness property, show the exponential decay of the solutions towards thermal equilibrium, and present a numerical example.

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The Nernst–Planck equations with steric effects for the ion concentrations  $u_i$  are given by

$$(1) \quad \partial_t u_i + \operatorname{div} J_i = 0, \quad J_i = -(\sigma \nabla u_i + z_i u_i \nabla \Phi + u_i \nabla p_i(u)) \quad \text{in } \Omega, \quad t > 0,$$

where  $\Omega \subset \mathbb{R}^d$  ( $d \geq 1$ ) is a bounded domain with Lipschitz boundary and

$$(2) \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j, \quad i = 1, \dots, n,$$

describes the potential associated to the  $i$ th species arising from steric effects. The parameters are the diffusion coefficient  $\sigma > 0$ , the ionic charges  $z_i \in \mathbb{R}$ , and the values  $a_{ij} \geq 0$  represent the strength of steric repulsion between the species. To ensure the parabolicity of the system, we suppose that the matrix  $(a_{ij})_{i,j=1}^n$  is symmetric and positive definite. We impose the initial and boundary conditions

$$(3) \quad u_i(0) = u_i^0 \quad \text{in } \Omega, \quad J_i \cdot \nu = 0 \quad \text{on } \partial\Omega, \quad t > 0, \quad i = 1, \dots, n,$$

where  $\nu$  is the exterior unit normal vector to  $\partial\Omega$ . The electric potential  $\Phi$  solves the Poisson equation with mixed Dirichlet–Neumann boundary conditions:

$$(4) \quad -\Delta \Phi = \sum_{i=1}^n z_i u_i \quad \text{in } \Omega, \quad \Phi = \Phi_D \quad \text{on } \Gamma_D, \quad \nabla \Phi \cdot \nu = 0 \quad \text{on } \Gamma_N,$$

where  $\Gamma_D \cup \Gamma_N = \partial\Omega$  and  $\Gamma_D \cap \Gamma_N = \emptyset$ . The right-hand side of (4) is the total ion charge. The no-flux boundary conditions mean that the ions cannot leave the domain, while the electric potential is assumed to be fixed on  $\Gamma_D$ , with  $\Phi_D$  being the applied potential, and  $\Gamma_N$  models insulating boundary parts.

**1.1. State of the art.** Without drift terms, equations (1)–(2) have been rigorously derived from moderately interacting particle systems in a mean-field-type limit [4]. A heuristic derivation including drift terms with a fixed potential for two species was presented in [11] together with a global existence analysis. The Poisson–Nernst–Planck model (1)–(2) was analyzed in [22] for two species and (biologically less realistic) homogeneous Dirichlet boundary conditions for the electric potential. Equations (1) for an arbitrary number of species and without potential terms were investigated in [27], but the existence proof was only sketched. An existence proof based on a finite-volume approximation for the same situation was presented in [28]. An analysis of the  $n$ -species model (1)–(4) is missing in the literature. In this paper, we fill this gap.

There exist other Nernst–Planck models modeling steric effects. In [35], the special case  $a_{ij} = \delta_{ij} a_i$  ( $\delta_{ij}$  is the Kronecker delta) was considered. This choice leads to nonlinear diffusion but does not contain cross-diffusion terms. Including the thermodynamic energy for the solvent in the free energy, the current densities become [29]

$$(5) \quad J_i = -(\sigma \nabla u_i - u_i \nabla \log u_0 + z_i u_i \nabla \Phi), \quad i = 1, \dots, n,$$

where  $u_0 = 1 - \sum_{j=1}^n u_j$  is the solvent concentration. In this model, the quantities  $u_i$  are mass fractions, and their sum equals one. The corresponding Poisson–Nernst–Planck

model was analyzed in [26], where the Poisson equation was replaced by the fourth-order Fermi–Poisson model [34]. Another approach is to allow for mobilities that depend on the solvent concentration, leading to

$$(6) \quad J_i = -(\sigma u_0 \nabla u_i - u_i \nabla u_0 + z_i u_0 u_i \nabla \Phi), \quad i = 1, \dots, n,$$

which avoids the logarithmic term but involves the degenerate diffusion  $u_0 \nabla u_i$ ; we refer to [3, 36] for a formal derivation and to [15] for an existence analysis. The systems with fluxes (5) or (6) yield a maximal concentration of ions,  $u_i \leq 1$ . It is argued in [16] that local concentrations can be large. According to [16, Sec. 5], this does not contradict the intuition that the percentage of space occupied by the ions cannot exceed one, since we are averaging the concentrations over some small neighborhood which keeps the local packing fraction below one.

Finally, we mention the approach of [14], where Nernst–Planck models with steric effects are derived by taking into account higher-order approximations of the Lennard–Jones term, leading to higher-order derivatives, which need to be added to equations (1).

In all the mentioned existence results, the matrix  $(a_{ij})$  is required to be positive definite. If the real part of at least one eigenvalue becomes negative for some value of the concentrations, and equations (1) fail to be parabolic in the sense of Petrovskii, which is a minimal condition for local existence of solutions. In this situation, the problem is ill-posed [13], and  $L^\infty(\Omega)$  blow-up in finite time is possible [18, Theorem 7]. If the matrix is positive semidefinite, system (1) is generally of hyperbolic–parabolic type. The case  $a_{ij} = a > 0$  and  $n = 2$  (with fixed potential terms) was investigated in [2, 11]. Formulated as a Lagrangian free-boundary problem, the two-species model may have more than one solution [12]. Without potential terms and for positive initial total concentrations, but for an arbitrary number of species, the existence and uniqueness of smooth solutions to the multi-species problem was proved in [9], while global dissipative measure-valued solutions were shown to exist in [20]. We discuss the special case of rank-one matrices  $(a_{ij})$  in Remark 12.

The uniqueness of weak solutions to cross-diffusion systems is generally a delicate problem. Often, only the weak–strong uniqueness property is proved. This means that any weak solution coincides with a strong solution with the same initial data, as long as the strong solution exists. This property was proved for, e.g., the Shigesada–Kawasaki–Teramoto population model [5], for a thin-film solar cell model [1, 19], for Maxwell–Stefan systems [23], and for fractional cross-diffusion equations [7], using the relative entropy method. Here, we extend this technique to equations (1)–(2).

**1.2. Entropy structure and main difficulties.** The analytical results are based on variants of the entropy method. The entropy structure follows from the free energy, consisting of the thermodynamic (Boltzmann) entropy, the electric energy, and the mixing (Rao) entropy:

$$(7) \quad H_{BR}(u) = \int_{\Omega} h_{BR}(u) dx, \quad \text{where}$$

$$h_{BR}(u) = \sigma \sum_{i=1}^n u_i (\log u_i - 1) + \frac{1}{2} |\nabla(\Phi - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij} u_i u_j + \sum_{i=1}^n z_i u_i \Phi_D.$$

We call  $H_{BR}(u)$  the (mathematical) Boltzmann–Rao entropy. The last term compensates the Dirichlet boundary condition for the potential. System (1)–(2) can be written as the formal gradient-flow equations

$$\partial_t u_i = \operatorname{div} \left( u_i \nabla \frac{\delta H_{BR}}{\delta u_i} \right), \quad i = 1, \dots, n,$$

where  $\delta H_{BR}/\delta u_i = \sigma \log u_i + z_i \Phi + p_i(u)$  is the variational derivative of  $H_{BR}$  with respect to  $u_i$  [15, Lemma 7]. This structure reveals that (see Theorem 1 for a proof)

$$\frac{d}{dt} H_{BR}(u) + \frac{1}{2} \sum_{i=1}^n \int_{\Omega} u_i |\nabla w_i|^2 dx \leq 0,$$

where  $w_i = \delta H_{BR}/\delta u_i$  is called the entropy variable (electro-chemical potential in thermodynamics). To derive uniform gradient bounds, we need to estimate the entropy production term  $\int_{\Omega} u_i |\nabla w_i|^2 dx$ . We show in Lemma 7 that

$$\sum_{i=1}^n \int_{\Omega} u_i |\nabla w_i|^2 dx \geq \sigma \sum_{i=1}^n \int_{\Omega} (4\sigma |\nabla \sqrt{u_i}|^2 + \alpha |\nabla u_i|^2) dx - C\sigma (H_{BR}(u) + 1)$$

for some constants  $\alpha, C > 0$ . This is the key estimate for the existence analysis. Note that we lose the gradient bounds if  $\sigma = 0$ . The entropy inequality yields an  $L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$  bound for  $u_i$ , an  $L^\infty(0, T; H^1(\Omega))$  bound for  $\Phi$ , and an  $L^2(0, T; L^2(\Omega))$  bound for  $\sqrt{u_i} \nabla w_i$ , which is sufficient for the existence analysis.

In the further analysis, we face two main difficulties. First, in the weak–strong uniqueness proof, to avoid issues with the logarithm, we do not use the Boltzmann–Rao entropy (7) but the Rao-type entropy

$$H_R(u) = \int_{\Omega} h_R(u) dx, \quad h_R(u) = \frac{1}{2} |\nabla(\Phi - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij} u_i u_j + \sum_{i=1}^n z_i u_i \Phi_D.$$

The time derivative of  $H_R$  is formally computed by taking the test function  $\phi_i = p_i(u) + z_i(\Phi - \Phi_D)$ . Unfortunately, this function is not admissible since we need the regularity  $\phi_i \in L^2(0, T; W^{1,4}(\Omega))$  in the weak formulation. This difficulty is overcome by extending the test function space and exploiting the regularity  $\sqrt{u_i} \nabla w_i \in L^2(\Omega_T)$ ; see Section 2.7 for details. Then the proof is based on the relative entropy

$$(8) \quad H_R(u|\bar{u}) = \int_{\Omega} (h_R(u) - h_R(\bar{u}) - h'_R(\bar{u}) \cdot (u - \bar{u})) dx,$$

where  $(u, \Phi)$  is a weak solution and  $(\bar{u}, \bar{\Phi})$  is a strong solution. The goal is to derive an inequality of the form

$$(9) \quad \frac{d}{dt} H_R(u|\bar{u}) \leq C H_R(u|\bar{u}) \quad \text{for } t > 0,$$

where  $C > 0$  is some constant. The difficulty is to make this inequality rigorous. For this, we write the relative entropy as the sum of  $H_R(u)$ ,  $H_R(\bar{u})$ , and some remainder terms. The solutions  $u$  and  $\bar{u}$  satisfy a Rao entropy inequality, while the remainder terms include the strong solution, which facilitates the computation of these expressions. Combining the estimations, we arrive eventually at (9).

The long-time behavior can be proved only if the stationary solution  $(u^\infty, \Phi^\infty)$  is in thermal equilibrium, which means that the stationary entropy variable  $w_i^\infty = \sigma \log u_i^\infty + z_i \Phi^\infty + p_i(u^\infty)$  vanishes. The relative entropy reads as

$$(10) \quad H_{BR}(u|u^\infty) = \int_{\Omega} (h_{BR}(u) - \bar{h}_{BR}(u^\infty) - h'_{BR}(u^\infty) \cdot (u - u^\infty)) dx.$$

To prove exponential decay, we need an estimate like (9) but with  $C < 0$  to achieve an exponential decay rate via Gronwall's lemma. The fact that the boundary conditions of  $u_i$  and  $\Phi$  are different leads to the second difficulty. Indeed, computing the time derivative of the relative entropy, we find that

$$\frac{d}{dt} H_{BR}(u|u^\infty) \leq - \sum_{i=1}^n \int_{\Omega} u_i |\nabla(w_i - w_i^\infty)|^2 dx,$$

and when expanding the square of  $\nabla w_i$ , the most delicate term is

$$I := 2\sigma \sum_{i=1}^n \int_{\Omega} z_i \nabla(u_i - u_i^\infty) \cdot \nabla(\Phi - \Phi^\infty) dx.$$

The positive definiteness of  $(a_{ij})$  provides the term  $\|\nabla(u_i - u_i^\infty)\|_{L^2(\Omega)}^2$  with a good sign. Thus, we may apply Young's inequality for  $I$  to absorb  $\|\nabla(u_i - u_i^\infty)\|_{L^2(\Omega)}^2$ , but the expression  $\|\nabla(\Phi - \Phi^\infty)\|_{L^2(\Omega)}^2$  contributes to the right-hand side with the wrong sign. Another idea is to integrate by parts and to use the Poisson equation as well as the boundary condition  $\nabla\Phi \cdot \nu = \nabla\Phi^\infty \cdot \nu = 0$  on  $\Gamma_N$ :

$$I = -2\sigma \int_{\Omega} \left( \sum_{i=1}^n z_i (u_i - u_i^\infty) \right)^2 dx + 2\sigma \sum_{i=1}^n \int_{\Gamma_D} (u_i - u_i^\infty) \nabla(\Phi - \Phi^\infty) \cdot \nu dx.$$

The boundary integral would vanish if  $u_i$  and  $u_i^\infty$  were satisfying the same Dirichlet boundary conditions. This situation holds true in semiconductor applications, where the long-time behavior of solution could be shown [10, 17]. Unfortunately, this is not the case here. To overcome this issue, we assume that  $\Phi$  satisfies Neumann conditions on the whole boundary, i.e.  $\Gamma_D = \emptyset$ . Then the delicate integral  $I$  is nonpositive and we can conclude the argument.

**1.3. Main results.** We impose the following assumptions:

- (A1) Domain:  $\Omega \subset \mathbb{R}^d$  ( $1 \leq d \leq 4$ ) is a bounded domain with Lipschitz boundary  $\partial\Omega = \Gamma_D \cup \Gamma_N$ , where  $\Gamma_D \cap \Gamma_N = \emptyset$  and  $\Gamma_N$  is open in  $\partial\Omega$ .
- (A2) Data:  $T > 0$ ,  $\sigma > 0$ ,  $z_i \in \mathbb{R}$  for  $i = 1, \dots, n$ , and  $(a_{ij})_{i,j=1}^n \subset \mathbb{R}^{n \times n}$  is symmetric and positive definite.

- (A3) Initial and boundary data:  $u_i^0 \in L^2(\Omega)$  satisfies  $u_i^0 > 0$  in  $\Omega$ . If  $\partial\Omega = \Gamma_N$ , we require that  $\sum_{i=1}^n \int_{\Omega} z_i u_i^0 dx = 0$ .
- (A4) Boundary data I: The boundary function  $\Phi_D$  on  $\Gamma_D$  can be extended to a function in  $H^1(\Omega) \cap L^\infty(\Omega)$  satisfying  $\Delta\Phi_D = 0$  in  $\Omega$  and  $\nabla\Phi_D \cdot \nu = 0$  on  $\Gamma_N$ .
- (A5) Boundary data II: The solution  $\phi$  to

$$-\Delta\phi = f \in L^2(\Omega) \quad \text{in } \Omega, \quad \phi = \Phi_D \quad \text{on } \Gamma_D, \quad \nabla\phi \cdot \nu = 0 \quad \text{on } \Gamma_N$$

satisfies  $\phi \in H^2(\Omega)$  and  $\|\phi\|_{H^2(\Omega)} \leq C(\|f\|_{L^2(\Omega)} + 1)$ , where  $C > 0$  depends on  $\Phi_D$ .

Assumption (A1) includes the case of homogeneous Neumann boundary conditions,  $\partial\Omega = \Gamma_N$ . The restriction to  $d \leq 4$  space dimensions is due to Sobolev embeddings. It can be removed in the existence analysis at the expense of lower regularity of  $u_i$ . The positive definiteness of  $(a_{ij})$  in Assumption (A2) helps us to derive  $H^1(\Omega)$  estimates for the solution. We discuss a special case of positive semidefinite matrices (namely rank-one matrices) in Remark 12 and the case  $\sigma = 0$  in Remark 13. Assumption (A4) is needed to define the Boltzmann–Rao entropy. The condition that  $\Phi_D$  satisfies an elliptic problem is needed to compute the entropy variables [15, Lemma 7]. Finally, Assumption (A5) is only needed for the weak–strong uniqueness and exponential decay results. Assumption (A5) is a regularity requirement for the solutions to the mixed Dirichlet–Neumann boundary-value problem; they are satisfied if, for instance, the boundaries  $\Gamma_D$  and  $\Gamma_N$  do not meet and the boundary data is sufficiently smooth [38].

We use the following notation. Set  $\Omega_T := \Omega \times (0, T)$ . The norm  $\|u\|_X$  of a vector-valued function  $u = (u_1, \dots, u_n)$  in some Banach space  $X$  is defined as  $\|u\|_X = \sum_{i=1}^n \|u_i\|_X$ . Furthermore, we introduce the Hilbert space

$$H_D^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D\}.$$

Our first main result concerns the existence of global weak solutions.

**Theorem 1** (Global existence). *Let Assumptions (A1)–(A4) hold. Then there exists a weak solution  $u = (u_1, \dots, u_n)$  to (1)–(4) satisfying  $u_i \geq 0$  in  $\Omega_T$ ,*

$$\sqrt{u_i}, u_i, \Phi \in L^2(0, T; H^1(\Omega)), \quad \partial_t u_i \in L^2(0, T; W^{1,4}(\Omega)'), \quad i = 1, \dots, n,$$

*and the initial data is satisfied in the sense of  $W^{1,4}(\Omega)'$ . If  $\partial\Omega = \Gamma_N$ , the potential satisfies  $\int_{\Omega} \Phi dx = 0$ . Moreover, the following entropy inequality holds:*

$$(11) \quad H_{BR}(u(t)) + \int_0^t \int_{\Omega} u_i |\nabla w_i|^2 dx ds \leq H_{BR}(u^0),$$

*where  $w_i = \sigma \log u_i + z_i \Phi + p_i(u)$  on  $\{u_i > 0\}$  and  $w_i = 0$  on  $\{u_i = 0\}$ .*

The theorem is proved by the Leray–Schauder fixed-point argument. For this, we approximate equations (1) by using an implicit Euler discretization, adding a higher-order regularization, and formulating the equations in terms of the entropy variable  $w_i$ , as in the boundedness-by-entropy method [24]. The mapping  $u \mapsto w$  is invertible and yields positive approximations of the concentrations; see Lemma 4. Uniform estimates are obtained from the discrete version of the Boltzmann–Rao entropy inequality (11); see Lemmas 6–8. The

Aubin–Lions lemma of [8] implies the strong convergence of a subsequence of approximating solutions, allowing us to identify the nonlinearities.

**Theorem 2** (Weak–strong uniqueness). *Let Assumptions (A1)–(A5) hold, let  $(u, \Phi)$  be a weak solution and  $(\bar{u}, \bar{\Phi})$  be a strong solution to (1)–(4) in the sense  $\nabla \bar{u}_i, \nabla \bar{\Phi} \in L^\infty(\Omega_T)$ , and both solutions satisfy the entropy inequality (11). Then  $u(t) = \bar{u}(t)$  and  $\Phi(t) = \bar{\Phi}(t)$  in  $\Omega$  for  $t > 0$ .*

As explained before, we use the relative entropy (8) to prove the theorem. Given a weak solution  $(u, \Phi)$  and a strong solution  $(\bar{u}, \bar{\Phi})$ , we write (see Lemma 14)

$$\begin{aligned} \frac{d}{dt} H_R(u|\bar{u}) &= \frac{dH_R}{dt}(u) + \frac{dH_R}{dt}(\bar{u}) - \frac{1}{2} \frac{d}{dt} \sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i \bar{u}_j + \bar{u}_i u_j) dx \\ &\quad - \frac{d}{dt} \int_{\Omega} \nabla(\Phi - \Phi_D) \cdot \nabla(\bar{\Phi} - \bar{\Phi}_D) dx. \end{aligned}$$

Compared to formulation (8), it is sufficient to suppose that  $\bar{u}$  satisfies the entropy inequality, while the minus sign in (8) in front of  $H_R(\bar{u})$  requires that  $\bar{u}$  fulfills the entropy equality. The time derivative of the remaining two integrals in the previous expression can be computed, as  $(\bar{u}, \bar{\Phi})$  is assumed to have sufficient regularity. After some computations, we end up with

$$\frac{d}{dt} H_R(u|\bar{u}) \leq C H_R(u|\bar{u}),$$

where  $C > 0$  depends on the  $L^\infty(0, T; W^{1,\infty}(\Omega))$  norms of  $\bar{u}$  and  $\bar{\Phi}$ . Gronwall’s lemma then shows that  $u(t) = \bar{u}(t)$  and  $\Phi(t) = \bar{\Phi}(t)$  in  $\Omega$  for  $t > 0$ .

Finally, we prove the exponential convergence of the weak solutions to the thermal equilibrium state in case  $\partial\Omega = \Gamma_N$ . We call  $(u^\infty, \Phi^\infty)$  a thermal equilibrium solution if the fluxes vanish, i.e.  $\nabla(\sigma \log u_i^\infty + z_i \Phi^\infty + p_i(u^\infty)) = 0$  in  $\Omega$ ,  $i = 1, \dots, n$ . A solution is given by  $u_i^\infty = \text{meas}(\Omega)^{-1} \int_{\Omega} u_i^0 dx$ , i.e.,  $u^\infty$  is constant in space. Then

$$0 = \nabla(\sigma \log u_i^\infty + z_i \Phi^\infty + p_i(u^\infty)) = z_i \nabla \Phi^\infty,$$

and  $\Phi^\infty$  is constant too. Because of the Neumann condition for  $\Phi$ , we have  $\int_{\Omega} \Phi^\infty dx = 0$ . This implies that  $\Phi^\infty = 0$ . In the numerical example of Section 5, we present the convergence to a nonconstant steady state if mixed boundary condition for  $\Phi$  are imposed.

**Theorem 3** (Exponential decay). *Let Assumptions (A1)–(A5) hold, let  $\partial\Omega = \Gamma_N$ , and let  $(u, \Phi)$  be a weak solution to (1)–(4). Then there exists a constant  $\lambda > 0$  such that*

$$\|u(t) - u^\infty\|_{L^2(\Omega)} + \|\nabla \Phi(t)\|_{L^2(\Omega)} \leq H_{BR}(u^0|u^\infty) e^{-\lambda \sigma t}, \quad t > 0.$$

The theorem is proved by differentiating the relative entropy (10) with respect to time. The entropy inequality (11) shows that

$$\frac{d}{dt} H_{BR}(u|u^\infty) = \frac{dH_{BR}}{dt}(u) \leq - \sum_{i=1}^n \int_{\Omega} u_i |\nabla w_i|^2 dx,$$

and the goal is to estimate the entropy production from above in terms of the relative entropy. For this step, we need pure Neumann conditions for  $\Phi$ . Then, using the logarithmic Sobolev and Poincaré–Wirtinger inequalities, we end up with

$$\frac{d}{dt} H_{BR}(u|u^\infty) \leq -\lambda\sigma H_{BR}(u|u^\infty),$$

where  $\lambda > 0$  depends on  $\alpha$ ,  $\max_{i,j=1,\dots,n} a_{ij}$ , and the constants of the logarithmic Sobolev and Poincaré–Wirtinger inequalities. Gronwall’s lemma finishes the proof.

The paper is organized as follows. The existence result is proved in Section 2. Section 3 is concerned with the proof of the weak–strong uniqueness property, and the exponential decay is shown in Section 4. Finally, we present a numerical example in Section 5.

## 2. GLOBAL EXISTENCE OF SOLUTIONS

The aim of this section is to prove Theorem 1. We first introduce an approximate problem in terms of the entropy variables, which is solved by means of the Leray–Schauder fixed-point theorem. Uniform estimates are derived from an approximate entropy inequality. These estimates allow us to use the Aubin–Lions compactness lemma to pass to the de-regularization limit.

**2.1. Preparations.** First, we show that the mapping between entropy variables and densities is invertible. We introduce the ionic charge vector  $z = (z_1, \dots, z_n) \in \mathbb{R}^n$ .

**Lemma 4.** *Let  $\sigma > 0$ . Introduce the function  $F : (0, \infty)^n \rightarrow \mathbb{R}^n$ ,  $F_i(u) = \sigma \log u_i + p_i(u)$ , where  $p_i$  is defined in (2). There exists a mapping  $u : \mathbb{R}^n \times \mathbb{R} \rightarrow (0, \infty)^n$ ,  $(w, \Phi) \mapsto u(w, \Phi)$ , such that  $u(w, \Phi) = F^{-1}(w - z\Phi)$ . Moreover,  $\Phi \mapsto \sum_{i=1}^n z_i u_i(w, \Phi)$  is a decreasing function.*

*Proof.* Taking into account that the range of the logarithm is the whole line, the range of  $F$  equals  $\mathbb{R}^n$ . The function  $F$  is strictly monotone since

$$(u - v) \cdot (F(u) - F(v)) = \sigma \sum_{i=1}^n (u_i - v_i) \log \frac{u_i}{v_i} + \sum_{i,j=1}^n a_{ij} (u_i - v_i)(u_j - v_j) > 0$$

for  $u, v \in (0, \infty)^n$  with  $u \neq v$  (this even holds if  $(a_{ij})$  is positive semidefinite), showing that  $F$  is one-to-one. Thus, the inverse  $F^{-1} : \mathbb{R}^n \rightarrow (0, \infty)^n$  exists and is strictly monotone too. By the inverse function rule, it is differentiable and  $(F^{-1})'(w) = (F'(u))^{-1}$ . Moreover,  $F'(u)$  and consequently  $F'(u)^{-1}$  are positive definite. We define  $u(w, \Phi) := F^{-1}(w - z\Phi)$ . Then

$$\frac{\partial}{\partial \Phi} \sum_{i=1}^n z_i u_i(w, \Phi) = - \sum_{i,j=1}^n z_i z_j (F'(u)^{-1})_{ij} \quad \text{with } u = u(w, \Phi)$$

is negative, which means that  $\Phi \mapsto \sum_{i=1}^n z_i u_i(w, \Phi)$  is decreasing.  $\square$

Lemma 4 shows that, with  $u = u(w, \Phi)$ ,

$$w_i = F_i(u) + z_i \Phi = \sigma \log u_i + p_i(u) + z_i \Phi, \quad i = 1, \dots, n.$$



**Lemma 5.** *Let  $w \in L^\infty(\Omega; \mathbb{R}^n)$  and  $\Phi_D \in L^\infty(\Omega)$ . Then there exists a unique weak solution  $\Phi \in H^1(\Omega) \cap L^\infty(\Omega)$  to*

$$(12) \quad -\Delta\Phi = \sum_{i=1}^n z_i u_i(w, \Phi) \quad \text{in } \Omega, \quad \Phi = \Phi_D \quad \text{on } \Gamma_D, \quad \nabla\Phi \cdot \nu = 0 \quad \text{on } \Gamma_N.$$

*Proof.* The existence and uniqueness of  $\Phi - \Phi_D \in H_D^1(\Omega)$  to (12) follows from the monotonicity of  $\Phi \mapsto -\sum_{i=1}^n z_i u_i(w, \Phi)$ . The boundedness of  $\Phi$  is a consequence of the Stampacchia truncation method [38, Sec. 2.3]. Indeed, let  $m > m_0 := \|\Phi_D\|_{L^\infty(\Omega)}$  and use  $(\Phi - m)^+ = \max\{0, \Phi - m\}$  as a test function in the weak formulation of (12):

$$\begin{aligned} \int_{\Omega} |\nabla(\Phi - m)^+|^2 dx &= \sum_{i=1}^n \int_{\Omega} z_i (u_i(w, \Phi) - u_i(w, m)) (\Phi - m)^+ dx \\ &+ \sum_{i=1}^n \int_{\Omega} z_i u_i(w, m) (\Phi - m)^+ dx \leq \sum_{i=1}^n \int_{\Omega} z_i u_i(w, m_0) (\Phi - m)^+ dx \\ &= C(\|w\|_{L^\infty(\Omega)}) \|(\Phi - m)^+\|_{L^2(\Omega)} g(m)^{1/2} \leq C \|\nabla(\Phi - m)^+\|_{L^2(\Omega)} g(m)^{1/2}, \end{aligned}$$

where  $g(m) = \text{meas}(\{\Phi > m\})$  and we used the Poincaré inequality. This shows that

$$\|\nabla(\Phi - m)^+\|_{L^2(\Omega)} \leq C g(m)^{1/2}.$$

By the Poincaré–Sobolev inequality, for  $2 < r < 2d/(d-2)$  ( $2 < r < \infty$  if  $d \leq 2$ ) and  $M > m$ ,

$$\begin{aligned} C \|\nabla(\Phi - m)^+\|_{L^2(\Omega)} &\geq \|(\Phi - m)^+\|_{L^r(\Omega)} \geq \left( \int_{\{\Phi > M\}} [(\Phi - m)^+]^r dx \right)^{1/r} \\ &\geq \left( \int_{\{\Phi > M\}} (M - m)^r dx \right)^{1/r} = (M - m) g(M)^{1/r}, \end{aligned}$$

and therefore,  $g(M) \leq C(M - m)^{-r} g(m)^{r/2}$ . (In this paper,  $C > 0$  is a generic constant whose value may change from line to line.) Since  $r/2 > 1$ , it follows from Stampacchia’s lemma [38, Lemma 2.9] that there exists  $M_0 > 0$  (depending on  $m_0$ ) such that  $g(M_0 + m_0) = 0$ . Consequently,  $\Phi \leq M_1 := M_0 + m_0$  in  $\Omega$ . We can prove  $\Phi \geq M_2$  for some  $M_2 \in \mathbb{R}$  in a similar way.  $\square$

This result also holds for homogeneous Neumann boundary conditions if  $\sum_{i=1}^n \int_{\Omega} z_i u_i^0 dx = 0$  in  $\Omega$ . (Instead of the Poincaré inequality, we need the Poincaré–Wirtinger inequality.) The solution  $\Phi$  is unique if we require that  $\int_{\Omega} \Phi dx = 0$ .

**2.2. Definition of an approximate problem.** Let  $T > 0$ ,  $N \in \mathbb{N}$ ,  $\tau = T/N > 0$ , and let  $m \in \mathbb{N}$  be such that  $m > d/2$ . This implies that the embedding  $H^m(\Omega) \hookrightarrow L^\infty(\Omega)$  is compact. We approximate the function  $w(x, k\tau)$  by the piecewise constant in time function  $w^k(x)$  and add a regularizing term. For this, let  $w^{k-1} \in L^\infty(\Omega; \mathbb{R}^n)$  be given and let  $\Phi^{k-1} - \Phi_D \in H_D^1(\Omega) \cap L^\infty(\Omega)$  be the unique solution to (12) with  $w = w^{k-1}$ . We

introduce  $u^{k-1} = u(w^{k-1}, \Phi^{k-1})$ , where  $u(w, \Phi)$  is defined in Lemma 4. Recall that  $u_i^k > 0$  in  $\Omega$  by construction. In particular,

$$(13) \quad w_i^k = \sigma \log u_i^k + z_i \Phi^k + \sum_{j=1}^n a_{ij} u_j^k, \quad \text{where } u_i^k = u_i(w^k, \Phi^k), \quad i = 1, \dots, n.$$

If  $k = 1$ , let  $\Phi^0 \in H^1(\Omega)$  be the unique solution to  $-\Delta \Phi^0 = \sum_{i=1}^n z_i u_i^0$  in  $\Omega$  with the boundary conditions in (4) and set  $w_i^0 = \sigma \log u_i^0 + z_i \Phi^0 + p_i(u^0)$ .

We wish to find  $w^k \in H^m(\Omega; \mathbb{R}^n)$  and  $\Phi^k - \Phi_D \in H_D^1(\Omega) \cap L^\infty(\Omega)$  such that

$$(14) \quad \begin{aligned} & \frac{1}{\tau} \int_{\Omega} (u(w^k, \Phi^k) - u(w^{k-1}, \Phi^{k-1})) \cdot \phi dx \\ & + \sum_{i=1}^n \int_{\Omega} u_i(w^k, \Phi^k) \nabla w_i^k \cdot \nabla \phi_i dx + \varepsilon b(w^k, \phi) = 0, \end{aligned}$$

$$(15) \quad \int_{\Omega} \nabla \Phi^k \cdot \nabla \psi dx = \int_{\Omega} \sum_{i=1}^n z_i u_i(w^k, \Phi^k) \psi dx$$

for all  $\phi \in H^m(\Omega; \mathbb{R}^n)$  and  $\psi \in H_D^1(\Omega)$ , where

$$(16) \quad b(w^k, \phi) = \int_{\Omega} \left( \sum_{|\alpha|=m} D^\alpha w^k \cdot D^\alpha \phi + w^k \cdot \phi \right) dx,$$

$\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$  is a multi-index,  $|\alpha| = \alpha_1 + \dots + \alpha_d$ , and  $D^\alpha = \partial^{|\alpha|} / \partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}$  is a partial derivative.

**2.3. Approximate entropy inequality.** Assuming the existence of a weak solution  $(w^k, \Phi^k)$  to (14)–(15), we derive the approximate entropy inequality which is used for the fixed-point argument. We set  $u^k := u(w^k, \Phi^k)$ .

**Lemma 6** (Approximate entropy inequality). *Let  $(w^k, \Phi^k)$  be a weak solution to (14)–(15). Then, with  $H_{BR}$  defined in (7),*

$$(17) \quad H_{BR}(u^k) + \tau \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla w_i^k|^2 dx + C\varepsilon\tau \|w^k\|_{H^m(\Omega)}^2 \leq H_{BR}(u^{k-1}).$$

*Proof.* We choose  $w^k \in H^m(\Omega; \mathbb{R}^n)$  as a test function in (14) and use the generalized Poincaré inequality [37, Chap. 2, Sec. 1.4], which gives  $b(w^k, w^k) \geq C \|w^k\|_{H^m(\Omega)}^2$ , to find that

$$\int_{\Omega} (u^k - u^{k-1}) \cdot w^k dx + \tau \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla w_i^k|^2 dx + C\varepsilon\tau \|w^k\|_{H^m(\Omega)}^2 \leq 0.$$

We rewrite the first term as

$$(18) \quad \int_{\Omega} (u^k - u^{k-1}) \cdot w^k dx = \sigma \sum_{i=1}^n \int_{\Omega} (u_i^k - u_i^{k-1}) \log u_i^k dx$$

$$\begin{aligned}
& + \sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i^k - u_i^{k-1})u_j^k dx + \sum_{i=1}^n \int_{\Omega} z_i(u_i^k - u_i^{k-1})(\Phi^k - \Phi_D) dx \\
& + \sum_{i=1}^n \int_{\Omega} z_i(u_i^k - u_i^{k-1})\Phi_D dx.
\end{aligned}$$

We estimate the integrals on the right-hand side term by term. The convexity of  $u \mapsto \sum_{i=1}^n u_i(\log u_i - 1)$  implies that

$$\sigma \sum_{i=1}^n \int_{\Omega} (u_i^k - u_i^{k-1}) \log u_i^k dx \geq \sigma \sum_{i=1}^n \int_{\Omega} (u_i^k(\log u_i^k - 1) - u_i^{k-1}(\log u_i^{k-1} - 1)) dx.$$

We deduce from the symmetry and positive semidefiniteness of  $(a_{ij})$  that

$$\begin{aligned}
\sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i^k - u_i^{k-1})u_j^k dx & = \sum_{i,j=1}^n \int_{\Omega} a_{ij} \left( u_i^k u_j^k - \frac{1}{2} u_i^{k-1} u_j^k - \frac{1}{2} u_i^k u_j^{k-1} \right) dx \\
& = \frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij} (u_i^k u_j^k - u_i^{k-1} u_j^{k-1}) dx + \frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij} (u_i^k - u_i^{k-1})(u_j^k - u_j^{k-1}) dx \\
& \geq \frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij} (u_i^k u_j^k - u_i^{k-1} u_j^{k-1}) dx.
\end{aligned}$$

Finally, taking into account the Poisson equation, we have

$$\begin{aligned}
\sum_{i=1}^n \int_{\Omega} z_i(u_i^k - u_i^{k-1})(\Phi^k - \Phi_D) dx & = \int_{\Omega} \nabla(\Phi^k - \Phi^{k-1}) \cdot \nabla(\Phi^k - \Phi_D) dx \\
& = \frac{1}{2} \int_{\Omega} (|\nabla(\Phi^k - \Phi_D)|^2 - |\nabla(\Phi^{k-1} - \Phi_D)|^2) dx + \frac{1}{2} \int_{\Omega} |\nabla(\Phi^k - \Phi^{k-1})|^2 dx \\
& \geq \frac{1}{2} \int_{\Omega} |\nabla(\Phi^k - \Phi_D)|^2 dx - \frac{1}{2} \int_{\Omega} |\nabla(\Phi^{k-1} - \Phi_D)|^2 dx.
\end{aligned}$$

Hence, by the definition of  $h_{BR}$  in (7), it follows from (18) that

$$\sum_{i=1}^n \int_{\Omega} (u_i^k - u_i^{k-1}) \cdot w_i^k dx \geq \int_{\Omega} (h_{BR}(u^k) - h_{BR}(u^{k-1})) dx.$$

We conclude that

$$H_{BR}(u^k) - H_{BR}(u^{k-1}) + \tau \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla w_i^k|^2 dx + C\varepsilon\tau \|w^k\|_{H^m(\Omega)}^2 \leq 0.$$

This finishes the proof.  $\square$

We can derive uniform gradient bounds from the entropy inequality. This is the key step of the proof.

**Lemma 7** (Entropy production estimate). *There exists  $C > 0$  independent of  $(\varepsilon, \tau)$  such that*

$$\begin{aligned} \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla w_i^k|^2 dx &\geq \sum_{i=1}^n \int_{\Omega} (4\sigma^2 |\nabla (u_i^k)^{1/2}|^2 + \alpha \sigma |\nabla u_i^k|^2 \\ &\quad + u_i^k |\nabla (p_i(u^k) + z_i \Phi^k)|^2) dx - C\sigma (H_{BR}(u^k) + 1). \end{aligned}$$

*Proof.* We expand  $u_i^k |\nabla w_i^k|^2$  by inserting definition (13) of  $w_i^k$ :

$$\begin{aligned} \sum_{i=1}^n u_i^k |\nabla w_i^k|^2 &= \sigma^2 \sum_{i=1}^n u_i^k |\nabla \log u_i^k|^2 + \sum_{i=1}^n u_i^k |\nabla (p_i(u^k) + z_i \Phi^k)|^2 \\ &\quad + 2\sigma \sum_{i=1}^n u_i^k \nabla \log u_i^k \cdot \nabla (p_i(u^k) + z_i \Phi^k) \\ &= 4\sigma^2 \sum_{i=1}^n |\nabla (u_i^k)^{1/2}|^2 + \sum_{i=1}^n u_i^k |\nabla (p_i(u^k) + z_i \Phi^k)|^2 \\ &\quad + 2\sigma \sum_{i,j=1}^n a_{ij} \nabla u_i^k \cdot \nabla u_j^k + 2\sigma \sum_{i=1}^n z_i \nabla u_i^k \cdot \nabla \Phi^k \\ &\geq 4\sigma^2 \sum_{i=1}^n |\nabla (u_i^k)^{1/2}|^2 + \sum_{i=1}^n u_i^k |\nabla (p_i(u^k) + z_i \Phi^k)|^2 \\ &\quad + \alpha \sigma \sum_{i=1}^n |\nabla u_i^k|^2 - \frac{\sigma}{\alpha} \sum_{i=1}^n z_i^2 |\nabla \Phi^k|^2, \end{aligned}$$

where we used  $\sum_{i,j=1}^n a_{ij} \xi_i \xi_j \geq \alpha |\xi|^2$  for  $\xi \in \mathbb{R}^n$  ( $\alpha > 0$  is the smallest eigenvalue of  $(a_{ij})$ ) and Young's inequality in the last step. The last term is estimated according to

$$\frac{\sigma}{\alpha} \sum_{i=1}^n z_i^2 |\nabla \Phi^k|^2 \leq C\sigma (h_{BR}(u^k) + 1),$$

where  $C > 0$  depends on the  $H^1(\Omega)$  norm of  $\Phi_D$ , which ends the proof.  $\square$

Lemmas 6 and 7 imply the following uniform bounds.

**Lemma 8** (Uniform bounds). *Let  $\tau > 0$  be sufficiently small. Then there exists  $C > 0$  independent of  $\varepsilon$  and  $\tau$  such that*

$$(19) \quad \sup_{k=1, \dots, N} \|u^k\|_{L^2(\Omega)} + \tau \sum_{k=1}^N \left( \sum_{i=1}^n \|(u_i^k)^{1/2}\|_{H^1(\Omega)}^2 + \|u^k\|_{H^1(\Omega)}^2 \right) \\ + \tau \sum_{k=1}^N \left( \sum_{i=1}^n \|(u_i^k)^{1/2} \nabla w_i^k\|_{L^2(\Omega)}^2 + \varepsilon \|w^k\|_{H^m(\Omega)}^2 \right) \leq C.$$

If Assumption (A5) holds then, for some constant  $C > 0$  independent of  $\varepsilon$  and  $\tau$ ,

$$(20) \quad \tau \sum_{i=1}^n \int_{\Omega} u_i^k (|\nabla p_i(u^k)|^2 + |\nabla \Phi^k|^2) dx \leq C.$$

*Proof.* We insert the entropy production estimate of Lemma 7 into the entropy inequality of Lemma 6,

$$(1 - \tau\sigma C)H_{BR}(u^k) + \tau \sum_{i=1}^n \int_{\Omega} (4\sigma^2 |\nabla(u_i^k)^{1/2}|^2 + \alpha\sigma |\nabla u_i^k|^2 + u_i^k |\nabla(p_i(u^k) + z_i \Phi^k)|^2) dx + C\varepsilon\tau \|w^k\|_{H^m(\Omega)}^2 \leq H_{BR}(u^{k-1}) + C\tau\sigma,$$

and sum the resulting inequality over  $k = 1, \dots, j$  for  $1 < j \leq N$ :

$$\begin{aligned} (1 - \tau\sigma C)H_{BR}(u^j) + \tau \sum_{k=1}^j \sum_{i=1}^n \int_{\Omega} (4\sigma^2 |\nabla(u_i^k)^{1/2}|^2 + \alpha\sigma |\nabla u_i^k|^2 + u_i^k |\nabla(p_i(u^k) + z_i \Phi^k)|^2) dx + C\varepsilon\tau \sum_{k=1}^j \|w^k\|_{H^m(\Omega)}^2 \\ \leq H_{BR}(u^0) + C\sigma\tau + C\tau \sum_{k=1}^{j-1} H_{BR}(u^k). \end{aligned}$$

Choosing  $0 < \tau < 1/(C\sigma)$ , the discrete Gronwall inequality [6] shows that for all  $j \leq N$ ,

$$H_{BR}(u^j) \leq \frac{H_{BR}(u^0) + C(T)}{1 - \tau\sigma C} e^{CT},$$

which leads to

$$(21) \quad H_{BR}(u^j) + C\tau\sigma \sum_{k=1}^j \left( \sigma \sum_{i=1}^n \|\nabla(u_i^k)^{1/2}\|_{L^2(\Omega)}^2 + \|\nabla u^k\|_{L^2(\Omega)}^2 \right) dx + \tau \sum_{k=1}^j \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla(p_i(u^k) + z_i \Phi^k)|^2 dx + C\varepsilon\tau \sum_{k=1}^j \|w^k\|_{H^m(\Omega)}^2 \leq C(u^0, T).$$

We deduce from the positive definiteness of  $(a_{ij})$  that  $\|u^j\|_{L^2(\Omega)}$  is bounded uniformly in  $(\varepsilon, \tau)$  and uniformly for  $j = 1, \dots, N$ . Then estimate (19) follows from the Poincaré–Wirtinger inequality.

Next, we prove estimate (20). We infer from (21) that

$$(22) \quad \tau \sum_{k=1}^N \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla p_i(u^k)|^2 dx \leq 2\tau \sum_{k=1}^N \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla(p_i(u^k) + z_i \Phi^k)|^2 dx + 2\tau \sum_{k=1}^N \sum_{i=1}^n \int_{\Omega} z_i^2 u_i^k |\nabla \Phi^k|^2 dx$$

$$\leq C + C\tau \sum_{k=1}^N \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla \Phi^k|^2 dx.$$

We use the fact that the embedding  $H^2(\Omega) \hookrightarrow W^{1,4}(\Omega)$  is continuous for  $d \leq 4$  to estimate

$$\begin{aligned} \tau \sum_{k=1}^N \int_{\Omega} u_i^k |\nabla \Phi^k|^2 dx &\leq \tau \sum_{k=1}^N \|u_i^k\|_{L^2(\Omega)} \|\nabla \Phi^k\|_{L^4(\Omega)}^2 \\ &\leq C\tau \sum_{k=1}^N \|u_i^k\|_{L^2(\Omega)} \|\Phi^k\|_{H^2(\Omega)}^2. \end{aligned}$$

To bound the  $H^2(\Omega)$  norm of  $\Phi^k$ , we deduce from Assumption (A5) that  $\|\Phi^k\|_{H^2(\Omega)} \leq C \sum_{i=1}^n \|u_i^k\|_{L^2(\Omega)} + C(\Phi_D)$ . Hence,

$$\begin{aligned} \tau \sum_{k=1}^N \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla \Phi^k|^2 dx &\leq C\tau \sum_{k=1}^N \sum_{i=1}^n \|u_i^k\|_{L^2(\Omega)}^3 + C(T) \\ &\leq CT \sum_{i=1}^n \left( \sup_{k=1, \dots, N} \|u_i^k\|_{L^2(\Omega)} \right)^3 + C(T) \leq C(T). \end{aligned}$$

Inserting this estimate into (22) concludes the proof.  $\square$

**2.4. Solution of the approximate problem.** We show that problem (14)–(15) possesses a weak solution.

**Lemma 9.** *Let  $w^{k-1} \in L^\infty(\Omega; \mathbb{R}^n)$  be given and let  $\Phi^{k-1} - \Phi_D \in H_D^1(\Omega) \cap L^\infty(\Omega)$  be the unique solution to the Poisson equation (12) with  $w = w^{k-1}$ . Then, for sufficiently small  $\tau > 0$ , there exists a solution  $w^k \in H^m(\Omega; \mathbb{R}^n)$ ,  $\Phi^k - \Phi_D \in H_D^1(\Omega) \cap L^\infty(\Omega)$  to (14)–(15).*

*Proof.* The idea is to use the Leray–Schauder fixed-point theorem. Let  $y \in L^\infty(\Omega; \mathbb{R}^n)$  and  $\delta \in [0, 1]$ . Let  $\Phi^k - \Phi_D \in H_D^1(\Omega) \cap L^\infty(\Omega)$  be the unique solution to

$$\int_{\Omega} \nabla \Phi^k \cdot \nabla \psi dx = \int_{\Omega} \sum_{i=1}^n z_i u_i(y, \Phi^k) \psi dx$$

for test functions  $\psi \in H_D^1(\Omega)$ , where  $u_i(y, \Phi)$  is defined in Lemma 4. Next, consider the linear problem

$$(23) \quad a(v, \phi) = F(\phi) \quad \text{for all } \phi \in H^m(\Omega; \mathbb{R}^n),$$

where

$$\begin{aligned} a(v, \phi) &= \delta \sum_{i=1}^n \int_{\Omega} u_i(y, \Phi^k) \nabla v_i \cdot \nabla \phi_i dx + \varepsilon b(v, \phi), \\ F(\phi) &= -\frac{\delta}{\tau} \int_{\Omega} (u(y, \Phi^k) - u(w^{k-1}, \Phi^{k-1})) \cdot \phi dx, \end{aligned}$$

recalling definition (16) of  $b$ . By the generalized Poincaré inequality, the bilinear form  $a$  is coercive on  $H^m(\Omega)$ :

$$a(v, v) = \delta \sum_{i=1}^n \int_{\Omega} u_i(y, \Phi^k) |\nabla v_i|^2 dx + \varepsilon b(v, v) \geq C\varepsilon \|v\|_{H^m(\Omega)}^2.$$

Moreover,  $a$  and  $F$  are continuous since  $u_i(y, \Phi^k) \in L^\infty(\Omega)$ . By the Lax–Milgram lemma, there exists a unique  $y \in H^m(\Omega; \mathbb{R}^n) \hookrightarrow L^\infty(\Omega; \mathbb{R}^n)$  to (23).

This defines the fixed-point operator  $S : L^\infty(\Omega; \mathbb{R}^n) \times [0, 1] \rightarrow L^\infty(\Omega; \mathbb{R}^n)$ . It holds that  $S(y, 0) = 0$  for all  $y \in L^\infty(\Omega; \mathbb{R}^n)$ . The continuity of  $S$  can be shown as in proof of Lemma 5 in [24]. The compactness of  $S$  follows from the compactness of the embedding  $H^m(\Omega; \mathbb{R}^n) \hookrightarrow L^\infty(\Omega; \mathbb{R}^n)$ . It remains to determine a uniform estimate for all fixed points of  $S(\cdot, \delta)$ . Let  $w^k \in H^m(\Omega; \mathbb{R}^n)$  be such a fixed point. If  $\delta = 0$ , there is nothing to show. Hence, let  $\delta > 0$ . Proceeding as in the proof of Lemma 6, we obtain the inequality

$$\delta H_{BR}(u^k) + C\varepsilon\tau \|w^k\|_{H^m(\Omega)}^2 \leq \delta H_{BR}(u^{k-1}) \leq H_{BR}(u^{k-1}),$$

where  $u^k = u(w^k, \Phi^k)$ . Choosing  $0 < \tau < 1/(C\sigma)$ , this provides a uniform estimate for  $w^k$  in  $H^m(\Omega; \mathbb{R}^n)$  and consequently in  $L^\infty(\Omega; \mathbb{R}^n)$ , which is the desired uniform bound. The Leray–Schauder theorem implies the existence of a fixed point of  $S(\cdot, 1)$ , which is a solution to (14), where  $\Phi^k$  solves (15).  $\square$

**2.5. Limit  $\varepsilon \rightarrow 0$ .** We perform first the limit  $\varepsilon \rightarrow 0$ . (The existence of a weak solution can be proved by performing the simultaneous limit  $(\varepsilon, \tau) \rightarrow 0$ , but we need the limit  $\varepsilon \rightarrow 0$  to show an inequality for the entropy  $H_R$ .) For this, we fix  $k \in \{1, \dots, n\}$  and set  $w_i^\varepsilon := w_i^k$ ,  $\Phi^\varepsilon := \Phi^k$ , and  $u_i^\varepsilon := u_i^k$ . The uniform estimates of Lemma 8 imply the existence of a subsequence, which is not relabeled, such that

$$\begin{aligned} (u_i^\varepsilon)^{1/2} &\rightharpoonup \sqrt{u_i}, \quad u_i^\varepsilon \rightharpoonup u_i \quad \text{weakly in } H^1(\Omega), \quad \nabla \Phi^\varepsilon \rightharpoonup \nabla \Phi \quad \text{weakly in } L^2(\Omega), \\ u_i^\varepsilon &\rightarrow u_i \quad \text{strongly in } L^2(\Omega), \quad \varepsilon w_i^\varepsilon \rightarrow 0 \quad \text{strongly in } H^m(\Omega) \quad \text{as } \varepsilon \rightarrow 0 \end{aligned}$$

for  $i = 1, \dots, n$ . This shows that

$$\begin{aligned} (u_i^\varepsilon)^{1/2} \nabla w_i^\varepsilon &= 2\sigma \nabla (u_i^\varepsilon)^{1/2} + z_i (u_i^\varepsilon)^{1/2} \nabla \Phi^\varepsilon + (u_i^\varepsilon)^{1/2} \sum_{j=1}^n a_{ij} \nabla u_j^\varepsilon \\ &\rightharpoonup 2\sigma \nabla \sqrt{u_i} + z_i \sqrt{u_i} \nabla \Phi + \sqrt{u_i} \sum_{j=1}^n a_{ij} \nabla u_j = \sqrt{u_i} \nabla w_i \end{aligned}$$

weakly in  $L^{4/3}(\Omega)$ , where we defined

$$w_i = \sigma \log u_i + z_i \Phi + \sum_{j=1}^n a_{ij} u_j \quad \text{on } \{u_i > 0\}, \quad w_i = 0 \quad \text{on } \{u_i = 0\}.$$

In fact, in view of the uniform  $L^2(\Omega)$  bound for  $(u_i^\varepsilon)^{1/2} \nabla w_i^\varepsilon$  from Lemma 8, the weak convergence holds even in  $L^2(\Omega)$ . Notice that  $\nabla w_i$  may not exist but  $\sqrt{u_i} \nabla w_i$  is a function in  $L^2(\Omega)$ . Since  $u_i \in H^1(\Omega) \hookrightarrow L^4(\Omega)$  for  $d \leq 4$ , we have  $u_i \nabla w_i \in L^{4/3}(\Omega)$ .

The convergences allow us to pass to the limit in the approximate problem (14)–(15), showing that  $u^k := u \in L^2(\Omega; \mathbb{R}^n)$  and  $\Phi^k - \Phi_D := \Phi - \Phi_D \in H_D^1(\Omega)$  is a solution to

$$(24) \quad \frac{1}{\tau} \int_{\Omega} (u^k - u^{k-1}) \cdot \phi dx + \sum_{i=1}^n \int_{\Omega} u_i^k \nabla w_i^k \cdot \nabla \phi_i dx = 0,$$

$$(25) \quad \int_{\Omega} \nabla \Phi^k \cdot \nabla \psi dx = \int_{\Omega} \sum_{i=1}^n z_i u_i^k \psi dx$$

for all  $\phi \in W^{1,4}(\Omega; \mathbb{R}^n)$  and  $\psi \in H_D^1(\Omega)$ . We wish to pass to the limit  $\varepsilon \rightarrow 0$  in the entropy inequality of Lemma 6. For this, we recall that  $u_i^\varepsilon \rightarrow u_i^k$  strongly in  $L^2(\Omega)$ , and  $\nabla \Phi^\varepsilon \rightarrow \nabla \Phi^k$ ,  $(u_i^\varepsilon)^{1/2} \nabla w_i^\varepsilon \rightharpoonup (u_i^k)^{1/2} \nabla w_i^k$  weakly in  $L^2(\Omega)$ . Therefore, by the weakly lower semicontinuity of convex continuous functions, the limit  $\varepsilon \rightarrow 0$  in (17) leads to

$$(26) \quad H_{BR}(u^k) + \tau \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla w_i^k|^2 dx \leq H_{BR}(u^{k-1}).$$

**Lemma 10.** *It holds that*

$$\begin{aligned} H_R(u^k) + \tau \sigma \sum_{i,j=1}^n \int_{\Omega} a_{ij} \nabla u_i^k \cdot \nabla u_j^k dx + \tau \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla (p_i(u^k) + z_i \Phi^k)|^2 dx \\ \leq H_R(u^{k-1}) - \tau \sigma \sum_{i=1}^n \int_{\Omega} z_i \nabla u_i^k \cdot \nabla \Phi^k dx, \end{aligned}$$

recalling definition (7) of  $H_R$ .

*Proof.* We wish to use  $\phi_i = p_i(u^k) + z_i \Phi^k$  as a test function in (24) but this function is not an element of  $W^{1,4}(\Omega)$ . In fact, we can extend the test function space for (24). Let  $V_i^k := \{\psi \in H^1(\Omega) : (u_i^k)^{1/2} \nabla \psi \in L^2(\Omega)\}$ . Then  $W^{1,4}(\Omega) \subset V_i^k$  (here we use  $u_i^k \in L^2(\Omega)$ ) and  $W^{1,4}(\Omega)$  is dense in  $V_i^k$ . Therefore, we can replace the test function space  $W^{1,4}(\Omega)$  by  $V_i^k$ . By estimate (20) (here we need Assumption (A5)),  $p_i(u^k)$  and  $\Phi^k$  are elements of  $V_i^k$ , such that we can use  $\phi_i$  as a test function in (24). Then

$$0 = I_1 + I_2 + I_3, \quad \text{where}$$

$$I_1 = \sum_{i=1}^n \int_{\Omega} (u_i^k - u_i^{k-1}) p_i(u^k) dx, \quad I_2 = \sum_{i=1}^n \int_{\Omega} z_i (u_i^k - u_i^{k-1}) \Phi^k dx,$$

$$I_3 = \tau \sum_{i=1}^n \int_{\Omega} u_i^k \nabla w_i^k \cdot \nabla (p_i(u^k) + z_i \Phi^k) dx.$$

As in the proof of (18), we find that

$$I_1 = \sum_{i,j=1}^n \int_{\Omega} a_{ij} (u_i^k - u_i^{k-1}) u_j^k dx \geq \frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij} (u_i^k u_j^k - u_i^{k-1} u_j^{k-1}) dx.$$



We use the Poisson equation (25) and integrate by parts to estimate the term  $I_2$ :

$$\begin{aligned}
I_2 &= \sum_{i=1}^n \int_{\Omega} (u_i^k - u_i^{k-1})(\Phi^k - \Phi_D) dx + \sum_{i=1}^n \int_{\Omega} z_i(u_i^k - u_i^{k-1})\Phi_D dx \\
&= - \int_{\Omega} \Delta(\Phi^k - \Phi^{k-1})(\Phi^k - \Phi_D) dx + \sum_{i=1}^n \int_{\Omega} z_i(u_i^k - u_i^{k-1})\Phi_D dx \\
&= \int_{\Omega} \nabla((\Phi^k - \Phi_D) - (\Phi^{k-1} - \Phi_D)) \cdot \nabla(\Phi^k - \Phi_D) dx + \sum_{i=1}^n \int_{\Omega} z_i(u_i^k - u_i^{k-1})\Phi_D dx \\
&\geq \left( \frac{1}{2} \int_{\Omega} |\nabla(\Phi^k - \Phi_D)|^2 dx + \sum_{i=1}^n \int_{\Omega} z_i u_i^k \Phi_D dx \right) \\
&\quad - \left( \frac{1}{2} \int_{\Omega} |\nabla(\Phi^{k-1} - \Phi_D)|^2 dx + \sum_{i=1}^n \int_{\Omega} z_i u_i^{k-1} \Phi_D dx \right).
\end{aligned}$$

This shows that  $I_1 + I_2 \geq H_R(u^k) - H_R(u^{k-1})$ . Finally, we rewrite  $I_3$ , decomposing  $w_i^k = \sigma \log u_i^k + (p_i(u^k) + z_i \Phi^k)$ :

$$\begin{aligned}
I_3 &= \tau \sum_{i=1}^n \int_{\Omega} u_i^k \nabla(\sigma \log u_i^k + (p_i(u^k) + z_i \Phi^k)) \cdot \nabla((p_i(u^k) + z_i \Phi^k)) dx \\
&= \tau \sum_{i=1}^n \int_{\Omega} u_i^k |\nabla(p_i(u^k) + z_i \Phi^k)|^2 dx + \tau \sigma \sum_{i,j=1}^n \int_{\Omega} a_{ij} \nabla u_i^k \cdot \nabla u_j^k dx \\
&\quad + \tau \sigma \sum_{i=1}^n \int_{\Omega} z_i \nabla u_i^k \cdot \nabla \Phi^k dx,
\end{aligned}$$

ending the proof.  $\square$

**2.6. Limit  $\tau \rightarrow 0$ .** 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  $x \in \Omega$  and  $t \in ((k-1)\tau, k\tau]$  and the shift operator  $(\sigma_{\tau} u^{(\tau)})(\cdot, t) = u^{k-1}$  for  $t \in ((k-1)\tau, k\tau]$ . Then equations (14)–(15) become

$$(27) \quad \frac{1}{\tau} \int_0^T \int_{\Omega} (u^{(\tau)} - \sigma_{\tau} u^{(\tau)}) \cdot \phi dx dt + \sum_{i=1}^n \int_0^T \int_{\Omega} u_i^{(\tau)} \nabla w_i^{(\tau)} \cdot \nabla \phi_i dx dt = 0,$$

$$(28) \quad \int_0^T \int_{\Omega} \nabla \Phi^{(\tau)} \cdot \nabla \psi dx dt = \int_0^T \int_{\Omega} \sum_{i=1}^n z_i u_i^{(\tau)} \psi dx dt$$

for  $\phi_i \in L^2(0, T; W^{1,4}(\Omega))$  and  $\psi \in L^2(0, T; H_D^1(\Omega))$ . We obtain from Lemma 8 the uniform estimates

$$\begin{aligned}
&\|u_i^{(\tau)}\|_{L^\infty(0,T;L^2(\Omega))} + \|u_i^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|(u_i^{(\tau)})^{1/2}\|_{L^2(0,T;H^1(\Omega))} \leq C, \\
&\|(u_i^{(\tau)})^{1/2} \nabla w_i^{(\tau)}\|_{L^2(\Omega_T)} + \|\Phi^{(\tau)}\|_{L^\infty(0,T;H^1(\Omega))} + \sqrt{\varepsilon} \|w_i^{(\tau)}\|_{L^2(0,T;H^m(\Omega))} \leq C,
\end{aligned}$$

$$(29) \quad \|(u_i^{(\tau)})^{1/2} \nabla p_i(u^{(\tau)})\|_{L^2(\Omega_T)} + \|(u_i^{(\tau)})^{1/2} \nabla \Phi^{(\tau)}\|_{L^2(\Omega_T)} \leq C,$$

where  $C > 0$  depends on  $T$  but not on  $\varepsilon$  and  $\tau$ . Estimate (29) holds under Assumption (A5) and is not needed for the existence analysis but for the derivation of the Rao-type entropy inequality.

We need a uniform bound for the discrete time derivative.

**Lemma 11** (Discrete time estimate). *There exists a constant  $C > 0$  independent of  $\varepsilon$  and  $\tau$  such that*

$$\tau^{-1} \|u_i^{(\tau)} - \sigma_\tau u_i^{(\tau)}\|_{L^2(0,T;W^{1,4}(\Omega)')} \leq C.$$

*Proof.* We use  $\phi_i \in L^2(0,T;W^{1,4}(\Omega))$  as a test function in (27):

$$\begin{aligned} \frac{1}{\tau} \left| \int_0^T \int_\Omega (u_i^{(\tau)} - \sigma_\tau u_i^{(\tau)}) \phi_i dx dt \right| &= \left| \int_0^T \int_\Omega u_i^{(\tau)} \nabla w_i^{(\tau)} \cdot \nabla \phi_i dx dt \right| \\ &\leq \|(u_i^{(\tau)})^{1/2}\|_{L^\infty(0,T;L^4(\Omega))} \|(u_i^{(\tau)})^{1/2} \nabla w_i^{(\tau)}\|_{L^2(\Omega_T)} \|\nabla \phi_i\|_{L^2(0,T;L^4(\Omega))} \\ &\leq C \|\nabla \phi_i\|_{L^2(0,T;L^4(\Omega))}, \end{aligned}$$

which finishes the proof.  $\square$

We apply the Aubin–Lions lemma in the version of [8] to conclude from the  $L^2(0,T;H^1(\Omega))$  bound for  $u^{(\tau)}$  and Lemma 11 that there exists a subsequence, which is not relabeled, such that

$$u_i^{(\tau)} \rightarrow u_i \quad \text{strongly in } L^2(\Omega_T) \text{ as } \tau \rightarrow 0.$$

Moreover, we obtain

$$\begin{aligned} \tau^{-1} (u_i^{(\tau)} - \sigma_\tau u_i^{(\tau)}) &\rightharpoonup \partial_t u_i \quad \text{weakly in } L^2(0,T;W^{1,4}(\Omega)'), \\ u_i^{(\tau)} &\rightharpoonup u_i, \quad \Phi^{(\tau)} \rightharpoonup \Phi \quad \text{weakly in } L^2(0,T;H^1(\Omega)). \end{aligned}$$

The linearity of  $p_i$  implies that

$$p_i(u^{(\tau)}) \rightharpoonup p_i(u) \quad \text{weakly in } L^2(0,T;H^1(\Omega)).$$

We infer that

$$\begin{aligned} (u_i^{(\tau)})^{1/2} \nabla w_i^{(\tau)} &= 2\sigma \nabla (u_i^{(\tau)})^{1/2} + z_i (u_i^{(\tau)})^{1/2} \nabla \Phi^{(\tau)} + (u_i^{(\tau)})^{1/2} \nabla p_i(u^{(\tau)}) \\ &\rightharpoonup 2\sigma \nabla \sqrt{u_i} + z_i \sqrt{u_i} \nabla \Phi + \sqrt{u_i} \nabla p_i(u) \quad \text{weakly in } L^2(0,T;L^{4/3}(\Omega)). \end{aligned}$$

In fact, by Lemma 8, this convergence holds in  $L^2(\Omega_T)$ . This implies that

$$\begin{aligned} u_i^{(\tau)} \nabla w_i^{(\tau)} &= (u_i^{(\tau)})^{1/2} \cdot (u_i^{(\tau)})^{1/2} \nabla w_i^{(\tau)} \\ &\rightharpoonup \sigma \nabla u_i + z_i u_i \nabla \Phi + u_i \nabla p_i(u) \quad \text{weakly in } L^2(0,T;L^{4/3}(\Omega)). \end{aligned}$$

Passing to the limit  $\tau \rightarrow 0$  in (27)–(28) yields

$$\int_0^T \langle \partial_t u_i, \phi_i \rangle dt + \int_0^T \int_\Omega u_i \nabla w_i \cdot \nabla \phi_i dx dt = 0,$$

$$\int_0^T \int_{\Omega} \nabla \Phi \cdot \nabla \psi dx dt = \int_0^T \int_{\Omega} \sum_{i=1}^n z_i u_i \psi dx dt$$

for test functions  $\phi_i \in L^2(0, T; W^{1,4}(\Omega))$  and  $\psi \in L^2(0, T; H_D^1(\Omega))$ , where  $i = 1, \dots, n$  and  $w_i$  is defined by

$$w_i = \sigma \log u_i + z_i \Phi + p_i(u) \quad \text{on } \{u_i > 0\}, \quad w_i = 0 \quad \text{on } \{u_i = 0\}.$$

It can be shown as in Step 3 of the proof of Lemma 5 in [24] that the initial conditions are satisfied in the sense of  $W^{1,4}(\Omega)'$ .

**2.7. Entropy inequalities.** We sum the entropy inequality (26) over  $k = 1, \dots, j$  with  $j \leq N$ :

$$H_{BR}(u^j) + \tau \sum_{k=1}^j \sum_{i=1}^n u_i^k |\nabla w_i^k|^2 dx \leq H_{BR}(u^0).$$

In terms of the piecewise constant in time function  $u^{(\tau)}$ , this inequality reads as

$$H_{BR}(u^{(\tau)}(t)) + \sum_{i=1}^n \int_0^t \int_{\Omega} u_i^{(\tau)} |\nabla w_i^{(\tau)}|^2 dx ds \leq H_{BR}(u^0).$$

The strong  $L^2(\Omega_T)$  convergence of  $(u^{(\tau)})$  as well as the weak  $L^2(\Omega_T)$  convergences of  $(\nabla \Phi^{(\tau)})$  and  $((u_i^{(\tau)})^{1/2} \nabla w_i^{(\tau)})$  lead to

$$H_{BR}(u(t)) + \int_0^t \int_{\Omega} u_i |\nabla w_i|^2 dx ds \leq H_{BR}(u^0).$$

This completes the proof of Theorem 1.

We wish to pass to the limit  $\tau \rightarrow 0$  in the entropy inequality of Lemma 10, which is needed for the weak–strong uniqueness property. For this, we require Assumption (A5). Summing this inequality over  $k = 1, \dots, j$  with  $j \leq N$  and writing the inequality in terms of  $u^{(\tau)}$ , we have

$$\begin{aligned} H_R(u^{(\tau)}(t)) - H_R(u^0) + \sigma \sum_{i,j=1}^n \int_0^t \int_{\Omega} a_{ij} \nabla u_i^{(\tau)} \cdot \nabla u_j^{(\tau)} dx ds \\ + \sum_{i=1}^n \int_0^t \int_{\Omega} u_i^{(\tau)} |\nabla (p_i(u^{(\tau)}) + z_i \Phi^{(\tau)})|^2 dx ds \\ \leq -\sigma \sum_{i=1}^n \int_0^t \int_{\Omega} z_i \nabla u_i^{(\tau)} \cdot \nabla \Phi^{(\tau)} dx ds. \end{aligned}$$

Using similar arguments as before, the limit  $\tau \rightarrow 0$  gives

$$(30) \quad H_R(u(t)) + \sigma \sum_{i,j=1}^n \int_0^t \int_{\Omega} a_{ij} \nabla u_i \cdot \nabla u_j dx ds + \sum_{i=1}^n \int_0^t \int_{\Omega} u_i |\nabla (p_i(u) + z_i \Phi)|^2 dx ds$$

$$\leq H_R(u^0) - \sigma \sum_{i=1}^n \int_0^t \int_{\Omega} z_i \nabla u_i \cdot \nabla \Phi dx ds.$$

**Remark 12** (Rank-one case). We have assumed that the matrix  $(a_{ij})$  is positive definite. One may ask whether we can also treat the case of positive semidefinite matrices. An idea is to use the technique of [2], extended in [9]. We only consider matrices  $(a_{ij})$  of rank one, i.e.  $a_{ij} = a > 0$  for  $i, j = 1, \dots, n$ . We also assume that  $\sigma = 0$  and  $z_i = z_0 \in \mathbb{R}$  for  $i = 1, \dots, n$ . We introduce the change of unknowns  $v := \sum_{i=1}^n u_i$  and  $v_i := u_i/v$  for  $i = 1, \dots, n$ . Summing equations (1) over  $i = 1, \dots, n$  gives the nonlinear drift-diffusion equation

$$(31) \quad \begin{aligned} \partial_t v &= \operatorname{div}(av \nabla v + z_0 v \nabla \Phi) \quad \text{in } \Omega, \quad t > 0, \\ \nabla v \cdot \nu &= 0 \quad \text{on } \partial\Omega, \quad v(\cdot, 0) = \sum_{i=1}^n u_i^0 \quad \text{in } \Omega, \end{aligned}$$

where the potential  $\Phi$  solves  $-\Delta \Phi = z_0 v$  in  $\Omega$  with mixed Dirichlet–Neumann boundary conditions. A computation shows that the relative concentrations satisfy the transport equation

$$\partial_t v_i = U \cdot \nabla v_i, \quad \text{where } U = \nabla(av + z_0 \Phi).$$

The transport equation can be solved by the method of characteristics if the transport velocity  $U$  is bounded and  $\operatorname{div} U$  is Hölder continuous. Thus, we need sufficient regularity for problem (31). Because of the porous-medium term in (31), we cannot expect classical solutions in general. However, the solutions are classical (for smooth initial data) if the potential is sufficiently regular and  $v$  is strictly positive. There are two issues. First, the mixed boundary conditions generally prevent  $\Phi$  to be a classical. This can be resolved by assuming that the Dirichlet and Neumann boundary parts do not meet [38]. Second, the positive lower bound is usually proved by using the Stampacchia truncation method. Unfortunately, this is delicate because of the different boundary conditions for  $v$  and  $\Phi$ . We leave details to future work.  $\square$

**Remark 13** (Vanishing linear diffusion). The existence result may be proved for  $\sigma = 0$ . In this case, the natural entropy is given by  $H_R$ , but the associated entropy inequality does not give suitable gradient estimates. We use instead the functional

$$H_1(u) = \int_{\Omega} \left( \sum_{i=1}^n u_i (\log u_i - 1) + \frac{1}{2} |\nabla(\Phi - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij} u_i u_j + \sum_{i=1}^n z_i u_i \Phi_D \right) dx.$$

In case  $\sigma = 0$ , the entropy variable becomes  $w_i = z_i \Phi + p_i(u)$ . Then, formally differentiating and applying Young’s inequality,

$$\frac{dH_1}{dt}(u) = - \sum_{i=1}^n \int_{\Omega} u_i \nabla(z_i \Phi + p_i(u)) \cdot \nabla(\log u_i + z_i \Phi + p_i(u)) dx$$

$$\begin{aligned}
&= - \sum_{i=1}^n \int_{\Omega} z_i \nabla u_i \cdot \nabla \Phi dx - \sum_{i,j=1}^n \int_{\Omega} a_{ij} \nabla u_i \cdot \nabla u_j dx \\
&\quad - \sum_{i=1}^n \int_{\Omega} u_i |\nabla(p_i(u) + z_i \Phi)|^2 dx \\
&\leq -\frac{\alpha}{2} \sum_{i=1}^n \int_{\Omega} |\nabla u_i|^2 dx + C \int_{\Omega} |\nabla \Phi|^2 dx.
\end{aligned}$$

Similarly as in the proof of Theorem 1, we arrive at the estimate

$$\frac{dH_{BR}}{dt}(u) + \frac{\alpha}{2} \sum_{i=1}^n \int_{\Omega} |\nabla u_i|^2 dx \leq C(H_{BR}(u) + 1),$$

which yields  $L^2(0, T; H^1(\Omega))$  bounds for  $u_i$  and an  $L^\infty(0, T; H^1(\Omega))$  bound for  $\Phi$ .

There is still an issue with the inversion of the mapping  $(w, \Phi) \mapsto u(w, \Phi)$ , since the logarithm is needed to ensure the positivity of  $u_i$ . This problem can be overcome by adding the term  $\delta \log u_i$ , i.e.  $w_i = \delta \log u_i + z_i \Phi + p_i(u)$ . Compared to the case  $\sigma > 0$ , we have to pass to the limit  $\delta \rightarrow 0$ ; see, e.g., the proof of [24, Theorem 4] for details. Still, we need to show that the limit  $\delta \rightarrow 0$  is possible in the modified approximate equations, and we leave details to the reader.  $\square$

### 3. WEAK–STRONG UNIQUENESS

In this section, we show Theorem 2. First, we rewrite the relative entropy (8).

**Lemma 14.** *It holds that*

$$\begin{aligned}
H_R(u|\bar{u}) &= H_R(u) + H_R(\bar{u}) - \frac{1}{2} \sum_{i=1}^n \int_{\Omega} a_{ij} (u_i \bar{u}_j + \bar{u}_i u_j) dx \\
&\quad - \int_{\Omega} \nabla(\Phi - \Phi_D) \cdot \nabla(\bar{\Phi} - \Phi_D) dx.
\end{aligned}$$

*Proof.* By definition (8) of  $H_R(u|\bar{u})$ ,

$$\begin{aligned}
H_R(u|\bar{u}) &= \int_{\Omega} \left( \frac{1}{2} |\nabla(\Phi - \Phi_D)|^2 - \frac{1}{2} |\nabla(\bar{\Phi} - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij} (u_i u_j - \bar{u}_i \bar{u}_j) \right. \\
&\quad \left. + \sum_{i=1}^n z_i (u_i - \bar{u}_i) \Phi_D \right) dx - \sum_{i=1}^n \int_{\Omega} \left( z_i \bar{\Phi} + \sum_{j=1}^n a_{ij} \bar{u}_j \right) (u_i - \bar{u}_i) dx \\
&= \int_{\Omega} \left( \frac{1}{2} |\nabla(\Phi - \Phi_D)|^2 - \frac{1}{2} |\nabla(\bar{\Phi} - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij} (u_i u_j + \bar{u}_i \bar{u}_j) \right) dx
\end{aligned}$$

$$- \sum_{i=1}^n \int_{\Omega} \left( z_i(u_i - \bar{u}_i)(\bar{\Phi} - \Phi_D) - \sum_{i,j=1}^n a_{ij}u_i\bar{u}_j \right) dx.$$

We use the Poisson equation to reformulate the term involving  $\bar{\Phi} - \Phi_D$ :

$$\begin{aligned} - \sum_{i=1}^n \int_{\Omega} z_i(u_i - \bar{u}_i)(\bar{\Phi} - \Phi_D) dx &= \int_{\Omega} \Delta(\Phi - \bar{\Phi})(\bar{\Phi} - \Phi_D) dx \\ &= \int_{\Omega} \Delta(\Phi - \Phi_D)(\bar{\Phi} - \Phi_D) dx - \int_{\Omega} \Delta(\bar{\Phi} - \Phi_D)(\bar{\Phi} - \Phi_D) dx \\ &= - \int_{\Omega} \nabla(\Phi - \Phi_D) \cdot \nabla(\bar{\Phi} - \Phi_D) dx + |\nabla(\bar{\Phi} - \Phi_D)|^2 dx. \end{aligned}$$

Thus, by the symmetry of  $(a_{ij})$ ,

$$\begin{aligned} H_R(u|\bar{u}) &= \int_{\Omega} \left( \frac{1}{2} |\nabla(\Phi - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij}u_iu_j \right) dx \\ &\quad + \int_{\Omega} \left( \frac{1}{2} |\nabla(\bar{\Phi} - \Phi_D)|^2 + \frac{1}{2} \sum_{i,j=1}^n a_{ij}\bar{u}_i\bar{u}_j \right) dx \\ &\quad - \int_{\Omega} \nabla(\Phi - \Phi_D) \cdot \nabla(\bar{\Phi} - \Phi_D) dx - \frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i\bar{u}_j + \bar{u}_i u_j) dx. \end{aligned}$$

Inserting the definitions of  $H_R(u)$  and  $H_R(\bar{u})$  concludes the proof.  $\square$

The solutions  $u$  and  $\bar{u}$  satisfy the entropy inequality (30). Furthermore, since the mixed terms  $u_i\bar{u}_j + \bar{u}_i u_j$  contain the strong solution and  $(a_{ij})$  is symmetric, we can compute

$$\begin{aligned} -\frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i\bar{u}_j + \bar{u}_i u_j) dx \Big|_0^t &= - \sum_{i,j=1}^n \int_0^t a_{ij} (\langle \partial_t u_i, \bar{u}_j \rangle + \langle \partial_t \bar{u}_i, u_j \rangle) ds \\ &= - \sum_{i=1}^n \int_0^t (\langle \partial_t u_i, p_i(\bar{u}) \rangle + \langle \partial_t \bar{u}_i, p_i(u) \rangle) ds \\ &= \sum_{i=1}^n \int_0^t \int_{\Omega} (u_i \nabla w_i \cdot \nabla p_i(\bar{u}) + \bar{u}_i \nabla \bar{w}_i \cdot \nabla p_i(u)) dx ds. \end{aligned}$$

where  $\bar{w}_i = \log \bar{u}_i + z_i \bar{\Phi} + p_i(\bar{u})$  on  $\{\bar{u}_i > 0\}$  and  $\bar{w}_i = 0$  on  $\{\bar{u}_i = 0\}$ . We insert the definitions of  $w_i$  and  $\bar{w}_i$ :

$$\begin{aligned} (32) \quad -\frac{1}{2} \sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i\bar{u}_j + \bar{u}_i u_j) dx \Big|_0^t &= \sigma \sum_{i,j=1}^n \int_0^t \int_{\Omega} a_{ij} (\nabla u_i \cdot \nabla \bar{u}_j + \nabla \bar{u}_i \cdot \nabla u_j) dx ds \\ &\quad + \sum_{i=1}^n \int_0^t \int_{\Omega} (z_i u_i \nabla \Phi \cdot \nabla p_i(\bar{u}) + z_i \bar{u}_i \nabla \bar{\Phi} \cdot \nabla p_i(u)) \end{aligned}$$

$$+ (u_i + \bar{u}_i) \nabla p_i(u) \cdot \nabla p_i(\bar{u}) dx ds.$$

Furthermore, using the Poisson equation,

$$\begin{aligned}
(33) \quad & - \int_{\Omega} \nabla(\Phi - \Phi_D) \cdot \nabla(\bar{\Phi} - \Phi_D) dx \Big|_0^t \\
&= - \int_0^t \int_{\Omega} (\nabla \partial_t \Phi \cdot \nabla(\bar{\Phi} - \Phi_D) + \nabla(\Phi - \Phi_D) \cdot \nabla \partial_t \bar{\Phi}) dx ds \\
&= - \sum_{i=1}^n \int_0^t z_i (\langle \partial_t u_i, \bar{\Phi} - \Phi_D \rangle + \langle \partial_t \bar{u}_i, \Phi - \Phi_D \rangle) ds \\
&= \sum_{i=1}^n \int_0^t \int_{\Omega} z_i u_i \nabla w_i \cdot \nabla(\bar{\Phi} - \Phi_D) dx ds + \sum_{i=1}^n \int_0^t \int_{\Omega} z_i \bar{u}_i \nabla \bar{w}_i \cdot \nabla(\Phi - \Phi_D) dx ds \\
&= \sum_{i=1}^n \int_0^t \int_{\Omega} z_i (\sigma \nabla u_i + u_i \nabla q_i) \cdot \nabla(\bar{\Phi} - \Phi_D) dx ds \\
&\quad + \sum_{i=1}^n \int_0^t \int_{\Omega} z_i (\sigma \nabla \bar{u}_i + \bar{u}_i \nabla \bar{q}_i) \cdot \nabla(\Phi - \Phi_D) dx ds,
\end{aligned}$$

where we have set  $q_i := p_i(u) + z_i \Phi$  and  $\bar{q}_i := p_i(\bar{u}) + z_i \bar{\Phi}$ . We add the inequalities for  $H_R(u(t))$  and  $H_R(\bar{u}(t))$  as well as the identities (32) and (33). Then some terms can be combined and after some computations, we end up with

$$\begin{aligned}
(34) \quad & H_R(u(t)|\bar{u}(t)) - H_R(u^0|\bar{u}^0) + \sigma \sum_{i,j=1}^n \int_0^t \int_{\Omega} a_{ij} \nabla(u_i - \bar{u}_i) \cdot \nabla(u_j - \bar{u}_j) dx ds \\
&\leq -\sigma \sum_{i=1}^n \int_0^t \int_{\Omega} z_i \nabla(u_i - \bar{u}_i) \cdot \nabla(\Phi - \bar{\Phi}) dx ds \\
&\quad - \sum_{i=1}^n \int_0^t \int_{\Omega} \{u_i |\nabla q_i|^2 + \bar{u}_i |\nabla \bar{q}_i|^2 - (u_i + \bar{u}_i) \nabla q_i \cdot \nabla \bar{q}_i\} dx ds \\
&= -\sigma \sum_{i=1}^n \int_0^t \int_{\Omega} z_i \nabla(u_i - \bar{u}_i) \cdot \nabla(\Phi - \bar{\Phi}) dx ds \\
&\quad - \sum_{i=1}^n \int_0^t \int_{\Omega} u_i |\nabla(q_i - \bar{q}_i)|^2 dx ds - \sum_{i=1}^n \int_0^t \int_{\Omega} (u_i - \bar{u}_i) \nabla \bar{q}_i \cdot \nabla(q_i - \bar{q}_i) dx ds.
\end{aligned}$$

By the positive definiteness, we have

$$\sigma \sum_{i,j=1}^n \int_0^t \int_{\Omega} a_{ij} \nabla(u_i - \bar{u}_i) \cdot \nabla(u_j - \bar{u}_j) dx ds \geq \alpha \sigma \sum_{i=1}^n \int_0^t \int_{\Omega} |\nabla(u_i - \bar{u}_i)|^2 dx ds.$$

We use Young's inequality for the first term on the right-hand side of (34):

$$\begin{aligned} -\sigma \sum_{i=1}^n \int_0^t \int_{\Omega} z_i \nabla(u_i - \bar{u}_i) \cdot \nabla(\Phi - \bar{\Phi}) dx ds &\leq \frac{\alpha\sigma}{2} \sum_{i=1}^n \int_0^t \int_{\Omega} |\nabla(u_i - \bar{u}_i)|^2 dx ds \\ &\quad + C(\alpha)\sigma \int_{\Omega} |\nabla(\Phi - \bar{\Phi})|^2 dx ds. \end{aligned}$$

The second term on the right-hand side of (34) is nonpositive and can be neglected. Finally, the last term in (34) is estimated according to

$$\begin{aligned} &-\sum_{i=1}^n \int_0^t \int_{\Omega} (u_i - \bar{u}_i) \nabla \bar{q}_i \cdot \nabla(q_i - \bar{q}_i) dx ds \\ &\leq \sum_{i=1}^n \|u_i - \bar{u}_i\|_{L^2(\Omega_T)} \|\nabla \bar{q}_i\|_{L^\infty(\Omega_T)} \|\nabla(p_i(u) - p_i(\bar{u})) + z_i \nabla(\Phi - \bar{\Phi})\|_{L^2(\Omega)} \\ &\leq C \sum_{i=1}^n \|u_i - \bar{u}_i\|_{L^2(\Omega_T)} \|\nabla \bar{q}_i\|_{L^\infty(\Omega_T)} (\|\nabla(u_i - \bar{u}_i)\|_{L^2(\Omega_T)} + \|\nabla(\Phi - \bar{\Phi})\|_{L^2(\Omega_T)}) \\ &\leq \frac{\alpha\sigma}{2} \sum_{i=1}^n \|\nabla(u_i - \bar{u}_i)\|_{L^2(\Omega)}^2 + C \sum_{i=1}^n \|u_i - \bar{u}_i\|_{L^2(\Omega)}^2 + C \|\nabla(\Phi - \bar{\Phi})\|_{L^2(\Omega)}^2, \end{aligned}$$

where  $C > 0$  depends on the  $L^\infty(\Omega_T)$  norm of  $\nabla \bar{q}_i$ . Adding these estimates and taking into account that

$$\sum_{i=1}^n \|u_i - \bar{u}_i\|_{L^2(\Omega)}^2 + \|\nabla(\Phi - \bar{\Phi})\|_{L^2(\Omega)}^2 \leq CH_R(u|\bar{u}),$$

we conclude from (34) that

$$H_R(u(t)|\bar{u}(t)) = H_R(u(t)|\bar{u}(t)) - H_R(u^0|\bar{u}^0) \leq C \int_0^t H_R(u|\bar{u}) ds,$$

where we used the fact that the initial data of the weak and strong solutions coincide by assumption,  $u^0 = \bar{u}^0$ . It follows from Gronwall's inequality that  $H(u(t)|\bar{u}(t)) = 0$  for  $t > 0$  and consequently  $u(t) = \bar{u}(t)$  and  $\Phi(t) = \bar{\Phi}(t)$  in  $\Omega$  for  $t > 0$ . This proves Theorem 2.

#### 4. EXPONENTIAL DECAY

We prove Theorem 3. Recall that  $\nabla \Phi \cdot \nu = 0$  on  $\partial\Omega$  in this proof. Differentiating the relative entropy  $H_{BR}(u|u^\infty)$ , defined in (10), with respect to time and taking into account mass conservation and the fact that  $u^\infty$  is constant, we find that

$$\frac{d}{dt} H_{BR}(u|u^\infty) = \frac{d}{dt} H_{BR}(u).$$



We infer from the entropy inequality (11) that

$$\begin{aligned}
(35) \quad \frac{d}{dt} H_{BR}(u|u^\infty) &\leq - \sum_{i=1}^n \int_{\Omega} u_i |\nabla w_i|^2 dx \\
&= - \sum_{i=1}^n \int_{\Omega} (4\sigma^2 |\nabla \sqrt{u_i}|^2 + u_i |\nabla(p_i(u) + z_i \Phi)|^2) dx \\
&\quad - 2\sigma \sum_{i=1}^n \int_{\Omega} (\nabla u_i \cdot \nabla p_i(u) + z_i \nabla u_i \cdot \nabla \Phi) dx.
\end{aligned}$$

(Strictly speaking, this inequality does not follow directly from (11). In fact, we can derive a similar inequality by replacing  $H_{BR}(u^0)$  by  $H_{BR}(u(s))$  with  $0 < s < t$ . Then dividing by  $s - t$  and passing to the limit  $s \rightarrow t$  yields (35).) Taking into account the positive definiteness, we obtain

$$-2\sigma \sum_{i=1}^n \int_{\Omega} \nabla u_i \cdot \nabla p_i(u) dx = -2\sigma \sum_{i,j=1}^n \int_{\Omega} a_{ij} \nabla u_i \cdot \nabla u_j dx \leq -2\alpha\sigma \sum_{i=1}^n \int_{\Omega} |\nabla u_i|^2 dx.$$

It follows from the Poincaré–Wirtinger inequality, using  $u_i^\infty = \text{meas}(\Omega)^{-1} \int_{\Omega} u_i dx$  (by mass conservation), that

$$\begin{aligned}
-2\sigma \sum_{i=1}^n \int_{\Omega} \nabla u_i \cdot \nabla p_i(u) dx &\leq -2\alpha\sigma C_P^{-1} \sum_{i=1}^n \int_{\Omega} (u_i - u_i^\infty)^2 dx \\
&\leq -C(a)\sigma \sum_{i,j=1}^n \int_{\Omega} a_{ij} (u_i - u_i^\infty)(u_j - u_j^\infty),
\end{aligned}$$

where  $C(a) = 2\alpha/(C_P \max_{i,j=1,\dots,n} |a_{ij}|)$ . We use the Poisson equation and the boundary condition  $\nabla \Phi \cdot \nu = 0$  on  $\partial\Omega$  to rewrite the last term on the right-hand side of (35):

$$\begin{aligned}
-2\sigma \sum_{i=1}^n \int_{\Omega} z_i \nabla u_i \cdot \nabla \Phi dx &= 2\sigma \int_{\Omega} \sum_{i=1}^n z_i u_i \Delta \Phi dx = -2\sigma \int_{\Omega} \left( \sum_{i=1}^n z_i u_i \right)^2 dx \\
&\leq -2\sigma \int_{\Omega} |\nabla \Phi|^2 dx,
\end{aligned}$$

where the last step is the usual elliptic estimate. By the logarithmic Sobolev inequality [25, Rem. 2.6],

$$-4\sigma^2 \sum_{i=1}^n \int_{\Omega} |\nabla \sqrt{u_i}|^2 dx \leq -4C_L \sigma^2 \sum_{i=1}^n \int_{\Omega} u_i \log \frac{u_i}{u_i^\infty} dx.$$

We combine the previous estimates to conclude from (35) that

$$\frac{d}{dt} H_{BR}(u|u^\infty) \leq - \sum_{i=1}^n \int_{\Omega} \left( 4C_L \sigma^2 u_i \log \frac{u_i}{u_i^\infty} + 2\sigma |\nabla \Phi|^2 \right)$$

$$\begin{aligned}
& + C(a)\sigma \sum_{i,j=1}^n \int_{\Omega} a_{ij}(u_i - u_i^{\infty})(u_j - u_j^{\infty}) dx \\
& \leq -\sigma \min\{2, 4C_L\sigma, C(a)\} H_{BR}(u|u^{\infty}).
\end{aligned}$$

Applying Gronwall's lemma proves the theorem. Notice that the decay rate vanishes if  $\sigma = 0$ .

## 5. NUMERICAL EXPERIMENT

We present a numerical result obtained by the software Netgen/NGSolve [33], where we use mixed Dirichlet–Neumann boundary conditions for the Poisson equation. The domain is the square  $\Omega = (0, 1)^2$  with Dirichlet conditions on the left and right sides of the square and Neumann conditions on the top and bottom sides. We consider three species. The potential on the left and right sides of the square is defined by  $\Phi_D = 0.1$ . The parameters are chosen as  $\sigma = 1$ ,  $z_1 = z_3 = -5$ ,  $z_2 = 5$ , and the matrix

$$(a_{ij}) = \begin{pmatrix} 2.5 & 1 & 1 \\ 1 & 1 & 0.5 \\ 1 & 0.5 & 0.5 \end{pmatrix}.$$

is positive definite. We choose the initial data

$$u_i(x, y) = \exp(-100(x - x_i)^2 - 100(y - y_i)^2) + 0.5, \quad i = 1, 2, 3,$$

where  $(x_1, y_1) = (0.25, 0.75)$ ,  $(x_2, y_2) = (0.5, 0.5)$ , and  $(x_3, y_3) = (0.75, 0.25)$ . For the numerical test, we have taken the mesh size 0.05 and the time step size  $4 \times 10^{-5}$ . Figure 1 shows the concentrations at the time steps  $N = 0$ ,  $N = 30$ , and  $N = 380$ . The last value corresponds to a solution that is close to the equilibrium state. At time step  $N = 380$ , the solution is rather flat in the interior of the domain, while the largest variations can be observed at the (Dirichlet) boundary. This is consistent with the numerical experiments of [13, Fig. 1A], where surface charge effects were observed at the boundary. We observe that the shape of the profile depends on the sign of the valence. The electric potential does not change significantly over time, as can be seen in Figure 2. This example shows that the concentrations converge to a (non-constant) steady state as  $t \rightarrow \infty$  in the case of mixed boundary conditions (which is expected). We note that the software is very sensible in situations where the drift or cross-diffusion terms are dominant such that in these cases a structure-preserving numerical scheme (to ensure the positivity of the densities) needs to be developed. This is left for future work.

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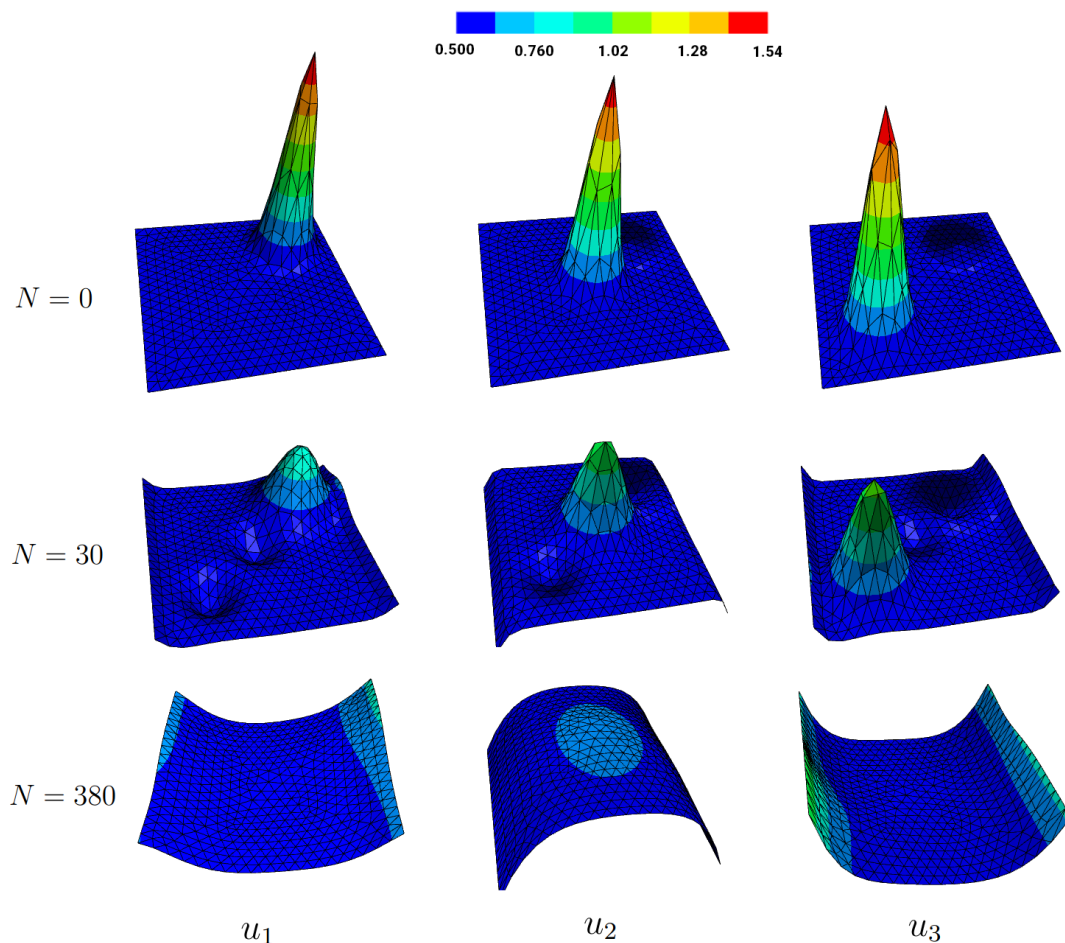


FIGURE 1. Ion concentrations  $u_1$  (left column),  $u_2$  (middle column), and  $u_3$  (right column) at time steps  $N = 0$  (top row),  $N = 30$  (middle row), and  $N = 380$  (bottom row).

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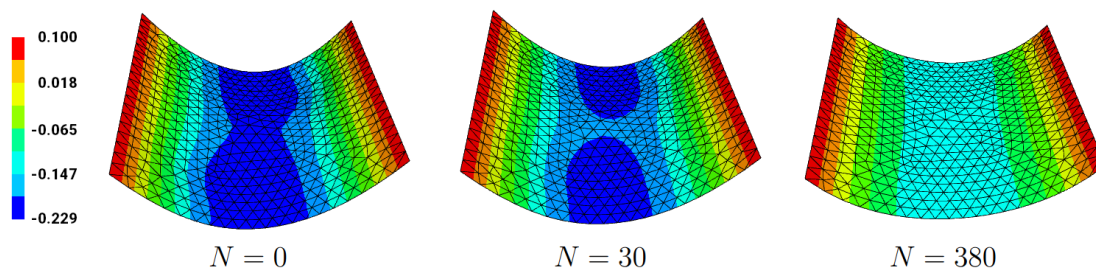


FIGURE 2. Electric potential  $\Phi$  at time steps  $N = 0$  (left),  $N = 30$  (middle), and  $N = 380$  (right).

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