Mathematical analysis of ionic solutions.

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Analytical and Numerical Aspects of Evolutions Equations

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Joint work with Dieter Bothe and Jürgen Saal

Contents

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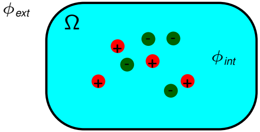
Introduction

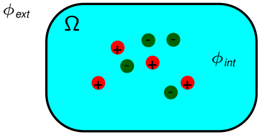
Motivation



Evolution of concentration c_i?

Introduction

Motivation



Evolution of concentration c_i?

Significance of *electrohydrodynamics:*

- *battery systems*
- *nanofiltration, e.g. desalination of water*
- *flow manipulation; e.g. electro-osmosis*
- *interface manipulation; e.g. optical lenses*
- ⋮ ⋮

Introduction

The model

Flux J_i of species i: $J_i = \underbrace{-D_i \nabla c_i}_{\text{diffusion}} \underbrace{- \frac{F}{RT} D_i q_i c_i \nabla \phi}_{\text{electromigration}} \underbrace{+ c_i u}_{\text{convection}},$

Electrostatic potential: $-\varepsilon \Delta \phi = F \sum_{i=1}^{N} q_i c_i$

Boundary conditions: $\langle J_i, \nu \rangle|_{\partial\Omega} = 0, \qquad (\partial_\nu \phi + \tau \phi)|_{\partial\Omega} = \xi$

Unknowns :		*Parameters* :	
c_i :	concentration	τ :	boundary capacity (> 0)
u :	velocity field	D_i :	diffusion coefficient (> 0)
(ϕ :	electrical potential)	q_i :	charge number ($\in \mathbb{Z}$)
(p :	pressure)		

Also: F Faraday constant, R ideal gas constant, T temperature, ε permittivity, (μ viscosity), all > 0.

Introduction

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The Navier-Stokes-Nernst-Planck-Poisson system (NSNPP)

$$
\left\{
\begin{aligned}
\partial_t u - \Delta u + (u\cdot\nabla)u + \nabla p &= -\textstyle\sum_{i=1}^N q_i c_i \nabla\phi && \textit{Navier-Stokes}\\
\operatorname{div} u &= 0 \\
\partial_t c_i + \operatorname{div}\underbrace{\left(-D_i\nabla c_i - D_i q_i c_i \nabla\phi + c_i u\right)}_{=J_i} &= 0, \quad i = 1,\dots,N && \textit{Nernst-Planck}\\
-\Delta\phi &= \textstyle\sum_{i=1}^N q_i c_i && \textit{Poisson}\\
u\big|_{\partial\Omega} &= 0 \\
\langle J_i, \nu\rangle\big|_{\partial\Omega} &= 0, \quad i = 1,\dots,N \\
(\partial_\nu\phi + \tau\phi)\big|_{\partial\Omega} &= \xi \\
u\big|_{t=0} &= u_0 \\
c_i\big|_{t=0} &= c_i^0, \quad i = 1,\dots,N
\end{aligned}
\right.
$$

considered on $(0, T)\times\Omega$ with $\Omega\subset\mathbb{R}^n$ bounded.

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References

- H. Amann, M. Renardy (1994), *Nonlin. Differ. Equ. Appl.*
  Electro-neutrality, i.e. $\sum_{i=1}^{N} q_i c_i \equiv 0$, small cross-diffusion; local well-posedn.
- Y.S. Choi, R. Lui (1995), *Arch. Rat. Mech. Anal.*
  NPP system, no bdy charge: global well-posedness and stability.
- A. Glitzky, R. Hünlich (1997), *Z. Angew. Math. Mech.*
  Electro-reaction-diffusion in heterostructures; global well-posedn. and stab.
- J. Wiedmann (1997), PhD thesis
  (NSNPP)+energy conservation+electro-neutrality; local well-posedness.
- M. Schmuck (2009), PhD thesis
  $D_1 = D_2 = \cdots = D_N$, well-posedness, numerical approach.

Today: No electro-neutrality, coupling with Navier-Stokes, varying diffusivities, boundary charge.

Main results

Global well-posedness in 2D

Theorem (Bothe, F., Saal, 2011)

Let $\Omega \subset \mathbb{R}^2$ be bounded with smooth boundary and $u^0 \in L^2_\sigma(\Omega)$, $0 \leq c^0 \in L^2(\Omega)$, and $\xi \in W^{3/2,2}(\partial\Omega)$. Then there is a weak solution

$$(u, c) \in L^\infty(0, \infty; L^2_\sigma(\Omega) \times L^2(\Omega)^N) \cap L^2_{loc}(0, \infty; W^{1,2}_{0,\sigma}(\Omega) \times W^{1,2}(\Omega)^N)$$

to (NSNPP), where $c \geq 0$.
This solution becomes strong instantaneously, i.e.

$$(u, c) \in W^{1,2}_{loc}(0, \infty; L^2_\sigma(\Omega) \times L^2(\Omega)^N) \cap L^2_{loc}(0, \infty; \mathcal{D}(A_S) \times W^{2,2}(\Omega)^N),$$

where $\mathcal{D}(A_S) = W^{2,2}(\Omega) \cap W^{1,2}_0(\Omega) \cap L^2_\sigma(\Omega)$ denotes the domain of the Stokes operator in $L^2_\sigma(\Omega)$. Moreover

$$\|c(t)\|_\infty \leq C, \quad \text{for } t \geq \delta > 0.$$

Theorem (Bothe, F., Saal, 2011)

Let $\Omega \subset \mathbb{R}^2$ be bounded with smooth boundary and $M_i > 0$, $i = 1, \dots, N$. Then there is a unique steady state solution

$$(u^\infty, c^\infty) \in \mathcal{D}(A_S) \times W^{2,2}(\Omega)^N$$

to (NSNPP) subject to $\int_\Omega c_i^\infty dx = M_i$, $i = 1, \dots, N$. It holds $u^\infty = 0$.
Suppose (u, c) is the global solution from the previous Theorem with initial values satisfying

$$\int_\Omega c_i^0 dx = M_i, \quad i = 1, \dots, N.$$

Then

$$\lim_{t \to \infty} \|u(t)\|_{W^{1,2}_{0,\sigma}(\Omega)} + \|c(t) - c^\infty\|_{W^{1,2}(\Omega)} = 0.$$

Main results

Exponential stability

Theorem (Bothe, F., Saal, 2011)

There are constants $C, \omega > 0$ *such that*

$$\|u(t)\|_2 + \|c(t) - c^\infty\|_2 \leq Ce^{-\omega t}.$$

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Exponential stability

Theorem (Bothe, F., Saal, 2011)

There are constants $C, \omega > 0$ *such that*

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Remarks

- *Global well-posedness without smallness restrictions on the data in 2D.*
- *Exponential convergence to the equilibrium state for **any** initial value in* L^2.
- *Global well-posedness open problem in 3D because of Navier-Stokes **and** Nernst-Planck.*

Sketch of proof

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Global well-posedness

1. Local well-posedness
   - Classical parabolic and Navier-Stokes theory.
   - Fixed-point arguments.
   - Smoothing by maximal regularity.
2. Global well-posedness
   - The system admits a Lyapunov functional

$$V(t) = E(u(t), c(t)) := \frac{1}{2}\|u\|_2^2 + \sum_{i=1}^{N} \int_\Omega (c_i \log c_i) dx + \frac{1}{2}\|\nabla\phi\|_2^2 + \frac{\tau}{2}\|\phi\|_{2,\partial\Omega}^2.$$

$$\dot{V}(t) = -D(u(t), c(t)) := -\|\nabla u\|_2^2 - \sum_{i=1}^{N} \int_\Omega \frac{d_i}{c_i} \exp(-2q_i\phi)|\nabla\zeta_i|^2 dx \leq 0,$$

   where $\zeta_i = c_i \exp(q_i\phi)$.
   - Energy estimates, Moser iteration. □

Sketch of proof

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Existence and uniqueness of steady states

- *Uniqueness*: characterization of steady states (u^∞, c^∞) with potential ϕ^∞:

$$u^\infty = 0, \qquad \zeta_i^\infty = c_i^\infty \exp(q_i \phi^\infty) = const.$$

- *Existence*: trajectories $(u(\cdot), c(\cdot))$ are relatively compact in L^2. Any accumulation point is a steady state.
- Note that due to $u^\infty = 0$ the function c^∞ is the unique solution to

$$\begin{aligned}
\operatorname{div}(-d_i \nabla c_i - d_i q_i c_i \nabla \phi) &= 0, && i = 1, \dots, N \\
\partial_\nu c_i + q_i c_i \partial_\nu \phi|_{\partial\Omega} &= 0, && i = 1, \dots, N, \\
-\Delta \phi &= \textstyle\sum_{i=1}^N q_i c_i, \\
\partial_\nu \phi + \tau \phi|_{\partial\Omega} &= \xi.
\end{aligned}$$

Sketch of proof

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Exponential stability

Define

$$\Psi(u(t), c(t)) := E(u(t), c(t)) - E(u^\infty, c^\infty)$$

$$= \frac{1}{2}\|u\|_2^2 + \sum_{i=1}^{N} \int_\Omega c_i \left(\log \frac{c_i}{c_i^\infty} - 1\right) + c_i^\infty dx + \frac{1}{2}\|\nabla(\phi - \phi^\infty)\|_2^2 + \frac{\tau}{2}\|\phi - \phi^\infty\|_{2,\partial\Omega}^2.$$

Then we have $\frac{\mathrm{d}}{\mathrm{d}t}\Psi(u(t), c(t)) = -D(u(t), c(t))$, where

$$D(u, c) = \|\nabla u\|_2^2 + \sum_{i=1}^{N} \frac{d_i}{c_i} \exp(-2q_i\phi)|\nabla\zeta_i|^2 dx \qquad (\zeta_i = c_i \exp(q_i\phi)).$$

It can be shown indirectly that there is $C > 0$ such that

$$\Psi(u, c) \leq CD(u, c).$$

Then with Gronwall

$$\Psi(u(t), c(t)) \leq C' e^{-\omega t}.$$

Sketch of proof

Exponential stability

Exponential decay to equilibrium

- Velocity:

$$\|u\|_2 \leq 2\Psi(u(t), c(t)) \leq Ce^{-\omega t}.$$

- Concentrations:
  From

$$\sum_i \|\sqrt{c_i} - \sqrt{c_i^\infty}\|_2^2 \leq \Psi(c),$$

  we deduce

$$\|c_i - c_i^\infty\|_2^2 = \|(c_i - c_i^\infty)(\sqrt{c_i} + \sqrt{c_i^\infty})(\sqrt{c_i} - \sqrt{c_i^\infty})\|_1 \leq C\Psi(c) \leq Ce^{-\omega t}.$$

Conclusion and Outlook

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Conclusion

- We considered (NSNPP) with boundary charge, varying diffusivities $D_i \neq D_j$ in general, and without electro-neutrality.
- (NSNPP) is globally well-posed in two dimensions.
- The global solution converges to uniquely determined equilibrium states with exponential speed.
- In the equilibrium state the velocity is zero.

Thank you !