



Analysis of a degenerate parabolic cross-diffusion system for ion transport [☆]



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ABSTRACT

A cross-diffusion system describing ion transport through biological membranes or nanopores in a bounded domain with mixed Dirichlet–Neumann boundary conditions is analyzed. The ion concentrations solve strongly coupled diffusion equations with a drift term involving the electric potential which is coupled to the concentrations through a Poisson equation. The global-in-time existence of bounded weak solutions and the uniqueness of weak solutions under moderate regularity assumptions are shown. The main difficulties of the analysis are the cross-diffusion terms and the degeneracy of the diffusion matrix, preventing the use of standard tools. The proofs are based on the boundedness-by-entropy method, extended to nonhomogeneous boundary conditions, and the uniqueness technique of Gajewski. A finite-volume discretization in one space dimension illustrates the large-time behavior of the numerical solutions and shows that the equilibration rates may be very small.

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1. Introduction

The transport of ions through membranes or nanopores can be described on the macroscopic level by the Poisson–Nernst–Planck equations, modeling ionic species and an electro-neutral solvent in the self-consistent field [19]. The equations can be derived in the mean-field limit from microscopic particle models [18] and lead to diffusion equations, satisfying Fick’s law for the fluxes. This ansatz breaks down in narrow ion channels if the finite size of the ions is taken into account. Including size exclusion, the mean-field model, derived from an on-lattice model in the diffusion limit [4,21] or taking into account the combined effect of the excess chemical potentials [17], leads to parabolic equations with cross-diffusion terms. The aim of this paper is to analyze the cross-diffusion system of [4].

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1.1. Model equations

The evolution of the ion concentrations (volume fractions) u_i and fluxes J_i of the i th species is governed by the equations

$$\partial_t u_i = \operatorname{div} J_i, \quad J_i = D_i(u_0 \nabla u_i - u_i \nabla u_0 + u_0 u_i (\beta z_i \nabla \Phi + \nabla W_i)) \quad (1)$$

for $i = 1, \dots, n$, where $u_0 = 1 - \sum_{i=1}^n u_i$ is the concentration (volume fraction) of the solvent. We have assumed that the molar masses are the same for all species. Varying molar masses are considered in, e.g., [6,8] in the context of the Maxwell–Stefan theory. The classical Nernst–Planck equations are obtained after setting $u_0 = 1$ [5]. They can be also coupled with fluidynamical equations; see, e.g., [24]. Modified Nernst–Planck models without volume filling, but including cross-diffusion terms, were suggested and analyzed in [13,16].

In equations (1), $D_i > 0$ denotes the diffusion coefficients, $\beta = q/(k_B \theta) > 0$ is the inverse thermal voltage (or inverse thermal energy) with the elementary charge q , the Boltzmann constant k_B , and the temperature θ , $z_i \in \mathbb{R}$ is the valence of the i th species, and $W_i = W_i(x)$ is an external potential. Note that Einstein’s relation between the diffusivity D_i and the mobility $\mu_i = qD_i/(k_B \theta) = D_i \beta$ holds. The electrical potential Φ is determined by the Poisson equation

$$-\lambda^2 \Delta \Phi = \sum_{i=1}^n z_i u_i + f, \quad (2)$$

where $\lambda > 0$ is the (scaled) permittivity, $\sum_{i=1}^n z_i u_i$ is the total charge density, and $f = f(x)$ is a permanent charge density.

Equations (1)–(2) are solved in the bounded domain $\Omega \subset \mathbb{R}^d$ ($d \geq 1$). Its boundary is supposed to consist of an insulating part Γ_N , on which no-flux boundary conditions are prescribed, and the union Γ_D of boundary contacts with external reservoirs, on which the concentrations are fixed. The electric potential is influenced by the voltage at Γ_E between two electrodes, and we assume for simplicity that $\Gamma_E = \Gamma_D$. This leads to the mixed Dirichlet–Neumann boundary conditions

$$J_i \cdot \nu = 0 \text{ on } \Gamma_N, \quad u_i = u_i^D \text{ on } \Gamma_D, \quad i = 1, \dots, n, \quad (3)$$

$$\nabla \Phi \cdot \nu = 0 \text{ on } \Gamma_N, \quad \Phi = \Phi^D \text{ on } \Gamma_D. \quad (4)$$

Finally, we prescribe the initial conditions

$$u_i(\cdot, 0) = u_i^0 \quad \text{in } \Omega, \quad i = 1, \dots, n. \quad (5)$$

Equations (1) can be written as the cross-diffusion system

$$\partial_t u_i = \operatorname{div} \left(\sum_{j=1}^n A_{ij}(u) \nabla u_j + D_i u_0 u_i \nabla F_i \right), \quad (6)$$

where $F_i = \beta z_i \Phi + W_i$ is the effective potential and the diffusion matrix $(A_{ij}(u))$ is defined by

$$A_{ii}(u) = D_i u_i, \quad A_{ij}(u) = D_i (u_0 + u_i), \quad j \neq i.$$

Mathematically, this system is strongly coupled with a nonsymmetric and generally not positive semidefinite diffusion matrix such that the existence of solutions to (6) is not trivial. A second difficulty is the fact that a maximum principle is generally not available for cross-diffusion systems, and the proof of nonnegativity

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