Poisson-Nernst-Planck System with Steric Effect

Peter Hirvonen
ongoing work with Ansgar Jüngel

TU WIEN

Model Equations

To model the influence of ion sizes for ion transport in ion channels, in [1] Lin and Eisenberg proposed the Poisson-Nernst-Planck equations with steric effect. This n-species Poisson-Nernst-Planck model for ion concentrations u_i is given by the following system of equations

$$\partial_t u_i = D_i \cdot \operatorname{div}\left(\nabla u_i + z_i u_i \nabla\Phi + u_i \sum_{j=1}^n a_{ij}\nabla u_j\right) =: D_i \operatorname{div} J_i$$

$$\Delta\Phi = -\sum_{i=1}^n z_i u_i$$

for $i = 1, \ldots, n$. We have the assumptions:

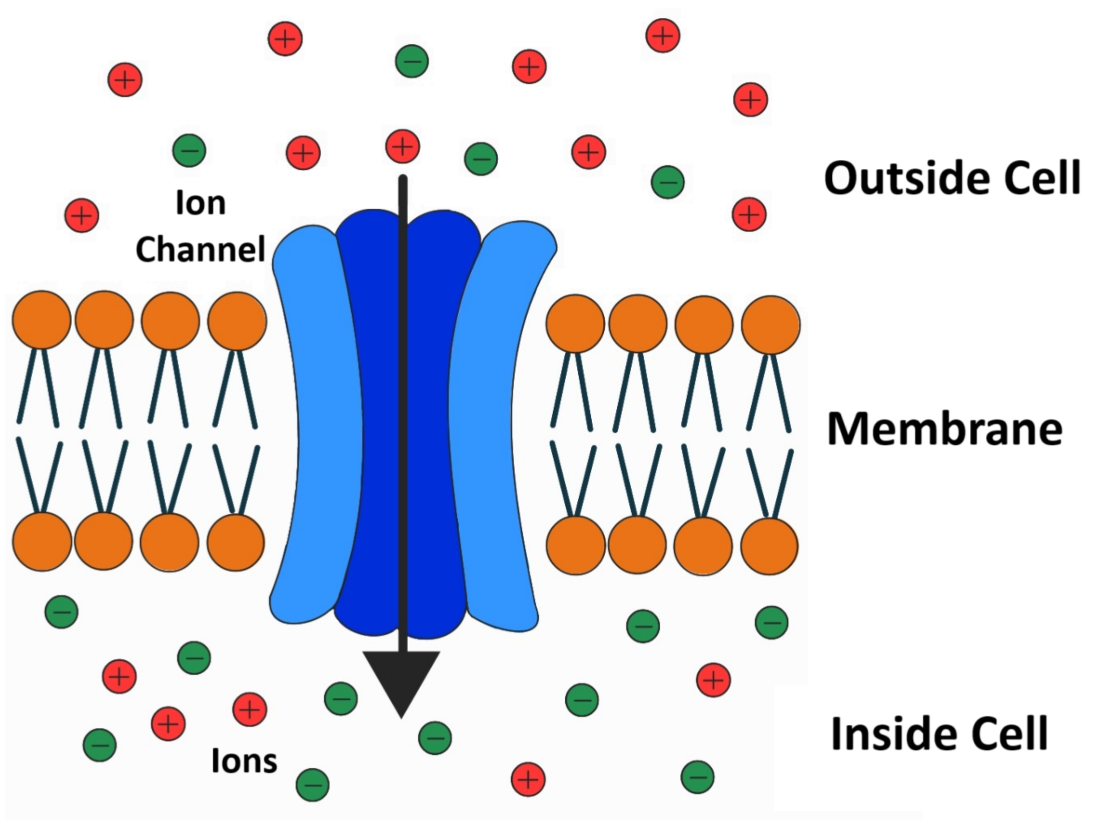
(A1) Domain: $\Omega \subseteq \mathbb{R}^d$ bounded with Lipschitz boundary $\partial\Omega = \Gamma_D \dot\cup \Gamma_N$ with $\operatorname{meas}(\Gamma_D) > 0$.

(A2) Data: $D_i > 0$, $z_i \in \mathbb{R}$, and $(a_{ij})_{i,j=1,\ldots,n}$ positive definite.

(A3) Initial Data: $u_i(0,x) = u_{i,0}(x) \in L^2(\Omega)$.

(A4) Boundary Conditions: $J_i \cdot \nu = 0$ on $\partial\Omega$, $\nabla\Phi \cdot \nu = 0$ on Γ_N, and $\Phi = \Phi^D$ on Γ_D, where $\Phi^D \in W^{1,\infty}(\Omega)$ is supposed to solve

$$\Delta\Phi^D = 0 \quad \text{in } \Omega, \quad \Phi^D \cdot \nu = 0 \quad \text{on } \Gamma_N.$$



Entropy-Structure

We define the entropy density

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + \frac{1}{2}|\nabla(\Phi - \Phi^D)|^2 + \frac{1}{2}\sum_{i,j=1}^n a_{ij}u_i u_j$$

and the entropy $H(u) = \int_\Omega h(u)dx$. Furthermore, we can define entropy variables

$$w_i - w_i^D = \frac{\partial h}{\partial u_i} = \log u_i + z_i(\Phi - \Phi^D) + \sum_{j=1}^n a_{ij}u_j,$$

where we differentiated formally and set $w_i^D = z_i\Phi^D$. By existence of an inverse to $u \mapsto w(u)$, we obtain a priori non-negativity of solutions. For the global existence proof, we will use an entropy inequality, which for constant Φ^D reads:

$$\frac{d}{dt}H(u) \leq -\sum_{i=1}^n \int_\Omega \frac{1}{u_i}\left|\nabla u_i + z_i u_i \nabla\Phi + u_i \sum_{j=1}^n a_{ij}\nabla u_j\right|^2 dx \leq 0.$$

This gives suitable gradient estimates after further calculations.

Existence of Global Weak Solutions

Theorem 1. *Consider the assumptions (A1)-(A4) from above. Let $q' = 2d+1$ and $q = (2d+2)/(2d+1)$. There exists a global weak solution (u, Φ) with*

- $u_1, \ldots, u_n \in L^2(0,T; H^1(\Omega))$,
- $\partial_t u_1, \ldots, \partial_t u_n \in L^{q'}(0,T; W^{1,q}(\Omega)')$,
- $\Phi \in L^2(0,T; H^1(\Omega))$,

to the weak problem

$$\int_0^T \langle \partial_t u_i, \varphi_i\rangle dt + \\ + \int_0^T \int_\Omega \left(\nabla u_i + z_i u_i \nabla\Phi + u_i \sum_{j=1}^n a_{ij}\nabla u_j\right) \cdot \nabla\varphi_i dx dt = 0, \tag{1}$$

$$\int_0^T \int_\Omega \nabla\Phi \cdot \nabla\theta dx dt = \int_0^T \int_\Omega \left(\sum_{i=1}^n z_i u_i\right) \theta dx dt, \tag{2}$$

for all $\varphi_i \in L^q(0,T; W^{1,q}(\Omega)), \theta \in L^2(0,T; H_D^1(\Omega)), i = 1, \ldots, n$.

Outline of Proof. We use the boundedness-by-entropy method, developed in [3], but slightly adapt the method to fit our case of coupled equation. □

Weak-Strong Uniqueness

Theorem 2. *Let (u, Φ) be a weak solution, and $(\bar u, \bar\Phi)$ be a strong solution, i.e. $\bar u_i, \bar\Phi \in L^\infty(0,T; W^{1,\infty}(\Omega))$, to (1)-(2) satisfying the same initial data. Then $u(t,x) = \bar u(t,x)$ as well as $\Phi(t,x) = \bar\Phi(t,x)$ for almost all $x \in \Omega$ and $t \in [0,T)$.*

Outline of Proof. We want to show a relative entropy inequality of the form

$$\frac{d}{dt}H(u, \Phi|\bar u, \bar\Phi) \leq C H(u, \Phi|\bar u, \bar\Phi), \tag{3}$$

where

$$H(u, \Phi|\bar u, \bar\Phi) = H(u|\bar u) + H(\Phi|\bar\Phi)$$

and

$$H(u|\bar u) = H(u) - H(\bar u) - H'(\bar u, \bar\Phi)(u - \bar u).$$

The novelty is the use of a relative Rao-entropy being an upper bound

$$H_R(u|\bar u) = \int_\Omega \sum_{i,j=1}^n a_{ij}(u_i - \bar u_i)(u_j - \bar u_j)dx \geq C\sum_{i=1}^n \|u_i - \bar u_i\|_{L^2(\Omega)}^2.$$

After proving (3), one can use Grönwall's inequality to show the result. □

Further Topics

Theorem 3. *Let $a_{ij} = \kappa > 0$ such that $(a_{ij})_{i,j=1,\ldots,n}$ is of rank one. Then for some $\alpha > 0$ there exists a classical solution $u \in C^{1+\alpha,1}(\bar\Omega_T; \mathbb{R}^d)$ under the conditions:*

$$\partial\Omega \in C^{2+\alpha}, \quad z_i = z, \quad \Phi \in C_b^2(\Omega), \quad \forall x \in \Omega : u_0(x) \geq c > 0.$$

Other interesting properties include:

- Long-time behaviour of solutions (work in progress).
- Boundedness of weak solutions (currently unsolved).

KEY REFERENCES

[1] Tai-Chia Lin and Robert (Bob) Eisenberg, A new approach to the lennard-jones potential and a new model: Pnp-steric equations, Communications in Mathematical Sciences **in the press** (2013), 149–173.

[2] Chia-Yu Hsieh, *Global existence of solutions for the poisson–nernst–planck system with steric effects*, Nonlinear Analysis: Real World Applications **50** (2019), 34–54.

[3] Ansgar Jüngel, *The boundedness-by-entropy method for cross-diffusion systems*, Nonlinearity **28** (2015), no. 6, 1963–2001.

CONTACT

Peter Hirvonen
TU Wien
Institute of Analysis and Scientific Computing

peter.hirvonen@tuwien.ac.at