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Energy estimates for continuous and discretized reaction-diffusion systems in heterostructures

Outline

- Model equations
- Weak formulation and energy functionals
- Energy estimates for the continuous problem
- Results for space and time discrete problem
- Concluding remarks

The model

X_i	species, $i = 1, \dots, m$	$\overline{u}_i$	reference densities
v_i	chemical potentials	$u_i = \overline{u}_i \mathrm{e}^{v_i}$	densities

- reversible reactions of mass action type

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m, \quad (\alpha, \beta) \in \mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$$

net rate $\quad k_{\alpha\beta}(\mathrm{e}^{v\cdot\alpha} - \mathrm{e}^{v\cdot\beta}), \qquad v = (v_1, \dots, v_m)$

net production rate of species X_i $\quad R_i := \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\mathrm{e}^{v\cdot\alpha} - \mathrm{e}^{v\cdot\beta})(\beta_i - \alpha_i)$

- mass fluxes $\quad j_i = -u_i \mathbf{S}_i(\cdot)\nabla v_i, \quad i = 1, \dots, m,$

anisotropies $\quad \mathbf{S}_i(x) = Q_i^T(x)\mathrm{diag}\big(\mu_i^k(x)\big)Q_i(x)$

continuity equations

$$\frac{\partial u_i}{\partial t} + \nabla \cdot j_i = R_i \text{ in } \mathbb{R}_+ \times \Omega, \quad \nu \cdot j_i = 0 \text{ on } \mathbb{R}_+ \times \Gamma,$$

$$u_i(0) = U_i \text{ in } \Omega, \quad i = 1, \dots, m.$$

Assumptions (A)

$\Omega \subset \mathbb{R}^N$ bounded Lipschitzian domain, $N \leq 3$, $\Gamma = \partial\Omega$;

$\mu_i^k \in L_+^\infty(\Omega)$, ess $\inf_\Omega \mu_i^k \geq \delta$, $k = 1, \ldots, N$, $i = 1, \ldots, m$;

$\overline{u}_i \in L_+^\infty(\Omega)$, $\overline{u}_i \geq \delta$, $U_i \in L_+^\infty(\Omega)$, $q_i \in \mathbb{Z}$, $i = 1, \ldots, m$;

$\mathcal{R} \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$ finite subset, $k_{\alpha\beta} \in L_+^\infty(\Omega)$, $\int_\Omega k_{\alpha\beta}\,\mathrm{d}x > 0$ for $(\alpha, \beta) \in \mathcal{R}$,
$\max\left\{\sum_{i=1}^m \alpha_i, \sum_{i=1}^m \beta_i\right\} \leq 3 \quad \forall (\alpha, \beta) \in \mathcal{R}$ if $N > 2$,
there are no "false" equilibria in the sense of Prigogine & Defay '54,
$\sum_{i=1}^m \int_\Omega U_i \kappa_i\,\mathrm{d}x > 0 \quad \forall \kappa \in \mathcal{S}^\perp$, $\kappa \geq 0$, $\kappa \neq 0$.

stoichiometric subspace $\qquad \mathcal{S} := \mathrm{span}\{\alpha - \beta : (\alpha, \beta) \in \mathcal{R}\}$

Weak formulation

$$v = (v_1, \dots, v_m) \in V = H^1(\Omega; \mathbb{R}^m), \quad u = (u_1, \dots, u_m) \in V^*$$

operators $A : V \cap L^\infty(\Omega, \mathbb{R}^m) \to V^*$, $E = (E_1, \dots, E_m) : V \to V^*$

$$\langle A\, v, \overline{v} \rangle_V := \int_\Omega \Big\{ \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i} \mathbf{S}_i \nabla v_i \cdot \nabla \overline{v}_i + \sum_{(\alpha,\ \beta) \in \mathcal{R}} k_{\alpha\beta} \Big(\mathrm{e}^{\alpha \cdot v} - \mathrm{e}^{\beta \cdot v} \Big) (\alpha - \beta) \cdot \overline{v} \Big\} \, \mathrm{d}x$$

$$\langle E v, \overline{v} \rangle_V := \int_\Omega \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i} \overline{v}_i \, \mathrm{d}x, \quad \overline{v} \in V$$

Problem (P)

$$\left. \begin{aligned} & u'(t) + Av(t) = 0,\ u(t) = Ev(t) \text{ f.a.a. } t \in \mathbb{R}_+,\ u(0) = U, \\ & u \in H^1_{\mathrm{loc}}(\mathbb{R}_+; V^*),\ v \in L^2_{\mathrm{loc}}(\mathbb{R}_+; V) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+; L^\infty(\Omega)^m). \end{aligned} \right\} \qquad \text{(P)}$$

Energy functionals

dissipation rate

$$D(v) = \int_\Omega \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i}\, \mathbf{S}_i \nabla v_i \cdot \nabla v_i \,\mathrm{d}x$$
$$+ \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(e^{v\cdot\alpha} - e^{v\cdot\beta})(\alpha-\beta)\cdot v \,\mathrm{d}x \geq 0 \quad \forall v \in V \cap L^\infty(\Omega, \mathbb{R}^m)$$

free energy

$$F(u) = \int_\Omega \sum_{i=1}^m \Big(u_i(\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i\Big)\,\mathrm{d}x$$

Results for the continuous problem (G./Hünlich '97, G./Gärtner '07)

- Invariants: (u,v) solution to (P) $\implies$

$$u(t) - U \in \mathcal{U} := \Big\{ u \in V^* : \ (\langle u_1, 1\rangle, \ldots, \langle u_m, 1\rangle) \in \mathcal{S} \Big\} \quad \forall\, t > 0.$$

- Thermodynamic equilibrium: There exists a unique solution (u^*, v^*) to

$$Av^* = 0, \quad u^* = Ev^*, \quad u^* - U \in \mathcal{U}. \tag{S}$$

  It holds $\nabla v^* = 0$ and $v^* \in \mathcal{S}^\perp$.

- Monotone decay of the free energy: Let (u,v) be a solution to Problem (P). Then

$$F(u(t_2)) \le F(u(t_1)) \le F(U) \quad \text{for } t_2 \ge t_1 \ge 0.$$

- Exponential decay of the free energy: Let (u,v) be a solution to Problem (P), and let (u^*, v^*) be the thermodynamic equilibrium. Then there exists a constant $\lambda > 0$ such that

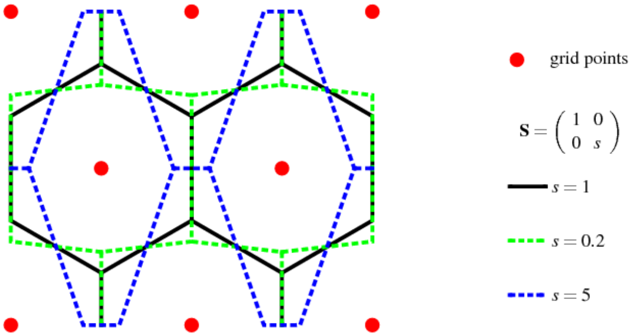
$$F(u(t)) - F(u^*) \le \mathrm{e}^{-\lambda t}(F(U) - F(u^*)) \quad \forall\, t \ge 0.$$

Space and time discretized problems

fixed set of grid points x^k, $k \in K$, for each species anisotropic Voronoi boxes

$$V_i^k = \{x \in \overline{\Omega} : \ d_i(x, x^k) \le d_i(x, x^l) \quad \forall l \in K\}, \ i = 1, \dots, m, \ k \in K$$

$$d_i(x, y)^2 := (x - y)^T \mathbf{S}_i^{-1} (x - y)$$



Space and time discretized problems

(B) $\overline{u}_i =$ const, $i = 1, \dots, m$, $k_{\alpha\beta} =$ const $(\alpha, \beta) \in \mathcal{R}$, $\tau =$ const,

$\mathbf{S}_i$ constant, symmetric, positive definite matrices.

- u_i^k mass of species X_i in V_i^k, $U_i^k = \int_{V_i^k} U_i \, \mathrm{d}x$, $\quad k \in K, i = 1, \dots, m$
- potentials v_i^k associated to grid points x^k
- discrete state equations $\quad u_i^k = \overline{u}_i \mathrm{e}^{v_i^k} |V_i^k|, \quad k \in K, \ i = 1, \dots, m$
- notation $\quad \vec{u} = (u_i^k)_{k \in K, \, i=1,\dots,m}, \quad \vec{v} = (v_i^k)_{k \in K, \, i=1,\dots,m}$

(C) $\mathcal{Z} = \{0, t_1, \dots, t_n, \dots\}$ partition of $\mathbb{R}_+$, $t_n \in \mathbb{R}_+$, $t_{n-1} < t_n$, $n \in \mathbb{N}$,

$t_n \to \infty$ as $n \to \infty$, $h_n = t_n - t_{n-1}$, $\sup_{n \in \mathbb{N}} h_n < \infty$.

Space and time discretized problems

Discretization scheme

$$\left.\begin{aligned}
&\frac{u_i^k(t_n)-u_i^k(t_{n-1})}{h_n} = -\sum_{l\in K} J_i^{kl}(t_n)|\partial V_i^k \cap \partial V_i^l| + R_i^k(t_n),\\
&k\in K,\ n\geq 1,\ i=1,\dots,m,\\
&\vec{u}(0)=\vec{U}.
\end{aligned}\right\}\qquad \text{(PD)}$$

discretized fluxes

$$J_i^{kl} = -\overline{u}_i\, Z_i^{kl}\, \frac{v_i^l - v_i^k}{|x^l - x^k|}\, |\mathbf{S}_i \nu_i^{kl}|, \quad \nu_i^{kl} \text{ outer unit normal of } V_i^k, \quad Z_i^{kl} = \frac{1}{2}(\mathrm{e}^{v_i^k} + \mathrm{e}^{v_i^l})$$

source terms from reactions

$$R_i^k = \sum_{\alpha,\beta\in\mathcal{R}} (\beta_i - \alpha_i) \sum_{k_1\in K} \cdots \sum_{k_{i-1}\in K} \sum_{k_{i+1}\in K} \cdots \sum_{k_m\in K} R_{\alpha\beta}[v_1^{k_1},\dots,v_{i-1}^{k_{i-1}}, v_i^k, v_{i+1}^{k_{i+1}},\dots,v_m^{k_m}]$$
$$\times |V_1^{k_1} \cap \cdots \cap V_{i-1}^{k_{i-1}} \cap V_i^k \cap V_{i+1}^{k_{i+1}} \cap \cdots \cap V_m^{k_m}|,$$

$$R_{\alpha\beta}[v_1^{k_1},\dots,v_m^{k_m}] = k_{\alpha\beta}\left(\mathrm{e}^{\sum_{i=1}^m \alpha_i v_i^{k_i}} - \mathrm{e}^{\sum_{i=1}^m \beta_i v_i^{k_i}}\right)$$

Discrete energy functionals

discrete version of E $\quad \widehat{E}\colon \mathbb{R}^{Mm} \to \mathbb{R}^{Mm}$, $\qquad (M = \#K)$

$$\widehat{E}\vec{v} = \Big(\big(\overline{u}_i \mathrm{e}^{v_i^k} |V_i^k| \big)_{k\in K} \Big)_{i=1,\dots,m}$$

discrete free energy

$$\widehat{F}(\vec{u}) = \sum_{i=1}^{m} \sum_{k\in K} \Big(u_i^k v_i^k - u_i^k + \overline{u}_i |V_i^k| \Big) \quad \text{for } \vec{u} = \widehat{E}\vec{v}$$

invariants: $(\vec{u}, \vec{v})$ solution to the discretized problem (PD) $\Longrightarrow$

$$\vec{u}(t_n) - \vec{U} \in \widehat{\mathcal{U}} = \Big\{ \vec{u} \in \mathbb{R}^{Mm} : \big(\sum_{k\in K} u_1^k, \dots, \sum_{k\in K} u_m^k \big) \in \mathcal{S} \Big\} \quad \forall n \in \mathbb{N}$$

Steady states of the discretized problem

Theorem 1. [Thermodynamic equilibrium]
We assume (A) and (B). Then there is a unique solution $(\vec{u}^*, \vec{v}^*)$ to Problem

$$\left.\begin{array}{l} \sum_{l \in K} J_i^{kl} |\partial V_i^k \cap \partial V_i^l| - R_i^k = 0, \; k \in K, \; i = 1, \dots, m, \\ \vec{u} = \widehat{E}\vec{v}, \quad \vec{u} - \vec{U} \in \widehat{\mathcal{U}}. \end{array}\right\} \qquad \text{(SD)}$$

This solution satisfies $\vec{v}^* \in \widehat{\mathcal{U}}^\perp$.

Idea of the proof

- introduce $G : \mathbb{R}^{Mm} \to \overline{\mathbb{R}}$,

$$G(\vec{v}) := \widehat{F}^*(\vec{v}) + I_{\widehat{\mathcal{U}}^\perp}(\vec{v}) - \langle \vec{U}, \vec{v} \rangle, \quad \vec{v} \in \mathbb{R}^{Mm},$$

  ($I_{\widehat{\mathcal{U}}^\perp}$characteristic function of $\widehat{\mathcal{U}}^\perp$). G is proper, lsc., strictly convex
- If $(\vec{u}, \vec{v})$ is a solution to (SD) then $\vec{v}$ is the unique minimizer of G. If $\vec{v}$ is a minimizer of G then $(\widehat{E}\vec{v}, \vec{v})$ is a solution to (SD).
- suffices to show that $G(\vec{v}) \to \infty$ if $\|\vec{v}\| \to \infty$ (indirect proof).

Discrete Poincaré like inequality (Glitzky '08)

Theorem 2. [Estimate of the free energy by the dissipation rate]
Let (A) and (B) be fulfilled. Moreover, let $(\vec{u}^*, \vec{v}^*)$ be the thermodynamic equilibrium according to Theorem 1. Then for every $\rho > 0$ there exists a constant $c_\rho > 0$ such that

$$\widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \leq c_\rho \widehat{D}(\vec{v})$$

for all $\vec{u} \in \mathcal{N}_\rho := \Big\{ \vec{u} = \widehat{E}\vec{v} \in \mathbb{R}^{Mm} : \ \widehat{F}(\vec{u}) - \widehat{F}(\vec{u}^*) \leq \rho, \ \vec{u} - \vec{U} \in \widehat{\mathcal{U}} \Big\}$.

$$\widehat{D}(\vec{v}) = \sum_{i=1}^{m} \sum_{k,l \in K,\, l<k} \overline{u}_i \, Z_i^{kl} \frac{(v_i^l - v_i^k)^2}{|x^l - x^k|} |\mathbf{S}_i \nu_i^{kl}| |\partial V_i^k \cap \partial V_i^l|$$

$$+ \sum_{(\alpha,\beta)\in\mathcal{R}} \sum_{k_1 \in K} \cdots \sum_{k_m \in K} R_{\alpha\beta}\big[v_1^{k_1}, \ldots, v_m^{k_m}\big] \sum_{i=1}^{m} (\alpha_i - \beta_i) v_i^{k_i} \, |V_1^{k_1} \cap \cdots \cap V_m^{k_m}| \geq 0.$$

Energy estimates for (PD)

Theorem 3. [Monotone end exponential decay of the free energy]
We assume (A), (B) and (C). Then the (fully implicit in time) discretization scheme (PD) is dissipative, i.e. solutions $(\vec{u}, \vec{v})$ to (PD) fulfil

$$\widehat{F}(\vec{u}(t_{n_2})) \leq \widehat{F}(\vec{u}(t_{n_1})) \leq \widehat{F}(\vec{U}) \quad \text{for all } t_{n_1} < t_{n_2}.$$

Moreover, there exists a $\lambda > 0$ such that

$$\widehat{F}(\vec{u}(t_n)) - \widehat{F}(\vec{u}^*) \leq \mathrm{e}^{-\lambda t_n} \big(\widehat{F}(\vec{U}) - \widehat{F}(\vec{u}^*)\big) \quad \forall n \geq 1.$$

Proof

- $\widehat{F} : \mathbb{R}^{Mm} \to \overline{\mathbb{R}}$ is convex, lsc., differentiable in arguments $\vec{u} > 0$.

  $$\vec{u} = \widehat{E}\vec{v} \Longrightarrow \vec{v} = \widehat{F}'(\vec{u}), \quad \widehat{F}(\vec{u}) - \widehat{F}(\vec{w}) \leq \widehat{F}'(\vec{u}) \cdot (\vec{u} - \vec{w}) \quad \forall \vec{w} \in \mathbb{R}^{Mm}$$

- $\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}(t_{l-1})) \leq \big(\vec{u}(t_l) - \vec{u}(t_{l-1})\big) \cdot \vec{v}(t_l) = -\widehat{D}(\vec{v}(t_l))$

Proof of Theorem 3

- let $\lambda \geq 0$, $n_2 > n_1 \geq 0$

$$\mathrm{e}^{\lambda t_{n_2}}\Big(\widehat{F}(\vec{u}(t_{n_2})) - \widehat{F}(\vec{u}^*)\Big) - \mathrm{e}^{\lambda t_{n_1}}\Big(\widehat{F}(\vec{u}(t_{n_1})) - \widehat{F}(\vec{u}^*)\Big)$$
$$\leq \sum_{l=n_1+1}^{n_2} h_l\,\mathrm{e}^{\lambda t_{l-1}}\Big\{\mathrm{e}^{\lambda h_l}\lambda\big(\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*)\big) - \widehat{D}(\vec{v}(t_l))\Big\}$$

- $\widehat{D}(\vec{v}(t_l)) \geq 0 \quad \forall l \geq 1,$ setting $\lambda = 0 \Longrightarrow$

$$\widehat{F}(\vec{u}(t_{n_2})) \leq \widehat{F}(\vec{u}(t_{n_1})) \leq \widehat{F}(\vec{U}) \quad \forall t_{n_2} > t_{n_1} \geq 0$$

- $\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*) \leq \widehat{F}(\vec{U}) - \widehat{F}(\vec{u}^*) =: \rho, \quad \vec{u}(t_l) \in \vec{U} + \widehat{\mathcal{U}} \Longrightarrow \vec{u}(t_l) \in N_\rho,\, l \geq 1,$
  Theorem 2 supplies $c_\rho > 0$ s.t.

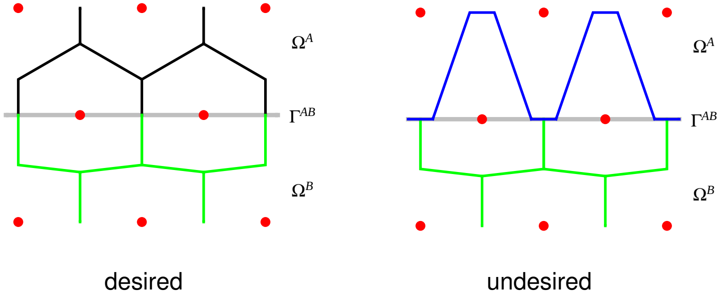
$$\widehat{F}(\vec{u}(t_l)) - \widehat{F}(\vec{u}^*) \leq c_\rho \widehat{D}(\vec{v}(t_l)) \quad \forall l$$

- choose $\lambda > 0$ s.t. $\lambda \mathrm{e}^{\lambda \overline{h}} c_\rho < 1$, $n_1 = 0$ □

Numerical treatment of heterostructures

$$\overline{\Omega} = \cup_{I\in\mathcal{I}}\overline{\Omega^I}, \quad \Gamma^{AB} = \overline{\Omega^A} \cap \overline{\Omega^B}, \quad \text{on } \Omega^I \text{ constant coefficients}$$

take grid $\{x^k : x^k \in \overline{\Omega}, k = 1, \ldots, \widetilde{M}\}$ respecting interfaces Γ^{AB}, $A,\ B \in \mathcal{I}$, $|\Gamma^{AB}| > 0$
especially endpoints of Γ^{AB} are grid points



Numerical treatment of heterostructures

on Ω^I $\qquad \mathbf{S}_i^I = {Q_i^I}^T \text{diag}(\mu_i^{kI}) Q_i^I$

$$\gamma := \max_{I \in \mathcal{I}} \max_{i=1,\dots,m} \arccos \frac{\min_k(\mu_i^{kI})}{\max_k(\mu_i^{kI})}$$

for $|\Gamma^{AB}| > 0$ let

$$\kappa^{AB} := \frac{\text{max. Euclidean dist. of directly neighboring grid points on het. interface } \Gamma^{AB}}{\text{min. Euclidean dist. of inner grid points to the het. interface } \Gamma^{AB}}$$

The restriction on the position of vertices on and close to interfaces and boundaries

$$\max_{A,B \in \mathcal{I},\, |\Gamma^{AB}|>0} \kappa^{AB} \leq \sqrt{2 - 2\sin\gamma}$$

allows to handle general heterostructures and boundary conditions. The described integration procedure can be applied independently on each Ω^I and the fluxes and potentials fulfill the continuity conditions.

Concluding remarks

Results remain true for (Glitzky '08)

- more general state equations $u_i = \overline{u}_i g_i(v_i - \overline{v}_i)$

  mass fluxes

$$j_i = -\overline{u}_i g_i'(v_i - \overline{v}_i)\mathbf{S}_i \nabla v_i$$

(inverse of the Hessian of the free energy for species X_i)

- charged species X_i with charge numbers q_i

  add Poisson equation for the electrostatic potential v_0

$$-\nabla \cdot (\mathbf{S}_0 \nabla v_0) = f + \sum_{i=1}^{m} q_i u_i \quad \text{on } \mathbb{R}_+ \times \Omega$$

$$\nu \cdot (\mathbf{S}_0 \nabla v_0) + \tau v_0 = f^\Gamma \quad \text{on } \mathbb{R}_+ \times \Gamma$$

mass fluxes

$$j_i = -\overline{u}_i g_i'(v_i - \overline{v}_i)\mathbf{S}_i \nabla (v_i + q_i v_0)$$

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