W I A S

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Ein stationäres Energiemodell mit mehreren Spezies

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Introduction

mass, charge and energy transport in heterogeneous semiconductor materials

mass and charge transport of charged and uncharged particles $\Longrightarrow$

continuity equations + Poisson equation

energy transport resulting in a variation of the lattice temperature $\Longrightarrow$

heat flow equation or balance equation for the densities of entropy or energy

heterogeneity: heterogeneous materials, mixed boundary conditions

fields of application:

- application of semiconductor devices
- semiconductor technology
- other problems in electrochemistry

restrict us to stationary case

global assertion: existence and uniqueness of thermodynamic equilibrium for special data

local result: unique steady state in a neighbourhood of thermodynamic equilibrium

Stationary energy model

$X_i, \; i = 1, \ldots, n$	- species	$\overline{u}_i$	- reference density
u_i	- particle density	E_i	- reference energy
ζ_i	- electrochemical potential	φ	- electrostatic potential
q_i	- charge number	T	- lattice temperature

ansatz for the state equations

$$u_i = \overline{u}_i(x, T)\, \mathrm{e}^{(\zeta_i - q_i\varphi + E_i(x,T))/T}, \quad i = 1, \ldots, n$$

reversible reactions

$$\alpha_1 X_1 + \ldots + \alpha_n X_n \rightleftharpoons \beta_1 X_1 + \ldots + \beta_n X_n$$

stoichiometric coefficients $(\alpha, \beta) = (\alpha_1, \ldots, \alpha_n, \beta_1, \ldots, \beta_n) \in \mathcal{R}$

reaction rates according to the mass action law

$$R_{\alpha\beta} = r_{\alpha\beta}(x, u, T, \varphi) \left(\mathrm{e}^{\sum_{i=1}^n \alpha_i \zeta_i / T} - \mathrm{e}^{\sum_{i=1}^n \beta_i \zeta_i / T} \right), \quad (\alpha, \beta) \in \mathcal{R}$$

Stationary energy model

ansatz for particle flux densities j_i and total energy flux density j_e

$$j_i = -\sum_{k=1}^{n} \sigma_{ik}(x,u,T)\left(\nabla\zeta_k + P_k(x,u,T)\nabla T\right), \quad i = 1,\dots,n$$

$$j_e = -\kappa(x,u,T)\nabla T + \sum_{i=1}^{n} \left(\zeta_i + P_i(x,u,T)T\right) j_i$$

σ_{ik}, κ - conductivities, P_i - transported entropies

$$\sigma_{ik} = \sigma_{ki}, \quad \sum_{i,k=1}^{n} \sigma_{ik}(x,u,T) y_i y_k \geq \sigma_0(u,T)\|y\|^2 \quad \forall y \in \mathbb{R}^n, \quad \kappa(x,u,T) \geq \kappa_0(u,T)$$

with $\sigma_0(u,T)$, $\kappa_0(u,T) > 0$ for all non-degenerated states u, T, no sign condition for P_i

Stationary energy model

n continuity equations, conservation law for the total energy, Poisson equation

$$
\left.
\begin{array}{rcl}
\nabla \cdot j_i & = & \displaystyle\sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta}, \quad i = 1, \dots, n \\
\nabla \cdot j_e & = & 0 \\
-\nabla \cdot (\varepsilon \nabla \varphi) & = & f + \displaystyle\sum_{i=1}^{n} q_i u_i
\end{array}
\right\} \quad \text{in } \Omega \subset \mathbb{R}^2
$$

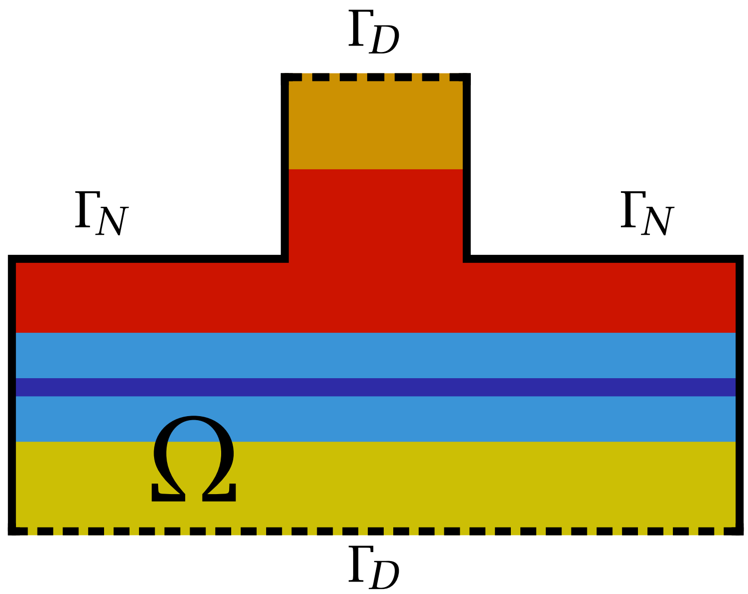
ε - dielectric permittivity
f - fixed charge density

Stationary energy model

mixed boundary conditions

$$-\nu \cdot j_i = g_i, \quad i = 1, \dots, n, \qquad -\nu \cdot j_e = g_{n+1}, \qquad \nu \cdot (\varepsilon \nabla \varphi) = g_{n+2} \qquad \text{on } \Gamma_N$$

$$\zeta_i = \zeta_i^D, \quad i = 1, \dots, n, \qquad T = T^D, \qquad \varphi = \varphi^D \qquad \text{on } \Gamma_D$$



Stationary energy model

Conservation of energy $\nabla \cdot j_e = 0$ frequently substituted by the heat flow equation

$$-\nabla \cdot (\kappa \nabla T) = H$$

where the source term

$$\begin{aligned} H &= -\sum_{i=1}^{n} \nabla \cdot ((\zeta_i + P_i T) j_i) \\ &= \sum_{i,k=1}^{n} \sigma_{ik} (\nabla \zeta_i + P_i \nabla T)(\nabla \zeta_k + P_k \nabla T) \\ &\quad - \sum_{i=1}^{n} T \, \nabla P_i \cdot j_i \\ &\quad - \sum_{i=1}^{n} (\zeta_i + P_i T) \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta} \end{aligned}$$

contains a lot of quadratic gradient terms

Stationary energy model

Reformulation by an entropy balance equation

entropy flux density

$$j_s = \frac{1}{T}\left(j_e - \sum_{i=1}^{n} \zeta_i\, j_i\right) = -\frac{\kappa}{T}\nabla T + \sum_{i=1}^{n} P_i\, j_i$$

for isothermal case, $\nabla T = 0$, $\Longrightarrow$

$$j_s = \sum_{i=1}^{n} P_i\, j_i$$

explains the meaning of P_i as transported entropies

Stationary energy model

entropy formulation

$$
\begin{pmatrix} j_1 \\ \vdots \\ j_n \\ j_s \end{pmatrix} = - \begin{pmatrix} \sigma_{11} & \cdots & \sigma_{1n} & \tau_1 \\ \vdots & \ddots & \vdots & \vdots \\ \sigma_{n1} & \cdots & \sigma_{nn} & \tau_n \\ \tau_1 & \cdots & \tau_n & \frac{\kappa}{T} + \tau_{n+1} \end{pmatrix} \begin{pmatrix} \nabla \zeta_1 \\ \vdots \\ \nabla \zeta_n \\ \nabla T \end{pmatrix}
$$

$$
\tau_i = \sum_{k=1}^{n} \sigma_{ik} P_k, \quad i = 1, ..., n, \quad \tau_{n+1} = \sum_{i,k=1}^{n} \sigma_{ik} P_i P_k
$$

matrix is symmetric, positive definite for non-degenerated states $\Longrightarrow$ Onsager's relations are fulfilled for fluxes $(j_1, \ldots, j_n, j_s)$ and generalized forces $(\nabla \zeta_1, \ldots, \nabla \zeta_n, \nabla T)$

Stationary energy model

entropy balance equation

$$\nabla \cdot j_s = d$$

entropy production rate

$$T\, d = -\sum_{i=1}^{n} j_i \cdot \nabla \zeta_i - j_s \cdot \nabla T + \sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta} \sum_{i=1}^{n} (\alpha_i - \beta_i)\zeta_i$$

$d \geq 0$, and for non-degenerated states

$$d = 0 \quad \Longleftrightarrow \quad \begin{cases} \nabla \zeta_i = 0, \quad i = 1, ..., n \\ \nabla T = 0 \\ \sum_{i=1}^{n} (\alpha_i - \beta_i)\zeta_i = 0 \quad \forall(\alpha,\beta) \in \mathcal{R} \end{cases}$$

conditions characterize thermodynamic equilibrium if a thermodynamic equilibrium satisfies the boundary conditions, the data has to fulfil

$$\zeta_i^D = \text{const}, \;\; i = 1, \ldots, n, \quad \textstyle\sum_{i=1}^n (\alpha_i - \beta_i)\zeta_i^D = 0 \;\; \forall(\alpha, \beta) \in \mathcal{R},$$

$$T^D = \text{const} > 0, \quad g_i = 0, \;\; i = 1, \ldots, n+1$$

corresponding equilibrium densities u_i are obtained by the state equations

$$u_i = \overline{u}_i(\cdot, T^D) \exp\left\{(\zeta_i^D - q_i\varphi + E_i(\cdot, T^D))/T^D\right\}, \quad i = 1, \ldots, n$$

where the electrostatic potential has to satisfy the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \varphi) = f + \sum_{i=1}^n q_i \overline{u}_i(\cdot, T^D) \exp\left\{(\zeta_i^D - q_i\varphi + E_i(\cdot, T^D))/T^D\right\}$$

$$\varphi = \varphi^D \text{ on } \Gamma_D, \quad \nu \cdot (\varepsilon \nabla \varphi) = g_{n+2} \text{ on } \Gamma_N$$

Stationary energy model

Onsager's relations for fluxes $(j_1, \ldots, j_n, j_e)$ and generalized forces $(\nabla\zeta_1, \ldots, \nabla\zeta_n, \nabla T)$ are not fulfilled

change of generalized forces to $(\nabla[\zeta_1/T], \ldots, \nabla[\zeta_n/T], \nabla[-1/T])$

$$\begin{pmatrix} j_1 \\ \vdots \\ j_n \\ j_e \end{pmatrix} = - \begin{pmatrix} \sigma_{11}T & \cdots & \sigma_{1n}T & \widetilde{\tau}_1 \\ \vdots & \ddots & \vdots & \vdots \\ \sigma_{n1}T & \cdots & \sigma_{nn}T & \widetilde{\tau}_n \\ \widetilde{\tau}_1 & \cdots & \widetilde{\tau}_n & \kappa T^2 + \widetilde{\tau}_{n+1} \end{pmatrix} \begin{pmatrix} \nabla[\zeta_1/T] \\ \vdots \\ \nabla[\zeta_n/T] \\ \nabla[-1/T] \end{pmatrix}$$

$$\widetilde{\tau}_i = \sum_{k=1}^{n} \sigma_{ik} T(\zeta_k + P_k T), \ \ i = 1, \ldots, n, \ \ \widetilde{\tau}_{n+1} = \sum_{i,k=1}^{n} \sigma_{ik} T(\zeta_i + P_i T)(\zeta_k + P_k T)$$

matrix is symmetric, positive definite for non-degenerated states $\Longrightarrow$ Onsager's relations are fulfilled for fluxes $(j_1, \ldots, j_n, j_e)$ and generalized forces $(\nabla[\zeta_1/T], \ldots, \nabla[\zeta_n/T], \nabla[-1/T])$

Stationary energy model

entropy production rate writes as

$$\begin{aligned} d = \; & -\sum_{i=1}^{n} j_i \cdot \nabla[\zeta_i/T] \\ & -j_e \cdot \nabla[-1/T] \\ & + \sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta} \sum_{i=1}^{n} (\alpha_i - \beta_i)\frac{\zeta_i}{T} \end{aligned}$$

again, $d \geq 0$, and for all non-degenerate states

$$d = 0 \quad \Longleftrightarrow \quad \begin{cases} \nabla[\zeta_i/T] = 0, \quad i = 1, \ldots, n \\ \nabla[-1/T] = 0 \\ \sum_{i=1}^{n} (\alpha_i - \beta_i)\frac{\zeta_i}{T} = 0 \quad \forall(\alpha,\beta) \in \mathcal{R} \end{cases}$$

conditions characterize thermodynamic equilibrium

Reformulation

introduce new variables

$$z = (z_1, \dots, z_{n+2}) = (\zeta_1/T, \dots, \zeta_n/T, -1/T, \varphi)$$

reformulate the state equations

$$u_i(x) = H_i(x, z), \quad i = 1, \dots, n$$

express reaction rates $R_{\alpha\beta}$ in the new variables

$$\begin{aligned} R_{\alpha\beta}(x, z) &= r_{\alpha\beta}(x, H_1(z), \dots, H_n(z), -1/z_{n+1}, z_{n+2}) \left(e^{\sum_{i=1}^n \alpha_i z_i} - e^{\sum_{i=1}^n \beta_i z_i} \right) \\ &= \tilde{r}_{\alpha\beta}(x, z) \left(e^{\sum_{i=1}^n \alpha_i z_i} - e^{\sum_{i=1}^n \beta_i z_i} \right), \qquad (\alpha, \beta) \in \mathcal{R} \end{aligned}$$

Reformulation

strongly coupled nonlinear elliptic system

$$-\nabla\cdot\begin{pmatrix} a_{11} & \cdots & a_{1,n+1} & 0 \\ \vdots & \ddots & \vdots & 0 \\ a_{n,1} & \cdots & a_{n,n+1} & 0 \\ a_{n+1,1} & \cdots & a_{n+1,n+1} & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}\begin{pmatrix} \nabla z_1 \\ \vdots \\ \nabla z_n \\ \nabla z_{n+1} \\ \nabla z_{n+2} \end{pmatrix} = \begin{pmatrix} R_1 \\ \vdots \\ R_n \\ 0 \\ f + \sum_{k=1}^n q_k H_k \end{pmatrix}$$

$$a_{ki} = a_{ik} = a_{ik}(x, z(x)),\ \ \varepsilon = \varepsilon(x)$$

$$R_i = \sum_{(\alpha,\beta)\in\mathcal{R}} (\beta_i - \alpha_i) R_{\alpha\beta}(x, z(x)),\ \ H_k = H_k(x, z(x))$$

mixed boundary conditions

$$z_i = z_i^D, \qquad i = 1, \ldots, n+2, \qquad \text{on } \Gamma_D$$

$$\nu\cdot\sum_{k=1}^{n+1} a_{ik}(z)\nabla z_k = g_i, \qquad i = 1, \ldots, n+1, \qquad \nu\cdot(\varepsilon\nabla z_{n+2}) = g_{n+2} \qquad \text{on } \Gamma_N$$

Outline of the results and methods

result:

local existence and uniqueness result near a thermodynamic equilibrium

methods:

- prove existence of thermodynamic equilibrium $u_i^* > 0,\ T^* > 0,\ \varphi^*$
- apply Implicit Function Theorem
- we obtain only local assertions (e.g. $T > 0$, $u_i > 0$ near thermodynamic equilibrium) but we needn't global assumptions

problems:

- suitable choice of function spaces and weak formulation
- supply requirements of Implicit Function Theorem
- properties of Nemyzki operators
- regularity results for strongly coupled elliptic systems with mixed boundary conditions
- technique works in 2D only

class (D)

Let $V = \mathbb{R}^n \times (-\infty, 0) \times \mathbb{R}$.

A function $b \colon \Omega \times V \to \mathbb{R}$ is of the class (D) iff it fulfills the following properties:

- b, $\partial_z b$ Caratheodory functions

  $z \mapsto b(x, z)$ is continuously differentiable f.a.a. $x \in \Omega$

  $x \mapsto b(x, z)$, $x \mapsto \partial_z b(x, z)$ are measurable $\forall\, z \in V$

- b, $\partial_z b$ (locally) uniformly bounded

  For every compact subset $K \subset V$ there exists an $M > 0$ such that

$$|b(x, z)| \leq M, \quad \|\partial_z b(x, z)\| \leq M \quad \forall z \in K, \text{ f.a.a. } x \in \Omega.$$

- b, $\partial_z b$ (locally) uniformly continuous

  For every compact subset $K \subset V$ and $\epsilon > 0$ there exists a $\delta > 0$ such that

$$|b(x, z^1) - b(x, z^2)| < \epsilon, \quad |\partial_z b(x, z^1) - \partial_z b(x, z^2)| < \epsilon$$

$\forall z^1,\ z^2 \in K$ with $|z^1 - z^2| < \delta$, f.a.a. $x \in \Omega$.

General assumptions

(A1) (domain)
Ω is a bounded Lipschitzian domain in $\mathbb{R}^2$, $\Gamma = \partial\Omega$,
Γ_D, Γ_N are disjoint open subsets of Γ, $\Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N}$, $\operatorname{mes} \Gamma_D > 0$,
$\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points

(A2) (boundedness and ellipticity of coefficients)
The functions $a_{ik} = a_{ki} \colon \Omega \times V \to \mathbb{R}$ are of the class (D), $i, k = 1, \ldots, n+1$.
For every compact subset $K \subset V$ there exists an $a_K > 0$ such that

$$\sum_{i,k=1}^{n+1} a_{ik}(x, z)\xi_i\xi_k \geq a_K \|\xi\|^2 \quad \forall z \in K,\ \forall \xi \in \mathbb{R}^{n+1}, \text{ f.a.a. } x \in \Omega$$

$\varepsilon \in L^\infty(\Omega)$, $0 < \varepsilon_0 \leq \varepsilon(x) \leq \varepsilon^0 < \infty$ a.e. in Ω,

(A3) (reaction terms in the continuity equations)
$\mathcal{R} \subset \mathbb{Z}_+^n \times \mathbb{Z}_+^n$, for $(\alpha, \beta) \in \mathcal{R}$ we define $R_{\alpha\beta} \colon \Omega \times V \to \mathbb{R}$ by

$$R_{\alpha\beta}(x, z) = \widetilde{r}_{\alpha\beta}(x, z) \left(\mathrm{e}^{\sum_{i=1}^n \alpha_i z_i} - \mathrm{e}^{\sum_{i=1}^n \beta_i z_i} \right)$$

where $\widetilde{r}_{\alpha\beta} \colon \Omega \times V \to \mathbb{R}_+$ is of the class (D)

General assumptions

(A4) (source terms in the Poisson equation)
$q_i \in \mathbb{Z}$, $H_i\colon \Omega \times V \to \mathbb{R}_+$ are of the class (D), $i = 1, \ldots, n$,
$h = -\sum_{i=1}^n q_i H_i\colon \Omega \times V \to \mathbb{R}$, $h(x, z_1, \ldots, z_{n+1}, \cdot)$ is monotonic increasing for all $(z_1, \ldots, z_{n+1}) \in \mathbb{R}^n \times (-\infty, 0)$, f.a.a $x \in \Omega$,

$$|h(x,z)| \le c_k \mathrm{e}^{c|z_{n+2}|}$$

$\forall (z_1, \ldots, z_{n+1}) \in [-k, k]^n \times [-k, -1/k]$, $z_{n+2} \in \mathbb{R}$, f.a.a. $x \in \Omega$.

For the data we suppose:

- There exists a $p > 2$ such that z_i^D on Γ_D are traces of functions $z_i^D \in W^{1,p}(\Omega)$, $i = 1, \ldots, n+2$, with $z_{n+1}^D < 0$ in Ω.
- $g_i \in L^\infty(\Gamma_N)$, $i = 1, \ldots, n+2$,
- $f \in L^\infty(\Omega)$

Weak formulation

Let $s \in [1, \infty)$, we define

$$X_s = (W_0^{1,s}(\Omega \cup \Gamma_N))^{n+2}$$
$$X_s^* = ((W_0^{1,s}(\Omega \cup \Gamma_N))^{n+2})^* = (W^{-1,s}(\Omega \cup \Gamma_N))^{n+2}$$
$$Y_s = (W^{1,s}(\Omega))^{n+2}$$

We set

$$z = Z + z^D, \quad w = (z^D, g, f)$$

Definition. Let $q \in (2, p]$ and $\tau > 1$. We define the open subset $M_{q,\tau} \subset X_q \times Y_p$ as

$$M_{q,\tau} = \Big\{(Z, z^D) \in X_q \times Y_p \text{ with } |Z_i + z_i^D| < \tau,\ i = 1, \dots, n, n+2, \\ -\tau < Z_{n+1} + z_{n+1}^D < -\tfrac{1}{\tau} \text{ on } \Omega \Big\}$$

Weak formulation

define $\quad F_{q,\tau}\colon M_{q,\tau} \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) \to X^*_{q'} \quad$ by

$$\begin{aligned}
\langle F_{q,\tau}(Z,w),\psi\rangle_{X_{q'}} &= \int_\Omega \Big\{ \sum_{i,k=1}^{n+1} a_{ik}(\cdot,z)\nabla z_k \cdot \nabla\psi_i + \varepsilon\nabla z_{n+2}\cdot\nabla\psi_{n+2}\Big\}\,\mathrm{d}x \\
&+ \int_\Omega \Big\{ \sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta}(\cdot,z) \sum_{i=1}^{n}(\alpha_i-\beta_i)\psi_i + h(\cdot,z)\psi_{n+2}\Big\}\,\mathrm{d}x \\
&- \int_\Omega f\psi_{n+2}\,\mathrm{d}x - \int_{\Gamma_N}\sum_{i=1}^{n+2} g_i\psi_i\,\mathrm{d}\Gamma, \quad \psi\in X_{q'}
\end{aligned}$$

$z = Z + z^D, \quad w = (z^D, g, f)$ $\qquad$ $q' = q/(q-1)$ dual exponent of q

Problem (P):

Find (q, τ, Z, w) such that $q \in (2, p]$, $\tau > 1$, $(Z, w) \in X_q \times Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)$,

$$(Z, z^D) \in M_{q,\tau}, \quad F_{q,\tau}(Z, w) = 0.$$

If (q, τ, Z, w) is a solution to (P) then $(\widetilde{q}, \widetilde{\tau}, Z, w)$ is a solution to (P) if $\widetilde{q} \leq q$, $\tau \leq \widetilde{\tau}$

Differentiability

Lemma 1. (Differentiability)
For all $\tau > 1$ and all exponents $p \geq q > 2$ the operator

$$F_{q,\tau}\colon M_{q,\tau} \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) \to X_{q'}^*$$

is continuously differentiable.

$$\begin{aligned}\langle \partial_Z F_{q,\tau}(Z,w)\overline{Z},\psi\rangle_{X_{q'}} &= \int_\Omega \sum_{i,k=1}^{n+1} \left\{a_{ik}(\cdot,z)\nabla \overline{Z}_k + \partial_z a_{ik}(\cdot,z)\cdot \overline{Z}\,\nabla z_k\right\}\cdot \nabla\psi_i \,\mathrm{d}x \\ &+ \int_\Omega \left\{\varepsilon\nabla\overline{Z}_{n+2}\cdot\nabla\psi_{n+2} + \partial_z h(\cdot,z)\cdot\overline{Z}\,\psi_{n+2}\right\}\mathrm{d}x \\ &+ \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} \partial_z R_{\alpha\beta}(\cdot,z)\cdot\overline{Z}\sum_{i=1}^{n}(\alpha_i-\beta_i)\psi_i\,\mathrm{d}x\end{aligned}$$

$\forall\, \overline{Z} \in X_q,\ \psi \in X_{q'}$

Thermodynamic equilibrium

$$Q = \Big\{ w = (z^D, g, f) \in W^{1,p}(\Omega)^{n+2} \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega):$$

$$g_i = 0,\ z_i^D = \text{const},\ i = 1, \ldots, n+1,\ z_{n+1}^D < 0,\ \sum_{i=1}^{n} (\alpha_i - \beta_i)\, z_i^D = 0\ \forall(\alpha, \beta) \in \mathcal{R} \Big\}$$

Theorem 1. (Existence and uniqueness of thermodynamic equilibria)
Let $w^* = (z^{D*}, g^*, f^*) \in Q$.
Then there exist $q_0 \in (2, p]$, $\tau > 1$ and $Z_{n+2}^* \in W_0^{1,q_0}(\Omega \cup \Gamma_N)$ such that

$$(Z^*, z^{D*}) = ((0, \ldots, 0, 0, Z_{n+2}^*), z^{D*}) \in M_{q_0,\tau}, \quad F_{q_0,\tau}(Z^*, w^*) = 0,$$

in other words, (q_0, τ, Z^*, w^*) is a solution to (P).

If $(\widetilde{q}, \widetilde{\tau}, \widetilde{Z}, w^*)$ is a solution to (P) then $\widetilde{Z} = Z^*$ in $X_{min\{q_0,\widetilde{q}\}}$.

For given $w^* = (z^{D*}, (0, \ldots, 0, 0, g_{n+2}^*), f^*) \in Q$ there exists a unique thermodynamic equilibrium $z^* = Z^* + z^{D*}$.

Sketch of the proof of Theorem 1

1. Solution of the Poisson equation: $\mathcal{E}\colon H_0^1(\Omega \cup \Gamma_N) \to H^{-1}(\Omega \cup \Gamma_N)$,

$$\langle \mathcal{E}(\phi), \overline{\phi} \rangle_{H_0^1(\Omega\cup\Gamma_N)} = \int_\Omega \varepsilon \nabla(\phi + z_{n+2}^{D*}) \cdot \nabla\overline{\phi} \,\mathrm{d}x - \int_{\Gamma_N} g_{n+2}^* \overline{\phi} \,\mathrm{d}\Gamma + \int_\Omega \big(h(\cdot, (0, \dots, 0, 0, \phi) + z^{D*}) - f^*\big) \overline{\phi} \,\mathrm{d}x \quad \forall \overline{\phi} \in H_0^1(\Omega \cup \Gamma_N)$$

is strongly monotone and hemicontinuous (Trudinger's imbedding result)
$\Longrightarrow$ unique solution $\phi = Z_{n+2}^*$ of $\mathcal{E}(\phi) = 0$

2. higher regularity: $Z_{n+2}^* \in W^{1,q_0}(\Omega \cup \Gamma_N)$ (Trudinger's imbedding result, Gröger's regularity result for elliptic equations with mixed boundary conditions)

Sketch of the proof of Theorem 1

3. Setting $Z^* = (0, \ldots, 0, 0, Z^*_{n+2})$, then for q_0 and suitable $\tau > 1$ we find

$$(Z^*, z^{D*}) \in M_{q_0,\tau}, \quad F_{q_0,\tau}(Z^*, w^*) = 0$$

$\Longrightarrow$ (q_0, τ, Z^*, w^*) is a solution to (P)

4. uniqueness: if $(\widetilde{q}, \widetilde{\tau}, \widetilde{Z}, w^*)$ would be a solution to (P), then for

$$\widehat{q} = \min\{q, \widetilde{q}\}, \quad \widehat{\tau} = \max\{\tau, \widetilde{\tau}\}$$

$(\widehat{q}, \widehat{\tau}, Z^*, w^*)$ and $(\widehat{q}, \widehat{\tau}, \widetilde{Z}, w^*)$ would be solutions to (P), too

- $0 = \langle F_{\widehat{q},\widehat{\tau}}(\widetilde{Z}, w^*) - F_{\widehat{q},\widehat{\tau}}(Z^*, w^*), (\widetilde{Z}_1, \ldots, \widetilde{Z}_{n+1}, 0)\rangle_{Xq'}$
  (A2), (A3) $\Longrightarrow \widetilde{Z}_i = 0, \ i = 1, \ldots, n+1$
- uniqueness of the solution of $\mathcal{E}(\phi) = 0 \quad \Longrightarrow \widetilde{Z}_{n+2} = Z^*_{n+2}$ •

Lemma 2. (Properties of the linearization in the thermodynamic equilibrium)

Let $w^* = (z^{D*}, g^*, f^*) \in Q$. Furthermore, let (q_0, τ, Z^*, w^*) with $Z^* = (0, \dots, 0, Z^*_{n+2})$ be the equilibrium solution to Problem (P) according to Theorem 1.

Then there exists a $q_1 \in (2, q_0]$ such that the Fréchet derivative

$$\partial_Z F_{q_1,\tau}(Z^*, w^*) \colon X_{q_1} \to X^*_{q_1'}$$

is an injective Fredholm Operator of index zero.

Sketch of the proof of Lemma 2

$$
\begin{aligned}
&\langle \partial_Z F_{q,\tau}(Z,w)\overline{Z},\psi\rangle_{X_{q'}} \\
&\quad = \int_\Omega \sum_{i,k=1}^{n+1} \left\{ a_{ik}(\cdot,z)\nabla \overline{Z}_k + \partial_z a_{ik}(\cdot,z)\cdot \overline{Z}\,\nabla z_k \right\}\cdot \nabla\psi_i \,\mathrm{d}x \\
&\quad + \int_\Omega \left\{ \varepsilon \nabla \overline{Z}_{n+2}\cdot \nabla \psi_{n+2} + \partial_z h(\cdot,z)\cdot \overline{Z}\,\psi_{n+2} \right\} \mathrm{d}x \\
&\quad + \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} \partial_z \widetilde{r}_{\alpha\beta}(\cdot,z)\cdot \overline{Z} \left(\mathrm{e}^{\sum_{i=1}^n \alpha_i z_i} - \mathrm{e}^{\sum_{i=1}^n \beta_i z_i} \right) \sum_{i=1}^n (\alpha_i-\beta_i)\psi_i \,\mathrm{d}x \\
&\quad + \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} \widetilde{r}_{\alpha\beta}(\cdot,z) \sum_{k=1}^n \left(\alpha_k \mathrm{e}^{\sum_{i=1}^n \alpha_i z_i} - \beta_k \mathrm{e}^{\sum_{i=1}^n \beta_i z_i} \right) \overline{Z}_k \sum_{i=1}^n (\alpha_i-\beta_i)\psi_i \,\mathrm{d}x \\
&\qquad\qquad \forall\, \overline{Z}\in X_q,\ \psi\in X_{q'}
\end{aligned}
$$

has to be calculated for $Z = Z^*$, $w = w^*$

Sketch of the proof of Lemma 2

1. linearization in thermodynamic equilibrium:

Let $q \in (2, q_0]$, since $(z^*, g^*, f^*) \in Q \Longrightarrow \partial_Z F_{q,\tau}(Z^*, w^*) = L_q + K_q$

$$\langle L_q \overline{Z}, \psi\rangle_{X_{q'}} = \int_\Omega \Big\{\sum_{i,k=1}^{n+1} a_{ik}(\cdot, z^*)\nabla \overline{Z}_k \cdot \nabla\psi_i + \varepsilon\nabla\overline{Z}_{n+2}\cdot\nabla\psi_{n+2}\Big\}\mathrm{d}x + \sum_{i=1}^{n+2}\int_\Omega \overline{Z}_i\,\psi_i\,\mathrm{d}x$$

- L_q is injective
- Gröger's regularity result $\Longrightarrow$ there exists $q_1 \in (2, q_0]$ such that L_q is surjective for all $q \in (2, q_1]$
- Banach's open mapping theorem $\Longrightarrow$ $L_q \colon X_q \to X_{q'}^*$ is an isomorphism for all $q \in (2, q_1]$

Sketch of the proof of Lemma 2

$$\langle K_q \overline{Z}, \psi \rangle_{X_{q'}} = \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} \tilde{r}_{\alpha\beta}(\cdot, z^*) \mathrm{e}^{\sum_{j=1}^n \alpha_j z_j^*} \sum_{i=1}^n (\alpha_i - \beta_i) \sum_{k=1}^n (\alpha_k - \beta_k) \overline{Z}_k \, \psi_i \, \mathrm{d}x$$

$$+ \int_\Omega \left\{ \partial_z h(\cdot, z^*) \cdot \overline{Z} \, \psi_{n+2} - \sum_{i=1}^{n+2} \overline{Z}_i \, \psi_i \right\} \mathrm{d}x$$

compact imbedding of $W^{1,q}(\Omega)$ into $L^\infty(\Omega) \Longrightarrow K_q$ is compact

2. Fredholm property:

criterion for Fredholm operators $\Longrightarrow$

$\partial_Z F_{q,\tau}(Z^*, w^*) = L_q + K_q$ is Fredholm operator of index 0 for all $q \in (2, q_1]$

3. injectivity of $\partial_Z F_{q_1,\tau}(Z^*, w^*)\colon X_{q_1} \to X^*_{q_1'}$: show injectivity on X_2, let $\overline{Z} \in X_2$

$$\left\langle \partial_Z F_{q_1,\tau}(Z^*, w^*)\overline{Z}, (\overline{Z}_1, \dots, \overline{Z}_{n+1}, 0)\right\rangle_{X_{q'}} = 0$$

strong ellipticity of $(a_{ik}(x, z^*))$, $\Gamma_D \neq \emptyset$, $\tilde{r}_{\alpha\beta}(x, z^*)\, \mathrm{e}^{\sum_{j=1}^n \alpha_j z_j^*} \geq 0 \ \forall(\alpha, \beta) \in \mathcal{R} \Longrightarrow$

$$\overline{Z}_i = 0, \ \ i = 1, \dots, n+1$$

use the test function $(0, \dots, 0, 0, \overline{Z}_{n+2}) \Longrightarrow$

$$\int_\Omega \left\{\varepsilon|\nabla \overline{Z}_{n+2}|^2 + \frac{\partial}{\partial z_{n+2}} h(\cdot, z^*)\, \overline{Z}_{n+2}^2\right\} \mathrm{d}x = 0$$

h is cont. differentiable, monotonic increasing in the argument z_{n+2} (see (A4)) $\Longrightarrow$

$\dfrac{\partial}{\partial z_{n+2}} h(x, z^*) \geq 0$ a.e. on Ω; together with $\varepsilon \geq \varepsilon_0$ a.e. on $\Omega \Longrightarrow \overline{Z}_{n+2} = 0$ •

Local existence and uniqueness result

Theorem 2. (Local existence and uniqueness of steady states)

Let $w^* = (z^{D*}, g^*, f^*) \in Q$. Furthermore, let (q_0, τ, Z^*, w^*) with $Z^* = (0, \dots, 0, Z^*_{n+2})$ be the equilibrium solution to Problem (P) according to Theorem 1.

Then there exists $q_1 \in (2, q_0]$ such that the following assertion holds: There exist neighbourhoods $U \subset X_{q_1}$ of Z^* and $W \subset Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)$ of $w^* = (z^{D*}, g^*, f^*)$ and a C^1-map $\Phi\colon W \to U$ such that $Z = \Phi(w)$ iff

$$F_{q_1,\tau}(Z, w) = 0, \quad (Z, z^D) \in M_{q_1,\tau}, \quad Z \in U, \quad w = (z^D, g, f) \in W.$$

For data $w = (z^D, g, f)$ near $w^* = (z^{D*}, g^*, f^*) \in Q$ there exists a unique solution $z = Z + z^D$ of the stationary energy model.

Conclusions

$$Q_1 = \Big\{ w = (z^D, g, f) \in Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) : \; g_i = 0, \; i = 1, \dots, n+1,$$
$$\int_{\Gamma_D} \sum_{i=1}^n (\alpha_i - \beta_i)\, z_i^D \, \mathrm{d}\Gamma = 0 \quad \forall (\alpha, \beta) \in \mathcal{R}, \quad z_{n+1}^D < 0 \Big\}.$$

$Q \subset Q_1$

Corollary 1.

Let $w = (z^D, g, f) \in Q_1$ be given. Then there are constants $q \in (2, p]$, $\tau > 1$, $\epsilon > 0$ such that the following assertions hold: If

$$\|\nabla z_i^D\|_{L^p(\Omega)} < \epsilon, \quad i = 1, \dots, n+1,$$

then there exists a $Z \in X_q$ such that (q, τ, Z, w) is a solution to (P). This solution lies in a neighbourhood of an equilibrium solution (q, τ, Z^*, w^*) to Problem (P), and in this neighbourhood there are no solutions $(q, \tau, \tilde{Z}, w)$ with $\tilde{Z} \neq Z$.

Proof of Corollary 1

- Let $w = (z^D, g, f) \in Q_1$, define

$$z_i^{D*} = \frac{1}{|\Gamma_D|}\int_{\Gamma_D} z_i^D \,\mathrm{d}\Gamma,\ i = 1, \ldots, n+1, \quad z_{n+2}^{D*} = z_{n+2}^D, \quad w^* = (z^{D*}, g, f)$$

$\Longrightarrow w^* \in Q$, let (q_0, τ, Z^*, w^*) be the equilibrium solution to (P)

- Theorem 2 guarantees $q \in (2, q_0]$, $\epsilon' > 0$ such that the equation $F_{q,\tau}(Z, w) = 0$ has a locally unique solution $Z \in X_q$ if

(1) $$\|w - w^*\|_{Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)} = \sum_{i=1}^{n+1} \|z_i^D - z_i^{D*}\|_{W^{1,p}(\Omega)} < \epsilon'.$$

- Since mean values of $z_i^D - z_i^{D*}$ on Γ_D vanish, Friedrich's inequality yields

$$\|z_i^D - z_i^{D*}\|_{W^{1,p}(\Omega)} \le c\,\|\nabla z_i^D\|_{L^p(\Omega)}, \quad i = 1, \ldots, n+1,$$

choosing ϵ in Corollary 1 sufficiently small inequality (1) can be fulfilled •

Conclusions

$$Q_2 = \left\{ w = (z^D, g, f) \in Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega) : z^D_{n+1} < 0 \right\}$$

$Q_1 \subset Q_2$

Corollary 2.

Let $w = (z^D, g, f) \in Q_2$ be given. Then there are constants $q \in (2, p]$, $\tau > 1$, $\epsilon > 0$ such that the following assertions hold: If

$$\|\nabla z_i^D\|_{L^p(\Omega)} < \epsilon, \quad i = 1, \ldots, n+1,$$

$$\|\sum_{i=1}^{n} (\alpha_i - \beta_i)\, z_i^D\|_{L^1(\Gamma_D)} < \epsilon \quad \forall (\alpha, \beta) \in \mathcal{R},$$

$$\|g_i\|_{L^\infty(\Gamma_N)} \le \epsilon, \quad i = 1, \ldots, n+1,$$

then there exists a $Z \in X_q$ such that (q, τ, Z, w) is a solution to (P). This solution lies in a neighbourhood of an equilibrium solution (q, τ, Z^*, w^*) to Problem (P), and in this neighbourhood there are no solutions $(q, \tau, \tilde{Z}, w)$ with $\tilde{Z} \neq Z$.

Proof of Corollary 2

stoichiometric subspace

$$\mathcal{S} = \text{span}\{\alpha - \beta : (\alpha, \beta) \in \mathcal{R}\} \subset \mathbb{R}^n, \qquad \mathbb{R}^n = \mathcal{S} \oplus \mathcal{S}^\perp$$

corresponding projection operators $\Pi_{\mathcal{S}} : \mathbb{R}^n \to \mathcal{S}$, $\Pi_{\mathcal{S}^\perp} : \mathbb{R}^n \to \mathcal{S}^\perp$

an indirect proof gives

(2) $$\|\lambda - \Pi_{\mathcal{S}^\perp}\lambda\|_{\mathbb{R}^n} = \|\Pi_{\mathcal{S}}\lambda\|_{\mathbb{R}^n} \le c \sum_{(\alpha,\beta)\in\mathcal{R}} |(\alpha - \beta)\cdot\lambda| \quad \forall \lambda \in \mathbb{R}^n$$

Proof of Corollary 2

Let $w = (z^D, g, f) \in Q_2$, define

$$\overline{z}_i^D = \frac{1}{|\Gamma_D|}\int_{\Gamma_D} z_i^D \,\mathrm{d}\Gamma,\ i = 1, \dots, n+1, \quad \lambda = (\overline{z}_1^D, \dots, \overline{z}_n^D),$$

$$(z_1^{D*}, \dots, z_n^{D*}) = \Pi_{\mathcal{S}^\perp}\lambda, \quad z_{n+1}^{D*} = \overline{z}_{n+1}^D, \quad z_{n+2}^{D*} = z_{n+2}^D,$$

$$w^* = (z^{D*}, (0, \dots, 0, g_{n+2}), f)$$

$\implies w^* \in Q$, let (q_0, τ, Z^*, w^*) be the equilibrium solution to (P)

Theorem 2 guarantees $q \in (2, q_0]$, $\epsilon' > 0$ such that the equation $F_{q,\tau}(Z, w) = 0$ has a locally unique solution $Z \in X_q$ if

$$(3) \qquad \|w - w^*\|_{Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)} = \sum_{i=1}^{n+1} \left\{ \|z_i^D - z_i^{D*}\|_{W^{1,p}(\Omega)} + \|g_i\|_{L^\infty(\Gamma_N)} \right\} < \epsilon'$$

Proof of Corollary 2

Friedrich's inequality and (2) for $\lambda = (\overline{z}_1^D, \ldots, \overline{z}_n^D) \Longrightarrow$

$$\begin{aligned}\sum_{i=1}^{n+1} \|z_i^D - z_i^{D*}\|_{W^{1,p}(\Omega)} &\le \sum_{i=1}^{n+1} \|z_i^D - \overline{z}_i^D\|_{W^{1,p}(\Omega)} + \sum_{i=1}^{n} \|\overline{z}_i^D - z_i^{D*}\|_{W^{1,p}(\Omega)} \\ &\le c\Big(\sum_{i=1}^{n+1} \|\nabla z_i^D\|_{L^p(\Omega)} + \sum_{(\alpha,\beta)\in\mathcal{R}} \|\sum_{i=1}^{n}(\alpha_i - \beta_i)\, z_i^D\|_{L^1(\Gamma_D)}\Big)\end{aligned}$$

$$\begin{aligned}&\|w - w^*\|_{Y_p \times L^\infty(\Gamma_N)^{n+2} \times L^\infty(\Omega)} \\ &\quad\le c\,\Big(\sum_{i=1}^{n+1} \big\{\|\nabla z_i^D\|_{L^p(\Omega)} + \|g_i\|_{L^\infty(\Gamma_N)}\big\} + \sum_{(\alpha,\beta)\in\mathcal{R}} \|\sum_{i=1}^{n}(\alpha_i - \beta_i)\, z_i^D\|_{L^1(\Gamma_D)}\Big)\end{aligned}$$

choosing ϵ in Corollary 2 sufficiently small inequality (3) can be fulfilled •

Conclusions

Interpretation

Let the source terms for the Poisson equation f, z_{n+2}^D, g_{n+2} be given. Then the stationary energy model has a solution, if

- driving forces for the fluxes induced by the boundary data
  (gradients $\nabla z_1^D, \ldots, \nabla z_{n+1}^D$)
- driving forces for all reactions evaluated on the boundary
  (affinities $\sum_{i=1}^n (\alpha_i - \beta_i) z_i^D$ on Γ_D)
- prescribed fluxes on the boundary
  ($g_1, \ldots, g_{n+1}$ on Γ_N)

are small enough. This solution is locally unique.

One could expect that uniqueness should be valid globally in this case. But such a result cannot be obtained by the Implicit Function Theorem.

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