A Poisson-Maxwell-Stefan model for isobaric isothermal electrically charged mixtures

Oliver Leingang,
Supervisor: Ansgar Jüngel.

Särkisaari, 8.8.2018
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- Macroscopic model and assumptions
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Goal: Analyse reaction diffusion models for electrically charged mixtures.

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Example: Electrolytes in electrochemical devices

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Photo of (flexible) Dye-sensitized Solar Cells [14], cropped. Photographer: Armin Kübelbeck, CC-BY-SA, Wikimedia Commons

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Electrolytes:

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Electrolytes:
- Solvent and dissolved positive and negative ions

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- Solvent and dissolved positive and negative ions
- Multicomponent mixture
- Solvent-Solute interaction
- Solute-Solute interactions

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Assume $\sum_{i=1}^N J_i = \sum_{i=1}^N r_i = 0$. Continuity and Poisson equation:

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Maxwell-Stefan equations

By assumption: \( \rho_N = 1 - \sum_{i=1}^{N-1} \rho_i \) and \( J_N = - \sum_{i=1}^{N-1} J_i \).
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General solution - Maxwell-Stefan equations:

\[
D_i = -\sum_{j \neq i} d_{ij}(\rho_j J_i - \rho_i J_j),
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with \( d_{ij} = 1/(|c|^2 M_i M_j D_{ij}) \).
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D_i = \nabla x_i + \beta (z_i x_i - \rho_i (z \cdot x)) \nabla \Phi
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Summary and open questions

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In short, with \( D' := (D_1, \ldots, D_{N-1}) \):

\[
D' = AJ', \ A \in \mathbb{R}^{N-1 \times N-1}.
\]
The Poisson-Maxwell-Stefan system

Let \( \rho' := (\rho_1, \ldots, \rho_{N-1}) \), then for \( \rho \in \mathbb{R}^N \), \( t > 0 \), \( y \in \Omega \), we have

\[
\partial_t \rho' = \text{div}(A^{-1}(\rho)D'(\rho, \Phi)) + r' (\rho), \quad \rho_N = 1 - \sum_{i=1}^{N-1} \rho_i,
\]

\[
D'(\rho, \Phi) = \left( \nabla x_i + \beta (z_i x_i - \rho_i (z \cdot x)) \right) \nabla \Phi \right)_{i=1}^{N-1},
\]

\[
-\lambda \Delta \Phi = \sum_{i=1}^{N} z_i c_i + f(y),
\]

For \( N = 3 \):

\[
A^{-1}(\rho) = \delta(\rho) \left( d_{23} + (d_{12} - d_{23}) \rho_1 (d_{13} - d_{12}) \rho_1 (d_{23} - d_{12}) \rho_2 d_{13} + (d_{12} - d_{13}) \rho_2 \right),
\]

\[
d_{ij} = 1 / (|c|_2 M_i M_j D_{ij}),
\]

\[
D_{ij} = D_{ji} > 0.
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$$- \lambda \Delta \Phi = \sum_{i=1}^{N} z_i c_i + f(y),$$

For $N = 3$:

$$A^{-1}(\rho) = \frac{1}{\delta(\rho)} \begin{pmatrix} d_{23} + (d_{12} - d_{23})\rho_1 & (d_{13} - d_{12})\rho_1 \\ (d_{23} - d_{12})\rho_2 & \rho_2 \\ d_{13} + (d_{12} - d_{13})\rho_2 & \rho_2 \end{pmatrix},$$

and $d_{ij} = 1/(|c|^2M_i M_j D_{ij})$, $D_{ij} = D_{ji} > 0$. 
### Known analytic results without electrical potential

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<th>Known Results</th>
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Known analytic results without electrical potential

- Bothe '11: Rigorous inversion of flux relation, \( D = AJ \), and local existence of solutions [1].
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A1 Domain and BC: $\Omega \subset \mathbb{R}^d$ is bounded with $\partial \Omega = \Gamma_{Di} \cup \Gamma_{Ne} \in C^{0,1}$, $\Gamma_{Di} \cap \Gamma_{Ne} = \emptyset$ and $\text{meas}(\Gamma_{Di}) > 0$. 
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with $\Phi^D \in H^1(\Omega) \cap L^\infty(\Omega)$.
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**A2** Initial data: \( \rho_1^0, \ldots, \rho_N^0 \geq 0 \text{ and } \sum_{i=1}^N \rho_i^0 = 1. \)
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A4 Production rates: \( r \in C([0, 1]^N; \mathbb{R}) \),

\[
\sum_{i=1}^N r_i(\rho) \log x_i \leq C_r \text{ for all } 0 < \rho_1, \ldots, \rho_N \leq 1.
\]
Global nonnegative weak solutions:

Theorem (O.L. and A. Jüngel, work in progress)

Let $A_1$-$A_4$ hold. There exist, for every $T > 0$, bounded weak solutions $\rho_1, \ldots, \rho_N \in [0,1]$ satisfying

$$\rho_i \in L^2(0,T;H^1(\Omega)), \quad \partial_t \rho_i \in L^2(0,T;(H^1(\Omega))'),$$

$$\Phi \in L^2(0,T;H^1(\Omega)), \quad i = 1, \ldots, N-1,$$

such that

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Define entropy by

\[ h(\rho) := |c| \sum_{i=1}^{N} x_i (\log x_i - 1) + |c| \]
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$$h(\rho) := |c| \sum_{i=1}^{N} x_i (\log x_i - 1) + |c| + \frac{\beta \lambda}{2} |\nabla(\Phi - \Phi^D)|^2.$$
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Entropy inequality ($r = 0$ and $\Phi_D$ constant):
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Entropy inequality ($r = 0$ and $\Phi_D$ constant):

\[ \frac{d}{dt} \int_{\Omega} h(\rho) dy \]
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\[ h(\rho) := |c| \sum_{i=1}^{N} x_i (\log x_i - 1) + |c| + \frac{\beta \lambda}{2} |\nabla (\Phi - \Phi^D)|^2. \]

Entropy inequality (\( r = 0 \) and \( \Phi^D \) constant):

\[ \frac{d}{dt} \int_{\Omega} h(\rho) \, dy = - \sum_{i,j=1}^{N-1} \int_{\Omega} B_{ij}(\rho) |c|^2 \left( \frac{D_j}{\rho_j} - \frac{D_N}{\rho_N} \right) \left( \frac{D_i}{\rho_i} - \frac{D_N}{\rho_N} \right) \, dy \]
Key idea: Entropy structure

Define entropy by

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with \( B(\rho) = (B_{ij}(\rho))_{i,j=1}^{N-1} \) symmetric, positive definite and bounded if \( \rho \in (0, 1]^N \).
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$$= \nabla \left( \frac{\log(x_i)}{M_i} - \frac{\log(x_N)}{M_N} + \beta \left( \frac{z_i}{M_i} - \frac{z_N}{M_N} \right) \Phi \right)$$
Boundedness by entropy method:

Define entropy variables for $i = 1, \ldots, N-1$, 
$$\omega_i := \log(x_iM_i) - \log(x_NM_N) + \beta(z_iM_i - z_NM_N)\Phi.$$ 
and show the inverse exists such that 
$$\rho'(\omega, \Phi) \in (0,1).$$

Rewrite equation: 
$$\partial_t \rho' = \text{div}(A^{-1}(\rho)D'(\rho, \Phi)) + r'\rho.$$ 
$$\partial_t \rho'(\omega, \Phi) = \text{div}(B(\rho'(\omega, \Phi))\nabla\omega) + r'(\rho(\omega, \Phi)).$$

Discretize with implicit Euler/Galerkin and regularize. Use discrete Entropy inequality to derive apriori estimate and pass to the limit $\Rightarrow$ existence of global weak solutions.
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FEM in entropy variables: Implementation

Galerkin-scheme in the proof allows for standard linear finite element spaces.

Nonlinearity and regularization:
\[
\frac{\partial}{\partial t} \rho'(\omega, \Phi) = \text{div} \left( B(\rho'(\omega, \Phi)) \nabla \omega \right) - \varepsilon \left( \omega - \omega^D \right)
\]

Recovering original variables:
\[
\rho_i = |c|M_i \left( 1 - s_0 \right) \frac{M_i}{M_N} e^{M_i \left( \omega_i - \beta \left( z_i M_i - z_N M_N \right) \Phi \right)}
\]

whereby \( s_0 \in [0, 1] \) is the solution of the fixed point problem
\[
F(s, \omega_i, \Phi) = \left( 1 - s \right) \sum_{i=1}^{N-1} \frac{M_i}{M_N} e^{M_i \left( \omega_i - \beta \left( z_i M_i - z_N M_N \right) \Phi \right)} - s = 0
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for \( i = 1, \ldots, N - 1 \).
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for \( i = 1, \ldots, N - 1. \)
Plot with equal molar mass and $N = 3$, $\beta = M_i = D_{ij} = 1$ for $i, j = 1, \ldots, 3$, $z_1 = z_2 = 1$, $z_3 = 0$, $\lambda = 0.01$. 

Equal molar mass
Different molar mass

Plot with different molar mass $M_1$ at time $t = 4$. 
Summary and open questions:

Summary

Global existence for the Poisson-Maxwell-Stefan system

New finite element scheme:
- "Convergence" of approximation follows by analytic proof
- Diffusion matrix is symmetric and positive definite
- Preserves lower and upper bounds
- Preserves a discrete version of the Entropy inequality

Open questions and challenges:
- Longtime behavior and decay rate
- Numerical analysis of the scheme
- Efficient implementation of the scheme for $d > 1$
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Thank you for your attention.


