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Energy estimates for electro–reaction–diffusion systems with partly fast kinetics

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Abstract

We start from a basic model for the transport of charged species in heterostructures containing the mechanisms diffusion, drift and reactions in the domain and at its boundary. Considering limit cases of partly fast kinetics we derive reduced models. This reduction can be interpreted as some kind of projection scheme for the weak formulation of the basic electro–reaction–diffusion system. We verify assertions concerning invariants and steady states and prove the monotone and exponential decay of the free energy along solutions to the reduced problem and to its fully implicit discrete-time version by means of the results of the basic problem. Moreover we make a comparison of prolongated quantities with the solutions to the basic model.

1 Motivation

In semiconductor technology the redistribution of dopants in semiconductor heterostructures is described by models where drift-diffusion processes of up to twenty different species (electrons, holes, dopants, differently charged vacancies, interstitials, and dopant-defect pairs) and more than hundred different reactions between these species like generation/recombination of defects, of electrons and holes, formation and collapse of dopant-defect pairs, ionization of defects and pairs are taken into account (see e.g. [3, 4, 7, 14]). Forced by such applications from semiconductor technology we are interested in reduced models where some of the present kinetic subprocesses are considered to be very fast. From a mathematical point of view such assumptions of fast subprocesses decrease the number of continuity equations which have to be taken into account. On the other hand, this reduction of the number of equations leads to additional nonlinearities in the remaining equations. Often there occur nonlocal constraints and nonlocal terms in the equations or in the boundary terms (see e.g. the model equations in [8, 12, 13]).

The first aim of the paper is to present a general scheme how to deduce the reduced models from a basic model where all subprocesses are nearly of the same rate. Second, we show that our scheme provides the possibility to carry over results concerning energy estimates for the basic problem to the reduced ones. These principles should be of interest also in other fields of applications of electro-reaction-diffusion systems.

The paper is organized as follows. In Section 2 we introduce a basic model for electro-reaction-diffusion processes and give some notation. The general assumptions and the weak formulation of the basic model are given in Section 3. In Section 4 we introduce our reduction scheme. Section 5 summarizes known results for the basic model which are relevant for the present paper. Assertions concerning invariants and steady states of the reduced problem are derived in Section 6, the proof of energy estimates for the reduced model is given in Section 7. In Section 8 we make a comparison between solutions of the reduced and the basic model. Section 9 provides energy estimates for a fully implicit time-discrete version of the reduced problem. Finally, in Section 10 we discuss four examples for the reduction of the model equations in the case of fast kinetic subprocesses in more detail.

2 A basic model for electro-reaction-diffusion processes in heterostructures

We consider a bounded domain Ω with boundary $\Gamma = \Gamma_N \cup \Gamma_D \cup \Gamma_0$ and $\operatorname{mes} \Gamma_0 = 0$. Let ν be the outer unit normal. We look at m electrically charged species X_i with charge numbers q_i and initial concentrations $U_i \colon \Omega \to \mathbb{R}_+$. Their concentrations $u_i \colon \mathbb{R}_+ \times \Omega \to \mathbb{R}_+$ as well as their chemical potentials $v_i \colon \mathbb{R}_+ \times \Omega \to \mathbb{R}$ are changing by chemical reactions taking place in Ω and at its boundary Γ, by diffusion processes and, in addition, by a drift which is caused by the inner electric field. The relation between concentrations and chemical potentials is assumed to be given by Boltzmann statistics

$$u_i = \overline{u}_i \, \mathrm{e}^{v_i}, \quad i = 1, \dots m,$$

where $\overline{u}_i \colon \Omega \to \mathbb{R}_+$ are given reference densities. The function $u_0 = \sum_{i=1}^m q_i u_i$ represents the charge density. By $v_0 \colon \mathbb{R}_+ \times \Omega \to \mathbb{R}$ we denote the electrostatic potential. Moreover, $\zeta_i := v_i + q_i v_0 \colon \mathbb{R}_+ \times \Omega \to \mathbb{R}$ corresponds to the electrochemical potential of the i-th species. All functions are suitably scaled.

The driving forces for the particle flux of the i-th species is the gradient of the electrochemical potential

$$j_i = -D_i u_i \nabla \zeta_i = -D_i \, u_i \nabla (v_i + q_i v_0), \quad i = 1, \dots m,$$

with given diffusivity $D_i \colon \Omega \to \mathbb{R}_+$.

We consider a finite set of mass action type reactions of the form

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m$$

and denote by $\mathcal{R}^\Omega$ and $\mathcal{R}^\Gamma$ the set of pairs (α, β) of stoichiometric coefficients $\alpha = (\alpha_1, \dots, \alpha_m)$, $\beta = (\beta_1, \dots, \beta_m)$ corresponding to all reactions running in Ω or at Γ. For each species the reaction rates R_i^Ω in the volume and R_i^Γ at the boundary are written as

$$R_i^\Sigma = \sum_{(\alpha,\, \beta) \in \mathcal{R}^\Sigma} R_{\alpha\beta}^\Sigma (\alpha_i - \beta_i), \quad i = 1, \dots, m,$$

$$R_{\alpha\beta}^\Sigma = k_{\alpha\beta}^\Sigma (x, v_0, \dots, v_m) \Big(\prod_{k=1}^m \mathrm{e}^{\zeta_k \alpha_k} - \prod_{k=1}^m \mathrm{e}^{\zeta_k \beta_k} \Big),$$

where the kinetic coefficients $k_{\alpha\beta}^\Sigma \colon \Sigma \times \mathbb{R}^{m+1} \to \mathbb{R}_+$ are fixed functions, $\Sigma = \Omega, \Gamma$.

Now we are able to formulate the electro–reaction–diffusion system modelling the transport of charged particles. Mass balance for each species coupled with a Poisson equation for the electrostatic potential v_0 lead to the following initial boundary value problem

$$\left.\begin{array}{rcll} \dfrac{\partial u_i}{\partial t} + \nabla \cdot j_i + R_i &=& 0 & \text{on } (0,\infty)\times\Omega, \\ \nu \cdot j_i &=& 0 & \text{on } (0,\infty)\times\Gamma, \\ u_i(0) &=& U_i & \text{on } \Omega\,,\ i=1,\dots,m, \\ -\nabla\cdot(\varepsilon\nabla v_0) &=& f^\Omega + \displaystyle\sum_{i=1}^m q_i u_i & \text{on } (0,\infty)\times\Omega, \\ \nu\cdot(\varepsilon\nabla v_0) + \tau v_0 &=& f^\Gamma & \text{on } (0,\infty)\times\Gamma_N, \\ v_0 &=& v_D & \text{on } (0,\infty)\times\Gamma_D, \end{array}\right\} \qquad (1)$$

where the initial densities $U_i \colon \Omega \to \mathbb{R}_+$, the dielectric permittivity $\varepsilon\colon \Omega \to \mathbb{R}_+$, the capacity $\tau\colon \Gamma_N \to \mathbb{R}_+$ are given. In many applications from semiconductor technology all physical parameters $\overline{u}_i$, D_i, $k^\Sigma_{\alpha\beta}$, ε, τ and f^Σ depend on the space variable in a non-smooth way.

Without loss of generality we will assume that $f^\Gamma = 0$ and $v_D = 0$ (otherwise we would have to use as a new variable the difference of v_0 and the solution $\widehat{v}_0$ of the Laplace equation

$$\begin{array}{rcll} -\nabla\cdot(\varepsilon\nabla\widehat{v}_0) &=& 0 & \text{on } (0,\infty)\times\Omega, \\ \nu\cdot(\varepsilon\nabla\widehat{v}_0) + \tau\widehat{v}_0 &=& f^\Gamma & \text{on } (0,\infty)\times\Gamma_N, \\ \widehat{v}_0 &=& v_D & \text{on } (0,\infty)\times\Gamma_D. \end{array}$$

Let us collect some notation which we use in the paper. We assume that $\Omega \subset \mathbb{R}^2$ is a bounded (strictly) Lipschitzian domain. The notation of function spaces $L^p(\Omega,\mathbb{R}^k)$, $H^1(\Omega,\mathbb{R}^k)$, $k\in\mathbb{N}$, corresponds to that in [16]. With regard to the definition of the space $H^1_0(\Omega\cup\Gamma_N)$ we refer to [6, Appendix]. If X is any Banach space X we write $\langle\cdot,\cdot\rangle_X$ for the corresponding dual pairing. By $\mathbb{R}^k_+$, L^p_+ we denote the cones of nonnegative elements. For the scalar product in $\mathbb{R}^k$ we use a centered dot. In our estimates positive constants, which depend at most on the data of our problem, are denoted by c.

3 Weak formulation of the basic model

Now we shall formulate a general evolution problem corresponding to the basic model problem introduced in Section 2. We summarize the assumptions concerning the data of the basic system our further considerations are based on:

$$\left.\begin{array}{l} \Omega \text{ is a bounded Lipschitzian domain in } \mathbb{R}^2\,,\ \Gamma := \partial\Omega, \\ \Gamma_D,\, \Gamma_N \text{ are disjoint open subsets of } \Gamma\,,\ \Gamma = \Gamma_D \cup \Gamma_N \cup (\overline{\Gamma_D} \cap \overline{\Gamma_N}), \\ \overline{\Gamma_D} \cap \overline{\Gamma_N} \text{ consists of finitely many points;} \end{array}\right\} \qquad (2)$$

$$\left.\begin{array}{l} q_i \in \mathbb{Z}\,,\ \overline{u}_i,\, U_i \in L^\infty(\Omega)\,,\ \overline{u}_i,\, U_i \ge c > 0, \\ D_i \in L^\infty(\Omega)\,,\ D_i \ge c > 0\,,\ i = 1,\dots,m, \\ U_0 := \sum_{i=1}^m q_i U_i\,,\ q := (q_1,\dots,q_m) \in \mathbb{Z}^m\,,\ f^\Omega \in L^2(\Omega), \\ \varepsilon \in L^\infty(\Omega)\,,\ \varepsilon \ge c > 0,\ \tau \in L^\infty_+(\Gamma_N)\,,\ \operatorname{mes}\Gamma_D + \|\tau\|_{L^1(\Gamma_N)} > 0; \end{array}\right\} \qquad (3)$$

$$\left.\begin{array}{l} \mathcal{R}^\Omega,\, \mathcal{R}^\Gamma \text{ are finite subsets of } \mathbb{Z}^m_+ \times \mathbb{Z}^m_+, \\ (\alpha - \beta)\cdot q = 0\ \ \forall (\alpha,\beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma, \\ \text{for } \Sigma = \Omega,\, \Gamma \text{ and } (\alpha,\beta) \in \mathcal{R}^\Sigma \text{ we define} \\ R^\Sigma_{\alpha\beta} := k^\Sigma_{\alpha\beta}(x,y)\,(\mathrm{e}^{\alpha\cdot\zeta} - \mathrm{e}^{\beta\cdot\zeta})\,,\ x \in \Sigma\,,\ y = (y_0, y_1, \cdots, y_m) \in \mathbb{R}^{m+1}, \\ \zeta_i := y_i + q_i y_0\,,\ i = 1,\dots,m, \text{ where} \\ k^\Sigma_{\alpha\beta} \colon \Sigma \times \mathbb{R}^{m+1} \to \mathbb{R}_+ \text{ satisfies the Carathéodory conditions,} \\ k^\Sigma_{\alpha\beta}(x,y) \ge c_R > 0 \text{ f.a.a. } x \in \Sigma,\ \forall y \in \mathbb{R}^{m+1} \text{ with } y_0 \in [-R,R]. \end{array}\right\} \qquad (4)$$

Finally, for the discussion of asymptotic properties we need a further assumption on the structure of the reaction system which will be introduced later on (see (6)).

For the weak formulation of our basic problem we use as variables the $m+1$ dimensional vectors of potentials and densities

$$v = (v_0, v_1, \dots, v_m)\,,\ u = (u_0, u_1, \dots, u_m).$$

The initial value for u has to be understood as $U = (U_0, \dots, U_m)$ with $U_0 = \sum_{i=1}^m q_i U_i$. We work with the function spaces

$$X := H^1_0(\Omega \cup \Gamma_N) \times H^1(\Omega, \mathbb{R}^m)\,,\ W := X \cap L^\infty(\Omega, \mathbb{R}^{m+1})$$

and define operators $A \colon W \to X^*$, $E_0 \colon H^1_0(\Omega \cup \Gamma_N) \to (H^1_0(\Omega \cup \Gamma_N))^*$, $E \colon X \to X^*$

by

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

$$+ \int_\Gamma \sum_{(\alpha,\,\beta)\in\mathcal{R}^\Gamma} R^\Gamma_{\alpha\beta}(\cdot, v)\,(\alpha-\beta)\cdot\overline{\zeta}\,\mathrm{d}\Gamma,$$

$$\langle E_0 v_0, \overline{v}_0\rangle_{H^1_0} := \int_\Omega \big\{ \varepsilon\nabla v_0\cdot\nabla\overline{v}_0 - f^\Omega\overline{v}_0 \big\}\,\mathrm{d}x + \int_{\Gamma_N} \tau v_0 \overline{v}_0\,\mathrm{d}\Gamma,$$

$$\langle Ev, \overline{v}\rangle_X := \langle E_0 v_0, \overline{v}_0\rangle_{H^1_0} + \int_\Omega \sum_{i=1}^m \overline{u}_i \mathrm{e}^{v_i}\overline{v}_i\,\mathrm{d}x, \quad \overline{v}\in X,$$

where $\zeta_i = v_i + q_i v_0$, $\overline{\zeta}_i = \overline{v}_i + q_i\overline{v}_0$, $i = 1, \ldots, m$. As in [10] a weak formulation of the basic problem (1) writes as

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

The concept of solution used in [9] is somewhat weaker.

The stoichiometric subspace $\mathcal{S}$ belonging to the system of volume and boundary reactions occurring in the basic model equations is given by

$$\mathcal{S} := \operatorname{span}\big\{\alpha-\beta:\ (\alpha,\beta)\in\mathcal{R}^\Omega\cup\mathcal{R}^\Gamma\big\}\subset\mathbb{R}^m.$$

Moreover we introduce the notation

$$\mathcal{U} := \Big\{ u\in X^*:\ u_0 = \sum_{i=1}^m q_i u_i\,,\ (\langle u_1, 1\rangle_{H^1}, \ldots, \langle u_m, 1\rangle_{H^1})\in\mathcal{S} \Big\}$$

and

$$\mathcal{U}^\perp = \Big\{ v\in X:\ \nabla\zeta = 0\,,\ \zeta\in\mathcal{S}^\perp\,,\ \zeta_i = v_i + q_i v_0\,,\ i = 1, \ldots, m \Big\}.$$

One easily verifies that $\langle u, v\rangle_X = 0$ for $u\in\mathcal{U}$, $v\in\mathcal{U}^\perp$. Solutions (u, v) to (P) fulfill the invariance property

$$u(t)\in\mathcal{U} + U \quad \forall t\in\mathbb{R}_+.$$

4 Reduction scheme for limit problems with partly fast kinetics

We derive weak formulations for reduced problems arising from our basic problem (P) under the general assumption that during the evolution process the vector of potentials $v = (v_0, \dots, v_m)$ underlies some restrictions which can be described in that way that the vector $v(t)$ lies in a closed subspace of X only. We assume that we are given a Banach space $\widetilde{X}$ and some linear operator $L\colon \widetilde{X} \to X$ such that all v from that closed subspace of X can be parametrized by means of some vector $\widetilde{v} \in \widetilde{X}$ with $v = L\widetilde{v}$. These assumptions are motivated by investigations concerning limits of fast kinetic subprocesses. For examples we refer to the reductions carried out in Section 10. Cf. e.g. the definitions of the operators L given in (19), (21), (22) and (23) and the corresponding choices for $\widetilde{X}$ in Subsection 10.1 – Subsection 10.4. Generally, for the operator L we now assume the fundamental properties

$$L\colon \widetilde{X} \to X \text{ linear, continuous, injective, } \operatorname{Im} L \text{ closed in } X,\ \mathcal{U}^\perp \subset \operatorname{Im} L. \tag{5}$$

Starting from our basic problem

$$u'(t) + Av(t) = 0, \quad u(t) = Ev(t) \quad \text{f.a.a. } t \in \mathbb{R}_+, \quad u(0) = U$$

we proceed by some kind of Galerkin procedure. We are looking for states $v \in \operatorname{Im} L$, $v = L\widetilde{v}$. And correspondingly we only consider test functions $h \in \operatorname{Im} L$, $h = L\widetilde{h}$, $\widetilde{h} \in \widetilde{X}$. This projection leads to

$$\begin{aligned}\langle u'(t) + Av(t), L\widetilde{h}\rangle_X &= \langle L^*u'(t) + L^*AL\widetilde{v}(t), \widetilde{h}\rangle_{\widetilde{X}} \\ &= 0 \quad \forall \widetilde{h} \in \widetilde{X},\ \text{f.a.a. } t \in \mathbb{R}_+,\end{aligned}$$

$$\begin{aligned}\langle u(t) - Ev(t), L\widetilde{h}\rangle_X &= \langle L^*u(t) - L^*EL\widetilde{v}(t), \widetilde{h}\rangle_{\widetilde{X}} \\ &= 0 \quad \forall \widetilde{h} \in \widetilde{X},\ \text{f.a.a. } t \in \mathbb{R}_+.\end{aligned}$$

This motivates the definitions

$$\widetilde{u} := L^*u, \quad \widetilde{A} = L^*AL, \quad \widetilde{E} = L^*EL.$$

Since $L^*\colon X^* \to \widetilde{X}^*$ is linear and continuous from $u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, X^*)$ it follows that $L^*u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}^*)$. Furthermore, $L^*u'(t) = (L^*u)'(t)$ f.a.a. $t \in \mathbb{R}_+$. In this notation we formulate the reduced problem $(\widetilde{\mathrm{P}})$ arising from the basic problem (P) under the additional assumptions concerning the fast kinetic subprocesses described by the operator L

$$\left.\begin{aligned}\widetilde{u}'(t) + \widetilde{A}\,\widetilde{v}(t) = 0\,,\ \widetilde{u}(t) = \widetilde{E}\,\widetilde{v}(t) \text{ f.a.a. } t \in \mathbb{R}_+\,,\ \widetilde{u}(0) = L^*U,\\ \widetilde{u} \in H^1_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}^*)\,,\ \widetilde{v} \in L^2_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}),\\ L\widetilde{v} \in L^2_{\mathrm{loc}}(\mathbb{R}_+, X) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1})).\end{aligned}\right\} \tag{$\widetilde{\mathrm{P}}$}$$

Our aim is to carry over as most as possible of the results from the basic problem (P) to the reduced problem $(\widetilde{\mathrm{P}})$. We assume the properties (5) for L to be satisfied.

5 Results for the basic problem (P)

In this section we summarize notation, properties and results on energy estimates for (P) which will be of importance for the analytical treatment of reduced model equations in the case of fast kinetics of some of the involved processes. For the proofs of the assertions stated in this section we refer to [9, 10].

Theorem 5.1 *We assume* (2) – (4). *There exists a unique steady state* (u^*, v^*) *of* (P) *in the sense that*

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

For the proof we refer to [9, Theorem 3.1]. Note that our concept of solutions implies that $U_i \geq c > 0,\ i = 1, \ldots, m$, and therefore the Slater condition in [9],

$$\sum_{i=1}^{m} \int_\Omega U_i \kappa_i \,\mathrm{d}x > 0 \ \text{ for all } \kappa \in \mathcal{S}^\perp, \quad \kappa \geq 0, \quad \kappa \neq 0$$

is automatically fulfilled.

For the steady state (u^*, v^*) we define the quantities $a_i^* := \mathrm{e}^{v_i^* + q_i v_0^*}, i = 1, \ldots, m$, $a^* := (a_1^*, \ldots, a_m^*)$. Using [9, Lemma 5.1] we obtain that $(a^*, v_0^*) \in \mathcal{M}$ where

$$\begin{aligned}\mathcal{M} \ &:= \ \Big\{(a, v_0) \in \mathbb{R}_+^m \times H_0^1(\Omega \cup \Gamma_N)\colon \prod_{i=1}^m a_i^{\alpha_i} = \prod_{i=1}^m a_i^{\beta_i}\ \forall (\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma,\\ &\qquad (E_0 v_0, u_1, \ldots, u_m) \in \mathcal{U} + U \text{ where } u_i := \overline{u}_i\, a_i\, \mathrm{e}^{-q_i v_0}\,,\ i = 1, \ldots, m, \Big\}.\end{aligned}$$

The operator E is a strictly monotone potential operator with potential $\Phi\colon X \to \mathbb{R}$,

$$\Phi(v) = \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla v_0|^2 - f^\Omega v_0 + \sum_{i=1}^m \overline{u}_i(\mathrm{e}^{v_i} - 1)\Big\}\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2}\, v_0^2 \,\mathrm{d}\Gamma,$$

Φ is continuous, strictly convex and subdifferentiable. The free energy $F\colon X^* \to \overline{\mathbb{R}}$ corresponds to the conjugate functional of Φ,

$$F(u) := \Phi^*(u) = \sup_{v \in X} \big\{\langle u, v\rangle_X - \Phi(v)\big\}, \quad u \in X^*.$$

If $u \in (H_0^1(\Omega \cup \Gamma_N))^* \times L_+^2(\Omega, \mathbb{R}^m)$ then the free energy at the state u is given by

$$F(u) = \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla v_0|^2 + \sum_{i=1}^m \big(u_i(\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i\big)\Big\}\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2}\, v_0^2 \,\mathrm{d}\Gamma,$$

where $E_0 v_0 = u_0$ (cf. [11, Lemma 3.2]). Next, we define the dissipation rate

$$D(v) := \langle A\, v, v\rangle_X, \quad v \in W.$$

Note that by the definition of the operator A the dissipation rate is nonnegative for all $v \in W$. Moreover, we have $D(v) = 0$ if and only if $v \in \mathcal{U}^\perp$ if and only if $Av = 0$. We cite the following result concerning the boundedness and the decay of the free energy from [10, Theorem 3.2].

Theorem 5.2 *We assume* (2) – (4)*. Let* (u, v) *be a solution to* (P)*. Then*

$$F(u(t_2)) \le F(u(t_1)) \le F(U) \quad \text{for } t_2 \ge t_1 \ge 0,$$
$$\|v_0(t)\|_{H^1} + \sum_{i=1}^m \|u_i(t) \ln u_i(t)\|_{L^1} + \int_0^t D(v(s))\, ds \le c \quad \forall t \in \mathbb{R}_+,$$

where c *depends only on the data.*

For assertions concerning the exponential decay of the free energy we need the additional assumption that

$$\mathcal{M} \subset \text{ int } \mathbb{R}^m_+ \times H^1_0(\Omega \cup \Gamma_N). \tag{6}$$

Theorem 5.3 *We assume* (2) – (4) *and* (6)*. Then for every* $R > 0$ *there exists a* $c_R > 0$ *such that*

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

for all $v \in M_R := \big\{v \in W\colon\ F(Ev) - F(u^*) \le R,\ Ev \in \mathcal{U} + U\big\}$.

Theorem 5.4 *Let* (2) – (4) *and* (6) *be satisfied. Then there exist constants* λ, $c > 0$ *depending only on the data such that*

$$F(u(t)) - F(u^*) \le e^{-\lambda t}(F(U) - F(u^*)),$$
$$\|v_0(t) - v_0^*\|_{H^1} + \sum_{i=1}^m \|u_i(t) - u_i^*\|_{L^1} \le c e^{-\lambda t/2} \quad \forall t \ge 0$$

if (u, v) *is a solution to* (P)*.*

For the proofs of the last two theorems we refer to [9, Theorem 5.2, Theorem 5.3]. Theorem 5.3 is based on an indirect proof such that the decay rate of the free energy in Theorem 5.4 can not be given explicitly. There are papers where for special situations an explicit rate of convergence is proved. Gajewski and Gärtner [5] did this for the van Roosbroeck system with magnetic field. Desvillettes and Fellner [2] provide an explicit rate of convergence for a reaction-diffusion system of two species and the reaction $2X_1 \rightleftharpoons X_2$ and one invariant and for a system of three species, the reaction $X_1 + X_2 \rightleftharpoons X_3$ and two invariants, respectively.

Additionally, in [10] we proved that (P) has at most one solution. Under some restrictions concerning the order of the reactions we there obtained solvability and global bounds for the solution to (P). Now we derive energy estimates for the reduced problem $(\widetilde{\text{P}})$.

6 Invariants and steady states for the reduced problem $(\widetilde{\mathbf{P}})$

We define

$$\widetilde{\mathcal{U}} := \Big\{ \widetilde{u} \in \widetilde{X}^* \colon \widetilde{u} = L^* u\,,\ u \in \mathcal{U} \Big\}$$

as well as

$$\widetilde{\mathcal{U}}^{\perp} = \Big\{ \widetilde{v} \in \widetilde{X} \colon v = L\widetilde{v} \in \mathcal{U}^{\perp} \Big\}.$$

We obtain the relation $\langle \widetilde{u}, \widetilde{v} \rangle_{\widetilde{X}} = 0 \quad \forall \widetilde{u} \in \widetilde{\mathcal{U}}\,,\ \forall \widetilde{v} \in \widetilde{\mathcal{U}}^{\perp}$.

Lemma 6.1 *Let $(\widetilde{u}, \widetilde{v})$ be a solution to $(\widetilde{\mathrm{P}})$. We suppose (2) – (4) for (P) and (5) for L. Then the invariance property*

$$\widetilde{u}(t) - L^* U \in \widetilde{\mathcal{U}} \quad \forall t \in \mathbb{R}_+$$

is fulfilled.

Proof. Let $\widetilde{h} \in \widetilde{\mathcal{U}}^{\perp}$ be arbitrarily given. Then $L\widetilde{h} \in \mathcal{U}^{\perp}$ and $\langle AL\widetilde{v}, L\widetilde{h} \rangle_X = 0$. Here we used that $\langle Av, \overline{v} \rangle = 0$ for $v \in W$, $\overline{v} \in \mathcal{U}^{\perp}$. We evaluate

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \widetilde{u}, \widetilde{h} \rangle_{\widetilde{X}} = \langle L^* A L \widetilde{v}, \widetilde{h} \rangle_{\widetilde{X}} = \langle AL\widetilde{v}, L\widetilde{h} \rangle_X = 0$$

which proves the assertion. □

The steady states for problem $(\widetilde{\mathrm{P}})$ are pairs $(\widetilde{u}^*, \widetilde{v}^*)$ fulfilling

$$\widetilde{A}\widetilde{v}^* = 0\,,\ \widetilde{u}^* = \widetilde{E}\widetilde{v}^*\,,\ \widetilde{u}^* - L^* U \in \widetilde{\mathcal{U}}\,,\ L\widetilde{v}^* \in W\,,\ \widetilde{v}^* \in \widetilde{X}.$$

Theorem 6.1 *We suppose (2) – (4) for (P) and the properties (5) for L.*
i) *Then (u^*, v^*) is a steady state of (P) if and only if $(\widetilde{u}^*, \widetilde{v}^*)$ is a steady state of $(\widetilde{\mathrm{P}})$ and $\widetilde{u}^* = L^* u^*$, $v^* = L\widetilde{v}^*$.*
ii) *There is exactly one steady state of $(\widetilde{\mathrm{P}})$.*

Proof. 1. ($\Longrightarrow$). If (u^*, v^*) is a steady state of (P) then $Av^* = 0$ which implies that $v^* \in \mathcal{U}^{\perp} \subset \operatorname{Im} L$. Since L is injective there exists a unique $\widetilde{v}^* \in \widetilde{X}$ with $v^* = L\widetilde{v}^*$. Next we define $\widetilde{u}^* := L^* u^*$ and obtain that $\widetilde{u}^* = L^* u^* = L^* E v^* = L^* E L \widetilde{v}^* = \widetilde{E}\widetilde{v}^*$. Moreover, $\widetilde{u}^* - L^* U = L^*(u^* - U) \in \widetilde{\mathcal{U}}$ and $\widetilde{A}\widetilde{v}^* = L^* A L \widetilde{v}^* = L^* A v^* = 0$.

2. ($\Longleftarrow$). If $(\widetilde{u}^*, \widetilde{v}^*)$ is a steady state of $(\widetilde{\mathrm{P}})$ we define $v^* := L\widetilde{v}^*\,,\ u^* := E\,L\widetilde{v}^*$. Then the relation $\widetilde{u}^* = \widetilde{E}\widetilde{v}^* = L^* E L \widetilde{v}^* = L^* u^*$ is satisfied. Furthermore, from $\widetilde{A}\widetilde{v}^* = 0$ it follows $0 = \langle \widetilde{A}\widetilde{v}^*, \widetilde{v}^* \rangle_{\widetilde{X}} = \langle AL\widetilde{v}^*, L\widetilde{v}^* \rangle_X = D(v^*)$. Thus $v^* \in \mathcal{U}^{\perp}$ and $Av^* = 0$. Next we show that $u^* - U \in \mathcal{U}$. Let $\overline{v} \in \mathcal{U}^{\perp} \subset \operatorname{Im} L$ be arbitrarily given. Then $\overline{v} = L\overline{\widetilde{v}}$, $\overline{\widetilde{v}} \in \widetilde{\mathcal{U}}^{\perp}$ and by $\widetilde{u}^* - L^* U \in \widetilde{\mathcal{U}}$ we conclude $\langle u^* - U, \overline{v} \rangle_X = \langle L^* u^* - L^* U, \overline{\widetilde{v}} \rangle_{\widetilde{X}} = \langle \widetilde{E}\widetilde{v}^* - L^* U, \overline{\widetilde{v}} \rangle_{\widetilde{X}} = \langle \widetilde{u}^* - L^* U, \overline{\widetilde{v}} \rangle_{\widetilde{X}} = 0$ which gives the assertion.

3. (Existence). The existence of a steady state of $(\widetilde{\mathrm{P}})$ follows by step 1 and Theorem 5.1.

4. (Uniqueness). If we would have two steady states of $(\widetilde{\mathrm{P}})$ $(\widetilde{u}^{*i}, \widetilde{v}^{*i})$, $i = 1, 2$, then by the second step $v^{*i} = L\widetilde{v}^{*i}$, $i = 1, 2$, would be components of the steady state of (P). By Theorem 5.1 the steady state of (P) is unique which means $v^{*1} = v^{*2}$. Since the operator L is injective it follows $\widetilde{v}^{*1} = \widetilde{v}^{*2}$. From $u^{*1} = u^{*2}$ we find $\widetilde{u}^{*1} = L^*u^{*1} = L^*u^{*2} = \widetilde{u}^{*2}$. $\square$

7 Energy estimates for the reduced problem $(\widetilde{\mathrm{P}})$

We define the energy functionals and carry over the convex structure from (P) to $(\widetilde{\mathrm{P}})$. At first we introduce the functional $\widetilde{\Phi}\colon \widetilde{X} \to \mathbb{R}$,

$$\widetilde{\Phi}(\widetilde{v}) := \Phi(L\widetilde{v}).$$

By the properties of L and Φ (cf. Section 5) this functional is continuous, strictly convex and subdifferentiable and the relation

$$\partial\widetilde{\Phi}(\widetilde{v}) = L^*\partial\Phi(L\widetilde{v}) = L^*EL\widetilde{v} = \widetilde{E}\widetilde{v}$$

holds. Again, the free energy $\widetilde{F}\colon \widetilde{X}^* \to \overline{\mathbb{R}}$ is defined as the conjugate functional of $\widetilde{\Phi}$,

$$\widetilde{F}(\widetilde{u}) := \widetilde{\Phi}^*(\widetilde{u}) = (\Phi L)^*(\widetilde{u}) = \sup_{\widetilde{v}\in\widetilde{X}} \Big\{ \langle \widetilde{u}, \widetilde{v}\rangle_{\widetilde{X}} - \Phi(L\widetilde{v}) \Big\}.$$

On the other hand, since Φ is convex and continuous (cf. [15, Sect. 3]) we have

$$\widetilde{F}(\widetilde{u}) = (L^*\Phi^*)(\widetilde{u}) = \inf \big\{ F(u)\colon u \in X^*,\ L^*u = \widetilde{u} \big\}, \tag{7}$$

where F is the free energy for the basic system. If $\widetilde{F}$ is subdifferentiable at $\widetilde{u}$, $\widetilde{u} = \widetilde{E}\widetilde{v}$ then we obtain

$$\widetilde{F}(\widetilde{u}) = F(u) \quad \text{where } u = \partial\Phi(L\widetilde{v}) = Ev. \tag{8}$$

Finally, we introduce the dissipation rate $\widetilde{D}\colon \widetilde{X} \cap \{\widetilde{v} \in \widetilde{X}\colon L\widetilde{v} \in W\} \to \mathbb{R}$ for the reduced system $(\widetilde{\mathrm{P}})$ by

$$\begin{aligned}\widetilde{D}(\widetilde{v}) &:= D(L\widetilde{v}) = \langle AL\widetilde{v}, L\widetilde{v}\rangle_X = \langle L^*AL\widetilde{v}, \widetilde{v}\rangle_{\widetilde{X}} \\ &= \langle \widetilde{A}\widetilde{v}, \widetilde{v}\rangle_{\widetilde{X}}, \qquad \widetilde{v} \in \widetilde{X} \cap \{\widetilde{v}\colon L\widetilde{v} \in W\}.\end{aligned}$$

Since D is nonnegative for all $v \in W$ it follows that $\widetilde{D}(\widetilde{v}) \geq 0$ for all $\widetilde{v}$ with $L\widetilde{v} \in W$.

The functional $\widetilde{F}$ is convex and lower semicontinuous. If $(\widetilde{u}, \widetilde{v})$ is a solution to $(\widetilde{\mathrm{P}})$ then $\partial\widetilde{F}(\widetilde{u}(t)) = \widetilde{v}(t)$ f.a.a. $t \in \mathbb{R}_+$. Moreover, $\partial\widetilde{F}(\widetilde{u}^*) = \widetilde{v}^* \in \widetilde{\mathcal{U}}^\perp$. Thus along any solution $(\widetilde{u},\widetilde{v})$ to $(\widetilde{\mathrm{P}})$ the function $t\mapsto \mathrm{e}^{\lambda t}\big(\widetilde{F}(\widetilde{u}(t))-\widetilde{F}(\widetilde{u}^*)\big)$ with $\lambda\in\mathbb{R}$ is absolutely continuous and we obtain (cf. [1, Lemma 3.3])

$$\begin{aligned}
&\mathrm{e}^{\lambda t}\;\big(\widetilde{F}(\widetilde{u}(t))-\widetilde{F}(\widetilde{u}^*)\big)-\big(\widetilde{F}(L^*U)-\widetilde{F}(\widetilde{u}^*)\big)\\
&\quad=\int_0^t \mathrm{e}^{\lambda s}\Big\{\lambda\big(\widetilde{F}(\widetilde{u}(s))-\widetilde{F}(\widetilde{u}^*)\big)+\langle \widetilde{u}'(s),\partial\widetilde{F}(\widetilde{u}(s))-\partial\widetilde{F}(\widetilde{u}^*)\rangle_{\widetilde{X}}\Big\}\,\mathrm{d}s\\
&\quad=\int_0^t \mathrm{e}^{\lambda s}\Big\{\lambda\big(\widetilde{F}(\widetilde{u}(s))-\widetilde{F}(\widetilde{u}^*)\big)-\langle \widetilde{A}(\widetilde{v}(s)),\widetilde{v}(s)-\widetilde{v}^*\rangle_{\widetilde{X}}\Big\}\,\mathrm{d}s\\
&\quad=\int_0^t \mathrm{e}^{\lambda s}\Big\{\lambda\big(\widetilde{F}(\widetilde{u}(s))-\widetilde{F}(\widetilde{u}^*)\big)-\langle \widetilde{A}(\widetilde{v}(s)),\widetilde{v}(s)\rangle_{\widetilde{X}}\Big\}\,\mathrm{d}s.
\end{aligned}\tag{9}$$

Theorem 7.1 *We suppose* (2) – (4) *for* (P) *and* (5) *for the operator* L. *Let* $(\widetilde{u},\widetilde{v})$ *be a solution to* $(\widetilde{\mathrm{P}})$. *Then*

$$\widetilde{F}(\widetilde{u}(t))+\int_0^t \widetilde{D}(\widetilde{v}(s))\,ds\le F(U)\quad \forall t\in\mathbb{R}_+.$$

Proof. 1. We set $\lambda=0$ in the relation (9). Since along solutions $(\widetilde{u},\widetilde{v})$ to $(\widetilde{\mathrm{P}})$ it is guaranteed that $L\widetilde{v}\in W$ for a.a. $s\in\mathbb{R}_+$ we have that $\langle\widetilde{A}(\widetilde{v}(s)),\widetilde{v}(s)\rangle_{\widetilde{X}}=\widetilde{D}(\widetilde{v}(s))\ge 0$ for a.a. $s\in\mathbb{R}_+$. This leads to the desired estimate if one takes into account that by (7) we have $\widetilde{F}(L^*U)\le F(U)$. □

Theorem 7.2 *Let* (2) – (4) *and* (6) *for* (P) *as well as* (5) *for the operator* L *be satisfied. Then there exists a constant* $\lambda>0$ *depending only on the data such that*

$$\widetilde{F}(\widetilde{u}(t))-\widetilde{F}(\widetilde{u}^*)\le e^{-\lambda t}(F(U)-\widetilde{F}(\widetilde{u}^*))\quad\forall t\ge 0 \tag{10}$$

if $(\widetilde{u},\widetilde{v})$ *is a solution to* $(\widetilde{\mathrm{P}})$.

Proof. If $(\widetilde{u},\widetilde{v})$ is a solution to $(\widetilde{\mathrm{P}})$ then for a.a. $s\in\mathbb{R}_+$ the following properties are fulfilled. We have $\widetilde{u}(s)=\widetilde{E}\widetilde{v}(s)$ and therefore by (8) and Theorem 6.1 and Theorem 7.1

$$\widetilde{F}(\widetilde{u}(s))-\widetilde{F}(\widetilde{u}^*)=F(EL\widetilde{v}(s))-F(u^*)\le F(U)-F(u^*)=:R.$$

Moreover $L\widetilde{v}(s)\in W$ and, since by Lemma 6.1 $L^*(EL\widetilde{v}(s)-U)=\widetilde{E}\widetilde{v}(s)-L^*U\in\widetilde{\mathcal{U}}$ we find $EL\widetilde{v}(s)-U\in\mathcal{U}$. Thus $L\widetilde{v}(s)$ belongs to a set M_R occurring in Theorem 5.3 on which there is given an estimate of the free energy by the dissipation rate. By Theorem 5.3 we conclude that

$$\widetilde{F}(\widetilde{u}(s))-\widetilde{F}(\widetilde{u}^*)=F(EL\widetilde{v}(s))-F(u^*)\le c_R D(L\widetilde{v})=c_R\widetilde{D}(\widetilde{v})=c_R\langle\widetilde{A}(\widetilde{v}(s)),\widetilde{v}(s)\rangle_{\widetilde{X}}.$$

Setting now $\lambda=1/c_R$ we thus obtain from (9) the estimate (10). □

8 Comparison with solutions to the basic problem

Let $(\widetilde{u}, \widetilde{v})$ be a solution to $(\widetilde{\mathrm{P}})$. We ask in what sense we can prescribe the behaviour of a solution to (P) by means of solutions to $(\widetilde{\mathrm{P}})$. For this purpose we define for quantities $\widetilde{v} \in \widetilde{X}$ and $\widetilde{u} \in \widetilde{X}^*$ quantities $\breve{v} \in X$ and $\breve{u} \in X^*$ by prolongation

$$\breve{v} := L\widetilde{v}, \quad \breve{u} := EL\widetilde{v}. \tag{11}$$

According to Theorem 6.1 we find by applying the transformation (11) to the steady state $(\widetilde{u}^*, \widetilde{v}^*)$ of $(\widetilde{\mathrm{P}})$ that

$$(\breve{u}^*, \breve{v}^*) = (EL\widetilde{v}^*, L\widetilde{v}^*) = (u^*, v^*) \tag{12}$$

corresponds to the steady state of (P). Additionally, cf. (8), for $\widetilde{u}$, where $\widetilde{F}$ is subdifferentiable, we have $\widetilde{F}(\widetilde{u}) = F(\breve{u})$. This means for the steady states $\widetilde{F}(\widetilde{u}^*) = F(u^*)$ and for solutions $(\widetilde{u}, \widetilde{v})$ to $(\widetilde{\mathrm{P}})$

$$\widetilde{F}(\widetilde{u}(t)) = F(\breve{u}(t)) \quad \text{f.a.a. } t \in \mathbb{R}_+. \tag{13}$$

Moreover we obtain the following conclusions from energy estimates for (P) and $(\widetilde{\mathrm{P}})$.

Theorem 8.1 *We suppose* (2) – (4) *and* (6) *for* (P) *as well as* (5) *for the operator L to be satisfied. Let (u, v) be a solution to* (P) *and let $(\breve{u}, \breve{v})$ be prolongated via* (11) *from a solution $(\widetilde{u}, \widetilde{v})$ to $(\widetilde{\mathrm{P}})$. Then there exist constants λ, $c > 0$ depending only on the data such that*

$$|F(\breve{u}(t)) - F(u(t))| \le ce^{-\lambda t},$$

$$\|\breve{v}_0(t) - v_0(t)\|_{H^1} + \sum_{i=1}^{m} \|\breve{u}_i(t) - u_i(t)\|_{L^1} \le ce^{-\lambda t/2} \quad \textit{f.a.a. } t \in \mathbb{R}_+.$$

Proof. Because of (12) and (13) we obtain by Theorem 7.2 that

$$F(\breve{u}(t)) - F(u^*) \le \mathrm{e}^{-\lambda t}(F(U) - F(u^*)) \quad \text{f.a.a } t \in \mathbb{R}_+. \tag{14}$$

Therefore Theorem 5.4 and the triangle inequality lead to the first estimate. For all $(\widehat{u}, \widehat{v}_0) \in X^* \times H_0^1(\Omega \cup \Gamma_N)$ with $\widehat{u} - u^* \in \mathcal{U}$ and $E_0\widehat{v}_0 = \widehat{u}_0$ the estimate

$$\|\widehat{v}_0 - v_0^*\|_{H^1}^2 + \sum_{i=1}^{m} \|\sqrt{\widehat{u}_i} - \sqrt{u_i^*}\|_{L^2}^2 \le c(F(\widehat{u}) - F(u^*)) \tag{15}$$

is valid (cf. [9, p.827]). By relation (11) we find $\breve{u}_0(t) = E_0(L\widetilde{v}(t))_0 = E_0\breve{v}_0(t)$. Next we show that $\breve{u}(t) - u^* \in \mathcal{U}$ f.a.a. $t \in \mathbb{R}_+$. Let $\overline{v} \in \mathcal{U}^\perp \subset \operatorname{Im} L$ be arbitrarily given. Then $\overline{v} = L\overline{\overline{v}}$, $\overline{\overline{v}} \in \widetilde{\mathcal{U}}^\perp$ and by Lemma 6.1 we conclude

$$\langle \breve{u}(t) - u^*, \overline{v}\rangle_X = \langle L^*\breve{u}(t) - L^*u^*, \overline{\overline{v}}\rangle_{\widetilde{X}} = \langle \widetilde{E}\widetilde{v}(t) - \widetilde{u}^*, \overline{\overline{v}}\rangle_{\widetilde{X}} = \langle \widetilde{u}(t) - \widetilde{u}^*, \overline{\overline{v}}\rangle_{\widetilde{X}} = 0 \text{ a.e.}$$

which gives the assertion. Thus we can apply inequality (15) to $(\breve{u}(t), \breve{v}_0(t))$ as well as to $(u(t), v_0(t))$ f.a.a. $t \in \mathbb{R}_+$. Together with (14) and Theorem 5.4 we obtain

$$\|\breve{v}_0(t) - v_0(t)\|_{H^1}^2 \le c\big(\|\breve{v}_0(t) - v_0^*\|_{H^1}^2 + \|v_0(t) - v_0^*\|_{H^1}^2\big) \le c\mathrm{e}^{-\lambda t} \quad \text{f.a.a. } t \in \mathbb{R}_+.$$

Analogously we find

$$\|\sqrt{\breve{u}_i(t)} - \sqrt{u_i(t)}\|_{L^2}^2 \le c\mathrm{e}^{-\lambda t} \quad \text{f.a.a. } t \in \mathbb{R}_+. \tag{16}$$

Using (13), Theorem 7.1 and the estimate $\sum_{i=1}^m \|\widehat{u}_i\|_{L^1} \le F(\widehat{u}) + c$ for elements $\widehat{u} = E\widehat{v}$ with $\widehat{v} \in X$ we have $\|\breve{u}_i(t)\|_{L^1} \le c$ a.e. in $\mathbb{R}_+$. From Theorem 5.2 it follows $\|u_i(t)\|_{L^1} \le c$ for all $t \in \mathbb{R}_+$. Therefore, using (16), we conclude for $i = 1, \ldots, m$ that

$$\begin{aligned}\|\breve{u}_i(t) - u_i(t)\|_{L^1} &\le \|\sqrt{\breve{u}_i(t)} - \sqrt{u_i(t)}\|_{L^2}\|\sqrt{\breve{u}_i(t)} + \sqrt{u_i(t)}\|_{L^2}\\ &\le c\mathrm{e}^{-\lambda t/2} \quad \text{a.e. in } \mathbb{R}_+. \qquad \square\end{aligned}$$

Remark 8.1 *If the assumptions of Theorem 8.1 are fulfilled and in addition $\widetilde{v}$ has the following regularity properties*

$$(L\widetilde{v})_0 \in C(\mathbb{R}_+, H^1), \quad (L\widetilde{v})_i \in C(\mathbb{R}_+, L^2) \cap C_{w^*}(\mathbb{R}_+, L^\infty), \quad i = 1, \ldots, m,$$

then the assertions of Theorem 8.1 hold for all $t \in \mathbb{R}_+$.

9 Energy estimates for a fully implicit time-discrete version of problem $(\widetilde{\mathrm{P}})$

Our aim is to approximate problem $(\widetilde{\mathrm{P}})$ by a discrete–time problem which saves the important property of monotonous and exponential decay of the free energy along trajectories of the discrete–time system to its equilibrium value. In [9, Section 6] we proved this property for the fully implicit discrete–time scheme corresponding to (P).

We assume that we are given sequences of partitions $\{Z_n\}_{n\in\mathbb{N}}$ of $\mathbb{R}_+$,

$$Z_n = \left\{t_n^0, t_n^1, \ldots, t_n^k, \ldots\right\}, \ t_n^0 = 0, \ t_n^k \in \mathbb{R}_+, \ t_n^{k-1} < t_n^k, \ k \in \mathbb{N}$$

with $t_n^k \to +\infty$ as $k \to \infty$. Let

$$h_n^k := t_n^k - t_n^{k-1}, \ S_n^k := (t_n^{k-1}, t_n^k], \ \overline{h}_n := \sup_{k\in\mathbb{N}} h_n^k.$$

For a given partition Z_n of $\mathbb{R}_+$ and a given Banach space B we introduce the space of piecewise constant functions

$$C_n(\mathbb{R}_+, B) := \Big\{\widetilde{u} : \mathbb{R}_+ \longrightarrow B \, : \, \widetilde{u}(t) = \widetilde{u}^k \quad \forall t \in S_n^k, \ \widetilde{u}^k \in B, \ k \in \mathbb{N}\Big\}.$$

We define the difference operator $\Delta_n : C_n(\mathbb{R}_+, \widetilde{X}^*) \longrightarrow C_n(\mathbb{R}_+, \widetilde{X}^*)$ by

$$(\Delta_n \widetilde{u})^k := \frac{1}{h_n^k}(\widetilde{u}^k - \widetilde{u}^{k-1}), \ \widetilde{u}^0 := \widetilde{U},$$

where $\widetilde{U} = L^*U$ is the initial value of problem $(\widetilde{\mathrm{P}})$. For $n \in \mathbb{N}$, we investigate the problem

$$\left.\begin{aligned} \Delta_n \widetilde{u}_n(t) + \widetilde{A}\widetilde{v}_n(t) = 0, \quad \widetilde{u}_n(t) = \widetilde{E}\widetilde{v}_n(t) \ \ \forall t \in \mathbb{R}_+, \\ \widetilde{v}_n \in C_n(\mathbb{R}_+, \widetilde{X}), \quad L\widetilde{v}_n \in C_n(\mathbb{R}_+, X) \cap C_n(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1})). \end{aligned}\right\} \qquad (\widetilde{\mathrm{P}}_n)$$

This fully implicit scheme can be written in more detail as

$$\widetilde{u}_n^k + h_n^k \widetilde{A}\widetilde{v}_n^k = \widetilde{u}_n^{k-1}, \ \ \widetilde{u}_n^k = \widetilde{E}\widetilde{v}_n^k, \ \ \widetilde{v}_n^k \in \widetilde{X}, \ \ L\widetilde{v}_n^k \in W, \ \ k \in \mathbb{N}, \ \ \widetilde{u}_n^0 = L^*U.$$

First, let us note that solutions of the discrete–time problems $(\widetilde{\mathrm{P}}_n)$ fulfil the same invariance property as solutions of the continuous problem $(\widetilde{\mathrm{P}})$,

$$\widetilde{u}_n(t) \in \widetilde{\mathcal{U}} + L^*U \quad \forall t \in \mathbb{R}_+. \tag{17}$$

This assertion proves as follows: Similar to Lemma 6.1 we obtain

$$\langle \Delta_n \widetilde{u}_n(s), \widetilde{h}\rangle_{\widetilde{X}} = 0 \quad \forall \widetilde{h} \in \widetilde{\mathcal{U}}^\perp, \forall s \in \mathbb{R}_+.$$

Thus

$$\int_0^{t_n^k} \Delta_n \widetilde{u}_n(s)\,\mathrm{d}s = \widetilde{u}_n^k - L^*U \in \widetilde{\mathcal{U}} \quad \forall k \in \mathbb{N}$$

which gives the assertion. Furthermore, each discrete–time problem $(\widetilde{\mathrm{P}}_n)$ has the same steady state $(\widetilde{u}^*, \widetilde{v}^*)$ as the continuous problem $(\widetilde{\mathrm{P}})$.

Theorem 9.1 *We suppose* (2) – (4) *for* (P) *as well as* (5) *for the operator L to be satisfied. Let $h > 0$ be given and let Z_n be any partition of $\mathbb{R}_+$ with $\overline{h}_n \le h$. Then the free energy $\widetilde{F}$ decreases monotonously along any solution $(\widetilde{u}_n, \widetilde{v}_n)$ to the discrete–time problem $(\widetilde{\mathrm{P}}_n)$, i.e.,*

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

If additionally (6) *is satisfied, then there exists a constant $\lambda > 0$ such that*

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

for any solution $(\widetilde{u}_n, \widetilde{v}_n)$ to $(\widetilde{\mathrm{P}}_n)$.

Proof. Let $(\widetilde{u}_n, \widetilde{v}_n)$ be a solution to $(\widetilde{\mathrm{P}}_n)$. Since $\widetilde{u}_n^l = \widetilde{E}\widetilde{v}_n^l$ we have $\widetilde{v}_n^l \in \partial\widetilde{F}(\widetilde{u}_n^l)$ which implies

$$\langle \widetilde{u}_n^l - \widetilde{w}, \widetilde{v}_n^l \rangle_{\widetilde{X}} \geq \widetilde{F}(\widetilde{u}_n^l) - \widetilde{F}(\widetilde{w}) \quad \forall \widetilde{w} \in \widetilde{X}^*.$$

We derive some discrete version of the estimate (9). Let $k > j \geq 0$ and $\lambda \geq 0$. Then we conclude that

$$\begin{aligned}
\mathrm{e}^{\lambda t_n^k}\big(\widetilde{F}(\widetilde{u}_n^k) - F(u^*)\big) &- \mathrm{e}^{\lambda t_n^j}\big(\widetilde{F}(\widetilde{u}_n^j) - F(u^*)\big) \\
&= \sum_{l=j+1}^{k} \Big\{ \big(\mathrm{e}^{\lambda t_n^l} - \mathrm{e}^{\lambda t_n^{l-1}}\big)\big(\widetilde{F}(\widetilde{u}_n^l) - F(u^*)\big) + \mathrm{e}^{\lambda t_n^{l-1}}\big(\widetilde{F}(\widetilde{u}_n^l) - \widetilde{F}(\widetilde{u}_n^{l-1})\big) \Big\} \\
&\leq \sum_{l=j+1}^{k} \Big\{ \mathrm{e}^{\lambda t_n^{l-1}}\big(\mathrm{e}^{\lambda h_n^l} - 1\big)\big(\widetilde{F}(\widetilde{u}_n^l) - F(u^*)\big) + \mathrm{e}^{\lambda t_n^{l-1}} \langle \widetilde{u}_n^l - \widetilde{u}_n^{l-1}, \widetilde{v}_n^l \rangle_{\widetilde{X}} \Big\} \\
&\leq \sum_{l=j+1}^{k} \Big\{ \mathrm{e}^{\lambda t_n^{l-1}}\, \mathrm{e}^{\lambda h}\, \lambda\, h_n^l \big(\widetilde{F}(\widetilde{u}_n^l) - F(u^*)\big) - \mathrm{e}^{\lambda t_n^{l-1}}\, h_n^l \langle \widetilde{A}\widetilde{v}_n^l, \widetilde{v}_n^l \rangle_{\widetilde{X}} \Big\} \\
&\leq \sum_{l=j+1}^{k} h_n^l\, \mathrm{e}^{\lambda t_n^{l-1}} \Big\{ \mathrm{e}^{\lambda h}\, \lambda \big(F(EL\widetilde{v}_n^l) - F(u^*)\big) - D(L\widetilde{v}_n^l) \Big\}.
\end{aligned}$$

At first, since the dissipation rate D is nonnegative, by setting $\lambda = 0$ we obtain

$$\widetilde{F}(\widetilde{u}_n^k) \leq \widetilde{F}(\widetilde{u}_n^j) \leq \widetilde{F}(L^*U) \leq F(U) \quad \forall k \geq j \geq 0$$

which means

$$\widetilde{F}(\widetilde{u}_n(t_2)) \leq \widetilde{F}(\widetilde{u}_n(t_1)) \leq F(U) \quad \forall t_2 > t_1 \geq 0.$$

Next, we fix $R > F(U) - F(u^*)$. Since $\widetilde{u}_n$ fulfils the invariance property (17) and $\widetilde{u}_n = \widetilde{E}\widetilde{v}_n$, we find that $EL\widetilde{v}_n^l - U \in \mathcal{U}$ and $L\widetilde{v}_n^l \in W$ for $l \in \mathbb{N}$. Thus the $L\widetilde{v}_n^l$, $l \in \mathbb{N}$, belong to the set M_R defined in Theorem 5.3. If we now choose $\lambda > 0$ such that $\lambda\, \mathrm{e}^{\lambda h} c_R \leq 1$ and set $j = 0$ Theorem 5.3 implies that

$$\widetilde{F}(\widetilde{u}_n^k) - F(u^*) \leq \mathrm{e}^{-\lambda t_n^k}\big(F(U) - F(u^*)\big) \quad \forall k \in \mathbb{N}$$

and the second assertion of the theorem follows. □

10 Examples for the reduction of the model equations in the case of fast kinetic subprocesses

10.1 Example 1: Some fast volume reactions

Our aim is to reduce the basic model under the assumption that the kinetic of a part of the involved reactions is very fast. In many applications by physical reasons such

assumptions are justified (see e.g. [7]). Let $\mathcal{R}_0^\Omega \subset \mathcal{R}^\Omega$ be a subset of fast volume reactions. Then
$$k_{\alpha\beta}^\Omega \to \infty \text{ a.e. in } \Omega \quad \forall (\alpha,\beta) \in \mathcal{R}_0^\Omega.$$
To guarantee that the reaction terms remain bounded a.e. in Ω we have to require
$$\mathrm{e}^{\alpha\cdot\zeta} = \mathrm{e}^{\beta\cdot\zeta} \quad \forall (\alpha,\beta) \in \mathcal{R}_0^\Omega. \tag{18}$$
Having in mind that $q \in \mathcal{S}^\perp$ (cf. (4)) the relations (18) mean that we have to look for states (u,v) where the vector of chemical potentials $v_{ch} = (v_1,\dots,v_m)$ fulfills the property
$$(\alpha-\beta)\cdot\zeta = (\alpha-\beta)\cdot v_{ch} = 0 \quad \forall (\alpha,\beta) \in \mathcal{R}_0^\Omega.$$
In other words, $v_{ch}(t,x) \in \mathcal{S}_0^\perp$ a.e. in $\mathbb{R}_+ \times \Omega$ where
$$\mathcal{S}_0 := \operatorname{span}\{\alpha-\beta : (\alpha,\beta) \in \mathcal{R}_0^\Omega\}.$$
$\mathcal{S}_0^\perp$ is a closed subset of $\mathbb{R}^m$. We introduce $M := \dim\, \mathcal{S}_0^\perp = m - \dim\, \mathcal{S}_0$. Then there exist a permutation matrix Π, a set of indices $\{i_1,\dots,i_M\}$ and a linear, injective mapping $\widetilde{L}\colon \mathbb{R}^M \to \mathbb{R}^m$ with $\operatorname{Im}\, \Pi^{-1}\widetilde{L} = \mathcal{S}_0^\perp$ such that a.e.
$$\Pi v_{ch} = \widetilde{L}\widetilde{v}_{ch} \quad \text{where} \quad \widetilde{v}_{ch} = (v_{i_1},\dots,v_{i_M}), \quad \widetilde{L}\widetilde{v}_{ch} = (\widetilde{v}_{ch}, (\widetilde{L}\widetilde{v}_{ch})_{M+1},\dots,(\widetilde{L}\widetilde{v}_{ch})_m).$$
By the closed range theorem, since the mapping $\widetilde{L}$ is injective, and $\operatorname{Im}\, \widetilde{L}$ is closed, the adjoint operator $\widetilde{L}^*$ is surjective. Pointwise we have $v_{ch} = \Pi^{-1}\widetilde{L}\widetilde{v}_{ch}$. The mapping $\Pi^{-1}\widetilde{L}$ can be carried over to an operator on space functions $\Pi^{-1}\widetilde{L}\colon (H^1)^M \to (H^1)^m$. Since Π is bijective and linear the operator $\Pi^{-1}\widetilde{L}$ is linear, injective and continuous. Thus the complete transformation of the potentials , $\widetilde{v} = (\widetilde{v}_0, \widetilde{v}_{ch})$ to $v = (v_0, v_{ch})$ is prescribed by $v = L\widetilde{v}$ where the operator
$$L := \begin{pmatrix} 1 & 0 \\ 0 & \Pi^{-1}\widetilde{L} \end{pmatrix} : H_0^1(\Omega\cup\Gamma_N) \times (H^1)^M \to H_0^1(\Omega\cup\Gamma_N) \times (H^1)^m \tag{19}$$
is linear, injective, continuous and $\operatorname{Im}\, L$ is closed. Again we obtain that the adjoint operator $L^*\colon (H_0^1(\Omega\cup\Gamma_N))^* \times (H^1)^{*m} \to (H_0^1(\Omega\cup\Gamma_N))^* \times (H^1)^{*M}$ is surjective.

Lemma 10.1 *The operator L has the property*
$$\mathcal{U}^\perp \subset \ Im\ L.$$

Proof. Let $v \in \mathcal{U}^\perp$ be given arbitrarily. Then $v = (0,\zeta) + (1,-q)v_0$. Because of (4) and $v \in \mathcal{U}^\perp$ we have $q,\, \zeta \in \mathcal{S}^\perp \subset \mathcal{S}_0^\perp = \operatorname{Im}\, \widetilde{L}$ such that $q = \widetilde{L}\widetilde{q}$, $\zeta = \widetilde{L}\widetilde{\zeta}$. Therefore $v = L(v_0, \widetilde{\zeta} - \widetilde{q}v_0) \in \operatorname{Im}\, L$. $\square$

10.2 Example 2: Some fast boundary reactions

Next, we reduce the basic model under the assumption that the kinetic of a part of the involved boundary reactions is very fast. Let $\mathcal{R}_0^\Gamma \subset \mathcal{R}^\Gamma$ be the subset of fast boundary reactions. Then

$$k^\Gamma_{\alpha\beta} \to \infty \text{ a.e. on } \Gamma \quad \forall(\alpha,\beta) \in \mathcal{R}_0^\Gamma.$$

Analogously we define

$$\mathcal{S}_0 := \operatorname{span}\{\alpha - \beta : \, (\alpha,\beta) \in \mathcal{R}_0^\Gamma\}. \tag{20}$$

By the same arguments as in the case of fast kinetics for volume reactions the limit case of fast boundary reactions now leads to conditions for the traces of the vector of chemical potentials

$$\gamma(v_{ch}) \in \mathcal{S}_0^\perp.$$

Here γ denotes the trace operator. Again we define $M := \dim \mathcal{S}_0^\perp$. Let $L' \colon (H^1)^M \to (H^1)^m$ be the linear, continuous, injective operator, let $\{i_1, \dots, i_M\}$ be the set of indices and let Π be the permutation operator as derived in Subsection 10.1 which would ensure that

$$\Pi v_{ch} = L'v', \quad v' = (v_{i_1}, \dots, v_{i_M}), \quad v_{ch} \in \mathcal{S}_0^\perp \text{ (a.e. on } \Omega)$$

for $\mathcal{S}_0$ defined in (20). Then we have $\gamma(v_{ch}) \in \mathcal{S}_0^\perp$, too. We define the operator

$$\begin{aligned} &L \colon H_0^1(\Omega \cup \Gamma_N) \times (H^1)^M \times (H_0^1(\Omega))^{m-M} \to H_0^1(\Omega \cup \Gamma_N) \times (H^1)^m, \\ &L\widetilde{v} = \big(\widetilde{v}_0, \Pi^{-1}(L'v' + (0, v''))\big), \quad \widetilde{v} = (\widetilde{v}_0, v', v''). \end{aligned} \tag{21}$$

By the properties of Π and L' the operator L is linear and continuous.

Lemma 10.2 *The operator L is injective.*

Proof. Since L is linear it suffices to show that from $L\widetilde{v} = 0$ it follows $\widetilde{v} = 0$: Let $L\widetilde{v} = 0$. Then $(L\widetilde{v})_0 = \widetilde{v}_0 = 0$. Since Π is bijective we have $L'v' + (0, v'') = 0$. Because of $L'v' = (v', (L'v')_{M+1}, \dots, (L'v')_m)$ we conclude that $(L'v')_i = v'_i = 0$, $i = 1, \dots, M$. This implies $L'v' = 0$ and thus $v'' = 0$, which in summary gives $\widetilde{v} = 0$. □

Lemma 10.3 *Im $L = \{v \in X \colon \gamma(v_{ch})(x) \in \mathcal{S}_0^\perp$ a.e. on $\Gamma\}$.*

Proof. 1. Let $v \in \operatorname{Im} L$. Then $v = (\widetilde{v}_0, \Pi^{-1}(L'v' + (0, v''))) = L\widetilde{v}$ where $\widetilde{v} = (\widetilde{v}_0, v', v'') \in H_0^1(\Omega \cup \Gamma_N) \times (H^1)^M \times (H_0^1(\Omega))^{m-M}$. Thus $v \in X$. Since $v'' \in (H_0^1(\Omega))^{m-M}$ we have $\gamma(\Pi^{-1}(0, v'')) = 0$. And therefore by the construction of the operators Π and L' it follows $\gamma(v_{ch}) = \gamma(\Pi^{-1}L'v') \in \mathcal{S}_0^\perp$ a.e. on Γ.

2. Let be $v \in X$ with $\gamma(v_{ch}) \in \mathcal{S}_0^\perp$. We set $\widetilde{v} = (\widetilde{v}_0, v', v'')$ with $\widetilde{v}_0 = v_0$, $v' = (v_{i_1}, \dots, v_{i_M})$ and

$$v''_j = (L'(v_{i_1}, \dots, v_{i_M}))_{j+M} - (\Pi v_{ch})_{j+M}, \quad j = 1, \dots, m-M,$$

and obtain that $v = L\widetilde{v}$. $\square$

Thus by Lemma 10.3 Im L is closed and the operator $L^*\colon H_0^1(\Omega\cup\Gamma_N)^* \times ((H^1)^*)^m \to H_0^1(\Omega\cup\Gamma_N)^* \times ((H^1)^*)^M \times (H_0^1(\Omega)^*)^{m-M}$ is surjective.

Lemma 10.4 *The operator L has the property*

$$\mathcal{U}^\perp \subset \textit{ Im } L.$$

Proof. Let $v \in \mathcal{U}^\perp$ be given arbitrarily. Then $v = (0, \zeta) + (1, -q)v_0 \in X$, where $\zeta \in \mathcal{S}^\perp$ is constant. By Lemma 10.3 we have to show that $v \in \{v \in X \colon \gamma(v_{ch})(x) \in \mathcal{S}_0^\perp$ a.e. on $\Gamma\} =$ Im L. First, since $\zeta =$ const and $\zeta \in \mathcal{S}^\perp \subset \mathcal{S}_0^\perp$ we find that $\gamma(\zeta) = \zeta \in \mathcal{S}_0^\perp$. Second, by (4) $q \in \mathcal{S}^\perp \subset \mathcal{S}_0^\perp$ and it results $\gamma(qv_0) = q\gamma(v_0) \in \mathcal{S}_0^\perp$ a.e. on Γ. Therefore we obtain $\gamma(\zeta - qv_0) = \gamma(v_{ch}) \in \mathcal{S}_0^\perp$ and $v \in X$ which together means that $v \in$ Im L. $\square$

10.3 Example 3: Fast diffusion of some species

Without loss of generality we now assume that for the last $m-k$ species

$$D_i \to \infty, \quad i = k+1, \dots, m,$$

(otherwise additionally permutation matrices must be used). To guarantee that the flux terms in the last $m-k$ continuity equations remain bounded a.e. in Ω we have to require that $\nabla\zeta_i = 0$ which means $v_i + q_i v_0 = \zeta_i =$ const a.e. in Ω, $i = k+1, \dots, m$. Thus the chemical potentials v_i may be expressed by $\zeta_i - q_i v_0$ for $i = k+1, \dots, m$. We define the operator

$$\begin{aligned} &L\colon H_0^1(\Omega\cup\Gamma_N) \times (H^1)^k \times \mathbb{R}^{m-k} \to H_0^1(\Omega\cup\Gamma_N) \times (H^1)^m, \\ &L\widetilde{v} := (v_0, v_1, \dots, v_k, \zeta_{k+1} - q_{k+1}v_0, \dots, \zeta_m - q_m v_0), \end{aligned} \tag{22}$$

where $\widetilde{v} = (\widetilde{v}_0, \dots \widetilde{v}_m) = (v_0, \dots, v_k, \zeta_{k+1}, \dots, \zeta_m)$. We get $v = L\widetilde{v}$ with a linear, continuous, injective operator L. Im $L = H_0^1(\Omega\cup\Gamma_N) \times (H^1)^k \times (H_0^1(\Omega\cup\Gamma_N) + \mathbb{R})^{m-k}$ is closed in X. Again the adjoint operator $L^*\colon (H_0^1(\Omega\cup\Gamma_N))^* \times (H^1)^{*m} \to (H_0^1(\Omega\cup\Gamma_N))^* \times (H^1)^{*k} \times \mathbb{R}^{m-k}$ is surjective and the relation

$$\mathcal{U}^\perp \subset \text{ Im } L$$

is satisfied. For the last assertion we argue as follows. Let $v \in \mathcal{U}^\perp$ be given arbitrarily. Then $\zeta_i = v_i + q_i v_0$ is constant for $i = 1, \dots, m$ and we obtain that $v = L(v_0, \dots, v_k, \zeta_{k+1}, \dots, \zeta_m) \in \text{Im } L$.

10.4 Example 4: Fast diffusion of some species and fast reactions between these species

An example for such a reduction is the elimination of electrons and holes from electro–reaction–diffusion systems prescribing problems from semiconductor technology by the assumptions that the diffusion of the electrons and holes as well as the generation/recombination of electrons and holes is very fast (D_n, $D_p \to \infty$, $k \to \infty$ in $k(\mathrm{e}^{\zeta_n+\zeta_p} - 1)$). These assumptions are very common in the modeling of dopant diffusion in semiconductor technology (see e.g. [14]). In [10, 11] we carried out this special reduction and investigated the concrete arising problem.

Without loss of generality we now assume that for the last $m-k$ species

$$D_i \to \infty, \quad i = k+1, \dots, m$$

(otherwise again permutation matrices have to be used). Moreover we suppose

$$k_{\alpha\beta} \to \infty \quad \forall (\alpha,\beta) \in \mathcal{R}_\diamond := \big\{ (\alpha,\beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma \colon \alpha_i = \beta_i = 0,\, i = 1, \dots, k \ \big\}.$$

To guarantee that the flux terms in the last $m-k$ continuity equations remain bounded a.e. in Ω we have to require that $\nabla \zeta_i = 0$ which means $v_i + q_i v_0 = \zeta_i =$ const a.e. in Ω, $i = k+1, \dots, m$. Thus the chemical potentials v_i may be expressed by $\zeta_i - q_i v_0$ for $i = k+1, \dots, m$. Moreover to keep the reaction terms for all reactions from $\mathcal{R}_\diamond$ bounded it is necessary that $\zeta \cdot \alpha = \zeta \cdot \beta$ for all $(\alpha,\beta) \in \mathcal{R}_\diamond$. If we define

$$\mathcal{S}_\diamond := \operatorname{span}\big\{ (\alpha_{k+1} - \beta_{k+1}, \dots, \alpha_m - \beta_m) \colon (\alpha,\beta) \in \mathcal{R}_\diamond \big\} \subset \mathbb{R}^{m-k}$$

then the relation $(\zeta_{k+1}, \dots, \zeta_m) \in {\mathcal{S}_\diamond}^\perp \subset \mathbb{R}^{m-k}$ must be satisfied. Let $K :=$ $\dim {\mathcal{S}_\diamond}^\perp = m - k -$ $\dim \mathcal{S}_\diamond$. Then there exists a linear, injective mapping $L_\diamond \colon \mathbb{R}^K \to \mathbb{R}^{m-k}$ and $\zeta^\diamond \in \mathbb{R}^K$ such that

$$(\zeta_{k+1}, \dots, \zeta_m) = L_\diamond \zeta^\diamond,$$

$\operatorname{Im} L_\diamond = {\mathcal{S}_\diamond}^\perp$ is closed and $L_\diamond^*$ is surjective. Let $M := k + K$. We define the operator

$$\begin{aligned} &L \colon H_0^1(\Omega \cup \Gamma_N) \times (H^1)^k \times \mathbb{R}^K \to H_0^1(\Omega \cup \Gamma_N) \times (H^1)^m, \\ &L\widetilde{v} := (v_0, v_1, \dots, v_k, (L_\diamond \zeta^\diamond)_1 - q_{k+1} v_0, \dots, (L_\diamond \zeta^\diamond)_{m-k} - q_m v_0), \end{aligned} \tag{23}$$

where $\widetilde{v} = (\widetilde{v}_0, \dots, \widetilde{v}_M) = (v_0, \dots, v_k, \zeta_1^\diamond, \dots, \zeta_K^\diamond)$. We thus obtain $v = L\widetilde{v}$ with a linear, continuous, injective operator L with closed range. For the injectivity one argues as follows: From $L\widetilde{v} = 0$ we obtain $v_0 = \cdots = v_k = 0$, $L_\diamond \zeta^\diamond = 0$. Since $L_\diamond$ is injective we find $\zeta^\diamond = 0$.

Again the operator $L^* \colon (H_0^1(\Omega \cup \Gamma_N))^* \times (H^1)^{*m} \to (H_0^1(\Omega \cup \Gamma_N))^* \times (H^1)^{*k} \times \mathbb{R}^K$ is surjective.

Lemma 10.5 *The operator L has the property*

$$\mathcal{U}^\perp \subset \ Im\ L.$$

Proof. Let $v \in \mathcal{U}^\perp$ be given arbitrarily. Then $\zeta_i = v_i + q_i v_0$ is constant and $\zeta \in \mathcal{S}^\perp$. Therefore $\zeta \perp (\alpha - \beta)$ for all $(\alpha, \beta) \in \mathcal{R}_\diamond$ which induces that the shorted vector

$$(\zeta_{k+1}, \ldots, \zeta_m) \in \mathcal{S}_\diamond{}^\perp = \text{ Im } L_\diamond.$$

Thus there exists an $\zeta^\diamond \in \mathbb{R}^K$ such that $(\zeta_{k+1}, \ldots, \zeta_m) = L_\diamond \zeta^\diamond$. Now, for $\widetilde{v} = (\widetilde{v}_0, \ldots, \widetilde{v}_M)$ with $\widetilde{v}_i = v_i$, $i = 0, \ldots, k$, and $\widetilde{v}_{k+i} = \zeta_i^\diamond$, $i = 1, \ldots, K$, we have $v = L\widetilde{v} \in \text{ Im } L$. $\square$

Remark 10.1 *In [12, 13] we considered pair diffusion models from semiconductor technology. These model equations can be obtained by a reduction from systems of type* (1) *by a suitable operator L with properties* (5)*. Also in [8] such a reduced model is investigated. But, in the three cited papers we did the required energy estimates for the reduced models by hand and did not use the principle introduced in the present paper in Section 6 – Section 8 to carry over the results concerning energy estimates for the basic system to the reduced one.*

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