Weierstraß-Institut für Angewandte Analysis und Stochastik

6th International Congress on
Industrial and Applied Mathematics
Zurich 16 - 20 July 2007

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Energy estimates for reaction-diffusion processes of charged species

Model equations

X_i	species, $i = 1, \ldots, m$	q_i	charge numbers
u_i	densities	v_i	chemical potentials
v_0	electrostatic potential	$\zeta_i = v_i + q_i v_0$	electrochemical potentials

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 $\quad k_{\alpha\beta}(\mathrm{e}^{\zeta\cdot\alpha} - \mathrm{e}^{\zeta\cdot\beta}), \quad \zeta = (\zeta_1, \ldots, \zeta_m)$

net production rate of species X_i

$$R_i := \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\mathrm{e}^{\zeta\cdot\alpha} - \mathrm{e}^{\zeta\cdot\beta})(\beta_i - \alpha_i)$$

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

Model equations

free energy

$$F(u) = F_{ch}(u) + F_{inter}(u) = \int_\Omega \sum_{i=1}^m \overline{u}_i f_i\left(\frac{u_i}{\overline{u}_i}\right) \mathrm{d}x + F_{inter}(u)$$

state equations

$$v_i = \frac{\partial F_{ch}}{\partial u_i}(u) = f_i'\left(\frac{u_i}{\overline{u}_i}\right), \quad u_i = \overline{u}_i (f_i')^{-1}(v_i) = \overline{u}_i g_i(v_i)$$

mass fluxes (Butta/Lebowitz'99, Giacomin/Lebowitz'00)

$$j_i = -\overline{u}_i g_i'(v_i) \mathbf{S}_i(\cdot)\nabla\zeta_i, \quad i = 1, \ldots, m,$$

$$\mathbf{S}_i(x) = Q_i^T(x)\mathrm{diag}\big(\mu_i^1(x), \mu_i^2(x)\big)Q_i(x) \quad \text{(Lades/Wachutka'97)}$$

Model equations

continuity equations

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

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

Poisson equation

$$-\nabla \cdot (\mathbf{S_0} \nabla v_0) = f + \sum_{i=1}^{m} q_i u_i \quad \text{in } \mathbb{R}_+ \times \Omega, \quad \nu \cdot (\mathbf{S_0} v_0) + \tau v_0 = f^\Gamma \quad \text{on } \mathbb{R}_+ \times \Gamma,$$

dielectric permittivity matrix

$$\mathbf{S_0}(x) = Q_0^T(x) \text{diag}(\varepsilon^1(x), \varepsilon^2(x)) Q_0(x)$$

$$u_0 = \sum_{i=1}^{m} q_i u_i$$

Assumptions

(A1) $\Omega \subset \mathbb{R}^2$ bounded Lipschitzian domain, $\Gamma = \partial\Omega$;

(A2) $g_i \in C^1(\mathbb{R}),\ \overline{u}_i \in L^\infty_+(\Omega),\ \overline{u}_i \ge \delta$,

$$\lim_{y\to\infty} \frac{1}{y} g_i(y) = +\infty,\ 0 < \delta \min\{1, g_i(y)\} \le g_i'(y) \le \delta^{-1} g_i(y),$$

$$\delta \min\{1, \exp(y)\} \le g_i(y) \le \delta^{-1}\exp(y),\ y \in \mathbb{R},\ i = 1,\ldots,m;$$

(A3) $\mu_i^k \in L^\infty_+(\Omega),$ ess $\inf_\Omega \mu_i^k \ge \delta,\ k = 1,2,\ i = 1,\ldots,m;$

(A4) $\mathcal{R} \subset \mathbb{Z}^m_+ \times \mathbb{Z}^m_+$ finite subset, $k_{\alpha\beta} \in L^\infty_+(\Omega),\ \int_\Omega k_{\alpha\beta}\, \mathrm{d}x > 0$ for $(\alpha,\beta) \in \mathcal{R}$,

no “false” equilibria in the sense of Prigogine;

(A5) $U_i \in L^\infty_+(\Omega),\ q_i \in \mathbb{Z},\ i = 1,\ldots,m,$

$$\int_\Omega \sum_{i=1}^m U_i \kappa_i \, \mathrm{d}x > 0 \quad \forall \kappa \in \mathcal{S}^\perp,\ \kappa \ge 0,\ \kappa \ne 0;$$

(A6) $\varepsilon^k \in L^\infty_+(\Omega),$ ess $\inf_\Omega \varepsilon^k \ge \delta,\ k = 1,2,\ \tau \in L^\infty_+(\Gamma),\ \int_\Gamma \tau\, \mathrm{d}\Gamma > 0,$

$f \in L^\infty(\Omega),\ f^\Gamma \in L^\infty(\Gamma).$

Weak formulation

$$v = (v_0, \dots, v_m) \in V = H^1(\Omega; \mathbb{R}^{m+1}), \quad u = (u_0, \dots, u_m) \in V^*$$

Problem P:

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

dissipation rate

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

free energy

$$F(u) = \int_\Omega \Big(\sum_{i=1}^m \overline{u}_i f_i\big(\frac{u_i}{\overline{u}_i}\big) + \frac{1}{2}\mathbf{S}_0 \nabla v_0 \cdot \nabla v_0 \Big) \,\mathrm{d}x + \int_\Gamma \frac{\tau}{2} v_0^2 \,\mathrm{d}\Gamma$$

Results for the continuous problem

(u, v) solution to (P) $\implies \quad u(t) \in U + \mathcal{U} \quad \forall t > 0$

$$\mathcal{U} := \Big\{ u \in V^* : \; u_0 = \sum_{i=1}^{m} q_i u_i, \; (\langle u_1, 1\rangle, \dots, \langle u_m, 1\rangle) \in \mathcal{S} \Big\}$$

Theorem 1. [Thermodynamic equilibrium] (G./Gröger/Hünlich’96)

Let (A1) – (A6) be fulfilled. There exists a unique solution (u^*, v^*) to

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

It holds $v^* \in V \cap L^\infty(\Omega)^{m+1}$, $\nabla \zeta^* = 0$ and $\zeta^* \in \mathcal{S}^\perp$.

Theorem 2. [Monotone decay of the free energy] (G./Gröger/Hünlich’96)

Let (A1) – (A6) be fulfilled and let (u, v) be a solution to Problem (P). Then

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

Results for the continuous problem

Theorem 3. [Estimate by the dissipation rate] (G./Gärtner'07)

Let (A1) – (A6) be fulfilled. Moreover, let (u^*, v^*) be the thermodynamic equilibrium. Then for every $R > 0$ there exists a constant $c_R > 0$ such that

$$F(u) - F(u^*) \le c_R D(v)$$

provided that $v \in V$, $u = Ev \in U + \mathcal{U}$, and $F(Ev) \le R$.

Theorem 4. [Exponential decay of the free energy] (G./Gärtner'07)

Let (A1) – (A6) be fulfilled, 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

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

Theorem 5. [Monotone and exponential decay of the free energy] (G.'07)

Let (A1) – (A6) be fulfilled. Let (u^*, v^*) be the thermodynamic equilibrium and let $h > 0$. Then the fully implicit time discretization scheme

$$u(nh) - u\big((n-1)h\big) + hAv(nh) = 0, \quad u(nh) = Ev(nh), \quad n \geq 1,$$
$$u(0) = U, \quad v(nh) \in V, \quad n \geq 0$$

is dissipative. Moreover, there exists a constant $\lambda > 0$ such that

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

Space and time discretized problems

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

$$V_i^k = \{x \in \overline{\Omega} : \, d_i(x, x^k) \le d_i(x, x^l) \quad \forall l \in K\}\,, \; i = 0, \dots, m\,, \; k \in K$$

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

u_i^k masses in V_i^k, potentials $v_0^k, \; v_i^k, \; \zeta_i^k$ associated to grid points x^k

$$u_i^k = \overline{u}_i g_i(v_i^k) |V_i^k|, \quad k \in K$$

$$\zeta_i^k = v_i^k + q_i \sum_{l \in K} \frac{|V_0^l \cap V_i^k|}{|V_i^k|} \, v_0^l, \quad i = 1, \dots, m$$

Space and time discretized problems

Theorem 6. [Dissipativeness of the discretization scheme] (G./Gärtner'07)

Let (A1) – (A6) be fulfilled. Moreover, let $\overline{u}_i$, $\mathbf{S}_i$, $k_{\alpha\beta}$ and τ be constant and let $h > 0$ be given. The following discrete problem is dissipative

$$P\vec{v}_0(nh) - \vec{f} = \vec{u}_0(nh), \quad n \geq 0,$$

$$\frac{u_i^k(nh) - u_i^k((n-1)h)}{h} = -\sum_{l \in K} J_i^{kl}(nh)|\partial V_i^k \cap \partial V_i^l| + R_i^k(nh),$$
$$k \in K,\ n \geq 1,\ i = 1, \ldots, m,$$

$$u_i^k(0) = U_i^k, \quad k \in K,\ i = 0, \ldots, m.$$

Space and time discretized problems

discretized Poisson equation

$$-\sum_{l\in K}\frac{v_0^l-v_0^k}{|x^l-x^k|}|\mathbf{S}_0\nu_0^{kl}||\partial V_0^k\cap\partial V_0^l|+\tau v_0^k|\partial V_0^k\cap\Gamma|-f^k=u_0^k,\quad k\in K,$$

where

$$f^k=\int_{V_0^k} f\,\mathrm{d}x+\int_{\partial V_0^k\cap\Gamma} f^\Gamma\,\mathrm{d}\Gamma,$$

$$u_0^k=\sum_{i=1}^m q_i\sum_{l\in K}\frac{|V_0^k\cap V_i^l|}{|V_i^l|}u_i^l,$$

ν_0^{kl} outer unit normal of V_0^k on $\partial V_0^k\cap\partial V_0^l$,

$$\vec{v}_0=(v_0^k)_{k\in K},\ \vec{f}=(f^k)_{k\in K},\ \vec{u}_0=(u_0^k)_{k\in K}$$

Space and time discretized problems

discretized fluxes

$$J_i^{kl} = -\overline{u}_i \, Z_i^{kl} \, \frac{\zeta_i^l - \zeta_i^k}{|x^l - x^k|} \, |\mathbf{S}_i \nu_i^{kl}|,$$

$$Z_i^{kl} = \begin{cases} \frac{g_i(v_i^l) - g_i(v_i^k)}{v_i^l - v_i^k} & \text{for } v_i^l \neq v_i^k \\ g_i'(v_i^k) & \text{for } v_i^l = v_i^k \end{cases}$$

source terms from reactions

$$R_i^k = \sum_{\alpha,\beta \in \mathcal{R}} (\beta_i - \alpha_i) \sum_{k_1 \in K} \cdots \sum_{k_{i-1} \in K} \sum_{k_{i+1} \in K} \cdots \sum_{k_m \in K} R_{\alpha\beta}[\zeta_1^{k_1}, \ldots, \zeta_{i-1}^{k_{i-1}}, \zeta_i^k, \zeta_{i+1}^{k_{i+1}}, \ldots, \zeta_m^{k_m}]$$
$$\times |V_1^{k_1} \cap \cdots \cap V_{i-1}^{k_{i-1}} \cap V_i^k \cap V_{i+1}^{k_{i+1}} \cap \cdots \cap V_m^{k_m}|,$$

$$R_{\alpha\beta}[\zeta_1^{k_1}, \ldots, \zeta_m^{k_m}] = k_{\alpha\beta} \left(\mathrm{e}^{\sum_{i=1}^m \alpha_i \zeta_i^{k_i}} - \mathrm{e}^{\sum_{i=1}^m \beta_i \zeta_i^{k_i}} \right)$$

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