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

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Motivation and Application

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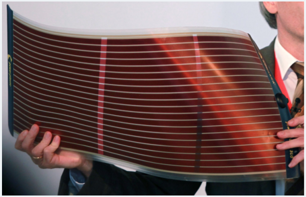

Photo of (flexible) Dye-sensitized Solar Cells [14], cropped. Photographer: Armin Kübelbeck, CC-BY-SA, Wikimedia Commons

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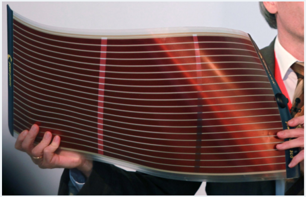

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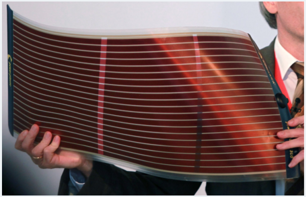

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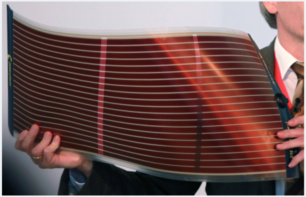

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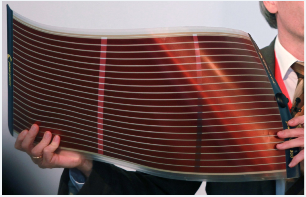

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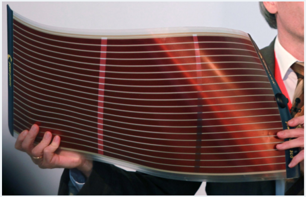

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By assumption: $\rho_N = 1 - \sum_{i=1}^{N-1} \rho_i$ and $J_N = -\sum_{i=1}^{N-1} J_i$.

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

$$D' = AJ',\ A \in \mathbb{R}^{N-1 \times N-1}.$$

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For $N = 3$:

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

and $d_{ij} = 1/(|c|^2 M_i M_j D_{ij})$, $D_{ij} = D_{ji} > 0$.

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- Daus, Jüngel and Tang '18: Exponential time decay with more involved reaction terms [7].

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A4 Production rates: $r \in C([0,1]^N; \mathbb{R})$, $\sum_{i=1}^N r_i(\rho) \log x_i \leq C_r$ for all $0 < \rho_1, \ldots, \rho_N \leq 1$.

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

such that $\rho_N = 1 - \sum_{i=1}^{N-1} \rho_i$.

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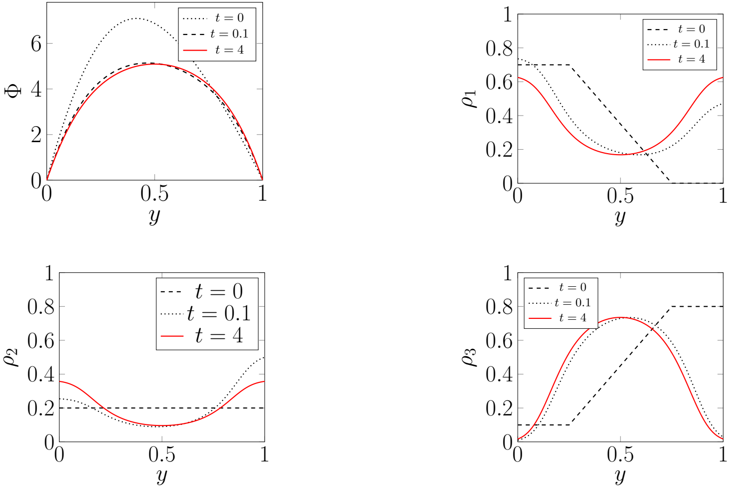
whereby $s_0 \in [0, 1]$ is the solution of the fixed point problem

$$F(s, \omega_i, \Phi) = \sum_{i=1}^{N-1} (1 - s)^{M_i/M_N} e^{M_i \left((\omega)_i - \beta\left(\frac{z_i}{M_i} - \frac{z_N}{M_N}\right)\Phi\right)} - s = 0,$$

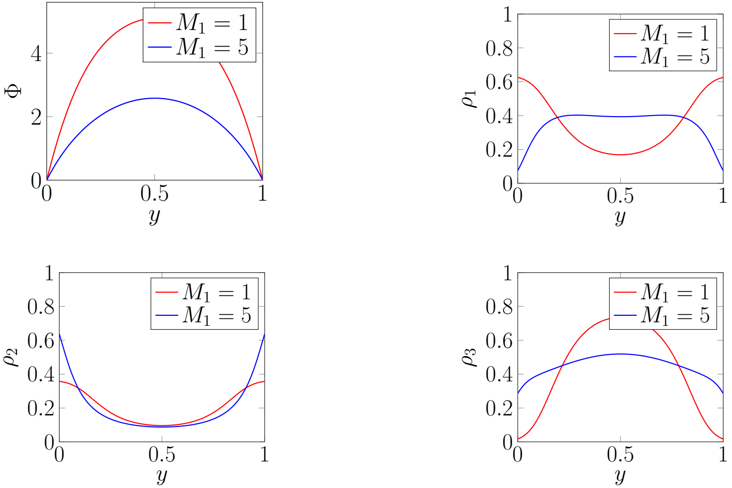
for $i = 1, \ldots, N - 1$.

Equal molar mass



Plot with equal molar mass and $N = 3$, $\beta = M_i = D_{ij} = 1$ for $i, j = 1, \ldots, 3$, $z_1 = z_2 = 1$, $z_3 = 0, \lambda = 0.01$.

Different molar mass



Plot with different molar mass M_1 at time $t = 4$.

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Thank you for your attention.

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