

Global estimates and asymptotics for electro–reaction–diffusion systems in heterostructures

A. Glitzky¹ and R. Hünlich

Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstr. 39, D–10117 Berlin, Germany

Abstract

We treat a wide class of electro–reaction–diffusion systems with nonsmooth data in two dimensional domains. Forced by applications in semiconductor technology a nonlinear and nonlocal Poisson equation is involved. We state global existence, uniqueness and asymptotic properties of solutions to the evolution problem. Essential tools in our investigations are energetic estimates, Moser iteration, regularization techniques and results for electro–diffusion systems with weakly nonlinear volume and boundary source terms. Especially, we discuss the connection between the existence of global lower bounds for the chemical potentials and the property that the energy functional decays exponentially to its equilibrium value as time tends to infinity.

AMS: 35B40, 35B45, 35D05, 35K45, 35K57, 78A35

KEY WORDS: Reaction–diffusion systems, drift–diffusion processes, motion of charged particles, global estimates, existence, uniqueness, asymptotic behaviour

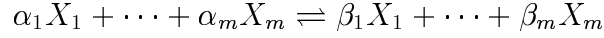
1 Introduction

In this paper we state global existence, uniqueness and asymptotic properties of solutions to evolution problems for electro–reaction–diffusion systems in heterostructures. First, we describe some concrete model equations which we are interested in.

Let Ω be a bounded domain, $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_0$ its boundary, $\text{mes } \Gamma_0 = 0$, ν the outer unit normal. We consider m electrically charged species X_i with charge numbers q_i and initial distributions $U_i: \Omega \rightarrow \mathbb{R}_+$. Their concentrations $u_i: \mathbb{R}_+ \times \Omega \rightarrow \mathbb{R}_+$ and their chemical potentials $v_i: \mathbb{R}_+ \times \Omega \rightarrow \mathbb{R}$ vary by diffusion processes, by chemical reactions running in Ω as well as on Γ and, finally, by a drift which is caused by the inner electric field. The charge density $u_0 = \sum_{i=1}^m q_i u_i$ occurs as source term for the electrostatic potential $\tilde{v}_0 = v_0 - \zeta_0$ where $v_0: \mathbb{R}_+ \times \Omega \rightarrow \mathbb{R}$ and $\zeta_0: \mathbb{R}_+ \rightarrow \mathbb{R}$ are some auxiliary quantities (cf. [17]).

¹Partly supported by the BMBF grant GA7FVB5–1.0M840.

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



and denote by \mathcal{R}^Ω and \mathcal{R}^Γ the sets of pairs (α, β) of stoichiometric coefficients $\alpha = (\alpha_1, \dots, \alpha_m)$, $\beta = (\beta_1, \dots, \beta_m)$ belonging to all reactions in Ω and on Γ , respectively. Mass conservation for each species yields the initial boundary value problem

$$\left. \begin{aligned} \frac{\partial u_i}{\partial t} + \nabla \cdot j_i + R_i^\Omega(\cdot, v_0, v_1, \dots, v_m, \zeta_0) &= 0 & \text{on } (0, \infty) \times \Omega, \\ \nu \cdot j_i - R_i^\Gamma(\cdot, v_0, v_1, \dots, v_m, \zeta_0) &= 0 & \text{on } (0, \infty) \times \Gamma, \\ u_i(0) &= U_i & \text{on } \Omega, \quad i = 1, \dots, m, \end{aligned} \right\} \quad (1.1)$$

$$\begin{aligned} u_i &= \bar{u}_i e^{v_i}, \quad j_i = -D_i u_i \nabla \zeta_i, \quad \zeta_i = v_i + q_i v_0, \quad i = 1, \dots, m, \\ R_i^\Sigma &= \sum_{(\alpha, \beta) \in \mathcal{R}^\Sigma} (\alpha_i - \beta_i) R_{\alpha\beta}^\Sigma, \quad \Sigma = \Omega, \Gamma, \quad i = 1, \dots, m, \\ R_{\alpha\beta}^\Sigma &= k_{\alpha\beta}^\Sigma(x, v_0, v_1, \dots, v_m, \zeta_0) \left(e^{\sum_{i=1}^m \alpha_i \zeta_i} - e^{\sum_{i=1}^m \beta_i \zeta_i} \right), \\ x \in \Sigma, \quad (v_0, v_1, \dots, v_m) &\in \mathbb{R}^{m+1}, \quad \zeta_0 \in \mathbb{R}, \quad (\alpha, \beta) \in \mathcal{R}^\Sigma, \quad \Sigma = \Omega, \Gamma, \end{aligned} \quad (1.2)$$

with given reference densities $\bar{u}_i: \Omega \rightarrow \mathbb{R}_+$, diffusivities $D_i: \Omega \rightarrow \mathbb{R}_+$ and kinetic coefficients $k_{\alpha\beta}^\Sigma: \Sigma \times \mathbb{R}^{m+2} \rightarrow \mathbb{R}_+$. The remaining quantities v_0, ζ_0 are obtained by the Poisson equation and by a charge conservation relation as follows (cf. [17]):

$$\left. \begin{aligned} -\nabla \cdot (\varepsilon \nabla v_0) + e_0(\cdot, v_0) &= \sum_{i=1}^m q_i u_i & \text{on } (0, \infty) \times \Omega, \\ v_0 &= \zeta_0 & \text{on } (0, \infty) \times \Gamma_D, \\ \nu \cdot (\varepsilon \nabla v_0) + \tau v_0 &= \tau \zeta_0 & \text{on } (0, \infty) \times \Gamma_N, \\ \int_\Omega e_0(\cdot, v_0) \, dx &= \int_\Omega \sum_{i=1}^m q_i u_i \, dx & \text{on } (0, \infty), \end{aligned} \right\} \quad (1.3)$$

$$e_0(x, y) = \sum_{i=1}^m q_i U_i(x) + f_0(x) + f_1(x) e^y - f_2(x) e^{-y}, \quad x \in \Omega, \quad y \in \mathbb{R}, \quad (1.4)$$

where the dielectric permittivity $\varepsilon: \Omega \rightarrow \mathbb{R}_+$, the capacity $\tau: \Gamma_N \rightarrow \mathbb{R}_+$ and the functions $f_0: \Omega \rightarrow \mathbb{R}$, $f_1, f_2: \Omega \rightarrow \mathbb{R}_+$ are given. Here homogeneous boundary conditions for \tilde{v}_0 are involved, since non-homogeneities not depending on time can be eliminated as in [17].

Assuming $\sum_{i=1}^m q_i (\alpha_i - \beta_i) = 0$ for all $(\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma$, $f_j = 0$, $j = 0, 1, 2$, and setting $\zeta_0 = 0$ we arrive at the standard problem of electro-diffusion with multiple reacting species as considered e. g. in [18]. The more complex form of (1.3) is motivated by problems arising in semiconductor technology we are mainly interested in. Moreover, in such problems all physical parameters \bar{u}_i , D_i , $k_{\alpha\beta}^\Sigma$, ε , τ , f_1 and f_2 depend on the space variable x in a

nonsmooth way. In general besides of the kinetic coefficients $k_{\alpha\beta}^{\Sigma}$ also the diffusivities D_i depend on the state variables. But such a dependency will be neglected in this paper.

A precise formulation of our model equations (1.1), (1.3) will be given in Section 2. Here we consider only the weak formulation of (1.3): For fixed t find (v_0, ζ_0) with $v_0 - \zeta_0 \in H_0^1(\Omega \cup \Gamma_N)$, $\zeta_0 \in \mathbb{R}$ such that

$$\left. \begin{aligned} \int_{\Omega} \left\{ \varepsilon \nabla v_0 \nabla h + \left(e_0(\cdot, v_0) - \sum_{i=1}^m q_i u_i \right) (h + \xi) \right\} dx + \int_{\Gamma_N} \tau (v_0 - \zeta_0) h \, d\Gamma = 0 \\ \forall (h, \xi) \in H_0^1(\Omega \cup \Gamma_N) \times \mathbb{R}. \end{aligned} \right\} \quad (1.3^*)$$

Setting $\bar{v}_0 = h + \xi$ we easily obtain the following equivalent formulation: Find $(v_0, \zeta_0) \in H \times \mathbb{R}$ such that

$$\left. \begin{aligned} \int_{\Omega} \left\{ \varepsilon \nabla v_0 \nabla \bar{v}_0 + \left(e_0(\cdot, v_0) - \sum_{i=1}^m q_i u_i \right) \bar{v}_0 \right\} dx + \\ \int_{\Gamma_N} \tau (v_0 - \pi(v_0)) (\bar{v}_0 - \pi(\bar{v}_0)) \, d\Gamma = 0 \quad \forall \bar{v}_0 \in H \quad \text{and} \quad \zeta_0 = \pi(v_0) \end{aligned} \right\} \quad (1.3^{**})$$

where

$$H = H_0^1(\Omega \cup \Gamma_N) + \mathbb{R}, \quad \pi(w) = \begin{cases} |\Gamma_D|^{-1} \int_{\Gamma_D} w \, d\Gamma & \text{if } |\Gamma_D| \neq 0, \\ \|\tau\|_{L^1(\Gamma_N)}^{-1} \int_{\Gamma_N} \tau w \, d\Gamma & \text{if } |\Gamma_D| = 0, \end{cases} \quad w \in H^1(\Omega). \quad (1.5)$$

An essential feature of the model equations (1.1), (1.3) is the fact that they allow *thermal equilibria* as steady states (see Section 5). Moreover, there is a convex functional which can be interpreted from the viewpoint of thermodynamics as *free energy*. This functional turns out to be a Lyapunov function of the system and ensures exponential decay of arbitrary perturbations of thermal equilibria, at least under some additional structural property of the underlying reaction system (see Section 5). Energetic estimates like in Subsection 3.3 and Subsection 5.3 are the basic key in deriving further global estimates and existence results.

If there are only two kinds of species with opposite sign of their charge (*electrons* and *holes*) we obtain the classical drift–diffusion model of carrier transport in semiconductors (the van Roosbroeck system, see [30]) as a special case of our model equations. Normally, here more general boundary conditions as in (1.1), (1.3) are of interest. Then the steady states need not correspond to thermal equilibria (see e. g. [1, 2, 24, 26, 31]). Starting from first results of Mock (see [28]) the transient problem has been extensively investigated by Gajewski and Gröger (see [12, 13, 14, 19, 22]).

As already mentioned we are mainly interested in electro–reaction–diffusion problems arising in semiconductor technology. Here more than two kinds of charged or uncharged species as well as a lot of chemical reactions have to be taken into account (see [23]). From this field of applications also the choice of our boundary conditions is motivated. Often the model equations (1.1), (1.3) are modified by assuming a local electro-neutrality condition

to determine the electrostatic potential (see [23, 31]). Special cases of this type where only one kind of species is electrically charged have been investigated in [16, 27].

Other applications of electro–reaction–diffusion systems come from the field of electrolysis. Whereas in papers of Amann (see [3, 4]) and Yu [33] the continuity equations are complemented by an electro-neutrality condition in papers of Choi and Lui (see [7, 8, 9]) the full system of continuity equations coupled with the Poisson equation is considered. Resulting from the special situation in electrolysis smooth kinetic coefficients and smooth domains are assumed. The application of corresponding techniques to the case of nonsmooth data in the situation of heterostructures as considered in this paper can not be expected, such that other techniques are needed.

Our investigation of the multiple species problem is based on methods used by Gajewski and Gröger for the van Roosbroeck system in heterostructures [14]. The main difference to [14] consists in the fact that we have in (1.1) no Dirichlet conditions and more general reactions. From this arise complications in deriving global lower bounds which we shall overcome by using an additional energetic estimate (see Subsection 5.3 and [15, 18]).

In Section 2 we summarize the assumptions on the data our further considerations are based on. Besides of assumptions concerning the principal structure of diffusion, drift and reaction terms there are requirements of a more technical character (two dimensional domains – cf. (2.1), growth condition for the source terms in the continuity equations – cf. (2.6), non-degeneracy condition of the reaction system – cf. (5.7)). Preliminary results concerning estimates for the solution to the possibly nonlinear and nonlocal Poisson equation, uniqueness of the solution to the evolution problem and first energetic estimates are collected in Section 3. Here we make essential use of assumption (2.1). Section 4 is devoted to existence results which are obtained by some regularization technique if the additional assumption (2.6) is fulfilled. Under the same assumption global upper bounds for the concentrations are established. The existence of global lower bounds as well as results concerning the asymptotic behaviour are shown in Section 5 where assumption (5.7) plays an important rôle. A more detailed representation of our investigations may be found in the report [17].

Let us collect some notation and results which are relevant for the paper. We assume that $\Omega \subset \mathbb{R}^2$ is a bounded (strictly) Lipschitzian domain. The notation of function spaces $L^p(\Omega, \mathbb{R}^k)$, $L^p(\Gamma, \mathbb{R}^k)$, $H^1(\Omega, \mathbb{R}^k)$, $k \in \mathbb{N}$, $L^\Psi(\Omega)$, corresponds to that in [25]. If there is no danger of misunderstanding we shall write shortly L^p instead of $L^p(\Omega, \mathbb{R}^k)$, and H^1 instead of $H^1(\Omega, \mathbb{R}^k)$. With regard to the definition of the spaces $H_0^1(\Omega \cup \Gamma_N)$, $W_0^{1,p}(\Omega \cup \Gamma_N)$ we refer to [20] or to [14, Appendix]. 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 . Analogously, $d: \mathbb{R}_+ \rightarrow \mathbb{R}_+$ stands for continuous, monotonously increasing functions with $\lim_{y \rightarrow \infty} d(y) = \infty$.

We apply Sobolev’s imbedding theorems (see [25]) as well as some other imbedding results. By a modified application of the Hölder inequality from [25, p. 317, formula (5)] we derive

$$\|w\|_{L^q(\Gamma)}^q \leq c_\Omega q \|w\|_{L^{2(q-1)}(\Omega)}^{q-1} \|w\|_{H^1(\Omega)} \quad \forall w \in H^1(\Omega), \quad q \geq 2. \quad (1.6)$$

By means of this trace inequality we get

$$\|w\|_{L^\infty(\Gamma)} \leq \|w\|_{L^\infty(\Omega)} \quad \forall w \in H^1(\Omega) \cap L^\infty(\Omega). \quad (1.7)$$

As a special case of the Gagliardo–Nirenberg inequality (see [11, 29]) we use the estimate

$$\|w\|_{L^p} \leq c_p \|w\|_{L^1}^{1/p} \|w\|_{H^1}^{1-1/p} \quad \forall w \in H^1(\Omega), \quad 1 < p < \infty. \quad (1.8)$$

As an extended form of Gagliardo–Nirenberg’s inequality one obtains that for any $\epsilon > 0$ and any $p \in (1, \infty)$ there exists a $c_{\epsilon,p} > 0$ such that

$$\|w\|_{L^p}^p \leq \epsilon \|w \ln |w|\|_{L^1} \|w\|_{H^1}^{p-1} + c_{\epsilon,p} \|w\|_{L^1} \quad \forall w \in H^1(\Omega). \quad (1.9)$$

In [5] this inequality is proved for bounded domains with smooth boundary and $p = 3$. An inspection of that proof yields the validity of (1.9) also for bounded Lipschitzian domains and $p \in (1, \infty)$, since (1.8) is true in this case, too. Finally, from Trudinger’s imbedding theorem (see [32]) we get

$$\|e^{|w|}\|_{L^p} \leq d_p (\|w\|_{H^1}) \quad \forall w \in H^1(\Omega), \quad 1 \leq p < \infty. \quad (1.10)$$

2 Formulation of the problem

In the sequel we shall formulate a general evolution problem which involves the concrete model problem introduced in Section 1. First we summarize the assumptions which our further considerations are based on:

$$\left. \begin{array}{l} \Omega \text{ is a bounded Lipschitzian domain in } \mathbb{R}^2, \quad \Gamma := \partial\Omega, \\ \Gamma_D, \Gamma_N \text{ are disjoint open subsets of } \Gamma, \quad \Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N}, \\ \overline{\Gamma_D} \cap \overline{\Gamma_N} \text{ consists of finitely many points;} \end{array} \right\} \quad (2.1)$$

$$\left. \begin{array}{l} q_i \in \mathbb{Z}, \quad \bar{u}_i, U_i \in L^\infty(\Omega), \quad \bar{u}_i, U_i \geq c > 0, \\ D_i \in L^\infty(\Omega), \quad D_i \geq c > 0, \quad i = 1, \dots, m; \\ U_0 := \sum_{i=1}^m q_i U_i; \\ \varepsilon \in L^\infty(\Omega), \quad \varepsilon \geq c > 0, \quad \tau \in L_+^\infty(\Gamma_N), \quad \text{mes } \Gamma_D + \|\tau\|_{L^1(\Gamma_N)} > 0; \end{array} \right\} \quad (2.2)$$

$$\left. \begin{array}{l} H \text{ is a linear closed subspace of } H^1(\Omega), \quad H_0^1(\Omega \cup \Gamma_N) \subset H; \\ \pi \in \mathcal{L}(H^1(\Omega), \mathbb{R}), \\ v - \pi(v) \in H_0^1(\Omega \cup \Gamma_N) \quad \forall v \in H, \\ \pi(h) \int_{\Gamma_N} \tau(v - \pi(v)) \, d\Gamma = 0 \quad \forall h \in H_0^1(\Omega \cup \Gamma_N), \quad \forall v \in H; \end{array} \right\} \quad (2.3)$$

$$\left. \begin{array}{l} e_0 : \Omega \times \mathbb{R} \rightarrow \mathbb{R} \text{ satisfies the Carathéodory conditions,} \\ |e_0(x, y)| \leq c e^{c|y|} \text{ f.a.a. } x \in \Omega, \quad \forall y \in \mathbb{R}, \quad c > 0, \\ e_0(x, y) - e_0(x, z) \geq b_0(x) (y - z) \text{ f.a.a. } x \in \Omega, \quad \forall y, z \in \mathbb{R} \text{ with } y \geq z, \\ b_0 \in L_+^\infty(\Omega), \quad \|b_0\|_{L^1} \geq c \|\pi\|, \quad c > 0; \end{array} \right\} \quad (2.4)$$

$$\left. \begin{aligned}
& \mathcal{R}^\Omega, \mathcal{R}^\Gamma \text{ are finite subsets of } \mathbb{Z}_+^m \times \mathbb{Z}_+^m; \\
& \text{for } \Sigma = \Omega, \Gamma \text{ and } (\alpha, \beta) \in \mathcal{R}^\Sigma \text{ we define} \\
& R_{\alpha\beta}^\Sigma := k_{\alpha\beta}^\Sigma(x, y, z) (e^{\alpha \cdot \zeta} - e^{\beta \cdot \zeta}), \quad x \in \Sigma, \quad y = (y_0, y_1, \dots, y_m) \in \mathbb{R}^{m+1}, \\
& \zeta_i := y_i + q_i y_0, \quad i = 1, \dots, m, \quad z \in \mathbb{R}, \text{ where} \\
& k_{\alpha\beta}^\Sigma: \Sigma \times \mathbb{R}^{m+1} \times \mathbb{R} \rightarrow \mathbb{R}_+ \text{ satisfies the Carathéodory conditions,} \\
& k_{\alpha\beta}^\Sigma(x, \cdot, \cdot) \text{ is locally Lipschitz continuous uniformly with respect to } x, \\
& k_{\alpha\beta}^\Sigma(x, y, z) \leq c e^{c(|y_0|+|z|)} \text{ f.a.a. } x \in \Sigma, \quad \forall (y, z) \in \mathbb{R}^{m+2}, \\
& k_{\alpha\beta}^\Sigma(x, y, z) \geq c_R > 0 \text{ f.a.a. } x \in \Sigma, \quad \forall (y, z) \in \mathbb{R}^{m+2} \text{ with } y_0, z \in [-R, R].
\end{aligned} \right\} \quad (2.5)$$

For the proof of existence results we shall additionally suppose that

$$\left. \begin{aligned}
& (e^{\alpha \cdot \zeta} - e^{\beta \cdot \zeta}) \max_{i=1, \dots, m} (\beta_i - \alpha_i) \leq c \left(\sum_{j=1}^m e^{n_\Sigma \zeta_j} + 1 \right) \\
& \forall \zeta \in \mathbb{R}^m, \quad \forall (\alpha, \beta) \in \mathcal{R}^\Sigma, \quad \Sigma = \Omega, \Gamma, \text{ with } n_\Omega = 2, n_\Gamma = 1, c > 0.
\end{aligned} \right\} \quad (2.6)$$

Finally, for the investigation of asymptotic properties we need a further assumption on the structure of the reaction system which will be introduced later on (see (5.7)).

Remark 2.1. The subspace H , see (2.3), equipped with the norm of $H^1(\Omega)$ will be regarded as a Hilbert space. Then it holds

$$H^* = \left\{ u_0 : u_0 = \tilde{u}_0|_H, \quad \tilde{u}_0 \in H^1(\Omega)^* \right\}.$$

If $\tilde{u}_0 \in H^1(\Omega)^*$ may be identified with a function $\tilde{u}_0 \in L^2(\Omega)$ then $u_0 = \tilde{u}_0|_H$ may also be identified with the function \tilde{u}_0 since $H_0^1(\Omega \cup \Gamma_N) \subset H$ and $H_0^1(\Omega \cup \Gamma_N)$ is dense in $L^2(\Omega)$.

Remark 2.2. By the assumptions (2.2)–(2.4) it follows that there exists a $c > 0$ such that

$$\|\nabla v_0\|_{L^2}^2 + \int_\Omega b_0 v_0^2 dx + \int_{\Gamma_N} \tau (v_0 - \pi(v_0))^2 d\Gamma \geq c \|v_0\|_{H^1}^2 \quad \forall v_0 \in H. \quad (2.7)$$

Remark 2.3. We define the function ϕ_0 by

$$\phi_0(x, y) := e_0(x, y)y - \int_0^y e_0(x, \eta) d\eta, \quad x \in \Omega, \quad y \in \mathbb{R}.$$

Often we will write only the second argument of the functions e_0 and ϕ_0 . By (2.4) we easily find the properties

$$e_0(y)(y - \bar{y}) - \int_{\bar{y}}^y e_0(\eta) d\eta \geq \frac{1}{2} b_0 (y - \bar{y})^2, \quad \phi_0(y) \geq \frac{1}{2} b_0 y^2 \quad \text{a.e. on } \Omega, \quad \forall y, \bar{y} \in \mathbb{R}. \quad (2.8)$$

Remark 2.4. For a special realization of H , π and e_0 we refer to (1.5) and (1.4).

Remark 2.5. The form of the reaction terms in (2.5) involves some important structural properties. First, it holds

$$R_{\alpha\beta}^\Sigma(x, y, z) \sum_{i=1}^m (\alpha_i - \beta_i)(y_i + q_i y_0) \geq 0 \text{ f.a.a. } x \in \Sigma, \forall (y, z) \in \mathbb{R}^{m+2}. \quad (2.9)$$

This will ensure the energetic estimates in Section 3. Furthermore, for $i = 1, \dots, m$

$$\begin{aligned} e^{-\zeta_i} (e^{\alpha\zeta} - e^{\beta\zeta})(\alpha_i - \beta_i) &\leq \alpha_i e^{\left\{(\alpha_i-1)\zeta_i + \sum_{j \neq i} \alpha_j \zeta_j\right\}} \text{ if } \alpha_i > \beta_i, \\ e^{-\zeta_i} (e^{\alpha\zeta} - e^{\beta\zeta})(\alpha_i - \beta_i) &\leq \beta_i e^{\left\{(\beta_i-1)\zeta_i + \sum_{j \neq i} \beta_j \zeta_j\right\}} \text{ if } \alpha_i < \beta_i. \end{aligned} \quad (2.10)$$

These relations are used for getting lower bounds in Section 4 and Section 5.

Remark 2.6. Condition (2.6) means only restrictions on the source terms of the continuity equations whereas sink terms may be of higher order.

In order to formulate our general evolution problem we use the variables

$$\begin{aligned} v &= (v_0, v_1, \dots, v_m) : \mathbb{R} \times \Omega \rightarrow \mathbb{R}^{m+1} \quad (\text{potentials}), \\ u &= (u_0, u_1, \dots, u_m) : \mathbb{R} \times \Omega \rightarrow \mathbb{R}^{m+1} \quad (\text{densities}). \end{aligned}$$

Analogously we set $U = (U_0, U_1, \dots, U_m)$ where $U_0 = \sum_{i=1}^m q_i U_i$ (cf. (2.2)). Since we want to take into account heterostructures the potentials must belong to a space of sufficiently smooth functions while the densities are regarded as elements of the corresponding dual space. We work with the function spaces

$$X := H \times H^1(\Omega, \mathbb{R}^m), \quad Y := L^2(\Omega, \mathbb{R}^{m+1}), \quad W := X \cap L^\infty(\Omega, \mathbb{R}^{m+1}).$$

We define the operators $A: W \times X \rightarrow X^*$, $E_0: H \rightarrow H^*$ and $E: X \rightarrow X^*$ by

$$\begin{aligned} \langle A(w, v), \bar{v} \rangle &:= \int_{\Omega} \left\{ \sum_{i=1}^m D_i \bar{u}_i e^{w_i} \nabla \zeta_i \nabla \bar{\zeta}_i + \sum_{(\alpha, \beta) \in \mathcal{R}^\Omega} R_{\alpha\beta}^\Omega(\cdot, w, \pi(w_0)) (\alpha - \beta) \cdot \bar{\zeta} \right\} dx \\ &+ \int_{\Gamma} \sum_{(\alpha, \beta) \in \mathcal{R}^\Gamma} R_{\alpha\beta}^\Gamma(\cdot, w, \pi(w_0)) (\alpha - \beta) \cdot \bar{\zeta} d\Gamma, \quad \bar{v} \in X, \end{aligned}$$

where $\zeta_i = v_i + q_i v_0$, $\bar{\zeta}_i = \bar{v}_i + q_i \bar{v}_0$, $i = 1, \dots, m$,

$$\langle E_0 v_0, \bar{v}_0 \rangle := \int_{\Omega} \left\{ \varepsilon \nabla v_0 \nabla \bar{v}_0 + e_0(v_0) \bar{v}_0 \right\} dx + \int_{\Gamma_N} \tau(v_0 - \pi(v_0)) (\bar{v}_0 - \pi(\bar{v}_0)) d\Gamma, \quad \bar{v}_0 \in H,$$

$$\langle E v, \bar{v} \rangle := \langle E_0 v_0, \bar{v}_0 \rangle + \int_{\Omega} \sum_{i=1}^m \bar{u}_i e^{v_i} \bar{v}_i dx, \quad \bar{v} \in X.$$

Then the problem which we are interested in reads as

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

Remark 2.7. Problem (P) includes the precise weak formulation of the model problem introduced in Section 1. Especially, by test functions of the form $(w, -q_1 w, \dots, -q_m w)$, $w \in H$, we obtain that for solutions (u, v) to (P) it holds

$$u_0(t) = \sum_{i=1}^m q_i u_i(t)|_H \text{ in } H^* \forall t \in \mathbb{R}_+. \quad (2.11)$$

Remark 2.8. If (u, v) is a solution to (P) then u, v have regularity properties which can be derived from the concept of solution only: $u \in C(\mathbb{R}_+, Y)$, $u \in C_{w^*}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1}))$, $v_0 \in C(\mathbb{R}_+, H)$, $v_i \in C(\mathbb{R}_+, L^2)$, $i = 1, \dots, m$, $v \in C_{w^*}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1}))$. Moreover, these regularity properties imply the validity of (2.11) in the sense of L^2 and the relations

$$\begin{aligned} E_0 v_0(t) &= u_0(t) \text{ in } H^* \forall t \in \mathbb{R}_+, \\ v_i(t) &= \ln(u_i(t)/\bar{u}_i) \text{ in } L^\infty(\Omega) \forall t \in \mathbb{R}_+, i = 1, \dots, m. \end{aligned} \quad (2.12)$$

3 Preliminary results

3.1 Estimates for the solution to the Poisson equation

First we note that because of (2.7), (2.8), (2.4) and (1.10) the operator $E_0: H \rightarrow H^*$ is strongly monotone, hemicontinuous, and therefore bijective.

Lemma 3.1. *Let the assumptions (2.1)–(2.4) be fulfilled. Then there exist constants $c > 0$, $q > 2$ and a continuous increasing function d such that for $v_0 \in H$ with $E_0 v_0 = u_0 \in L^2(\Omega)$*

$$\|v_0\|_{L^\infty} \leq c \left(\|u_0 \ln |u_0|\|_{L^1} + d(\|v_0\|_{H^1}) + 1 \right), \quad (3.1)$$

$$\|v_0\|_{W^{1,q}} \leq c \left(\|u_0\|_{L^{2q/(2+q)}} + d(\|v_0\|_{H^1}) + 1 \right). \quad (3.2)$$

Proof. Let $v_0 \in H$ be the solution to $E_0 v_0 = u_0$. Then $w := v_0 - \pi(v_0) \in H_0^1(\Omega \cup \Gamma_N)$ and for $h \in H_0^1(\Omega \cup \Gamma_N)$ it holds $\pi(h) \int_{\Gamma_N} \tau w \, d\Gamma = 0$, cf. (2.3). Since $H_0^1(\Omega \cup \Gamma_N) \subset H$ it follows from the weak formulation of the Poisson equation that

$$\int_{\Omega} \varepsilon \nabla w \nabla h \, dx + \int_{\Gamma_N} \tau w h \, d\Gamma = \int_{\Omega} (u_0 - e_0(\cdot, v_0)) h \, dx \quad \forall h \in H_0^1(\Omega \cup \Gamma_N).$$

Because of the last assumption in (2.2) we can now apply to this equation results of Gröger for elliptic equations [21, Theorem 1] and [20, Theorem 1] and obtain

$$\begin{aligned} \|v_0\|_{L^\infty} &\leq c \left(\|u_0 - e_0(\cdot, v_0)\|_{L^\Psi} + \|v_0\|_{H^1} \right), \quad \Psi(s) = (1+s) \ln(1+s) - s \text{ for } s \geq 0, \\ \|v_0\|_{W^{1,q}} &\leq c \left(\|u_0 - e_0(\cdot, v_0)\|_{(W_0^{1,q/(q-1)}(\Omega \cup \Gamma_N))^*} + \|v_0\|_{H^1} \right) \quad \text{for some } q > 2. \end{aligned}$$

Because of (2.4) and (1.10) the remaining norms of $u_0 - e_0(\cdot, v_0)$ can be estimated in such a way that the assertions follow. \square

3.2 Uniqueness

From now up to the end of Section 5 we suppose the assumptions (2.1)–(2.5) to be fulfilled.

Theorem 3.1. *There exists at most one solution to (P) .*

Proof. It suffices to prove uniqueness on every finite time interval $S := [0, T]$. Let (u^j, v^j) , $j = 1, 2$, be solutions to (P). Then there exists a constant c such that

$$\|u^j(t)\|_{L^\infty}, \|v^j(t)\|_{L^\infty}, \|v^j(t)\|_{L^\infty(\Gamma)}, |\pi(v_0^j(t))|, \|v_0^j(t)\|_{W^{1,q}} \leq c \text{ f.a.a. } t \in S, \quad j = 1, 2,$$

where $q > 2$ (cf. Lemma 3.1). Let $\tilde{u} := u^1 - u^2$, $\tilde{v} := v^1 - v^2$. Testing $E_0 v_0^1(t) - E_0 v_0^2(t) = \tilde{u}_0(t)$ by $\tilde{v}_0(t)$ we obtain by the strong monotonicity of E_0 that

$$\|\tilde{v}_0(t)\|_{H^1} \leq c \sum_{i=1}^m \|\tilde{u}_i(t)\|_{L^2} \text{ f.a.a. } t \in S. \quad (3.3)$$

Let $z_i := \tilde{u}_i/\bar{u}_i$, $i = 1, \dots, m$. We use $(0, z_1, \dots, z_m) \in L^2(S, X)$ as test function for (P) and take into account that $R_{\alpha\beta}^\Sigma(x, \cdot, \cdot)$ is uniformly locally Lipschitz continuous. The norms of \tilde{v}_i in $L^2(\Omega)$ and $L^2(\Gamma)$ can be estimated by the corresponding norms of z_i . With inequality (3.3) and $r := 2q/(q-2)$ we conclude as follows

$$\begin{aligned} \sum_{i=1}^m \left\{ \|z_i(t)\|_{L^2}^2 + \int_0^t \|z_i\|_{H^1}^2 ds \right\} &\leq c \int_0^t \sum_{i=1}^m \left\{ \|z_i\|_{L^r} \|\nabla v_0^1\|_{L^q} \|\nabla z_i\|_{L^2} \right. \\ &\quad \left. + \|\nabla \tilde{v}_0\|_{L^2} \|\nabla z_i\|_{L^2} + \|z_i\|_{L^2}^2 + \|\tilde{v}_0\|_{H^1}^2 + \|z_i\|_{L^2(\Gamma)}^2 \right\} ds \\ &\leq \int_0^t \sum_{i=1}^m \left\{ \frac{1}{2} \|z_i\|_{H^1}^2 + c \left(\|v_0^1\|_{W^{1,q}}^r \|z_i\|_{L^2}^2 + \|z_i\|_{L^2}^2 \right) \right\} ds \\ &\leq \int_0^t \sum_{i=1}^m \left\{ \frac{1}{2} \|z_i\|_{H^1}^2 + c \|z_i\|_{L^2}^2 \right\} ds \quad \forall t \in S. \end{aligned}$$

Gronwall's lemma yields $z_i = 0$ on S , $i = 1, \dots, m$. With (3.3) the assertion follows. \square

3.3 Energetic estimates

In this subsection we collect results on energetic estimates which can be obtained similar to the techniques in [15, 18]. We define the functional $\Phi: X \rightarrow \mathbb{R}$,

$$\Phi(v) := \int_{\Omega} \left\{ \frac{\varepsilon}{2} |\nabla v_0|^2 + \int_0^{v_0} e_0(y) dy + \sum_{i=1}^m \bar{u}_i (e^{v_i} - 1) \right\} dx + \int_{\Gamma_N} \frac{\tau}{2} (v_0 - \pi(v_0))^2 d\Gamma.$$

By (1.10) this functional is continuous, Gâteaux differentiable and it holds $\partial\Phi = E$. Since E is strictly monotone Φ is strictly convex. Its conjugate functional $F: X^* \rightarrow \overline{\mathbb{R}}$,

$$F(u) := \sup_{v \in X} \left\{ \langle u, v \rangle - \Phi(v) \right\},$$

is proper, lower semicontinuous and convex. It holds $u = Ev = \partial\Phi(v)$ if and only if $v \in \partial F(u)$, cf. [10]. F may be interpreted as the free energy of the reaction–diffusion system.

Lemma 3.2. *If $u \in H^* \times L_+^2(\Omega, \mathbb{R}^m)$ then the value of $F(u)$ can be calculated as*

$$F(u) = \int_{\Omega} \left\{ \frac{\varepsilon}{2} |\nabla v_0|^2 + \phi_0(v_0) + \sum_{i=1}^m \left(u_i \ln \frac{u_i}{\bar{u}_i} - 1 \right) + \bar{u}_i \right\} dx + \int_{\Gamma_N} \frac{\tau}{2} (v_0 - \pi(v_0))^2 d\Gamma$$

where v_0 fulfils the relation $E_0 v_0 = u_0$. The functional $F|_{H^* \times L_+^2(\Omega, \mathbb{R}^m)}$ is continuous.

For the proof we refer to [17, Lemma 3.2].

Along any solution (u, v) to (P) the function $t \mapsto F(u(t))$ is absolutely continuous and it holds (see [6])

$$\frac{d}{dt} F(u(t)) = -D(v(t)) \text{ f.a.a. } t \in \mathbb{R}_+$$

where the dissipation rate D is given by $D(v) := \langle A(v, v), v \rangle$, $v \in W$. By the definition of the operator A and by (2.9) the dissipation rate is nonnegative for all $v \in W$. This together with (3.1), (2.11) and (1.7) ensures the following result.

Theorem 3.2. *Let (u, v) be a solution to (P). Then*

$$\begin{aligned} F(u(t_2)) &\leq F(u(t_1)) \leq F(U) \quad \text{for } t_2 \geq t_1 \geq 0, \\ \|v_0(t)\|_{H^1} + \sum_{i=1}^m \|u_i(t) \ln u_i(t)\|_{L^1} + \int_0^t D(v(s)) ds &\leq c \quad \forall t \in \mathbb{R}_+, \\ \|v_0(t)\|_{L^\infty}, \|v_0(t)\|_{L^\infty(\Gamma)}, |\pi(v_0(t))| &\leq c \quad \forall t \in \mathbb{R}_+ \end{aligned}$$

where c depends only on the data.

4 Existence

4.1 The regularized problem (\mathbf{P}_N)

In the sequel we consider a problem on an arbitrarily fixed time interval $S := [0, T]$ which arises from (P) by regularizing the reaction and boundary terms. Let, for $N \in \mathbb{R}_+$, $\rho_N : \mathbb{R}^{m+2} \rightarrow [0, 1]$ be a fixed Lipschitz continuous function such that

$$\rho_N(y, z) := \begin{cases} 0 & \text{if } |(y, z)|_\infty \geq N, \\ 1 & \text{if } |(y, z)|_\infty \leq N/2 \end{cases}, \quad |(y, z)|_\infty := \max\{|y_0|, \dots, |y_m|, |z|\}.$$

We define the operator $A_N : W \times X \rightarrow X^*$ by

$$\begin{aligned} \langle A_N(w, v), \bar{v} \rangle &:= \int_{\Omega} \left\{ \sum_{i=1}^m D_i \bar{u}_i e^{w_i} \nabla \zeta_i \nabla \bar{\zeta}_i \right. \\ &\quad \left. + \sum_{(\alpha, \beta) \in \mathcal{R}^\Omega} \rho_N(w, \pi(w_0)) R_{\alpha\beta}^\Omega(\cdot, w, \pi(w_0)) (\alpha - \beta) \cdot \bar{\zeta} \right\} dx \\ &\quad + \int_{\Gamma} \sum_{(\alpha, \beta) \in \mathcal{R}^\Gamma} \rho_N(w, \pi(w_0)) R_{\alpha\beta}^\Gamma(\cdot, w, \pi(w_0)) (\alpha - \beta) \cdot \bar{\zeta} d\Gamma, \quad \bar{v} \in X. \end{aligned}$$

The operator E is not changed. Now we are looking for solutions to the regularized problem

$$\left. \begin{aligned} u'(t) + A_N(v(t), v(t)) &= 0, \quad u(t) = Ev(t) \text{ f.a.a. } t \in S, \quad u(0) = U, \\ u &\in H^1(S, X^*), \quad v \in L^2(S, X) \cap L^\infty(S, L^\infty(\Omega, \mathbb{R}^{m+1})). \end{aligned} \right\} \quad (\mathbf{P}_N)$$

4.2 Solvability of (\mathbf{P}_N)

Theorem 4.1. *For each $N \in \mathbb{R}_+$ there exists a unique solution to (\mathbf{P}_N) .*

Proof. For fixed $N \in \mathbb{R}_+$, $\Sigma = \Omega, \Gamma$, $i = 1, \dots, m$, we define $g_i^\Sigma: \Sigma \times \mathbb{R}^{m+1} \times \mathbb{R} \rightarrow \mathbb{R}$ by

$$g_i^\Sigma(x, y, z) := \rho_N(y, z) \sum_{(\alpha, \beta) \in \mathcal{R}^\Sigma} R_{\alpha\beta}^\Sigma(x, y, z)(\beta_i - \alpha_i).$$

Then g_i^Σ satisfies the Carathéodory conditions and the following properties can be verified:

$$\begin{aligned} |g_i^\Sigma(x, y, z)| &\leq c_\Sigma \text{ f.a.a. } x \in \Sigma, \quad \forall (y, z) \in \mathbb{R}^{m+2}, \\ |g_i^\Sigma(x, y, z) - g_i^\Sigma(x, \bar{y}, \bar{z})| &\leq L_\Sigma |(y - \bar{y}, z - \bar{z})|_\infty \\ \text{f.a.a. } x \in \Sigma, \quad \forall (y, z), (\bar{y}, \bar{z}) &\in \mathbb{R}^{m+2}, \\ \sum_{i=1}^m g_i^\Sigma(x, y, z)(y_i + q_i y_0) &\geq 0 \text{ f.a.a. } x \in \Sigma, \quad \forall (y, z) \in \mathbb{R}^{m+2}, \\ g_i^\Sigma(x, y, z) &\leq c_\Sigma e^{y_i} \text{ f.a.a. } x \in \Sigma, \quad \forall (y, z) \in \mathbb{R}^{m+2} \text{ with } y_i \leq 0. \end{aligned}$$

Thus we can apply [17, Theorem 6.1] for electro-diffusion systems with weakly nonlinear volume and boundary source terms to obtain the assertion. \square

4.3 Estimates for the solution to (\mathbf{P}_N)

We are going to find estimates for solutions to (\mathbf{P}_N) which do not depend on N . In this paper we prove such estimates under the additional assumption (2.6). At first, note that for the solution to (\mathbf{P}_N) the relation (2.11) is valid. The dissipation rate corresponding to (\mathbf{P}_N) , $D_N(v) := \langle A_N(v, v), v \rangle$, is nonnegative for all $v \in W$. Therefore the results of Theorem 3.2 remain true for the solution to (\mathbf{P}_N) and with Lemma 3.1 we find that

$$F(u(t)) \leq c, \quad \|u_i(t) \ln u_i(t)\|_{L^1}, \quad \|u_i(t)\|_{L^1} \leq c, \quad i = 1, \dots, m, \quad \forall t \in S, \quad (4.1)$$

$$\begin{aligned} \|v_0(t)\|_{L^\infty}, \quad \|v_0(t)\|_{L^\infty(\Gamma)}, \quad |\pi(v_0(t))| &\leq c_{4.2}, \\ \|v_0(t)\|_{W^{1,q}} &\leq c \left(\sum_{i=1}^m \|u_i(t)\|_{L^{2q/(2+q)}} + 1 \right) \quad \forall t \in S. \end{aligned} \quad (4.2)$$

All these estimates in (4.1) and (4.2) are independent of N and T . Next we look for upper bounds for the concentrations. We intend to use the Moser iteration and start with some preliminary estimate.

Lemma 4.1. *Additionally we suppose (2.6). Then there exist constants $c, c_{4.3} > 0$ depending only on the data, but not on N and T , such that for the solution (u, v) to (P_N)*

$$\|u_i(t)\|_{L^2} \leq c, \quad i = 1, \dots, m, \quad \|v_0(t)\|_{W^{1,q}} \leq c_{4.3} \quad \forall t \in S. \quad (4.3)$$

Proof. Let $K := \max \{1, \|U_1/\bar{u}_1\|_{L^\infty}, \dots, \|U_m/\bar{u}_m\|_{L^\infty}\}$, $z_i := (u_i/\bar{u}_i - K)^+$, $i = 1, \dots, m$. We use the test function $2e^t(0, z_1, \dots, z_m)$ for (P_N) . By (2.6) the source terms in the volume and boundary reactions are of at most second and first order, respectively. Moreover $|\rho_N| \leq 1$. With (4.2), (1.6), the Hölder and Young inequalities we find that

$$\begin{aligned} e^t \sum_{i=1}^m \|z_i(t)\|_{L^2}^2 &\leq \int_0^t e^s \sum_{i=1}^m \left\{ -\delta \|z_i\|_{H^1}^2 \right. \\ &\quad \left. + c \left(\|z_i\|_{L^3}^3 + 1 + \left(1 + \sum_{j=1}^m \|z_j\|_{L^{r'}}\right) \|z_i\|_{H^1} (\|z_i\|_{L^r} + 1) \right) \right\} ds \quad \forall t \in S \end{aligned}$$

with $r = 2q/(q-2)$, $r' = 2q/(q+2)$, q from (3.2) and some $\delta > 0$. For $\|z_i\|_{L^3}^3$ we apply (1.9) with $p = 3$, $\epsilon := \delta/(4 \sum_{i=1}^m \|z_i \ln z_i\|_{L^\infty(S, L^1)} + 1)$. Moreover, from (1.9) with $p = r$ and $p = r'$, respectively, from (1.8) and Young's inequality we find a constant $c > 0$ such that

$$\begin{aligned} &\sum_{i=1}^m \left(1 + \sum_{j=1}^m \|z_j\|_{L^{r'}}\right) \|z_i\|_{H^1} (\|z_i\|_{L^r} + 1) \\ &\leq \sum_{i=1}^m \left(\epsilon \sum_{j=1}^m \|z_j \ln z_j\|_{L^1} + \frac{\delta}{2} \right) \|z_i\|_{H^1}^2 + c \left(1 + \sum_{i=1}^m \|z_i \ln z_i\|_{L^1}^{2r'/(r'-1)}\right) \end{aligned}$$

with ϵ defined as above. Thus we can continue our estimates by

$$e^t \sum_{i=1}^m \|z_i(t)\|_{L^2}^2 \leq \int_0^t e^s \sum_{i=1}^m \left\{ \left(2\epsilon \sum_{j=1}^m \|z_j \ln z_j\|_{L^1} - \frac{\delta}{2}\right) \|z_i\|_{H^1}^2 + c \left(\|z_i \ln z_i\|_{L^1}^{2r'/(r'-1)} + 1\right) \right\} ds.$$

By the choice of ϵ the factor in front of $\|z_i\|_{H^1}^2$ is nonpositive and with (4.1) we arrive at

$$e^t \sum_{i=1}^m \|z_i(t)\|_{L^2}^2 \leq c \int_0^t e^s \sum_{i=1}^m \left(\|z_i \ln z_i\|_{L^\infty(S, L^1)}^{2r'/(r'-1)} + 1\right) ds \leq c e^t \quad \forall t \in S$$

which gives the estimate for $u_i(t)$. Since $r' < 2$, by (4.2) the result for $v_0(t)$ follows. \square

Theorem 4.2. *Additionally we assume (2.6). Then there exists a constant $c_{4.4} > 0$ depending only on the data, but not on N and T , such that for the solution (u, v) to (P_N)*

$$\|u_i(t)/\bar{u}_i\|_{L^\infty} \leq c_{4.4} \quad \forall t \in S, \quad i = 1, \dots, m. \quad (4.4)$$

The same estimate holds for the $L^\infty(\Gamma)$ -norms of $u_i(t)/\bar{u}_i$ for a.a. $t \in S$.

Proof. The proof is based on Moser iteration. In [14] such techniques are used for the van Roosbroeck equations. Since our system contains more general volume and boundary reaction terms we obtain Moser exponents differing from those in [14]. Let z_i be defined

as in the proof of Lemma 4.1, and let $w_i := z_i^{p/2}$ where $p \geq 4$. We use the test function $pe^t(0, z_1^{p-1}, \dots, z_m^{p-1})$ for (P_N) and define

$$\kappa := c_{4,3}^{2r} + 1 \text{ where } r = 2q/(q-2), \text{ } q \text{ from (3.2)}. \quad (4.5)$$

Having in mind (2.6) and $|\rho_N| \leq 1$ we obtain for all $t \in S$

$$e^t \sum_{i=1}^m \int_{\Omega} |w_i(t)|^2 dx \leq \int_0^t e^s \sum_{i=1}^m \left\{ -\delta \|w_i\|_{H^1}^2 + cp \left(\|\nabla v_0\|_{L^q} \|\nabla w_i\|_{L^2} (\|w_i\|_{L^r} + 1) + \|w_i\|_{L^{2(p+1)/p}}^{2(p+1)/p} + \|w_i\|_{L^2(\Gamma)}^2 + 1 \right) \right\} ds.$$

By (1.6), (1.8) and Young's inequality we obtain the iteration formula

$$\sum_{i=1}^m \|z_i(t)\|_{L^p}^p + 1 \leq c_{4,6} p^{2r} \kappa \left(\sum_{i=1}^m \sup_{s \in S} \|z_i(s)\|_{L^{p/2}}^{p/2} + 1 \right)^{2p/(p-2)} \quad \forall t \in S, \text{ } p \geq 4 \quad (4.6)$$

where $c_{4,6} > 1$ depends only on the data and κ, r are defined in (4.5). Now we set $p = 2^k$, $k \in \mathbb{N}$, $k \geq 2$. From the corresponding recursion formula (4.6) we conclude that

$$a_k \leq (2^{4r} \kappa c_{4,6} a_1)^{c_{\theta} 2^k}, \quad a_k := \sum_{i=1}^m \sup_{s \in S} \|z_i(s)\|_{L^{2^k}}^{2^k} + 1, \quad c_{\theta} := \prod_{j=1}^{\infty} \frac{2^j}{2^j - 1}.$$

Passing to the limit $k \rightarrow \infty$ we obtain

$$\sum_{i=1}^m \|z_i(t)\|_{L^{\infty}} \leq \sqrt{m} \left(2^{4r} \kappa c_{4,6} \left(\sum_{i=1}^m \sup_{s \in S} \|z_i(s)\|_{L^2}^2 + 1 \right) \right)^{c_{\theta}} \quad \forall t \in S.$$

With Lemma 4.1 and (1.7) the desired estimates are verified. \square

We intend to estimate the concentrations from below (or the negative part of the chemical potentials from above) by Moser iteration, too. Corresponding estimates for the van Roosbroeck equations were given in [14, Lemma 4.6].

Lemma 4.2. *Let the estimate (4.4) for the solution (u, v) to (P_N) be fulfilled. Then there exists a constant $c > 0$ such that the recursion formula*

$$e^t \|(v_i + K)^-(t)\|_{L^p}^p \leq c \int_0^t e^s p^{2r} \kappa \left(\|(v_i + K)^-(s)\|_{L^{p/2}}^p + 1 \right) ds$$

$$\forall p \geq 2, \quad \forall t \in S, \quad i = 1, \dots, m,$$

holds where $K := \max \{1, \ln \|\bar{u}_1/U_1\|_{L^{\infty}}, \dots, \ln \|\bar{u}_m/U_m\|_{L^{\infty}}\}$, κ, r from (4.5) and c depends on the data, but not on N, T and p .

Proof. Let $z := (\ln(u_i/\bar{u}_i) + K)^-$. For $p \geq 2$ we take the test function which has the i -th component $-pe^t z^{p-1} \bar{u}_i/u_i$, the other components shall be zero. From the L^{∞} -estimates for u_j/\bar{u}_j , $j = 1, \dots, m$, and v_0 on Ω and at Γ and from the structure of the volume

and boundary reactions (see (2.10)) it follows that $R_{\alpha\beta}^{\Sigma}(\alpha_i - \beta_i)z^{p-1}\bar{u}_i/u_i \leq cz^{p-1}$. Since $|\rho_N| \leq 1$ estimates like in [14, p. 24] give the recursion formula

$$e^t \|z(t)\|_{L^p}^p \leq \int_0^t e^s c p^{2r} \kappa \left(\|z\|_{L^{p/2}}^p + 1 \right) ds \quad \forall t \in S, \quad (4.7)$$

which proves the lemma. \square

Lemma 4.3. *Under the assumption of Lemma 4.2 there exists a constant $c > 0$ depending only on the data, but not on N and T , such that for the solution (u, v) to (P_N)*

$$\|(v_i + K)^-(t)\|_{L^1} \leq c e^{cT} \quad \forall t \in S, \quad i = 1, \dots, m.$$

Proof. Using the notation of Lemma 4.2 we continue the estimation in (4.7) for $p = 2$ by

$$e^t \|z(t)\|_{L^1}^2 \leq c e^t \|z(t)\|_{L^2}^2 \leq c \int_0^t e^s (\|z(s)\|_{L^1}^2 + 1) ds \quad \forall t \in S$$

and apply Gronwall's Lemma to obtain that $\|z(t)\|_{L^1} \leq c e^{cT}$, $t \in S$. \square

Theorem 4.3. *Let the estimate (4.4) for the solution (u, v) to (P_N) be fulfilled. Then there exists an increasing function $d_{4.8} > 0$ depending only on the data, but not on N , such that*

$$\|v_i^-(t)\|_{L^\infty} \leq d_{4.8}(T) \quad \forall t \in S, \quad i = 1, \dots, m. \quad (4.8)$$

The same estimate holds for the $L^\infty(\Gamma)$ -norms of $v_i^-(t)$ for a.a. $t \in S$.

Proof. We use the notation of Lemma 4.2 again. Similar as in the proof of Lemma 4.6 in [14] we find from (4.7) that

$$\|z(t)\|_{L^\infty} \leq c_{4.9} \kappa \left(\sup_{s \in S} \|z(s)\|_{L^1} + 1 \right) \quad \forall t \in S. \quad (4.9)$$

Thus Lemma 4.3 supplies the estimate $\|z(t)\|_{L^\infty} \leq d(T)$. Together with (1.7) we obtain a lower bound for $\ln u_i(t)/\bar{u}_i$ on Ω and at Γ depending only on the data and on T . \square

4.4 Existence result and global estimates

Theorem 4.4. *Under the additional assumption (2.6) there exists a (unique) solution (u, v) to problem (P) . It holds*

$$\|u_i(t)/\bar{u}_i\|_{L^\infty} \leq c_{4.4} \quad \forall t \in \mathbb{R}_+, \quad i = 1, \dots, m. \quad (4.10)$$

The same estimate is valid for the $L^\infty(\Gamma)$ -norms of $u_i(t)/\bar{u}_i$ for a.a. $t \in \mathbb{R}_+$. Moreover

$$\operatorname{ess\,inf}_{x \in \Omega} u_i(t) \geq \operatorname{ess\,inf}_{x \in \Omega} \bar{u}_i e^{-d_{4.8}(t)} \quad \forall t \in \mathbb{R}_+, \quad i = 1, \dots, m. \quad (4.11)$$

Proof. We define a mapping from \mathbb{R}_+ to $L^\infty(\Omega, \mathbb{R}^{m+1}) \times L^\infty(\Omega, \mathbb{R}^{m+1})$ by

$$\begin{aligned} (u(t), v(t)) &:= (u_{\widetilde{N}(t)}(t), v_{\widetilde{N}(t)}(t)) \text{ for } t > 0, \\ (u(0), v(0)) &:= (U, E_0^{-1}U_0, \ln[U_1/\bar{u}_1], \dots, \ln[U_m/\bar{u}_m]) \end{aligned}$$

where $(u_{\widetilde{N}(t)}, v_{\widetilde{N}(t)})$ solves $(P_{\widetilde{N}(t)})$ on $S := [0, t]$ and $\widetilde{N}(t) := 2 \max\{c_{4.2}, \ln c_{4.4}, d_{4.8}(t)\}$. Since $\widetilde{N}(t) \geq \widetilde{N}(s)$ for $t \geq s$ and since the solution to each problem (P_N) is unique we get $(u_{\widetilde{N}(s)}(s), v_{\widetilde{N}(s)}(s)) = (u_{\widetilde{N}(t)}(s), v_{\widetilde{N}(t)}(s))$, $s \leq t$. Thus we obtain that $(u, v)|_{[0, t]}$ is a solution to $(P_{\widetilde{N}(t)})$ on $[0, t]$. By the choice of $\widetilde{N}(t)$ we guarantee that the operators $A_{\widetilde{N}(t)}$ and A coincide on the solution to $(P_{\widetilde{N}(t)})$. Therefore (u, v) is a solution to (P) . Uniqueness has been proved in Theorem 3.1. The estimates follow from Theorem 4.2, Theorem 4.3. \square

The lower bound obtained in (4.11) depends on t , especially it tends to zero if $t \rightarrow \infty$. But one might ask if there is a positive constant as global lower bound for the concentrations. This question is closely related to the asymptotic behaviour of the solution to (P) which will be discussed in the next section.

5 Global lower bounds and asymptotics

5.1 Steady states

In this section we suppose the general assumptions (2.1)–(2.5). Further assumptions will be specified later on. First, we introduce some spaces:

$$\begin{aligned} \mathcal{S} &:= \text{span}\{\alpha - \beta : (\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma\}, \\ \mathcal{U} &:= \left\{ u \in X^* : u_0 = \sum_{i=1}^m q_i u_i|_H, (\langle u_1, 1 \rangle, \dots, \langle u_m, 1 \rangle) \in \mathcal{S} \right\}, \\ \mathcal{U}^\perp &= \left\{ v \in X : \nabla \zeta = 0, \zeta \in \mathcal{S}^\perp \text{ where } \zeta_i = v_i + q_i v_0, i = 1, \dots, m \right\}. \end{aligned}$$

Having in mind Remark 2.7 and using the test function $(0, 1, \dots, 1)$ we obtain for a solution (u, v) to (P) the following invariance property

$$u(t) \in \mathcal{U} + U \quad \forall t \in \mathbb{R}_+. \quad (5.1)$$

Therefore it makes sense to look for steady states (u^*, v^*) to (P) which fulfil the property $u^* \in \mathcal{U} + U$. As in [18, Theorem 3.1], [15, Theorem 3.2] we obtain the following result.

Theorem 5.1. *There exists a unique steady state (u^*, v^*) to (P) in the sense that*

$$A(v^*, v^*) = 0, \quad u^* = E v^*, \quad u^* \in \mathcal{U} + U, \quad v^* \in W. \quad (5.2)$$

The element u^ is the unique minimizer of F on $\mathcal{U} + U$, while the element v^* is the unique minimizer of $\Phi - \langle U, \cdot \rangle$ on \mathcal{U}^\perp . Furthermore*

$$u^*, v^* \in L^\infty(\Omega, \mathbb{R}^{m+1}), \quad u_i^* \geq c > 0 \text{ a.e. on } \Omega, \quad a_i^* := e^{v_i^* + q_i v_0^*} = \text{const} > 0, \quad i = 1, \dots, m.$$

5.2 Asymptotics of the free energy

According to Theorem 3.2 we already know that the free energy along trajectories of (P) remains bounded and decays monotonously. Now we want to investigate the asymptotic behaviour of the free energy in more detail. Let (u^*, v^*) be the steady state (5.2) and let (u, v) be a solution to (P). Because of $v^* \in \mathcal{U}^\perp$ and $u(t) - u^* \in \mathcal{U}$, $t \in \mathbb{R}_+$, we get

$$\sum_{i=1}^m \|\sqrt{u_i(t)/u_i^*} - 1\|_{L^2}^2 + \|v_0(t) - v_0^*\|_{H^1}^2 \leq c(F(u(t)) - F(u^*)) \quad \forall t \in \mathbb{R}_+. \quad (5.3)$$

Here we used the properties (2.7) and (2.8).

Theorem 5.2. *Let (u, v) be a solution to (P) and define*

$$a(t) := (a_1(t), \dots, a_m(t)), \quad a_i(t) := u_i(t)/\bar{u}_i e^{q_i v_0(t)}, \quad t \in \mathbb{R}_+, \quad i = 1, \dots, m.$$

Then there exists a sequence $\{t_k\}_{k \in \mathbb{N}}$, $t_k \in \mathbb{R}_+$, with $t_k \rightarrow \infty$ such that $\sqrt{a_i(t_k)} \rightarrow \sqrt{a_i^\bullet}$ in $H^1(\Omega)$, $v_0(t_k) \rightarrow v_0^\bullet$ in H , $u(t_k) \rightarrow u^\bullet$ in Y where (a^\bullet, v_0^\bullet) belongs to the set

$$\begin{aligned} \mathcal{M} := & \left\{ (a, v_0) \in \mathbb{R}_+^m \times H : \prod_{i=1}^m a_i^{\alpha_i} = \prod_{i=1}^m a_i^{\beta_i} \quad \forall (\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma, \right. \\ & \left. (E_0 v_0, u_1, \dots, u_m) \in \mathcal{U} + U \text{ where } u_i := \bar{u}_i a_i e^{-q_i v_0}, \quad i = 1, \dots, m \right\} \end{aligned}$$

and it holds $u_0^\bullet = E_0 v_0^\bullet$, $u_i^\bullet = \bar{u}_i a_i^\bullet e^{-q_i v_0^\bullet}$. Moreover $F(u(t)) \rightarrow F(u^\bullet)$ as $t \rightarrow \infty$.

Proof. Let (u, v) be a solution to (P). Then $\sqrt{a_i(t)} \in H^1(\Omega)$ for a.a. $t \in \mathbb{R}_+$ and by Theorem 3.2 we obtain that

$$D(v(t)) \geq c \widetilde{D}(a(t)) \quad \text{f.a.a. } t \in \mathbb{R}_+ \text{ with some } c > 0, \quad (5.4)$$

$$\begin{aligned} \widetilde{D}(a) := & \int_{\Omega} \left\{ \sum_{i=1}^m \left| \nabla \sqrt{a_i/a_i^*} \right|^2 + \sum_{(\alpha, \beta) \in \mathcal{R}^\Omega} \left[\prod_{i=1}^m \sqrt{a_i/a_i^*}^{\alpha_i} - \prod_{i=1}^m \sqrt{a_i/a_i^*}^{\beta_i} \right]^2 \right\} dx \\ & + \int_{\Gamma} \sum_{(\alpha, \beta) \in \mathcal{R}^\Gamma} \left[\prod_{i=1}^m \sqrt{a_i/a_i^*}^{\alpha_i} - \prod_{i=1}^m \sqrt{a_i/a_i^*}^{\beta_i} \right]^2 d\Gamma. \end{aligned} \quad (5.5)$$

Moreover, by the definition of a_i and a_i^* (cf. Theorem 5.1)

$$\sqrt{a_i/a_i^*} - 1 = e^{q_i(v_0 - v_0^*)/2} (\sqrt{u_i/u_i^*} - 1) + e^{q_i(v_0 - v_0^*)/2} - 1,$$

which yields with (5.3) and Theorem 3.2 for $i = 1, \dots, m$ that

$$\|\sqrt{a_i(t)/a_i^*} - 1\|_{L^2}^2 + \|v_0(t) - v_0^*\|_{H^1}^2 \leq c(F(u(t)) - F(u^*)) \leq c \quad \forall t \in \mathbb{R}_+. \quad (5.6)$$

Because of $\|D(v)\|_{L^1(\mathbb{R}_+)} < \infty$ (cf. Theorem 3.2) and (5.4) we find a sequence $t_k \rightarrow \infty$ with $\widetilde{D}(a(t_k)) \rightarrow 0$ as $t_k \rightarrow \infty$. This together with the relations (5.4), (5.5) and (5.6)

enables us to show similarly to step ii) in the proof of Theorem 5.2 in [18] that, at least for a subsequence, it holds

$$\sqrt{a_i(t_k)} \rightarrow \sqrt{a_i^\bullet} \text{ in } H^1, \quad a_i^\bullet \in \mathbb{R}_+, \quad i = 1, \dots, m, \quad \prod_{i=1}^m a_i^{\alpha_i} = \prod_{i=1}^m a_i^{\beta_i} \quad \forall (\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma,$$

$v_0(t_k) \rightharpoonup v_0^\bullet$ in $H^1(\Omega)$, $v_0^\bullet \in H$, $u(t_k) \rightarrow u^\bullet$ in Y , $u_i^\bullet = \bar{u}_i a_i^\bullet e^{-q_i v_0^\bullet}$, $i = 1, \dots, m$, and $Ev(t_k) \rightharpoonup (E_0 v_0^\bullet, u_1^\bullet, \dots, u_m^\bullet)$ in X^* . Thus $u_0^\bullet = E_0 v_0^\bullet$ and since $\mathcal{U} + U$ is weakly closed we have $(a^\bullet, v_0^\bullet) \in \mathcal{M}$. Testing $u_0(t_k) - u_0^\bullet = E_0 v_0(t_k) - E_0 v_0^\bullet$ by $v_0(t_k) - v_0^\bullet$ and using the convergence results just mentioned we find the strong convergence $v_0(t_k) \rightarrow v_0^\bullet$ in H . By $u^\bullet \in H^* \times L_+^2(\Omega, \mathbb{R}^m)$ and the continuity result in Lemma 3.2 we get $F(u(t_k)) \rightarrow F(u^\bullet)$. The monotonous decay of the free energy (Theorem 3.2) gives $F(u(t)) \rightarrow F(u^\bullet)$ as $t \rightarrow \infty$. \square

Let us make some remarks concerning the set \mathcal{M} . If (u, v) is a steady state in the sense of (5.2) then $a_i := e^{v_i + q_i v_0} = \text{const} > 0$ and it holds $\prod_{i=1}^m a_i^{\alpha_i} = \prod_{i=1}^m a_i^{\beta_i}$ for all $(\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma$. Moreover we have $(E_0 v_0, u_1, \dots, u_m) \in \mathcal{U} + U$. Thus $(a, v_0) \in \mathcal{M}$. On the other hand, let be $(a, v_0) \in \mathcal{M}$ and $a_i > 0$, $i = 1, \dots, m$, then (u, v) defined by $u_0 := E_0 v_0$, $u_i := \bar{u}_i a_i e^{-q_i v_0}$, $v_i := \ln a_i - q_i v_0$, $i = 1, \dots, m$, is a steady state in the sense of (5.2).

If there are elements $(a, v_0) \in \mathcal{M}$ with $a \notin \text{int } \mathbb{R}_+^m$ then we have no correspondence of such elements to a steady state (u, v) in the sense of (5.2). To exclude such situations we might assume that

$$\mathcal{M} \subset \text{int } \mathbb{R}_+^m \times H. \quad (5.7)$$

Then by Theorem 5.1 $\mathcal{M} = \{(a^*, v_0^*)\}$ follows.

Remark 5.1. For the van Roosbroeck system relation (5.7) is fulfilled. But (5.7) can be verified also for more complicated reaction systems considered in [23].

5.3 Exponential decay of the free energy

The additional assumption (5.7) leads to sharper asymptotic results. Without the knowledge of global a priori bounds for the concentrations from above and below away from zero it is possible to show that the free energy along trajectories of the system (P) decays exponentially to its steady state value. This result can be obtained by the same methods as in [18, Theorem 5.3] (or as in [15], where the nonlinearity e_0 of the Poisson equation is included, but not the nonlocal term π).

Theorem 5.3. *Let (5.7) be satisfied. Then there exists a $\lambda > 0$ depending only on the data such that*

$$F(u(t)) - F(u^*) \leq e^{-\lambda t} (F(u) - F(u^*)) \quad \forall t \geq 0 \quad (5.8)$$

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

Next, we collect estimates resulting from (5.8) which will be of importance for the start of global a priori estimates for the concentrations from below by positive constants.

Corollary 5.1. *Let (u, v) be a solution to (P) and let (5.8) be satisfied. Then there exists a constant $c > 0$ depending only on the data such that for $i = 1, \dots, m$ it holds*

$$\begin{aligned} & \|\sqrt{u_i(t)/u_i^*} - 1\|_{L^2}, \|\sqrt{a_i(t)/a_i^*} - 1\|_{L^2} \leq c e^{-\lambda t/2}, \\ & \|v_0(t) - v_0^*\|_{H^1}, \|u_i(t) - u_i^*\|_{L^1}, \|a_i(t) - a_i^*\|_{L^1} \leq c e^{-\lambda t/2} \quad \forall t \in \mathbb{R}_+. \end{aligned} \quad (5.9)$$

Moreover there exists a constant $c_{5.10} > 0$ depending only on the data such that

$$\begin{aligned} & \|v_0 - v_0^*\|_{L^2(\mathbb{R}_+, H^1)}, \|v_0 - v_0^*\|_{L^1(\mathbb{R}_+, L^1)}, \|v_0 - v_0^*\|_{L^1(\mathbb{R}_+, L^1(\Gamma))} \leq c_{5.10}, \\ & \|u_i/u_i^* - 1\|_{L^1(\mathbb{R}_+, L^1)}, \|u_i/u_i^* - 1\|_{L^1(\mathbb{R}_+, L^1(\Gamma))} \leq c_{5.10}, \quad i = 1, \dots, m. \end{aligned} \quad (5.10)$$

Proof. By the L^∞ -estimates for v_0 and v_0^* and since $u_i(t)/u_i^* \in H^1(\Omega)$ f.a.a. $t \in \mathbb{R}_+$ we have f.a.a. t

$$\begin{aligned} |u_i(t)/u_i^* - 1| & \leq c \left(|a_i(t)/a_i^* - 1| + |v_0(t) - v_0^*| \right) \\ & \leq c \left(\left| \sqrt{a_i(t)/a_i^*} - 1 \right|^2 + \left| \sqrt{a_i(t)/a_i^*} - 1 \right| + |v_0(t) - v_0^*| \right) \quad \text{a.e. in } \Omega, \Gamma. \end{aligned} \quad (5.11)$$

Thus all assertions in (5.9) are a consequence of (5.8), (5.3) and (5.6). From (5.9) the first four estimates in (5.10) follow immediately. With (5.11) and the trace inequality (1.6) we obtain

$$\|u_i/u_i^* - 1\|_{L^1(\Gamma)} \leq c \left\{ \|\sqrt{a_i/a_i^*} - 1\|_{H^1}^2 + \|\sqrt{a_i/a_i^*} - 1\|_{L^2}^{2/3} + \|v_0 - v_0^*\|_{H^1} \right\}.$$

Since $\|D(v)\|_{L^1(\mathbb{R}_+)} \leq c$ we find by (5.4) and (5.9) that $\|\sqrt{a_i/a_i^*} - 1\|_{L^2(\mathbb{R}_+, H^1)} \leq c$. This together with (5.9) proves the last assertion in (5.10). \square

5.4 Global lower bounds for the chemical potentials

Next we are looking for lower bounds for the chemical potentials, in other words, for positive lower bounds for the concentrations, which do not depend on time. Corresponding estimates for the van Roosbroeck equations were given in [14, Lemma 4.6]. But the main difference to our problem is the fact that there essentially Dirichlet boundary conditions for the continuity equations are used to find a start of the iteration process. This fails in our setting.

In what follows besides of (2.1)–(2.5) we shall suppose that there is a constant $c_{5.12}$ depending only on the data such that

$$\|u_i\|_{L^\infty(\mathbb{R}_+, L^\infty(\Omega))}, \|u_i/\bar{u}_i\|_{L^\infty(\mathbb{R}_+, L^\infty(\Gamma))} \leq c_{5.12}, \quad i = 1, \dots, m, \quad (5.12)$$

and that (5.8) is satisfied if (u, v) is a solution to problem (P). At first we prove a lemma which provides a suitable start for the Moser iteration.

Lemma 5.1. *Let (u, v) be a solution to (P) and let (5.12) and (5.8) be fulfilled. Then there exists a constant $c > 0$ depending only on the data such that*

$$\|v_i^-(t)\|_{L^1} \leq c, \quad \forall t \in \mathbb{R}_+, \quad i = 1, \dots, m.$$

Proof. For fixed $i \in \{1, \dots, m\}$ the functional $\Theta: H^1 \rightarrow \overline{\mathbb{R}}$, given by

$$\Theta(w) := \int_{\Omega} u_i^*(x) \vartheta(w(x)) \, dx, \quad \vartheta(y) = \begin{cases} -\ln(1-y) & \text{if } y \leq 0, \\ +\infty & \text{if } y > 0 \end{cases}, \quad u_i^* \text{ from (5.2)}$$

is convex and lower semicontinuous. Its conjugate $G := \Theta^*: (H^1)^* \rightarrow \overline{\mathbb{R}}$ is proper, convex and lower semicontinuous. If (u, v) is a solution to (P) then $G(u_i(t))$ may be written as

$$G(u_i(t)) = \int_{\Omega} \left\{ u_i^* \left(\ln \frac{u_i}{u_i^*} \right)^-(t) - (u_i - u_i^*)^-(t) \right\} \, dx.$$

Since $-\bar{z}(t) := -(1 - u_i^*/u_i(t))^- \in \partial G(u_i(t))$ for a.a. $t \in \mathbb{R}_+$ Brézis' formula ([6]) yields

$$G(u_i(t)) - G(U_i) = - \int_0^t \langle u_i'(s), \bar{z}(s) \rangle_{H^1} \, ds = \int_0^t \langle A(v, v), (0, \dots, \bar{z}, \dots, 0) \rangle \, ds \quad \forall t \in \mathbb{R}_+.$$

Let $z := (\ln(u_i/u_i^*))^-$. Since $\zeta_i^* = \text{const}$ (see Theorem 5.1) we can evaluate

$$u_i \nabla(v_i + q_i v_0) \nabla \bar{z} = u_i \nabla[(v_i - v_i^* + q_i(v_0 - v_0^*)) \nabla \bar{z}] = -u_i^* (\nabla z)^2 + u_i^* q_i \nabla(v_0 - v_0^*) \nabla z.$$

Taking into account the boundedness of u_i^* from above and below we derive for $t \in \mathbb{R}_+$

$$\begin{aligned} G(u_i(t)) &\leq \int_0^t \left\{ -\delta \|\nabla z\|_{L^2}^2 + c \|\nabla(v_0 - v_0^*)\|_{L^2} \|\nabla z\|_{L^2} \right. \\ &\quad + \int_{\Omega} \sum_{(\alpha, \beta) \in \mathcal{R}^{\Omega}} k_{\alpha\beta}^{\Omega} [e^{\alpha\zeta} - e^{\beta\zeta}] (\alpha_i - \beta_i) \left(1 - \frac{u_i^*}{u_i}\right)^- \, dx \\ &\quad \left. + \int_{\Gamma} \sum_{(\alpha, \beta) \in \mathcal{R}^{\Gamma}} k_{\alpha\beta}^{\Gamma} [e^{\alpha\zeta} - e^{\beta\zeta}] (\alpha_i - \beta_i) \left(1 - \frac{u_i^*}{u_i}\right)^- \, d\Gamma \right\} \, ds + G(U_i) \end{aligned} \quad (5.13)$$

where $\delta > 0$. By assumption (2.2) the initial value $G(U_i)$ is finite. We decompose Ω into $\Omega_+(s) := \{x \in \Omega : u_i(s, x) \geq u_i^*(x)\}$ and $\Omega_-(s) := \{x \in \Omega : u_i(s, x) < u_i^*(x)\}$. On Ω_+ reaction terms multiplied by the test function vanish. On Ω_- we have

$$\left(e^{\alpha\zeta} - e^{\beta\zeta} \right) \left(1 - \frac{u_i^*}{u_i} \right)^- = e^{\alpha\zeta^*} \left[\prod_{j=1}^m \left(\frac{u_j}{u_j^*} e^{q_j(v_0 - v_0^*)} \right)^{\alpha_j} - \prod_{j=1}^m \left(\frac{u_j}{u_j^*} e^{q_j(v_0 - v_0^*)} \right)^{\beta_j} \right] \left(\frac{u_i}{u_i^*} - 1 \right).$$

The expression in the brackets as function of $(u_1/u_1^*, \dots, u_m/u_m^*, v_0 - v_0^*)$ is Lipschitz continuous on $[0, C]^m \times [-C, C]$, and at $(1, \dots, 1, 0)$ its value is zero. Since u_j/\bar{u}_j , $j = 1, \dots, m$, and v_0 are globally bounded (see (5.12) and Theorem 3.2) we get for a.a. $s \in \mathbb{R}_+$

$$\left| e^{\alpha\zeta(s)} - e^{\beta\zeta(s)} \right| |\alpha_i - \beta_i| \leq c \left(\sum_{j=1}^m |u_j(s)/u_j^* - 1| + |v_0(s) - v_0^*| \right) \quad \text{a.e. on } \Omega_-.$$

Next, for $\alpha_i > \beta_i$ (then $\alpha_i \geq 1$) we estimate (cf. also (2.10))

$$\begin{aligned} & \left(e^{\alpha_i \zeta} - e^{\beta_i \zeta} \right) (\alpha_i - \beta_i) \frac{u_i^*}{u_i} \\ & \leq (\alpha_i - \beta_i) e^{\alpha_i \zeta^*} \left[e^{q \cdot \alpha (v_0 - v_0^*)} \left(\frac{u_i}{u_i^*} \right)^{\alpha_i - 1} \prod_{j \neq i} \left(\frac{u_j}{u_j^*} \right)^{\alpha_j} - e^{q \cdot \beta (v_0 - v_0^*)} \prod_{j=1}^m \left(\frac{u_j}{u_j^*} \right)^{\beta_j} \right]. \end{aligned}$$

Arguing as above we find for a.a. $s \in \mathbb{R}_+$

$$\left(e^{\alpha_i \zeta(s)} - e^{\beta_i \zeta(s)} \right) (\alpha_i - \beta_i) \frac{u_i^*}{u_i(s)} \leq c \left(\sum_{j=1}^m |u_j(s)/u_j^* - 1| + |v_0(s) - v_0^*| \right) \quad \text{a.e. on } \Omega_-.$$

Similar estimates are obtained for $\alpha_i < \beta_i$. The same arguments hold for the boundary terms. Applying (5.10) we continue estimate (5.13) by

$$\begin{aligned} G(u_i(t)) & \leq c \left\{ 1 + \|v_0 - v_0^*\|_{L^2(\mathbb{R}_+, H^1)}^2 + \|v_0 - v_0^*\|_{L^1(\mathbb{R}_+, L^1)} + \|v_0 - v_0^*\|_{L^1(\mathbb{R}_+, L^1(\Gamma))} \right. \\ & \quad \left. + \sum_{j=1}^m \left(\|u_j/u_j^* - 1\|_{L^1(\mathbb{R}_+, L^1)} + \|u_j/u_j^* - 1\|_{L^1(\mathbb{R}_+, L^1(\Gamma))} \right) \right\} \leq c \quad \forall t \in \mathbb{R}_+. \end{aligned}$$

Thus $\|z(\cdot)\|_{L^1}$ as well as $\|v_i^-(\cdot)\|_{L^1}$ is bounded on \mathbb{R}_+ . \square

Theorem 5.4. *Let (u, v) be a solution to (P) and let (5.12) and (5.8) be fulfilled. Then there exists a constant $c_{5.14} > 0$ depending only on the data such that*

$$\|v_i^-(t)\|_{L^\infty} \leq c_{5.14}, \quad \text{ess inf}_{x \in \Omega} u_i(t) \geq \text{ess inf}_{x \in \Omega} \bar{u}_i e^{-c_{5.14} t} \quad \forall t \in \mathbb{R}_+, \quad i = 1, \dots, m. \quad (5.14)$$

A corresponding estimate holds for the $L^\infty(\Gamma)$ -norms of $v_i^-(t)$ for a.a. $t \in \mathbb{R}_+$.

Proof. Arguing as in the proof of Theorem 4.3 with $z(t) := (\ln(u_i(t)/\bar{u}_i) + K)^-$ and K defined in Lemma 4.2 we obtain inequality (4.9) for all $t \in \mathbb{R}_+$. Lemma 5.1 supplies the global boundedness of $\|z(t)\|_{L^\infty}$. With (2.12) and (1.7) the other assertions follow. \square

Corollary 5.2. *Let (u, v) be a solution to (P) and let (5.12) and (5.14) be fulfilled. Then by [18, Theorem 5.1] relation (5.8) is satisfied. Thus, if global upper bounds are known the existence of global lower bounds is equivalent to the fact that the free energy decays exponentially to its steady state value $F(u^*)$.*

5.5 Asymptotics of the densities and potentials

Theorem 5.5. *Let (u, v) be a solution to (P) and let (5.12) and (5.14) be fulfilled. Then for $p \in [1, +\infty)$ there exist constants $c, \lambda_p > 0$ depending only on the data such that*

$$\|u_i(t) - u_i^*\|_{L^p}, \quad \|v_i(t) - v_i^*\|_{L^p} \leq c e^{-\lambda_p t} \quad \forall t \geq 0, \quad i = 0, \dots, m.$$

Proof. Because of Corollary 5.2 the estimates (5.9) are valid. From (5.12) and (5.9) we obtain for $p \in [1, +\infty)$, $i = 1, \dots, m$,

$$\|u_i(t) - u_i^*\|_{L^p}^p \leq \|u_i(t) - u_i^*\|_{L^1} \|u_i(t) - u_i^*\|_{L^\infty}^{p-1} \leq c^p e^{-\lambda t/2} \quad \forall t \in \mathbb{R}_+.$$

Analogously, because of (5.9) and Theorem 3.2 we estimate

$$\|v_0(t) - v_0^*\|_{L^p}^p \leq \|v_0(t) - v_0^*\|_{L^1} \|v_0(t) - v_0^*\|_{L^\infty}^{p-1} \leq c^{p-1} \|v_0(t) - v_0^*\|_{H^1} \leq c^p e^{-\lambda t/2} \quad \forall t \in \mathbb{R}_+.$$

The same is true for v_i , $i = 1, \dots, m$, since by (2.12), (5.12) and (5.14) we find

$$\|v_i(t) - v_i^*\|_{L^1} = \|\ln u_i(t) - \ln u_i^*\|_{L^1} \leq c \|u_i(t)/u_i^* - 1\|_{L^1} \quad \forall t \in \mathbb{R}_+. \quad \square$$

5.6 Summary

Now we summarize our results which we have obtained under the assumptions (2.1)–(2.5) completed by the growth condition (2.6) and non-degeneracy requirement (5.7).

Theorem 5.6. *We assume (2.1)–(2.5), (2.6) and (5.7). Then there is a unique solution to (P). For this solution global estimates as in (5.12) and (5.14) are satisfied. Moreover the results on the asymptotic behaviour as in Theorem 5.3 and Theorem 5.5 are valid.*

References

1. F. Alabau, *A method for proving uniqueness theorems for the stationary semiconductor device and electrochemistry equations*, *Nonlinear Anal.* **18** (1992), 861–872.
2. ———, *On the existence of multiple steady-state solutions in the theory of electrodiffusion. Part I: The nonelectroneutral case. Part II: A constructive method for the electroneutral case*, *Rapport Interne 96007*, *Mathématiques Appliquées de Bordeaux*, Université Bordeaux, 1996.
3. H. Amann, *Nonhomogeneous linear and quasilinear elliptic and parabolic boundary value problems*, *Function Spaces, Differential Operators and Nonlinear Analysis* (H.-J. Schmeisser and H. Triebel, eds.), *Teubner-Texte zur Mathematik*, vol. 133, Teubner, Stuttgart - Leipzig, 1993, pp. 9–126.
4. H. Amann and M. Renardy, *Reaction-diffusion problems in electrolysis*, *Nonlinear Differ. Equ. Appl.* **1** (1994), 91–117.
5. P. Biler, W. Hebisch, and T. Nadzieja, *The Debye system: Existence and large time behavior of solutions*, *Nonlinear Anal.* **23** (1994), 1189–1209.
6. H. Brézis, *Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert*, *North-Holland Math. Studies*, no. 5, North-Holland, Amsterdam, 1973.
7. Y. S. Choi and R. Lui, *Analysis of an electrochemistry model with zero-flux boundary conditions*, *Applicable Analysis* **49** (1993), 277–288.
8. ———, *Global stability of solutions of an electrochemistry model with multiple species*, *J. Differential Equations* **116** (1995), 306–317.
9. ———, *Multi-dimensional electrochemistry model*, *Arch. Rational Mech. Anal.* **130** (1995), 315–342.
10. I. Ekeland and R. Temam, *Convex analysis and variational problems*, *Studies in Mathematics and its Applications*, vol. 1, North-Holland, Amsterdam, 1976.

11. E. Gagliardo, *Ulteriori proprietà di alcune classi di funzioni in più variabili*, Ricerche Mat. **8** (1959), 24–51.
12. H. Gajewski, *On existence, uniqueness and asymptotic behavior of solutions of the basic equations for carrier transport in semiconductors*, Z. Angew. Math. Mech. **65** (1985), 101–108.
13. ———, *On the uniqueness of solutions to the drift–diffusion–model of semiconductor devices*, Mathematical Models and Methods in Applied Sciences **4** (1994), 121–133.
14. H. Gajewski and K. Gröger, *Initial boundary value problems modelling heterogeneous semiconductor devices*, Surveys on analysis, geometry and mathematical physics (B.-W. Schulze and H. Triebel, eds.), Teubner-Texte zur Mathematik, vol. 117, Teubner, Leipzig, 1990, pp. 4–53.
15. A. Glitzky, K. Gröger, and R. Hünlich, *Free energy and dissipation rate for reaction diffusion processes of electrically charged species*, Applicable Analysis **60** (1996), 201–217.
16. ———, *Discrete-time methods for equations modelling transport of foreign-atoms in semiconductors*, Nonlinear Anal. **28** (1997), 463–487.
17. A. Glitzky and R. Hünlich, *Electro–reaction–diffusion systems in heterostructures*, Report, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, 1997.
18. ———, *Energetic estimates and asymptotics for electro–reaction–diffusion systems*, Z. Angew. Math. Mech. (to appear).
19. K. Gröger, *Initial boundary value problems for semiconductor device theory*, Z. Angew. Math. Mech. **67** (1987), 345–355.
20. ———, *A $W^{1,p}$ -estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann. **283** (1989), 679–687.
21. ———, *Boundedness and continuity of solutions to linear elliptic boundary value problems in two dimensions*, Math. Ann. **298** (1994), 719–728.
22. K. Gröger and J. Rehberg, *Uniqueness for the two–dimensional semiconductor equations in case of high carrier densities*, Math. Z. **213** (1993), 523–530.
23. A. Höfler and N. Strecker, *On the coupled diffusion of dopants and silicon point defects*, Technical Report 94/11, ETH Integrated Systems Laboratory, Zurich, 1994.
24. J. W. Jerome, *Analysis of charge transport. A mathematical study of semiconductor devices*, Springer, Berlin - Heidelberg - New York, 1996.
25. A. Kufner, O. John, and S. Fučík, *Function spaces*, Academia, Prague, 1977.
26. P. A. Markowich, C. A. Ringhofer, and C. Schmeiser, *Semiconductor equations*, Springer, Wien - New York, 1990.
27. W. Merz, K. Pulverer, and E. Wilczok, *Single species dopant diffusion in silicon. Numerical and analytical treatment*, The Mathematical Scientist (to appear).
28. M. S. Mock, *An initial value problem from semiconductor device theory*, SIAM J. Math. Anal. **5** (1974), 597–612.
29. L. Nirenberg, *An extended interpolation inequality*, Ann. Scuola Norm. Sup. Pisa **20** (1966), 733–737.
30. W. V. van Roosbroeck, *Theory of flow of electrons and holes in germanium and other semiconductors*, Bell Syst. Techn. J. **29** (1950), 560–607.
31. I. Rubinstein, *Electro–diffusion of ions*, SIAM Studies in Applied Mathematics, vol. 11, SIAM, Philadelphia, 1990.
32. N. S. Trudinger, *On imbeddings into Orlicz spaces and some applications*, J. of Mathematics and Mechanics **17** (1967), 473–483.
33. Xun Yu, *Steady state solution for electrochemical processes with multiple reacting species*, Quart. Appl. Math. **53** (1995), 507–525.