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Electro–reaction–diffusion systems in heterostructures

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Abstract

The paper is devoted to the mathematical investigation of a general class of electro–reaction–diffusion systems with nonsmooth data which arises in applications to semiconductor technology. Besides of a basic problem, a reduced problem is considered which is obtained if the kinetics of the free carriers is fast. For two dimensional domains we prove a global existence and uniqueness result. In addition, asymptotic properties of solutions are studied. Basic ideas are energy estimates, Moser iteration, regularization techniques and an existence result for electro–diffusion systems with weakly nonlinear volume and boundary source terms which is proved in the paper, too. The relationship between the property that the energy functional decays exponentially in time to its equilibrium value and the existence of global positive lower bounds for the densities of the species is investigated. We illustrate relations between the model and its reduced version in general and for concrete examples. Finally, we discuss the special features of heterostructures for simplified model problems.

1 Introduction

1.1 The basic model

This paper is devoted to the investigation of evolution problems for electro–reaction–diffusion systems in heterostructures. We start with a more detailed explanation of 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, $\operatorname{mes}\Gamma_0 = 0$, ν the outer unit normal. We consider m mobile, electrically charged species X_i with charge numbers q_i. Let initial particle densities $U_i\colon \Omega \to \mathbb{R}_+$ of these species, fixed charge densities $f^\Omega\colon \Omega \to \mathbb{R}$, $f^\Gamma\colon \Gamma_N \to \mathbb{R}$ and the electrostatic potential $v_0^\Gamma\colon \Gamma_D \to \mathbb{R}$ as data of our problem be given. The particle densities $u_i\colon \mathbb{R}_+ \times \Omega \to \mathbb{R}_+$ of the species X_i and their chemical potentials $v_i\colon \mathbb{R}_+ \times \Omega \to \mathbb{R}$ will vary in time 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 whereby the charge density of the mobile species $u_0 = \sum_{i=1}^m q_i u_i$ will be an additional source term for the electrostatic potential $v_0\colon \mathbb{R}_+ \times \Omega \to \mathbb{R}$. All quantities are suitably scaled.

The relations between the densities and the chemical potentials (the so called state equations) are assumed to be given by the Boltzmann statistics

$$u_i = \overline{u}_i\, \mathrm{e}^{v_i} \text{ on } \mathbb{R}_+ \times \Omega,\ i = 1, \ldots, m, \tag{1.1}$$

where $\overline{u}_i\colon \Omega \to \mathbb{R}_+$ is some reference density of the i–th species. In order to describe the underlying kinetic processes the electrochemical potentials

$$\zeta_i = v_i + q_i v_0 \text{ on } \mathbb{R}_+ \times \overline{\Omega},\ i = 1, \ldots, m, \tag{1.2}$$

are introduced. Their gradients are assumed to be the driving forces of the particle fluxes

$$j_i = -D_i\, u_i\, \nabla\zeta_i \text{ on } \mathbb{R}_+ \times \Omega,\ i = 1, \ldots, m, \tag{1.3}$$

with given diffusivities $D_i\colon \Omega \to \mathbb{R}_+$. Finally, a finite number of mass action type reactions of the form

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

is considered where $\alpha = (\alpha_1, \ldots, \alpha_m)$, $\beta = (\beta_1, \ldots, \beta_m)$ denote the vectors of stoichiometric coefficients of such a reaction. Let $\mathcal{R}^\Omega$ and $\mathcal{R}^\Gamma$ denote the sets of all pairs (α, β) belonging to all reactions in Ω and on Γ, respectively. The corresponding reaction rates $R^\Omega_{\alpha\beta}$ and $R^\Gamma_{\alpha\beta}$ are assumed to be given as

$$\left.\begin{aligned} &R^\Sigma_{\alpha\beta} = k^\Sigma_{\alpha\beta}(x, v_0, v_1, \cdots, v_m)\left(\mathrm{e}^{\sum_{i=1}^m \alpha_i\zeta_i} - \mathrm{e}^{\sum_{i=1}^m \beta_i\zeta_i}\right), \\ &x \in \Sigma,\ (v_0, v_1, \ldots, v_m) \in \mathbb{R}^{m+1},\ (\alpha, \beta) \in \mathcal{R}^\Sigma,\ \Sigma = \Omega, \Gamma, \end{aligned}\right\} \tag{1.4}$$

with kinetic coefficients $k^\Sigma_{\alpha\beta}\colon \Sigma \times \mathbb{R}^{m+1} \to \mathbb{R}_+$.

Now we are able to formulate the basic equations of our model. Balancing the number of particles for each species we get the initial boundary value problem

$$\left.\begin{aligned} \frac{\partial u_i}{\partial t} + \nabla\cdot j_i + \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} (\alpha_i - \beta_i)\, R^\Omega_{\alpha\beta} &= 0 \quad \text{on } (0,\infty)\times\Omega, \\ \nu\cdot j_i - \sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma} (\alpha_i - \beta_i)\, R^\Gamma_{\alpha\beta} &= 0 \quad \text{on } (0,\infty)\times\Gamma, \\ u_i(0) &= U_i \quad \text{on } \Omega,\ i = 1, \ldots, m. \end{aligned}\right\} \tag{1.5}$$

The electrostatic potential implicitly here occuring via (1.3), (1.4) and (1.2) is obtained from the elliptic boundary value problem

$$\begin{aligned} -\nabla\cdot(\varepsilon\,\nabla v_0) &= f^\Omega + \sum_{i=1}^m q_i u_i \quad \text{on } (0,\infty)\times\Omega, \\ v_0 &= v_0^\Gamma \quad \text{on } (0,\infty)\times\Gamma_D, \\ \nu\cdot(\varepsilon\,\nabla v_0)+\tau v_0 &= f^\Gamma \quad \text{on } (0,\infty)\times\Gamma_N \end{aligned} \tag{1.6}$$

where the dielectric permittivity $\varepsilon\colon\Omega\to\mathbb{R}_+$ and the capacity $\tau\colon\Gamma_N\to\mathbb{R}_+$ are given.

Motivated by problems arising in semiconductor technology we are interested in the investigation of heterostructures. Then all physical parameters $\overline{u}_i$, D_i, $k^\Sigma_{\alpha\beta}$, ε and τ depend on the space variable x in a nonsmooth way. In general besides of the kinetic coefficients $k^\Sigma_{\alpha,\beta}$ also the diffusivities D_i depend on the state variables. But such a dependency is not considered in this paper.

If problem (1.5), (1.6) has a sufficiently smooth solution then the relations (1.6) must be fulfilled for $t=0$, too. We set $V_0=v_0(0)$ and introduce new quantities

$$\begin{gathered} \widetilde{v}_0 := v_0 - V_0,\ \widetilde{v}_i := v_i + q_i V_0, \\ \widetilde{\overline{u}}_i := \overline{u}_i \mathrm{e}^{-q_i V_0},\ \widetilde{k}^\Sigma_{\alpha\beta}(x,\widetilde{v}_0,\cdots,\widetilde{v}_i,\cdots) := k^\Sigma_{\alpha\beta}(x,\widetilde{v}_0+V_0(x),\cdots,\widetilde{v}_i-q_iV_0(x),\cdots). \end{gathered} \tag{1.7}$$

Then after omitting the tilde all relations (1.1) – (1.5) remain unchanged whereas (1.6) has to be replaced by

$$\left.\begin{aligned} -\nabla\cdot(\varepsilon\,\nabla v_0)+e_0 &= \sum_{i=1}^m q_i u_i \quad \text{on } (0,\infty)\times\Omega, \\ v_0 &= 0 \quad \text{on } (0,\infty)\times\Gamma_D, \\ \nu\cdot(\varepsilon\,\nabla v_0)+\tau v_0 &= 0 \quad \text{on } (0,\infty)\times\Gamma_N \end{aligned}\right\} \tag{1.8}$$

where

$$e_0 = \sum_{i=1}^m q_i U_i. \tag{1.9}$$

Qualitative properties of the functions $\overline{u}_i, k^\Sigma_{\alpha\beta}$ as assumed in Section 2 remain valid if the data $f^\Omega, f^\Gamma, v_0^\Gamma$ for the original Poisson equation (1.6) are given in an appropriate way.

A precise formulation of the basic model equations (1.5), (1.8) will be given in Section 2. Here let us only mention the weak formulation of the Poisson equation (1.8): For fixed $t\in(0,\infty)$ find $v_0\in H_0^1(\Omega\cup\Gamma_N)$ such that

$$\left.\begin{aligned} &\int_\Omega \Big\{\varepsilon\nabla v_0\cdot\nabla h + \Big(e_0-\sum_{i=1}^m q_i u_i\Big)h\Big\}\,\mathrm{d}x + \int_{\Gamma_N}\tau v_0 h\,\mathrm{d}\Gamma = 0 \\ &\forall h\in H_0^1(\Omega\cup\Gamma_N). \end{aligned}\right\} \tag{1.10}$$

In general one has to require that each reaction conserves the electric charge what means

$$\sum_{i=1}^m q_i(\alpha_i-\beta_i) = 0 \quad \forall(\alpha,\beta)\in\mathcal{R}^\Omega\cup\mathcal{R}^\Gamma. \tag{1.11}$$

Then, multiplying the continuity equations in (1.5) by q_i, integrating by parts and summing up, we get

$$\int_\Omega \sum_{i=1}^m q_i u_i(t,x)\,\mathrm{d}x = \int_\Omega \sum_{i=1}^m q_i U_i(x)\,\mathrm{d}x \quad \forall t>0 \tag{1.12}$$

such that the total electric charge of all mobile species is conserved, too. In our further investigations of the basic model equations (1.5), (1.8) we do not make explicit use of (1.11). But this assumption as well as its consequence (1.12) are of interest in deriving some reduced model equations.

1.2 The reduced model

Again motivated by problems arising in semiconductor technology let us consider the situation that there are two special species X_{m-1} with $q_{m-1} = -1$ (*electrons*) and X_m with $q_m = +1$ (*holes*) and that in Ω there runs among other reactions a generation–recombination reaction of the form

$$X_{m-1} + X_m \rightleftharpoons 0 \tag{1.13}$$

with the reaction rate

$$R = k\left(\mathrm{e}^{\zeta_{m-1}+\zeta_m} - 1\right).$$

This reaction obviously conserves the charge. In addition we assume (1.11) to be fulfilled for all other reactions, too. The special character of the species X_{m-1}, X_m consists in the fact, that their kinetic coefficients D_{m-1}, D_m and k are large compared with those of the other species. Therefore it makes sense to consider the limit case

$$D_{m-1},\, D_m,\, k \to \infty. \tag{1.14}$$

If we want the fluxes j_{m-1}, j_m as well as the reaction rate R to remain bounded we have to require that

$$\nabla\zeta_{m-1} = \nabla\zeta_m = 0,\ \zeta_{m-1} + \zeta_m = 0 \text{ on } \mathbb{R}_+ \times \Omega.$$

Then $\zeta := \zeta_{m-1}$ depends only on time t and it holds

$$v_{m-1} = v_0 + \zeta,\ v_m = -(v_0+\zeta),\ \zeta_{m-1} = \zeta,\ \zeta_m = -\zeta. \tag{1.15}$$

Using (1.1) the electron and hole densities are expressed as

$$u_{m-1} = \overline{u}_{m-1}\mathrm{e}^{v_0+\zeta},\ u_m = \overline{u}_m \mathrm{e}^{-(v_0+\zeta)}. \tag{1.16}$$

All left hand quantities in (1.15), (1.16) will be known if v_0 and ζ are known. Therefore we may omit in (1.5) the continuity equations for $i = m-1, m$. Substituting into the reaction rates occuring in the remaining continuity equations the relations (1.15) and taking into account (1.11) we obtain

$$\begin{aligned} &R^\Sigma_{\alpha\beta} = k^\Sigma_{\alpha\beta}(x, v_0, v_1, \cdots, v_{m-2}, v_0+\zeta, -v_0-\zeta) \times \\ &\mathrm{e}^{-\zeta\sum_{i=1}^m \alpha_i q_i}\left(\mathrm{e}^{\sum_{i=1}^{m-2}\alpha_i(\zeta_i + q_i\zeta)} - \mathrm{e}^{\sum_{i=1}^{m-2}\beta_i(\zeta_i+q_i\zeta)}\right), \\ &x \in \Sigma,\ (v_0, v_1, \ldots, v_{m-2}) \in \mathbb{R}^{m-1},\ \zeta \in \mathbb{R},\ \Sigma = \Omega, \Gamma. \end{aligned} \tag{1.4*}$$

Thus we get a reduced initial boundary value problem for the first $m-2$ species still involving the variables v_0 and ζ. These variables may be found from the Poisson equation (1.8) and from the conservation relation (1.12). Substituting there the relations (1.16) we obtain

$$\begin{aligned} -\nabla\cdot(\varepsilon\,\nabla v_0)+e_0(\cdot,v_0+\zeta) &= \sum_{i=1}^{m-2} q_i u_i && \text{on } (0,\infty)\times\Omega,\\ v_0 &= 0 && \text{on } (0,\infty)\times\Gamma_D,\\ \nu\cdot(\varepsilon\,\nabla v_0)+\tau v_0 &= 0 && \text{on } (0,\infty)\times\Gamma_N,\\ \int_\Omega e_0(\cdot,v_0+\zeta)\,\mathrm{d}x &= \int_\Omega \sum_{i=1}^{m-2} q_i u_i\,\mathrm{d}x && \text{on } (0,\infty) \end{aligned} \tag{1.8*}$$

where

$$e_0(x,y)=\sum_{i=1}^{m} q_i U_i(x)+\overline{u}_{m-1}(x)\,\mathrm{e}^{y}-\overline{u}_m(x)\,\mathrm{e}^{-y},\ x\in\Omega,\ y\in\mathbb{R}. \tag{1.9*}$$

In order to determine v_0 and ζ thus we arrive at a boundary value problem for a nonlinear Poisson equation constrained by a nonlocal condition. The corresponding weak formulation reads as follows: For fixed t find $(v_0,\zeta)\in H_0^1(\Omega\cup\Gamma_N)\times\mathbb{R}$ such that

$$\begin{aligned} &\int_\Omega\Big\{\varepsilon\nabla v_0\cdot\nabla h+\Big(e_0(\cdot,v_0+\zeta)-\sum_{i=1}^{m-2}q_iu_i\Big)\,(h+\xi)\Big\}\,\mathrm{d}x+\int_{\Gamma_N}\tau v_0 h\,\mathrm{d}\Gamma=0\\ &\forall(h,\xi)\in H_0^1(\Omega\cup\Gamma_N)\times\mathbb{R}. \end{aligned} \tag{1.10*}$$

Together with (1.5) (where one has to replace m by $m-2$ and (1.4) by (1.4*)) we have found the reduced model equations for the first $m-2$ species which we are interested in. In the reduced model the real kinetics of the species X_{m-1}, X_m is neglected with the exception of the charge conservation relation containing the initial values U_{m-1}, U_m which besides of the reference densities $\overline{u}_{m-1}, \overline{u}_m$ must be given.

Now we want to reformulate the reduced model equations in such a way that their structure becomes more similar to that of the basic model equations. We set $\widetilde{m}=m-2$ and introduce the variables

$$\widetilde{v}_0:=v_0+\zeta,\quad \widetilde{u}_i:=u_i,\ \widetilde{v}_i:=v_i,\ \widetilde{\zeta}_i:=\zeta_i+q_i\zeta,\ i=1,\ldots,\widetilde{m}. \tag{1.17}$$

Again as in (1.1), (1.2) it holds

$$\widetilde{u}_i=\overline{u}_i\mathrm{e}^{\widetilde{v}_i},\ \widetilde{\zeta}_i=\widetilde{v}_i+q_i\widetilde{v}_0,\ i=1,\ldots,\widetilde{m},$$

and instead of (1.5) we obtain

$$\left.\begin{aligned} \frac{\partial\widetilde{u}_i}{\partial t}+\nabla\cdot\widetilde{j}_i+\sum_{(\widetilde{\alpha},\widetilde{\beta})\in\widetilde{\mathcal{R}}^\Omega}(\widetilde{\alpha}_i-\widetilde{\beta}_i)\,\widetilde{R}^\Omega_{\widetilde{\alpha}\widetilde{\beta}} &= 0 \quad \text{on } (0,\infty)\times\Omega,\\ \nu\cdot\widetilde{j}_i-\sum_{(\widetilde{\alpha},\widetilde{\beta})\in\widetilde{\mathcal{R}}^\Gamma}(\widetilde{\alpha}_i-\widetilde{\beta}_i)\,\widetilde{R}^\Gamma_{\widetilde{\alpha}\widetilde{\beta}} &= 0 \quad \text{on } (0,\infty)\times\Gamma,\\ \widetilde{u}_i(0) &= U_i \quad \text{on } \Omega,\ i=1,\ldots,\widetilde{m}. \end{aligned}\right\} \tag{1.5**}$$

Here as in (1.3) it holds

$$\widetilde{j}_i=-D_i\,\widetilde{u}_i\,\nabla\widetilde{\zeta}_i,\ i=1,\ldots,\widetilde{m},$$

since $\nabla\zeta = 0$ and because of (1.4*) we find that

$$\left.\begin{aligned}
&\widetilde{R}^{\Sigma}_{\widetilde{\alpha}\widetilde{\beta}} = \widetilde{k}^{\Sigma}_{\widetilde{\alpha}\widetilde{\beta}}(x,\widetilde{v}_0,\widetilde{v}_1,\cdots,\widetilde{v}_{\widetilde{m}},\zeta)\left(\mathrm{e}^{\sum_{i=1}^{\widetilde{m}}\widetilde{\alpha}_i\widetilde{\zeta}_i} - \mathrm{e}^{\sum_{i=1}^{\widetilde{m}}\widetilde{\beta}_i\widetilde{\zeta}_i}\right),\\
&x\in\Sigma,\ (\widetilde{v}_0,\widetilde{v}_1,\ldots,\widetilde{v}_{\widetilde{m}})\in\mathbb{R}^{\widetilde{m}+1},\ \zeta\in\mathbb{R},\ (\widetilde{\alpha},\widetilde{\beta})\in\widetilde{\mathcal{R}}^{\Sigma},\ \Sigma=\Omega,\Gamma,\\
&\widetilde{k}^{\Sigma}_{\widetilde{\alpha}\widetilde{\beta}}(x,\widetilde{v}_0,\widetilde{v}_1,\cdots,\widetilde{v}_{\widetilde{m}},\zeta) = \sum_{\substack{(\alpha,\beta)\in\mathcal{R}^{\Sigma}\\ \alpha_i=\widetilde{\alpha}_i,\,\beta_i=\widetilde{\beta}_i,\,i=1,\ldots,\widetilde{m}}} k^{\Sigma}_{\alpha\beta}(x,\widetilde{v}_0-\zeta,\widetilde{v}_1,\cdots,\widetilde{v}_{\widetilde{m}},\widetilde{v}_0,-\widetilde{v}_0)\,\mathrm{e}^{-\zeta\sum_{i=1}^{m}\alpha_i q_i},\\
&\widetilde{\mathcal{R}}^{\Sigma} =\\
&\left\{(\widetilde{\alpha},\widetilde{\beta})\in\mathbb{Z}_+^{\widetilde{m}}\times\mathbb{Z}_+^{\widetilde{m}}\colon (\widetilde{\alpha},\widetilde{\beta})\neq(0,0),\ \widetilde{\alpha}_i=\alpha_i,\ \widetilde{\beta}_i=\beta_i,\ i=1,\ldots,\widetilde{m},\ (\alpha,\beta)\in\mathcal{R}^{\Sigma}\right\}.
\end{aligned}\right\}\quad(1.4^{**})$$

The only essential difference between (1.4**) and (1.4) is that the kinetic coefficients $\widetilde{k}^{\Sigma}_{\widetilde{\alpha}\widetilde{\beta}}$ additionally depend on ζ. The constrained Poisson problem (1.8*) is transformed to

$$\left.\begin{aligned}
-\nabla\cdot(\varepsilon\,\nabla\widetilde{v}_0)+e_0(\cdot,\widetilde{v}_0) &= \sum_{i=1}^{\widetilde{m}} q_i\widetilde{u}_i && \text{on } (0,\infty)\times\Omega,\\
\widetilde{v}_0 &= \zeta && \text{on } (0,\infty)\times\Gamma_D,\\
\nu\cdot(\varepsilon\,\nabla\widetilde{v}_0)+\tau\widetilde{v}_0 &= \tau\zeta && \text{on } (0,\infty)\times\Gamma_N,\\
\int_\Omega e_0(\cdot,\widetilde{v}_0)\,\mathrm{d}x &= \int_\Omega\sum_{i=1}^{\widetilde{m}} q_i\widetilde{u}_i\,\mathrm{d}x && \text{on } (0,\infty)
\end{aligned}\right\}\quad(1.8^{**})$$

with the corresponding weak formulation: Find $(\widetilde{v}_0,\zeta)\in\left\{(h+\eta,\eta)\colon h\in H_0^1(\Omega\cup\Gamma_N),\ \eta\in\mathbb{R}\right\}\subset(H_0^1(\Omega\cup\Gamma_N)+\mathbb{R})\times\mathbb{R}$ such that

$$\begin{aligned}
&\int_\Omega\left\{\varepsilon\nabla\widetilde{v}_0\cdot\nabla\widetilde{h}+\left(e_0(\cdot,\widetilde{v}_0)-\sum_{i=1}^{\widetilde{m}}q_i\widetilde{u}_i\right)\widetilde{h}\right\}\mathrm{d}x+\int_{\Gamma_N}\tau(\widetilde{v}_0-\zeta)\,(\widetilde{h}-\xi)\,\mathrm{d}\Gamma=0\\
&\forall(\widetilde{h},\xi)\in\left\{(h+\eta,\eta)\colon h\in H_0^1(\Omega\cup\Gamma_N),\ \eta\in\mathbb{R}\right\}.
\end{aligned}$$

Under some assumptions which we shall formulate in the next section (see (2.1), (2.2)) the following equivalent formulation can be derived: Find $(\widetilde{v}_0,\zeta)\in H\times\mathbb{R}$ such that

$$\left.\begin{aligned}
&\int_\Omega\left\{\varepsilon\nabla\widetilde{v}_0\cdot\nabla\widetilde{h}+\left(e_0(\cdot,\widetilde{v}_0)-\sum_{i=1}^{\widetilde{m}}q_i\widetilde{u}_i\right)\widetilde{h}\right\}\mathrm{d}x+\\
&\int_{\Gamma_N}\tau(\widetilde{v}_0-\pi(\widetilde{v}_0))\,(\widetilde{h}-\pi(\widetilde{h}))\,\mathrm{d}\Gamma=0\quad\forall\widetilde{h}\in H,\quad\zeta=\pi(\widetilde{v}_0)
\end{aligned}\right\}\quad(1.10^{**})$$

where

$$\begin{aligned}
&H = H_0^1(\Omega\cup\Gamma_N)+\mathbb{R}\subset H^1(\Omega),\\
&\pi(w)=\begin{cases}(\operatorname{mes}\Gamma_D)^{-1}\displaystyle\int_{\Gamma_D} w\,\mathrm{d}\Gamma & \text{if } \operatorname{mes}\Gamma_D\neq 0,\\ \|\tau\|^{-1}_{L^1(\Gamma_N)}\displaystyle\int_{\Gamma_N}\tau\,w\,\mathrm{d}\Gamma & \text{if } \operatorname{mes}\Gamma_D=0,\end{cases}\qquad w\in H^1(\Omega).
\end{aligned}\quad(1.18)$$

Although the variational equation in (1.10**) contains an additional nonlinear term in the volume integral as well as a nonlocal term in the boundary integral this equation has the same principal structure as (1.10). After inserting the relation $\zeta = \pi(\widetilde{v}_0)$ into (1.4**) the kinetic coefficients $\widetilde{k}^{\Sigma}_{\underset{\sim}{\alpha\beta}}$ depend only on the variables $\widetilde{v}_0, \ldots \widetilde{v}_{\widetilde{m}}$ (nonlocally with respect to $\widetilde{v}_0$). Thus after introducing new variables our reduced model equations (1.5**) and (1.8**) do not differ essentially from the basic model equations (1.5) and (1.8) what makes it possible to investigate both models in a unified way.

1.3 Comments

An essential feature of the model equations (1.5), (1.8) and (1.5**), (1.8**), respectively, is the fact that they allow *thermal equilibria* as steady states (see Subsection 5.1). 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). Energy estimates like in Subsection 3.3 and Subsection 5.3 are the basic key in deriving 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 [53]) as a special case of our model equations (1.5), (1.8). Normally, here more general boundary conditions are of interest. Then the steady states do not correspond to thermal equilibria (see e.g. [1, 2, 41, 49, 54]). Starting from first results of Mock (see [51]) the transient problem has been extensively investigated by Gajewski and Gröger (see [17, 18, 19, 20, 21, 29, 32]).

As already mentioned in the preceding subsections we are mainly interested in electro–reaction–diffusion problems arising in semiconductor technology. Here more then two kinds of charged or uncharged species as well as a lot of chemical reactions have to be taken into account. An overview of corresponding model equations, especially in the reduced form (1.5**), (1.8**), may be found in [38]. From this field of applications also the choice of our boundary conditions is motivated. Often the model equations (1.5**), (1.8**) are once more reduced by assuming a local electroneutrality condition to determine the electrostatic potential (see [38, 54]). Special cases of this type where (besides of electrons and holes) only one kind of species is electrically charged have been investigated in [23, 25, 50].

Other applications of electro–reaction–diffusion systems come from the field of electrolysis. Whereas in papers of Amann (see [3, 4]) and Yu [60] the continuity equations are completed by an electroneutrality condition in papers of Choi and Lui (see [7, 8, 9, 10, 11]) and Jüngel [42] the full system of continuity equations coupled with the Poisson equation is considered. Resulting from the special situation in electrolysis all these authors work with smooth kinetic coefficients and mainly with smooth domains. The application of some of their techniques to the case of nonsmooth data in the situation of heterostructures as considered in our paper can not be expected, such that other techniques are needed.

Our investigation of the multiple species problem is based on methods developed by Gajewski and Gröger for the van Roosbroeck system in heterogeneous semiconductor structures [21]. The main difference to [21] consists in the fact that we have no Dirichlet conditions for the continuity equations and more general reaction terms. From this arise some complications in deriving global lower bounds which we shall overcome by using an additional energy estimate (see Subsection 5.3 and [24, 26]).

1.4 Contents of the paper

In Section 2 we give a precise formulation of the problems introduced in the preceding subsections (cf. problem (P) below). There we summarize also 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 ore less technical character (two dimensional domains – cf. (2.1), growth condition for the source terms in the continuity equations – cf. (2.6), nondegeneracy condition of the reaction system – cf. (5.9)). Preliminary results concerning estimates for the solution of the possibly nonlinear and nonlocal Poisson equation, uniqueness of the solution of the evolution problem and first energy 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 (cf. problem ($\mathrm{P_N}$)) if the additional assumption (2.6) is fulfilled. Furthermore under the same assumption global upper bounds for the densities are established. The existence of global lower bounds as well as results concerning the asymptotic behaviour are obtained in Section 5 where assumption (5.9) plays an important rôle.

Section 6 contains existence and uniqueness results for electro–diffusion systems with weakly nonlinear source terms (cf. problem ($\mathrm{P_G}$)) which may be of interest by their selves. Here these results ensure the solvability of the regularized problem ($\mathrm{P_N}$) which is considered in Section 4 to construct the solution of problem (P).

In Section 7 we discuss relations between the basic and the reduced models. As was to be expected we can prove that both models are asymptotically equivalent.

In the last section we present some examples, especially for the case of heterostructures, which are motivated from applications to semiconductor technology.

1.5 Technicalities

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 [45]. 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 [31] or to [21, Appendix]. Let us note that $H_0^1(\Omega\cup\Gamma_N) = H^1(\Omega)$ if $\Gamma_N = \partial\Omega$. By $\mathbb{Z}_+^k$, $\mathbb{R}_+^k$, 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, $d\colon \mathbb{R}_+ \to \mathbb{R}_+$ stands for continuous, monotonously increasing functions with $\lim_{y\to\infty} d(y) = \infty$.

We shall apply Sobolev's imbedding theorems (see [45]) as well as some further imbedding results. First, by a modified application of the Hölder inequality from [45, p. 317, formula (5)] we derive

$$\|w\|^q_{L^q(\Gamma)} \le c_{1.19}\, \|w\|^{q-1}_{L^{2(q-1)}(\Omega)} \|w\|_{H^1(\Omega)} \quad \forall w \in H^1(\Omega),\ q \ge 2 \text{ with } c_{1.19} = c_\Omega\, q. \tag{1.19}$$

For $w \in H^1(\Omega)\cap L^\infty(\Omega)$ from (1.19) we find

$$\|w\|_{L^q(\Gamma)} \le \|w\|_{L^\infty(\Omega)} \Big(\frac{|\Omega|^{1/2} c_\Omega\, q\, \|w\|_{H^1(\Omega)}}{\|w\|_{L^\infty(\Omega)}}\Big)^{1/q}$$

and passing to the limit $q \to \infty$ we get

$$\|w\|_{L^\infty(\Gamma)} \le \|w\|_{L^\infty(\Omega)} \quad \forall w \in H^1(\Omega) \cap L^\infty(\Omega). \tag{1.20}$$

As a special case of the Gagliardo–Nirenberg inequality (see [16, 52]) we use the following result:

$$\|w\|_{L^p} \le c_p \, \|w\|_{L^1}^{1/p} \|w\|_{H^1}^{1-1/p} \quad \forall w \in H^1(\Omega),\ 1 < p < \infty. \tag{1.21}$$

Especially, for p from compact intervals

$$\|w\|_{L^p} \le c\, \|w\|_{L^1}^{1/p} \|w\|_{H^1}^{1-1/p} \quad \forall w \in H^1(\Omega),\ p_1 \le p \le p_2 \text{ with } c \le \max\{c_{p_1}, c_{p_2}, 1\}^{1/p_1}.$$

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

$$\|w\|_{L^p}^p \le \epsilon \, \|w \ln |w|\|_{L^1} \, \|w\|_{H^1}^{p-1} + c_{\epsilon,p} \, \|w\|_{L^1} \quad \forall w \in H^1(\Omega). \tag{1.22}$$

In [5] this inequality is proved for bounded domains with smooth boundary and $p = 3$. An inspection of that proof yields the validity of (1.22) also for bounded Lipschitzian domains and $p \in (1, \infty)$, since (1.21) is true in this case, too. Finally, from Trudinger's imbedding theorem (see [57]) we get

$$\|\mathrm{e}^{|w|}\|_{L^p} \le d_p(\|w\|_{H^1}) \quad \forall w \in H^1(\Omega),\ 1 \le p < \infty. \tag{1.23}$$

2 The problem

2.1 Assumptions

In the next subsection we shall formulate a general evolution problem which involves the concrete model problems discussed in Section 1. Here we summarize all assumptions which our further considerations are based on:

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

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

$$\left.\begin{array}{l}H \text{ is a linear closed subspace of } H^1(\Omega),\ H^1_0(\Omega \cup \Gamma_N) \subset H;\\ \pi \in \mathcal{L}(H^1(\Omega), \mathbb{R});\\ v - \pi(v) \in H^1_0(\Omega \cup \Gamma_N)\ \forall v \in H,\\ \pi(h) \int_{\Gamma_N} \tau(v - \pi(v))\, \mathrm{d}\Gamma = 0\ \forall h \in H^1_0(\Omega \cup \Gamma_N),\ \forall v \in H;\end{array}\right\} \tag{2.3}$$

$$\left.\begin{array}{l}e_0 \colon \Omega \times \mathbb{R} \to \mathbb{R} \text{ satisfies the Carathéodory conditions,}\\ |e_0(x, y)| \le c\, \mathrm{e}^{c|y|} \text{ f.a.a. } x \in \Omega, \forall y \in \mathbb{R},\ c > 0,\\ e_0(x, y) - e_0(x, z) \ge b_0(x)\,(y - z) \text{ f.a.a. } x \in \Omega,\ \forall y, z \in \mathbb{R} \text{ with } y \ge z,\\ b_0 \in L^\infty_+(\Omega),\ \|b_0\|_{L^1} \ge c\,\|\pi\|,\ c > 0;\end{array}\right\} \tag{2.4}$$

$$\left.\begin{array}{l}\mathcal{R}^\Omega, \mathcal{R}^\Gamma \text{ are finite subsets of } \mathbb{Z}^m_+ \times \mathbb{Z}^m_+;\\ \text{for } \Sigma = \Omega, \Gamma \text{ and } (\alpha, \beta) \in \mathcal{R}^\Sigma \text{ we define}\\ R^\Sigma_{\alpha\beta} := k^\Sigma_{\alpha\beta}(x, y, z)\, (\mathrm{e}^{\alpha\cdot\zeta} - \mathrm{e}^{\beta\cdot\zeta}),\ x \in \Sigma,\ y = (y_0, y_1, \cdots, y_m) \in \mathbb{R}^{m+1},\\ \zeta_i := y_i + q_i y_0,\ i = 1, \dots, m,\ z \in \mathbb{R},\ \text{where}\\ k^\Sigma_{\alpha\beta} \colon \Sigma \times \mathbb{R}^{m+1} \times \mathbb{R} \to \mathbb{R}_+ \text{ satisfies the Carathéodory conditions,}\\ k^\Sigma_{\alpha\beta}(x, \cdot, \cdot) \text{ is locally Lipschitz continuous uniformly with respect to } x,\\ k^\Sigma_{\alpha\beta}(x, y, z) \le c\mathrm{e}^{c\,(|y_0| + |z|)} \text{ f.a.a. } x \in \Sigma,\ \forall (y, z) \in \mathbb{R}^{m+2},\\ k^\Sigma_{\alpha\beta}(x, y, z) \ge b^\Sigma_{\alpha\beta,R}(x) \text{ f.a.a. } x \in \Sigma, \forall (y, z) \in \mathbb{R}^{m+2} \text{ with } y_0, z \in [-R, R],\\ b^\Sigma_{\alpha\beta,R} \in L^\infty_+(\Sigma),\, \|b^\Sigma_{\alpha\beta,R}\|_{L^1(\Sigma)} > 0.\end{array}\right\} \tag{2.5}$$

For the proof of existence results we shall additionally suppose that

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

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 (5.9)).

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

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

If $\widetilde{u}_0 \in H^1(\Omega)^*$ may be identified with a function $\widetilde{u}_0 \in L^2(\Omega)$,

$$\langle \widetilde{u}_0, h\rangle_{H^1} = \int_\Omega \widetilde{u}_0\, h\,\mathrm{d}x \ \forall h \in H^1(\Omega),$$

then for $u_0 = \widetilde{u}_0|_H$ we obtain

$$\langle u_0, h\rangle_H = \langle \widetilde{u}_0, h\rangle_{H^1} = \int_\Omega \widetilde{u}_0\, h\,\mathrm{d}x \ \forall h \in H,$$

and u_0 may also be identified with the function $\widetilde{u}_0 \in L^2(\Omega)$ since $H^1_0(\Omega\cup\Gamma_N) \subset H$ and $H^1_0(\Omega\cup\Gamma_N)$ lies 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

$$\|\nabla v_0\|^2_{L^2} + \int_\Omega b_0\, v_0^2\,\mathrm{d}x + \int_{\Gamma_N} \tau(v_0 - \pi(v_0))^2\,\mathrm{d}\Gamma \ge c\|v_0\|^2_{H^1}\ \forall v_0 \in H. \tag{2.7}$$

Remark 2.3. We define the function ϕ_0 by

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

By (2.4) we easily find the following properties of e_0 and ϕ_0:

$$\begin{aligned}
&(e_0(x,y) - e_0(x,\overline{y}))\,(y-\overline{y}) \ge b_0(x)\,(y-\overline{y})^2,\\
&e_0(x,y)(y-\overline{y}) - \int_{\overline{y}}^y e_0(x,\eta)\,\mathrm{d}\eta \ge \tfrac12 b_0(x)\,(y-\overline{y})^2,\\
&\phi_0(x,y) \ge \tfrac12 b_0(x)\,y^2,\\
&\int_0^y e_0(x,\eta)\,\mathrm{d}\eta \ge \tfrac12 b_0(x)\,y^2 + e_0(x,0)y\ \ \text{f.a.a. } x \in \Omega,\ \forall y,\overline{y} \in \mathbb{R}.
\end{aligned} \tag{2.8}$$

Often we will write only the second argument of the functions e_0 and ϕ_0.

Remark 2.4. For a special realization of H, π and e_0 we refer to (1.18) and (1.9*).

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

$$\begin{gathered}
R^\Sigma_{\alpha\beta}(x,y,z)\sum_{i=1}^m(\alpha_i-\beta_i)(y_i+q_iy_0) \ge 0\\
\text{f.a.a. } x \in \Sigma,\ \forall y = (y_0,\dots,y_m) \in \mathbb{R}^{m+1},\ \forall z \in \mathbb{R}.
\end{gathered} \tag{2.9}$$

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

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

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

Remark 2.6. For example, the assumption (2.6) is fulfilled for a reaction with stoichiometric coefficients $(\alpha, \beta) \in \mathcal{R}^\Sigma$ if $\sum_{j=1}^m \alpha_j = 0$ or $\sum_{j=1}^m \beta_j = 0$. Another possibility is that $\max\{\sum_{j=1}^m \alpha_j, \sum_{j=1}^m \beta_j\} \le n_\Sigma$. Let us note that condition (2.6) means only restrictions on the source terms of the continuity equations whereas sink terms may be of higher order. In the van Roosbroeck system which is a special case of our more general setting the source terms are of order zero.

2.2 Formulation of the problem (P)

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

$$v = (v_0, v_1, \ldots, v_m) : \mathbb{R}_+ \times \Omega \to \mathbb{R}^{m+1} \quad \text{(potentials)},$$
$$u = (u_0, u_1, \ldots, u_m) \colon \mathbb{R}_+ \times \Omega \to \mathbb{R}^{m+1} \quad \text{(densities)}.$$

Analogously we set $U = (U_0, U_1, \ldots, U_m)$ 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

$$X := H \times H^1(\Omega, \mathbb{R}^m), \;\; Y := L^2(\Omega, \mathbb{R}^{m+1})$$

and their duals X^*, $Y^* = Y$. In addition, let

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

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

$$\langle A(w,v), \overline{v}\rangle := \int_\Omega \Big\{ \sum_{i=1}^m D_i \overline{u}_i \mathrm{e}^{w_i} \nabla \zeta_i \cdot \nabla \overline{\zeta}_i + \sum_{(\alpha,\,\beta) \in \mathcal{R}^\Omega} R^\Omega_{\alpha\beta}(\cdot, w, \pi(w_0))\, (\alpha - \beta) \cdot \overline{\zeta} \Big\}\, \mathrm{d}x$$
$$+ \int_\Gamma \sum_{(\alpha,\,\beta) \in \mathcal{R}^\Gamma} R^\Gamma_{\alpha\beta}(\cdot, w, \pi(w_0))\, (\alpha - \beta) \cdot \overline{\zeta}\, \mathrm{d}\Gamma, \quad \overline{v} \in X,$$

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

$$\langle E_0 v_0, \overline{v}_0 \rangle := \int_\Omega \Big\{ \varepsilon \nabla v_0 \cdot \nabla \overline{v}_0 + e_0(\cdot, v_0) \overline{v}_0 \Big\}\, \mathrm{d}x + \int_{\Gamma_N} \tau (v_0 - \pi(v_0))(\overline{v}_0 - \pi(\overline{v}_0))\, \mathrm{d}\Gamma, \;\; \overline{v}_0 \in H,$$

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

Then the problem which we are interested in reads as

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

Remark 2.7. Problem (P) includes the precise weak formulation of the model problems introduced in Section 1. The 0–th components of the equations $u' + A(v, v) = 0$ and $u = Ev$ represent the continuity equation for the charge density and the (possibly nonlinear, nonlocal) Poisson equation (1.10) and (1.10**), respectively. The other components of these equations are the weak form of (1.5) and (1.1), respectively.

Remark 2.8. By test functions of the form $(w, -q_1 w, \dots, -q_m w)$, $w \in H$, we obtain that for solutions (u, v) of (P) it holds

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

Remark 2.9. If (u, v) is a solution of (P) then u, v have the following regularity properties: $u \in C(\mathbb{R}_+, Y)$, $u \in C_{w^*}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1}))$, $v_0 \in C(\mathbb{R}_+, H)$, $v_i \in C(\mathbb{R}_+, L^2)$, $i = 1, \dots, m$, $v \in C_{w^*}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{m+1}))$. These regularity properties imply the relations

$$\left.\begin{aligned} &u_0(t) = E_0 v_0(t) \text{ in } H^*,\\ &u_i(t) = \overline{u}_i \, \mathrm{e}^{v_i(t)} \text{ in } L^\infty(\Omega),\ i = 1, \dots, m,\\ &u_0(t) = \sum_{i=1}^{m} q_i u_i(t) \text{ in } L^\infty(\Omega) \end{aligned}\right\} \quad \forall t \in \mathbb{R}_+. \tag{2.12}$$

Remark 2.10. Because of (2.7), (2.8) the operator $E_0 \colon H \longrightarrow H^*$ is strongly monotone. Therefore there exists a constant $c > 0$ such that

$$\|v_0(t)\|_{H^1},\ |\pi(v_0(t))| \le c\Big(1 + \sum_{i=1}^{m} \|u_i(t)\|_{L^2}\Big) \ \forall t \in \mathbb{R}_+ \tag{2.13}$$

if (u, v) is a solution of (P). Finally let us note that the operator $E \colon X \longrightarrow X^*$ is strictly monotone.

3 Preliminary results

3.1 Estimates for the solution of the Poisson equation

Lemma 3.1. *Let the assumptions* (2.1)–(2.4) *be fulfilled. Then there exist constants* $c > 0$, $q > 2$ *and a continuous increasing positive function* d *such that*

$$\|v_0\|_{L^\infty} \le c\big(\|u_0 \ln|u_0|\|_{L^1} + d(\|v_0\|_{H^1}) + 1\big), \tag{3.1}$$

$$\|v_0\|_{W^{1,q}} \le c\big(\|u_0\|_{L^{2q/(2+q)}} + d(\|v_0\|_{H^1}) + 1\big) \tag{3.2}$$

if $v_0 \in H$ *and* $E_0 v_0 = u_0 \in L^2(\Omega)$.

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

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

Because of the last assumption in (2.2) we can now apply to this equation results of Gröger for elliptic equations [31, Theorem 1] and [30, Theorem 1] and obtain

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

Because of (2.4) and (1.23) we can estimate the Orlicz norm of $u_0 - e_0(\cdot, v_0)$ by

$$\|u_0 - e_0(\cdot, v_0)\|_{L^\Psi} \le c\,(\|u_0 \ln|u_0|\|_{L^1} + d(\|v_0\|_{H^1}) + 1),$$

and the first assertion of the lemma is proved. Moreover, using the Sobolev imbedding theorem as well as Trudinger's result (1.23) we get

$$\|u_0 - e_0(\cdot, v_0)\|_{(W_0^{1,q/(q-1)}(\Omega \cup \Gamma_N))^*} \le c\,(\|u_0\|_{L^{2q/(2+q)}} + d(\|v_0\|_{H^1}) + 1)$$

which completes the proof. □

3.2 Uniqueness result

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 of* (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 of (P). Then there exists a constant c such that

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

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

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

Let $z_i := \widetilde{u}_i / \overline{u}_i$, $i = 1, \dots, m$. We use $(0, z_1, \dots, z_m) \in L^2(S, X)$ as test function for (P) and take into account that $R^{\Sigma}_{\alpha\beta}(x, \cdot, \cdot)$ is uniformly locally Lipschitz continuous. The norms of $\widetilde{v}_i$ 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

$$\begin{aligned}
&\sum_{i=1}^m \Big\{ \|z_i(t)\|_{L^2}^2 + \int_0^t \|z_i\|_{H^1}^2 \mathrm{d}s \Big\} \\
&\quad \leq c \int_0^t \sum_{i=1}^m \Big\{ \|z_i\|_{L^r} \|\nabla v_0^1\|_{L^q} \|\nabla z_i\|_{L^2} \\
&\qquad\qquad + \|\nabla \widetilde{v}_0\|_{L^2} \|\nabla z_i\|_{L^2} + \|z_i\|_{L^2}^2 + \|\widetilde{v}_0\|_{H^1}^2 + \|z_i\|_{L^2(\Gamma)}^2 \Big\} \mathrm{d}s \\
&\quad \leq \int_0^t \sum_{i=1}^m \Big\{ \tfrac{1}{4} \|z_i\|_{H^1}^2 + c\big(\|z_i\|_{L^2}^{2/r} \|\nabla v_0^1\|_{L^q} \|z_i\|_{H^1}^{2-2/r} + \|z_i\|_{L^2}^2 \big) \Big\} \mathrm{d}s \\
&\quad \leq \int_0^t \sum_{i=1}^m \Big\{ \tfrac{1}{2} \|z_i\|_{H^1}^2 + c\big(\|v_0^1\|_{W^{1,q}}^r \|z_i\|_{L^2}^2 + \|z_i\|_{L^2}^2 \big) \Big\} \mathrm{d}s \\
&\quad \leq \int_0^t \sum_{i=1}^m \Big\{ \tfrac{1}{2} \|z_i\|_{H^1}^2 + c \|z_i\|_{L^2}^2 \Big\} \mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

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

3.3 Energy estimates

In this subsection we collect results on energy estimates which can be obtained similar to the techniques in [26, Section 4]. We define the functional $\Phi \colon X \longrightarrow \mathbb{R}$,

$$\Phi(v) := \int_\Omega \Big\{ \tfrac{\varepsilon}{2} |\nabla v_0|^2 + \int_0^{v_0} e_0(y)\,\mathrm{d}y + \sum_{i=1}^m \overline{u}_i \left(\mathrm{e}^{v_i} - 1\right) \Big\} \mathrm{d}x + \int_{\Gamma_N} \tfrac{\tau}{2} (v_0 - \pi(v_0))^2 \,\mathrm{d}\Gamma.$$

Because of (1.23) this functional is continuous, Gâteaux differentiable and it holds $\partial \Phi = E$. Since E is strictly monotone the functional Φ is strictly convex. Its conjugate functional $F \colon X^* \longrightarrow \overline{\mathbb{R}}$,

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

is proper, lower semicontinuous and convex. It holds $u = Ev = \partial \Phi(v)$ if and only if $v \in \partial F(u)$. 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*

$$F(u) = \int_\Omega \Big\{ \tfrac{\varepsilon}{2} |\nabla v_0|^2 + \phi_0(v_0) \Big\} \mathrm{d}x + \int_{\Gamma_N} \tfrac{\tau}{2} (v_0 - \pi(v_0))^2 \,\mathrm{d}\Gamma + \sum_{i=1}^m F_i(u_i)$$

where v_0 fulfils the relation $E_0 v_0 = u_0$ and

$$F_i(u_i) = \int_\Omega \Big\{\big(u_i(\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i\Big\} \,\mathrm{d}x, \quad u_i \in L^2_+(\Omega).$$

Moreover the functional $F|_{H^* \times L^2_+(\Omega,\mathbb{R}^m)}$ is continuous.

Proof. 1. We define $\Phi_0 \colon H \longrightarrow \mathbb{R}$, $\Phi_i \colon H^1(\Omega) \longrightarrow \mathbb{R}$, $i = 1, \dots, m$, by

$$\begin{aligned}\Phi_0(v_0) &:= \int_\Omega \Big\{\tfrac{\varepsilon}{2}|\nabla v_0|^2 + \int_0^{v_0} e_0(y)\,\mathrm{d}y\Big\}\,\mathrm{d}x + \int_{\Gamma_N} \tfrac{\tau}{2}(v_0 - \pi(v_0))^2 \,\mathrm{d}\Gamma,\\ \Phi_i(v_i) &:= \int_\Omega \overline{u}_i(\mathrm{e}^{v_i} - 1)\,\mathrm{d}x.\end{aligned}$$

Then $\Phi(v) = \sum_{i=0}^m \Phi_i(v_i)$ and obviously $F(u) = \Phi^*(u) = \sum_{i=0}^m \Phi_i^*(u_i)$.

2. Since E_0 is strongly monotone and hemicontinuous (here Trudinger's result (1.23) is used) E_0 is surjective (see e.g. [22, 47, 62]) such that for $u_0 \in H^*$ there exists $v_0 \in H$ with $u_0 = E_0 v_0$ and Φ_0 is subdifferentiable in v_0. Therefore (cf. [12, 61])

$$\Phi_0^*(u_0) = \langle E_0 v_0, v_0\rangle - \Phi_0(v_0) = \int_\Omega \Big\{\tfrac{\varepsilon}{2}|\nabla v_0|^2 + \phi_0(v_0)\Big\}\,\mathrm{d}x + \int_{\Gamma_N} \tfrac{\tau}{2}\,(v_0 - \pi(v_0))^2 \,\mathrm{d}\Gamma.$$

The continuity of Φ_0^* on H now results from the strong monotonicity of E_0 and the continuity of Φ_0.

3. Next we prove the continuity of F_i. Let $w_n, w \in L^2_+(\Omega)$ and $w_n \to w$ in $L^2(\Omega)$. Because of $|\eta \ln \eta| \le \mathrm{e}^{-1} + \eta^2$ for $\eta \ge 0$ we obtain by Fatou's lemma that

$$\begin{aligned}2\int_\Omega (\tfrac{1}{\mathrm{e}} + w^2)\,\mathrm{d}x &\le \liminf_{n\to\infty} \int_\Omega (\tfrac{2}{\mathrm{e}} + w^2 + w_n^2 - |w_n \ln w_n - w \ln w|)\,\mathrm{d}x\\ &\le 2\int_\Omega (\tfrac{1}{\mathrm{e}} + w^2)\,\mathrm{d}x - \limsup_{n\to\infty} \int_\Omega |w_n \ln w_n - w \ln w|\,\mathrm{d}x\end{aligned}$$

which ensures that $\lim_{n\to\infty} \int_\Omega |w_n \ln w_n - w \ln w|\,\mathrm{d}x = 0$. Together with $w_n \to w$ in $L^2(\Omega)$ this proves the continuity of F_i.

4. It remains to show that $\Phi_i^*(u_i) = F_i(u_i)$ if $u_i \in L^2_+(\Omega)$, $i = 1, \dots, m$. Let $u_i \in L^2_+(\Omega)$ and let $w_n \in H^1(\Omega)$, $w_n \ge 0$ and $w_n \to u_i/\overline{u}_i$ in $L^2(\Omega)$. Moreover, let $\delta > 0$ sufficiently small. We define $v_{in} := \ln(w_n + \delta) \in H^1(\Omega)$ and $u_{in} := \overline{u}_i\,(w_n + \delta)$. Then $u_{in} \ge \delta \overline{u}_i$ and $u_{in} \to u_i + \delta \overline{u}_i$ in $L^2(\Omega)$. Since the function $f(\eta) := \ln(\eta + \delta)$, $\eta \ge 0$, is Lipschitz continuous with Lipschitz constant δ^{-1} we find that

$$\langle u_i - u_{in}, v_{in}\rangle \to -\int_\Omega \delta \overline{u}_i \ln(u_i/\overline{u}_i + \delta)\,\mathrm{d}x \quad \text{as } n \to \infty. \tag{3.4}$$

By the subdifferentiability of Φ_i in v_{in} it follows

$$\Phi_i^*(u_{in}) = \langle u_{in}, v_{in}\rangle - \Phi_i(v_{in}) = F_i(u_{in})$$

which yields

$$\Phi_i^*(u_i) = \sup_{\overline{v}_i \in H^1(\Omega)} \{\langle u_i, \overline{v}_i\rangle - \Phi_i(\overline{v}_i)\} \ge \langle u_i, v_{in}\rangle - \Phi_i(v_{in}) = \langle u_i - u_{in}, v_{in}\rangle + F_i(u_{in}).$$

Because of the lower semicontinuity of Φ_i^*, the continuity of F_i and of (3.4) after passing to the limit $n \to \infty$ we obtain

$$\begin{aligned}\Phi_i^*(u_i + \delta\overline{u}_i) &\le \liminf_{n\to\infty} \Phi_i^*(u_{in}) = \lim_{n\to\infty} F_i(u_{in}) = F_i(u_i + \delta\overline{u}_i) \\ &\le \Phi_i^*(u_i) + \int_\Omega \delta\overline{u}_i \ln(u_i/\overline{u}_i + \delta)\,\mathrm{d}x.\end{aligned}$$

Again using the lower semicontinuity of Φ_i^*, the continuity of F_i and the estimate

$$|\delta\ln(\eta+\delta)| \le \begin{cases} \delta|\ln\delta| & \text{if } \ 0 \le \eta \le 1/2, \\ \delta(\mathrm{e}^{-1} + \eta) & \text{if } \ \eta > 1/2 \end{cases}$$

by passing to the limit $\delta \to 0$ the assertion follows. □

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

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

where the dissipation rate D is given by

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

Note that by the definition of the operator A and by (2.9) the dissipation rate is nonnegative for all $v \in W$. This ensures the following result.

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

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

where c *depends only on the data.*

The following corollary is a direct consequence of Theorem 3.2, (3.1), (2.11) and (1.20).

Corollary 3.1. *There is a constant* $c_{3.5} > 0$ *depending only on the data such that*

$$\|v_0(t)\|_{L^\infty}, \ \|v_0(t)\|_{L^\infty(\Gamma)}, \ |\pi(v_0(t))| \le c_{3.5} \quad \forall t \in \mathbb{R}_+ \tag{3.5}$$

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

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 terms. Let, for $N \in \mathbb{R}_+$, $\rho_N\colon \mathbb{R}^{m+2} \to [0,1]$ be a fixed Lipschitz continuous function such that

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

We define the operator $A_N\colon W \times X \longrightarrow X^*$ by

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

where $\zeta_i = v_i + q_i v_0,\ \overline{\zeta}_i = \overline{v}_i + q_i \overline{v}_0,\ i = 1,\dots,m$. The operator E is not changed. Now we are looking for solutions of the following regularized problem

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

4.2 Solvability of $(\mathbf{P_N})$

Theorem 4.1. *For each $N \in \mathbb{R}_+$ there exists a unique solution of* $(\mathrm{P_N})$.

Proof. We intend to apply Theorem 6.1. For fixed $N\in\mathbb{R}_+$, $\Sigma = \Omega,\Gamma,\ i = 1,\dots,m$, we define functions $g_i^\Sigma\colon \Sigma\times\mathbb{R}^{m+1}\times\mathbb{R}\to\mathbb{R}$ by

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

Obviously g_i^Σ satisfies the Carathéodory conditions. Since $R^\Sigma_{\alpha\beta}(x,\cdot,\cdot)$ are uniformly locally Lipschitz continuous and ρ_N is a Lipschitz continuous function with $\rho_N(y,z) = 0$ for $|(y,z)|_\infty \geq N$ the function $g_i^\Sigma(x,\cdot,\cdot)$ is uniformly Lipschitz continuous. The property (2.9) yields

$$\sum_{i=1}^m g_i^\Sigma(x,y,z)\,(y_i + q_i y_0) \geq 0 \text{ for a.a. } x\in\Sigma,\ \forall (y,z)\in\mathbb{R}^{m+2}$$

since $\rho_N(y,z)\geq 0$. Moreover, since $\rho_N(y,z) = 0$ for $|(y,z)|_\infty \geq N$ we find the estimate

$$|g_i^\Sigma(x,y,z)| \leq \sum_{(\alpha,\,\beta)\in\mathcal{R}^\Sigma} \max_{(y,z)\in[-N,N]^{m+2}} |R^\Sigma_{\alpha\beta}(x,y,z)||\alpha_i - \beta_i| \text{ for a.a. } x\in\Sigma,\ \forall (y,z)\in\mathbb{R}^{m+2}$$

the right hand side of which is bounded by some constant depending on N. At last using (2.10) one proves easily that

$$g_i^\Sigma(x,y,z) \le c^\Sigma \mathrm{e}^{y_i} \text{ for a.a. } x \in \Sigma,\ \forall (y,z) \in \mathbb{R}^{m+2} \text{ with } y_i \le 0.$$

Thus the functions g_i^Σ, $\Sigma = \Omega, \Gamma$, $i = 1, \dots, m$, fulfil the assumptions (6.1), and we can apply Theorem 6.1 to obtain the assertion. □

4.3 Estimates for the solution of ($\mathrm{P_N}$)

We are going to find estimates for solutions of ($\mathrm{P_N}$) 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 of ($\mathrm{P_N}$) the relation (2.11) is valid. The dissipation rate corresponding to ($\mathrm{P_N}$), $D_N(v) := \langle A_N(v,v), v\rangle$, is nonnegative for all $v \in W$. Therefore the results of Theorem 3.2 remain true for the solution of ($\mathrm{P_N}$) and

$$\begin{aligned} &F(u(t)) \le c, \quad \|v_0(t)\|_{H^1} \le c \quad \forall t \in S, \\ &\|u_i(t)\|_{L^1},\ \|u_i(t)\ln u_i(t)\|_{L^1} \le c \quad \forall t \in S,\ i = 1, \dots, m. \end{aligned} \tag{4.1}$$

By Lemma 3.1 we find that

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

All these estimates in (4.1) and (4.2) are independent of N and of the length T of the time interval S.

Next we look for upper bounds for the densities. These will not depend on T. We intend to use the Moser technique and start with some preliminary estimate.

Lemma 4.1. *Additionally we suppose* (2.6)*. Then there exists a constant $c > 0$ depending only on the data, but not on N and T, such that for the solution (u,v) of* ($\mathrm{P_N}$)

$$\sum_{i=1}^m \|u_i(t)\|_{L^2} \le c \quad \forall t \in S.$$

Proof. Let $K := \max\{1, \|U_1/\overline{u}_1\|_{L^\infty}, \dots, \|U_m/\overline{u}_m\|_{L^\infty}\}$ and $z_i := (u_i/\overline{u}_i - K)^+$, $i = 1, \dots, m$. We use the test function

$$2\mathrm{e}^t(0, z_1, \dots, z_m) \in L^2(S, X)$$

for ($\mathrm{P_N}$). Note that by (2.6) the source terms in the volume and boundary reactions are of at most second and first order, respectively. Moreover, the factor ρ_N in front of the source terms can be estimated by 1. With the inequalities (4.1) and (4.2) we find by using the trace inequality

(1.19), the Hölder and Young inequalities that for all $t \in S$

$$\begin{aligned}\mathrm{e}^t \sum_{i=1}^m \|z_i(t)\|_{L^2}^2 \le \int_0^t \mathrm{e}^s \sum_{i=1}^m \Big\{ &- \delta \|z_i\|_{H^1}^2 + c\big(\|z_i\|_{L^2(\Gamma)}^2 + \|z_i\|_{L^1(\Gamma)} + \|z_i\|_{L^1} \\ &+ \|z_i\|_{L^2}^2 + \|z_i\|_{L^3}^3 + \|\nabla v_0\|_{L^q} \|u_i/\overline{u}_i\|_{L^r} \|\nabla z_i\|_{L^2}\big)\Big\}\, \mathrm{d}s \\ \le \int_0^t \mathrm{e}^s \sum_{i=1}^m \Big\{ &- \tfrac{\delta}{2} \|z_i\|_{H^1}^2 + \overline{c}\,\big(\|z_i\|_{L^3}^3 + 1 \\ &+ \big(1 + \sum_{j=1}^m \|z_j\|_{L^{r'}}\big) \|z_i\|_{H^1} (\|z_i\|_{L^r} + 1)\big)\Big\}\, \mathrm{d}s\end{aligned}$$

with $r = 2q/(q-2)$, $r' = 2q/(q+2)$, q from (3.2) and some positive constant δ. For $\|z_i\|_{L^3}^3$ we apply inequality (1.22) with $p = 3$, $\epsilon := \delta/(\overline{c} + 8\overline{c} \sum_{i=1}^m \|z_i \ln z_i\|_{L^\infty(S,L^1)})$. Moreover, from (1.22) with $p = r$ and $p = r'$, respectively, from Gagliardo–Nirenberg's inequality (1.21) and Young's inequality we find a constant $c > 0$ such that

$$\begin{aligned}&\sum_{i=1}^m \big(1 + \sum_{j=1}^m \|z_j\|_{L^{r'}}\big) \|z_i\|_{H^1} (\|z_i\|_{L^r} + 1) \\ &\qquad \le \sum_{i=1}^m \Big(\epsilon \sum_{j=1}^m \|z_j \ln z_j\|_{L^1} + \tfrac{\delta}{4}\Big) \|z_i\|_{H^1}^2 + c\Big(1 + \sum_{i=1}^m \|z_i \ln z_i\|_{L^1}^{2r'/(r'-1)}\Big)\end{aligned}$$

with ϵ defined as above. In addition, here we used the relation $y \le y \ln |y| + c$ for $y \ge 0$ and the fact that $2 < 2r/(r-1) < 2r'/(r'-1)$. Thus we can continue our estimates by

$$\mathrm{e}^t \sum_{i=1}^m \|z_i(t)\|_{L^2}^2 \le \int_0^t \mathrm{e}^s \sum_{i=1}^m \Big\{ \big(2\epsilon\, \overline{c} \sum_{j=1}^m \|z_j \ln z_j\|_{L^1} - \tfrac{\delta}{4}\big) \|z_i\|_{H^1}^2 + c\big(\|z_i \ln z_i\|_{L^1}^{2r'/(r'-1)} + 1\big)\Big\}\, \mathrm{d}s.$$

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

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

which implies the desired estimate for $\sum_{i=1}^m \|u_i(t)\|_{L^2}$. $\square$

Remark 4.1. Since $r' = 2q/(q+2) < 2$, by relation (4.2) and Lemma 4.1 there are constants c, $c_{4.3} > 0$ depending only on the data, not on N and T, such that for the solution (u, v) of $(\mathrm{P_N})$

$$\sum_{i=1}^m \|u_i(t)\|_{L^{r'}} \le c, \quad \|v_0(t)\|_{W^{1,q}} \le c_{4.3} \quad \forall t \in S. \tag{4.3}$$

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) of* $(\mathrm{P_N})$

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

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

Proof. The proof is based on Moser iteration. In [21] such techniques are used for the van Roosbroeck equations. But our system contains more general volume and boundary reaction terms only fulfilling assumption (2.6). Therefore we obtain Moser exponents differing from those in [21]. Let $z_i := (u_i/\overline{u}_i - K)^+$ with K defined in the proof of Lemma 4.1, $w_i := z_i^{p/2}$ where $p \geq 4$. Since $v_i \in L^2(S, H^1) \cap L^\infty(S, L^\infty)$ we have

$$pe^t\,(0, z_1^{p-1}, \ldots, z_m^{p-1}) \in L^2(S, X)$$

and we can take it as a test function for $(\mathrm{P_N})$. We define

$$\kappa := c_{4.3}^{2r} + 1 \text{ where } r = 2q/(q-2),\ q \text{ from (3.2)}. \tag{4.5}$$

Note that volume and boundary reaction terms satisfy the restrictions (2.6) and $|\rho_N| \leq 1$. Since K is a constant defined by the data and $u_i \leq z_i + K$ we have for all $t \in S$

$$\begin{aligned}
&\mathrm{e}^t \sum_{i=1}^m \int_\Omega \overline{u}_i |w_i(t)|^2 \,\mathrm{d}x \\
&\leq \int_0^t \mathrm{e}^s \sum_{i=1}^m \Big\{ \int_\Omega \Big\{ -\delta|\nabla w_i|^2 + cp\big(|w_i|^2 + u_i|\nabla v_0||\nabla z_i^{p-1}| + (u_i^2+1)z_i^{p-1}\big)\Big\}\,\mathrm{d}x \\
&\qquad\qquad + cp\int_\Gamma (u_i+1)z_i^{p-1}\,\mathrm{d}\Gamma\Big\}\,\mathrm{d}s \\
&\leq \int_0^t \mathrm{e}^s \sum_{i=1}^m \Big\{ -\delta\|w_i\|_{H^1}^2 + cp\big(\|\nabla v_0\|_{L^q}\|\nabla w_i\|_{L^2}(\|w_i\|_{L^r}+1) \\
&\qquad\qquad + \|w_i\|_{L^{2(p+1)/p}}^{2(p+1)/p} + \|w_i\|_{L^2(\Gamma)}^2 + 1\big)\Big\}\,\mathrm{d}s.
\end{aligned}$$

We apply for r and $\widetilde{p} := 2(p+1)/p$, $p \geq 4$, Gagliardo–Nirenberg's inequality (1.21). Since $\widetilde{p} \in (2, 5/2]$ for $p \geq 4$, the constant $c_{\widetilde{p}}$ can be estimated from above by means of $\max\{c_2, c_{5/2}, 1\}^{1/2}$. We continue

$$\begin{aligned}
&\mathrm{e}^t \sum_{i=1}^m \int_\Omega \overline{u}_i |w_i(t)|^2 \,\mathrm{d}x \\
&\leq \int_0^t \mathrm{e}^s \sum_{i=1}^m \Big\{ -\tfrac{\delta}{2}\|w_i\|_{H^1}^2 + cp^{2r}(\|\nabla v_0\|_{L^q}^{2r}+1)(\|w_i\|_{L^1}^2+1) \\
&\qquad\qquad + cp\big(\|w_i\|_{H^1}^{(p+2)/p}\|w_i\|_{L^1} + \|w_i\|_{H^1}^{3/2}\|w_i\|_{L^1}^{1/2} + 1\big)\Big\}\,\mathrm{d}s \\
&\leq \int_0^t \mathrm{e}^s \sum_{i=1}^m c\Big\{p^{2r}\kappa(\|w_i\|_{L^1}^2+1) + p^4\|w_i\|_{L^1}^{2p/(p-2)} + p^4\|w_i\|_{L^1}^2 + 1\Big\}\,\mathrm{d}s \\
&\leq cp^{2r}\kappa\int_0^t \mathrm{e}^s \sum_{i=1}^m (\|w_i\|_{L^1}^{2p/(p-2)}+1)\,\mathrm{d}s \;\leq\; cp^{2r}\kappa\mathrm{e}^t\sum_{i=1}^m (\sup_{s\in S}\|z_i(s)\|_{L^{p/2}}^{p^2/(p-2)}+1).
\end{aligned}$$

Therefore we obtain the estimate

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

with $c_{4.6} > 1$ depending only on the data. Let

$$a_k := \sum_{i=1}^m \sup_{s\in S}\|z_i(s)\|_{L^{2^k}}^{2^k} + 1, \quad k = 1, 2, \ldots.$$

Now we set $p = 2^k$, $k \in \mathbb{N}$, $k \geq 2$. From (4.6) we conclude that

$$a_k \leq (2^{2r})^k \, (\kappa \, c_{4.6}) \, a_{k-1}^{\left\{\frac{2^k}{2^{k-1}-1}\right\}}$$
$$\leq \Big[(2^{2r})^{\left\{\sum_{i=0}^{k-2}(k-i)2^i\right\}} \, (\kappa \, c_{4.6})^{\left\{\sum_{i=0}^{k-2} 2^i\right\}} \, a_1^{\left\{2^{k-1}\right\}} \Big]^{\prod_{j=1}^{k-1} \frac{2^j}{2^j-1}}.$$

The last inequality can be proved by induction. Note that the product $c_\theta := \prod_{j=1}^{\infty} \frac{2^j}{2^j-1}$ is finite and all of its factors are greater than 1. Moreover

$$\sum_{i=0}^{k-2} 2^i \leq 2^{k-1}, \quad \sum_{i=0}^{k-2} (k-i)\, 2^i \leq 2^{k+1}, \quad k \geq 2$$

such that

$$a_k \leq (2^{4r} \kappa \, c_{4.6} \, a_1)^{c_\theta 2^k}.$$

Thus we arrive at

$$\sum_{i=1}^{m} \|z_i(t)\|_{L^{2^k}} \leq \sqrt{m}\, (2^{4r} \kappa \, c_{4.6} (\sum_{i=1}^{m} \sup_{s \in S} \|z_i(s)\|_{L^2}^2 + 1))^{c_\theta} \quad \forall t \in S,\ k \geq 2.$$

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

$$\sum_{i=1}^{m} \|z_i(t)\|_{L^\infty} \leq \sqrt{m}\, (2^{4r} \kappa \, c_{4.6} (\sum_{i=1}^{m} \sup_{s \in S} \|z_i(s)\|_{L^2}^2 + 1))^{c_\theta} \quad \forall t \in S.$$

Writing this inequality in terms of u_i and applying the result of Lemma 4.1 we find the desired estimates in Ω. The estimates at the boundary follow from (1.20). □

We intend to estimate the densities from below (or the negative parts of the chemical potentials from above) by Moser iteration, too. Corresponding estimates for the van Roosbroeck equations were given in [21, Lemma 4.6]. Our more general reaction and boundary terms do not produce new difficulties in proving the recursion formula since estimates from above are already known.

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

$$\mathrm{e}^t \|(v_i + K)^-(t)\|_{L^p}^p \leq c \int_0^t \mathrm{e}^s p^{2r} \kappa (\|(v_i + K)^-(s)\|_{L^{p/2}}^p + 1)\, \mathrm{d}s$$
$$\forall p \geq 2, \quad \forall t \in S, \quad i = 1, \dots, m,$$

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

Proof. Let $z := (\ln(u_i/\overline{u}_i) + K)^-$. For $p \geq 2$ we take the test function which has the i–th component

$$-p\mathrm{e}^t z^{p-1} \overline{u}_i / u_i,$$

the other components shall be zero. Note that from the L^∞–estimates for v_0, $u_j/\overline{u}_j$, $j = 1, \dots, m$, on Ω and at Γ and from the structure of the volume and boundary reactions (see (2.10)) it follows that

$$R_{\alpha\beta}^{\Sigma}(\alpha_i - \beta_i) z^{p-1} \frac{\overline{u}_i}{u_i} = k_{\alpha\beta}^{\Sigma} \Big[\prod_{j=1}^{m} (\frac{u_j}{\overline{u}_j} \mathrm{e}^{q_j v_0})^{\alpha_j} - \prod_{j=1}^{m} (\frac{u_j}{\overline{u}_j} \mathrm{e}^{q_j v_0})^{\beta_j} \Big] z^{p-1} \frac{\overline{u}_i}{u_i} (\alpha_i - \beta_i) \leq c\, z^{p-1}.$$

Moreover, the factor ρ_N in front of the reaction terms can be estimated by 1. Now estimates like in [21, p. 24] (trace and imbedding results, the Gagliardo–Nirenberg and Hölder inequalities) give the recursion formula

$$\mathrm{e}^t \|z(t)\|_{L^p}^p \le \int_0^t \mathrm{e}^s c p^{2r} \kappa \big(\|z\|_{L^{p/2}}^p + 1 \big)\, \mathrm{d}s \quad \forall t \in S \tag{4.7}$$

which proves the lemma. □

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) of* ($\mathrm{P_N}$)

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

(*with K defined in Lemma 4.2*).

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

$$\mathrm{e}^t \|z(t)\|_{L^1}^2 \le c\mathrm{e}^t \|z(t)\|_{L^2}^2 \le c \int_0^t \mathrm{e}^s (\|z(s)\|_{L^1}^2 + 1)\, \mathrm{d}s \quad \forall t \in S$$

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

Theorem 4.3. *For the solution (u, v) of* ($\mathrm{P_N}$) *we assume the validity of estimate* (4.4). *Then there exists a continuous increasing function $d_{4.8} > 0$ depending only on the data, but not on N, such that*

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

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 [21] we find from (4.7) that

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

Together with Lemma 4.3 this supplies the estimate $\|z(t)\|_{L^\infty} \le d(T)$. Thus we obtain a lower bound for $\ln u_i(t)/\overline{u}_i$ depending only on the data and on T. This procedure can be done for $i = 1, \dots, m$. The estimate for the boundary norms follows from (1.20). □

4.4 Existence result

Theorem 4.4. *Under the additional assumption* (2.6) *there exists a* (*unique*) *solution of problem* (P).

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

$$(u(t), v(t)) := (u_{\widetilde{N}(t)}(t), v_{\widetilde{N}(t)}(t)) \text{ for } t > 0,$$

$$(u(0), v(0)) := (U, E_0^{-1} U_0, \ln[U_1/\overline{u}_1], \dots, \ln[U_m/\overline{u}_m])$$

where $(u_{\widetilde{N}(t)}, v_{\widetilde{N}(t)})$ is the solution of $(\mathrm{P}_{\widetilde{\mathrm{N}}(\mathrm{t})})$ on $S := [0,t]$ and

$$\widetilde{N}(t) := 2\max\{c_{4.2}, \ln c_{4.4}, d_{4.8}(t)\}. \tag{4.10}$$

Since $\widetilde{N}(t) \geq \widetilde{N}(s)$ for $t \geq s$ and since the solution of each problem $(\mathrm{P_N})$ 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 the pair of time functions $(u,v)|_{[0,t]}$ is a solution of $(\mathrm{P}_{\widetilde{\mathrm{N}}(\mathrm{t})})$ 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 of $(\mathrm{P}_{\widetilde{\mathrm{N}}(\mathrm{t})})$ (see (4.1), (4.2), Theorem 4.2, Theorem 4.3). Therefore (u,v) defined here is a solution of (P). Uniqueness has been proved in Theorem 3.1. □

4.5 Global estimates

Theorem 4.5. *Under the assumption* (2.6) *for the solution* (u,v) *of* (P) *it holds*

$$\|u_i(t)/\overline{u}_i\|_{L^\infty} \leq c_{4.4} \quad \forall t \in \mathbb{R}_+, \quad i = 1,\ldots,m. \tag{4.11}$$

The same estimate is valid for the $L^\infty(\Gamma)$*–norms of* $u_i(t)/\overline{u}_i$ *for a.a.* $t \in \mathbb{R}_+$*. Furthermore it holds*

$$\operatorname*{ess\,inf}_{x\in\Omega} u_i(t) \ \geq \operatorname*{ess\,inf}_{x\in\Omega} \overline{u}_i\, \mathrm{e}^{-d_{4.8}(t)} \quad \forall t \in \mathbb{R}_+, \quad i = 1,\ldots,m. \tag{4.12}$$

Proof. Let (u,v) be the solution of (P) and $t \in \mathbb{R}_+$ be arbitrarily given. Then $(u,v)|_{[0,t]}$ is the solution of $(\mathrm{P}_{\widetilde{\mathrm{N}}(\mathrm{t})})$ on $S = [0,t]$ with $\widetilde{N}(t)$ defined in (4.10). Thus Theorem 4.2 gives

$$\|u_i(t)/\overline{u}_i\|_{L^\infty} \leq c_{4.4}, \quad i = 1,\ldots,m,$$

which leads to the desired $L^\infty(\Omega)$–estimate in (4.11). The corresponding estimate for the boundary norms again follows from (1.20). Additionally, Theorem 4.3 gives

$$\|(\ln(u_i/\overline{u}_i))^-(t)\|_{L^\infty}, \leq d_{4.8}(t),\ i = 1,\ldots,m.$$

This leads to

$$u_i(t) \geq \overline{u}_i\, \mathrm{e}^{-d_{4.8}(t)} \quad \text{f.a.a. } x \in \Omega$$

which proves the last assertion. □

The lower bound obtained in (4.12) depends on t, especially it tends to zero if $t \to \infty$. Thus it makes sense to ask if there is a positive constant lower bound for the densities. This question is closely related to the asymptotic behaviour of the solution of (P) which will be discussed in the next section.

5 Global lower bounds and asymptotics

5.1 Invariants and 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. By $\mathcal{S} \subset \mathbb{R}^m$ we denote the stoichiometric subspace belonging to all volume and boundary reactions,

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

We define

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

and $\mathcal{U}^\perp := \{v \in X : \langle u, v\rangle = 0 \; \forall u \in X^*\}$. One easily verifies that

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

Having in mind Remark 2.8 and using the test function $(0, 1, \dots, 1)$ we obtain for a solution (u, v) of (P) the following invariance property

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

Remark 5.1. Let $\kappa \in \mathcal{S}^\perp$ and define

$$I_\kappa(u) := \sum_{i=1}^m \kappa_i \langle u_i, 1\rangle, \; u \in X^*.$$

If (u, v) is a solution of (P) we find by (5.1) that

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

Thus each $\kappa \in \mathcal{S}^\perp$ generates an invariant of the reaction–diffusion system. If (1.11) should be fulfilled then $q = (q_1, \dots, q_m) \in \mathcal{S}^\perp$ and the corresponding invariant would represent the total electric charge.

According to (5.1) it makes sense to look for steady states (u^*, v^*) of (P) which fulfil the property $u^* \in \mathcal{U} + U$.

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

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

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

$$u^*, \, v^* \in L^\infty(\Omega, \mathbb{R}^{m+1}), \; v^* \in L^\infty(\Gamma, \mathbb{R}^{m+1}),$$

$$u_i^* \geq c > 0 \text{ a.e. on } \Omega, \; a_i^* := \mathrm{e}^{v_i^* + q_i v_0^*} = \text{const} > 0, \, i = 1, \dots, m.$$

For the proof we refer to [26, Theorem 3.1] or to [24, Theorem 3.2]. Because of (2.2) the assumption concerning the initial values required there is fulfilled.

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 of (P). Because of $v^* \in \mathcal{U}^\perp$ and $u(t) - u^* \in \mathcal{U}$, $t \in \mathbb{R}_+$, we get

$$\begin{aligned} F(u(t)) - F(u^*) &= \int_\Omega \Big\{ \sum_{i=1}^m \Big\{ u_i(t)(\ln \frac{u_i(t)}{u_i^*} - 1) + u_i^* \Big\} \\ &\quad + \int_{v_0^*}^{v_0(t)} (e_0(v_0(t)) - e_0(y))\,\mathrm{d}y + \tfrac{\varepsilon}{2} |\nabla (v_0(t) - v_0^*)|^2 \Big\}\,\mathrm{d}x \\ &\quad + \int_{\Gamma_N} \tfrac{\tau}{2} (v_0(t) - v_0^* - \pi(v_0(t) - v_0^*))^2\,\mathrm{d}\Gamma \\ &\geq c \Big(\sum_{i=1}^m \| \sqrt{u_i(t)/u_i^*} - 1 \|_{L^2}^2 + \| v_0(t) - v_0^* \|_{H^1}^2 \Big) \quad \forall t \in \mathbb{R}_+. \end{aligned} \tag{5.3}$$

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

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

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

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

$$\begin{aligned} \mathcal{M} := \Big\{ (a, v_0) \in \mathbb{R}_+^m \times H \colon \prod_{i=1}^m a_i^{\alpha_i} = \prod_{i=1}^m a_i^{\beta_i}\ \forall (\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma, \\ (E_0 v_0, u_1, \ldots, u_m) \in \mathcal{U} + U \text{ where } u_i := \overline{u}_i\, a_i\, \mathrm{e}^{-q_i v_0},\ i = 1, \ldots, m \Big\} \end{aligned} \tag{5.4}$$

and it holds $u_0^\bullet = E_0 v_0^\bullet$, $u_i^\bullet = \overline{u}_i a_i^\bullet \mathrm{e}^{-q_i v_0^\bullet}$, $i = 1, \ldots, m$. *Moreover,* $F(u(t)) \to F(u^\bullet)$ *as* $t \to +\infty$.

Proof. 1. Let (u, v) be a solution of (P). Then for $a_i = \mathrm{e}^{\zeta_i}$ it holds $\sqrt{a_i(t)} \in H^1(\Omega)$ for a.a. $t \in \mathbb{R}_+$ and by Corollary 3.1 we obtain that

$$\mathrm{e}^{v_i} |\nabla \zeta_i|^2 \geq c \Big| \nabla \sqrt{a_i} \Big|^2.$$

For all $(\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma$ it holds

$$(\mathrm{e}^{\alpha \cdot \zeta} - \mathrm{e}^{\beta \cdot \zeta})\,(\alpha - \beta) \cdot \zeta \geq c \Big[\prod_{i=1}^m \sqrt{a_i}^{\,\alpha_i} - \prod_{i=1}^m \sqrt{a_i}^{\,\beta_i} \Big]^2$$

and using Corollary 3.1 again we find that

$$D(v(t)) \geq c\, \widetilde{D}(a(t)) \qquad \text{f.a.a. } t \in \mathbb{R}_+ \text{ with some } c > 0 \tag{5.5}$$

where

$$\begin{aligned}\widetilde{D}(a) := \int_\Omega \Big\{ \sum_{i=1}^m \big|\nabla\sqrt{a_i}\big|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} b^\Omega_{\alpha\beta,R}\Big[\prod_{i=1}^m \sqrt{a_i}^{\alpha_i} - \prod_{i=1}^m \sqrt{a_i}^{\beta_i}\Big]^2\Big\}\,\mathrm{d}x \\ + \int_\Gamma \sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma} b^\Gamma_{\alpha\beta,R}\Big[\prod_{i=1}^m \sqrt{a_i}^{\alpha_i} - \prod_{i=1}^m \sqrt{a_i}^{\beta_i}\Big]^2\,\mathrm{d}\Gamma\end{aligned} \tag{5.6}$$

with $R = c_{3.5}$.

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

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

which yields with (5.3) and Corollary 3.1 that

$$\begin{aligned}&\|\sqrt{a_i(t)/a_i^*} - 1\|^2_{L^2} + \|v_0(t) - v_0^*\|^2_{H^1} \le c(\|\sqrt{u_i(t)/u_i^*} - 1\|^2_{L^2} + \|v_0(t) - v_0^*\|^2_{H^1}) \\ &\le c(F(u(t)) - F(u^*)) \le c(F(U) - F(u^*)) \quad \forall t\in\mathbb{R}_+,\ i = 1,\dots,m.\end{aligned} \tag{5.7}$$

These estimates will be used in some of the next proofs, too. Here they ensure that

$$\|\sqrt{a_i(t)}\|^2_{L^2} + \|v_0(t)\|^2_{H^1} \le c \quad \forall t\in\mathbb{R}_+. \tag{5.8}$$

3. Because of $\|\widetilde{D}(a)\|_{L^1(\mathbb{R}_+)} < \infty$ (cf. Theorem 3.2 and (5.5)) there exists a sequence $t_k \to +\infty$ such that $\widetilde{D}(a(t_k)) \to 0$. This implies $\nabla\sqrt{a_i(t_k)} \to 0$ in L^2, and since $\|\sqrt{a_i(t_k)}\|_{L^2} \le c$ (cf. (5.8)) we conclude that $\sqrt{a(t_k)} \to \sqrt{a^\bullet}$ in $H^1(\Omega,\mathbb{R}^m)$ with $\sqrt{a^\bullet}\in\mathbb{R}^m$. Next, by (5.6) and Fatou's lemma we obtain

$$\prod_{i=1}^m \sqrt{a_i^\bullet}^{\alpha_i} = \prod_{i=1}^m \sqrt{a_i^\bullet}^{\beta_i}, \quad \prod_{i=1}^m a_i^{\bullet\alpha_i} = \prod_{i=1}^m a_i^{\bullet\beta_i} \quad \forall(\alpha,\beta)\in\mathcal{R}^\Omega\cup\mathcal{R}^\Gamma.$$

4. By (5.8) it holds $\|v_0(t_k)\|_{H^1} \le c$. Therefore, at least for a subsequence, $v_0(t_k) \rightharpoonup v_0^\bullet$ in $H^1(\Omega)$, $v_0(t_k) \to v_0^\bullet$ in $L^2(\Omega)$.

5. We set $u_i^\bullet = \overline{u}_i a_i^\bullet \mathrm{e}^{-q_i v_0^\bullet}$ and $u_0^\bullet = \sum_{i=1}^m q_i u_i^\bullet$. Since

$$\|u_i(t_k) - u_i^\bullet\|_{L^2} \le c(\|\sqrt{a_i(t_k)} - \sqrt{a_i^\bullet}\|^2_{L^4} + \|\sqrt{a_i(t_k)} - \sqrt{a_i^\bullet}\|_{L^2} + \|v_0(t_k) - v_0^\bullet\|_{L^2})$$

we obtain that $u(t_k) \to u^\bullet$ in Y.

6. It holds $E_0 v_0(t_{k+l}) - E_0 v_0(t_k) = u_0(t_{k+l}) - u_0(t_k)$. By the strong monotonicity of E_0 and because of $u_0(t_k) \to u^\bullet$ in H^*, $v_0(t_k) \rightharpoonup v_0^\bullet$ in $H^1(\Omega)$ we have $v_0(t_k) \to v_0^\bullet$ in $H^1(\Omega)$, too. Since E_0 is demicontinuous we find

$$E_0 v(t_k) \rightharpoonup E_0 v_0^\bullet \text{ in } H^*, \quad E_0 v_0^\bullet = u_0^\bullet.$$

7. Since $(E_0 v_0(t_k), u_1(t_k), \dots, u_m(t_k)) \rightharpoonup (E_0 v_0^\bullet, u_1^\bullet, \dots, u_m^\bullet)$ in X^* and $u(t_k) \in \mathcal{U} + U$ it results $u^\bullet = (E_0 v_0^\bullet, u_1^\bullet, \dots, u_m^\bullet) \in \mathcal{U} + U$. Thus we finally get $(a^\bullet, v_0^\bullet) \in \mathcal{M}$.

8. Because of $u^\bullet \in H^* \times L^2_+(\Omega,\mathbb{R}^m)$ and the continuity result in Lemma 3.2 we obtain that $F(u(t_k)) \to F(u^\bullet)$. The monotonous decay of the free energy (see Theorem 3.2) leads to $F(u(t)) \to F(u^\bullet)$ as $t \to +\infty$. □

Remark 5.2. If (u,v) is a steady state in the sense of (5.2) then $a_i := \mathrm{e}^{v_i+q_i v_0} = \text{const} > 0$ 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 $u_0 := E_0 v_0$, $u_i := \overline{u}_i\, a_i\, \mathrm{e}^{-q_i v_0}$, $v_i := \ln a_i - q_i v_0$, $i = 1, \dots, m$, is a steady state in the sense of (5.2). If there are elements $(a, v_0) \in \mathcal{M}$ with $a \notin \operatorname{int} \mathbb{R}_+^m$ then we have no correspondence of such elements to a steady state (u,v) in the sense of (5.2).

In order to exclude the situation which has been mentioned at the end of Remark 5.2 we shall assume that

$$\mathcal{M} \subset \operatorname{int} \mathbb{R}_+^m \times H. \tag{5.9}$$

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

Remark 5.3. For the van Roosbroeck system assumption (5.9) is fulfilled. But (5.9) can be verified also for more complicated reaction systems considered in [38] (cf. the examples in Section 8, too).

Corollary 5.1. *Let the additional assumption* (5.9) *be fulfilled and let* (u,v) *be a solution of* (P). *Then* $v_0(t) \to v_0^*$ *in* H, $\sqrt{a_i(t)} \to \sqrt{a_i^*}$, $\sqrt{u_i(t)} \to \sqrt{u_i^*}$ *in* $L^2(\Omega)$ *and* $a_i(t) \to a_i^*$, $u_i(t) \to u_i^*$ *in* $L^1(\Omega)$, $i = 1, \dots, m$, *as* $t \to +\infty$.

Proof. Continuing the proof of Theorem 5.2 and using assumption (5.9) we now have $a^\bullet = a^*$, $v_0^\bullet = v_0^*$, $u^\bullet = u^*$ and $F(u(t)) \to F(u^*)$ as $t \to +\infty$. By the inequalities (5.3) and (5.7) we find the assertions for $\sqrt{u_i(t)}$, $\sqrt{a_i(t)}$ and $v_0(t)$. With

$$\|u_i(t) - u_i^*\|_{L^1} \le \|\sqrt{u_i(t)} - \sqrt{u_i^*}\|_{L^2} \|\sqrt{u_i(t)} + \sqrt{u_i^*}\|_{L^2}, \ \|\sqrt{u_i(t)}\|_{L^2} \le c \ \forall t \in \mathbb{R}_+ \tag{5.10}$$

and corresponding estimates for a_i we verify the last two assertions. □

5.3 Exponential decay of the free energy

The additional assumption (5.9) leads to sharper asymptotic results. Without the knowledge of global a priori bounds for the densities 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 equilibrium value. The proof is based on an estimate of the free energy from above by the dissipation rate. The following result can be obtained by the same methods as in [26, Theorem 5.2] (or in [24, Theorem 4.2], there the nonlinearity e_0 of the Poisson equation is included, but not the nonlocal term π).

Theorem 5.3. *We assume* (5.9). *Then for every* $R > 0$ *there exists a* $c_R > 0$ *such that*

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

for all $v \in M_R$ *where*

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

Theorem 5.3 enables us to improve the global stability results given in Corollary 5.1.

Theorem 5.4. *Let* (5.9) *be satisfied. Then there exists a* $\lambda > 0$ *depending only on the data such that*

$$F(u(t)) - F(u^*) \le \mathrm{e}^{-\lambda t}\,(F(U) - F(u^*)) \quad \forall t \ge 0 \tag{5.11}$$

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

For the proof we refer to [26, Theorem 5.3]. Next, we collect some estimates resulting from (5.11) which will be of importance for the start of global a priori estimates for the densities from below by positive constants.

Corollary 5.2. *Let* (u,v) *be a solution of* (P) *and let* (5.11) *be satisfied. Then there exists a constant* $c > 0$ *depending only on the data such that for* $i = 1,\dots,m$ *it holds*

$$\begin{aligned} &\|\sqrt{u_i(t)/u_i^*} - 1\|_{L^2},\ \|\sqrt{a_i(t)/a_i^*} - 1\|_{L^2} \le c\,\mathrm{e}^{-\lambda t/2}, \\ &\|v_0(t) - v_0^*\|_{H^1},\ \|u_i(t) - u_i^*\|_{L^1},\ \|a_i(t) - a_i^*\|_{L^1} \le c\,\mathrm{e}^{-\lambda t/2}\ \forall t \in \mathbb{R}_+. \end{aligned} \tag{5.12}$$

Moreover there exists a constant $c_{5.13} > 0$ *depending only on the data such that*

$$\begin{aligned} &\|v_0 - v_0^*\|_{L^2(\mathbb{R}_+,H^1)},\ \|v_0 - v_0^*\|_{L^1(\mathbb{R}_+,L^1)},\ \|v_0 - v_0^*\|_{L^1(\mathbb{R}_+,L^1(\Gamma))} \le c_{5.13}, \\ &\|u_i/u_i^* - 1\|_{L^1(\mathbb{R}_+,L^1)},\ \|u_i/u_i^* - 1\|_{L^1(\mathbb{R}_+,L^1(\Gamma))} \le c_{5.13},\ i = 1,\dots,m. \end{aligned} \tag{5.13}$$

Proof. The assertions in (5.12) are a consequence of (5.11), (5.7) and (5.10). From (5.12) the first four estimates in (5.13) follow immediately. 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. $t \in \mathbb{R}_+$

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

With the trace inequality (1.19) we obtain

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

Since $\|D(v)\|_{L^1(\mathbb{R}_+)} \le c$ we find by (5.5) and (5.12) that $\|\sqrt{a_i/a_i^*} - 1\|_{L^2(\mathbb{R}_+,H^1)} \le c$. This together with (5.12) proves the last assertion in (5.13). □

5.4 Global lower bounds for the chemical potentials

Next we are looking for global lower bounds for the chemical potentials, in other words, for positive global lower bounds for the densities. We want to do this similarly to Lemma 4.2 and Theorem 4.3. Lemma 4.3 must be improved since now we have to look for a lower bound which is independent of the length of the time interval. Corresponding estimates for the van Roosbroeck equations were given in [21, 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 $c_{5.14}$ depending only on the data such that

$$\|u_i\|_{L^\infty(\mathbb{R}_+,L^\infty(\Omega))},\ \|u_i/\overline{u}_i\|_{L^\infty(\mathbb{R}_+,L^\infty(\Gamma))} \le c_{5.14}, \quad i = 1,\dots,m, \tag{5.14}$$

and that (5.11) is satisfied if (u, v) is a solution of 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 of* (P) *and let* (5.14) *and* (5.11) *be fulfilled. Then there exists a constant $c > 0$ depending only on the data such that*

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

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

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

where u_i^* is the i–th component of the steady state (5.2) is convex and lower semicontinuous. Its conjugate $G := \Theta^* \colon (H^1)^* \to \overline{\mathbb{R}}$ is proper, convex and lower semicontinuous. If (u, v) is a solution of (P) then $G(u_i(t))$ may be written as

$$G(u_i(t)) = \int_\Omega \Big\{ u_i^* \, (\ln \frac{u_i}{u_i^*})^-(t) - (u_i - u_i^*)^-(t) \Big\}\, \mathrm{d}x.$$

The function $\overline{z} := (1 - u_i^*/u_i)^-$ belongs to $L^2_{\mathrm{loc}}(\mathbb{R}_+, H^1)$ and for a.a. $t \in \mathbb{R}_+$ we have that $-\overline{z}(t) \in \partial G(u_i(t))$. Thus the Brézis formula (see [6]) yields

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

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

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

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

$$\begin{aligned} G(u_i(t)) \le \int_0^t \Big\{ &- \delta\, \|\nabla z\|_{L^2}^2 + c \|\nabla (v_0 - v_0^*)\|_{L^2} \|\nabla z\|_{L^2} \\ &+ \int_\Omega \sum_{(\alpha,\,\beta) \in \mathcal{R}^\Omega} k_{\alpha\beta}^\Omega \, [\mathrm{e}^{\alpha\cdot\zeta} - \mathrm{e}^{\beta\cdot\zeta}] (\alpha_i - \beta_i) (1 - \frac{u_i^*}{u_i})^-\, \mathrm{d}x \\ &+ \int_\Gamma \sum_{(\alpha,\,\beta) \in \mathcal{R}^\Gamma} k_{\alpha\beta}^\Gamma \, [\mathrm{e}^{\alpha\cdot\zeta} - \mathrm{e}^{\beta\cdot\zeta}] (\alpha_i - \beta_i) (1 - \frac{u_i^*}{u_i})^-\, \mathrm{d}\Gamma \Big\}\, \mathrm{d}s + G(U_i) \end{aligned} \tag{5.15}$$

where $\delta > 0$. By assumption (2.2) the initial value $G(U_i)$ is finite. We decompose Ω into

$$\Omega_+(s) := \{x \in \Omega : u_i(s,x) \ge u_i^*(x)\}, \quad \Omega_-(s) := \{x \in \Omega : u_i(s,x) < u_i^*(x)\}.$$

On Ω_+ reaction terms multiplied by the test function vanish. Since $(a^*, v_0^*) \in \mathcal{M}$, $a_i^* = u_i^*/\overline{u}_i \mathrm{e}^{q_i v_0^*}$, $i = 1, \dots, m$, and $\alpha - \beta \in \mathcal{S}$, $\zeta^* \in \mathcal{S}^\perp$ we have in Ω_-

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

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 $[0,R]^m \times [-R,R]$, $R > 0$, and at $(1, \dots, 1, 0)$ its value is zero. Since $u_j/\overline{u}_j$, $j = 1, \dots, m$, and v_0 are globally bounded (see (5.14) and Corollary 3.1) we get f.a.a. $s \in \mathbb{R}_+$

$$\big|\mathrm{e}^{\alpha\cdot\zeta(s)} - \mathrm{e}^{\beta\cdot\zeta(s)}\big|\, |\alpha_i - \beta_i| \le c \Big(\sum_{j=1}^m |u_j(s)/u_j^* - 1| + |v_0(s) - v_0^*| \Big) \quad \text{a.e. on } \Omega_-.$$

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

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

Again the term in the brackets is Lipschitz continuous in $(u_1/u_1^*,\dots,u_m/u_m^*,v_0-v_0^*)$ on $[0,R]^m\times[-R,R]$, $R>0$, at $(1,\dots,1,0)$ its value is zero and f.a.a. $s\in\mathbb{R}_+$

$$
(\mathrm{e}^{\alpha\cdot\zeta(s)} - \mathrm{e}^{\beta\cdot\zeta(s)})(\alpha_i-\beta_i)\,\frac{u_i^*}{u_i(s)} \le c\Big(\sum_{j=1}^{m}|u_j(s)/u_j^*-1| + |v_0(s)-v_0^*|\Big) \quad \text{a.e. on } \Omega_-.
$$

Similar estimates are obtained for $\alpha_i < \beta_i$. The same arguments hold for the boundary terms. Applying (5.13) we continue estimate (5.15) by

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

From the definition of G we thus obtain that $\|z(\cdot)\|_{L^1}$ is bounded on $\mathbb{R}_+$. Since

$$
v_i^-(t) = \big(\ln\frac{u_i}{\overline{u}_i}\big)^-(t) \le z(t) + \big(\ln\frac{u_i^*}{\overline{u}_i}\big)^-
$$

the assertion of Lemma 5.1 follows. □

Theorem 5.5. *Let* (u,v) *be a solution of* (P) *and let* (5.14) *and* (5.11) *be fulfilled. Then there exists a constant* $c_{5.16}>0$ *depending only on the data such that*

$$
\|v_i^-(t)\|_{L^\infty} \le c_{5.16},\ \operatorname*{ess\,inf}_{x\in\Omega} u_i(t) \ge \operatorname*{ess\,inf}_{x\in\Omega}\overline{u}_i\,\mathrm{e}^{-c_{5.16}}\ \forall t\in\mathbb{R}_+,\ i=1,\dots,m. \tag{5.16}
$$

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 $z(t) := (\ln(u_i(t)/\overline{u}_i)+K)^-$ and K defined in Lemma 4.2 we obtain inequality (4.9) for all $t\in\mathbb{R}_+$, $i=1,\dots,m$, since $c_{4.9}$ does not depend on the length of the time interval. By Lemma 5.1 we therefore obtain the global boundedness of $\|z(t)\|_{L^\infty}$. The estimates for the boundary norms follow from (1.20). □

Corollary 5.3. *Let* (u,v) *be a solution of* (P) *and let* (5.14) *and* (5.16) *be fulfilled. Then by* [26, Theorem 5.1] *relation* (5.11) *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 5.6. *Let* (u, v) *be a solution of* (P) *and let* (5.14) *and* (5.16) *be fulfilled. Then there exist constants* c, $\lambda_p > 0$ *depending only on the data such that*

$$\sum_{i=0}^{m} \|u_i(t) - u_i^*\|_{L^p} \le c\,\mathrm{e}^{-\lambda_p t} \quad \forall\, t \ge 0,$$
$$\sum_{i=0}^{m} \|v_i(t) - v_i^*\|_{L^p} \le c\,\mathrm{e}^{-\lambda_p t} \quad \forall\, t \ge 0 \quad \text{where } p \in [1, +\infty).$$

Proof. Because of Corollary 5.3 the estimates (5.12) are valid. By (5.14), (2.12) and by (5.12) we obtain for $p \in [1, +\infty)$, $i = 1, \ldots, m$

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

Since by (5.12) $\|v_0(t) - v_0^*\|_{H^1} \le c\,\mathrm{e}^{-\lambda t/2}$ and by Corollary 3.1 $\|v_0(t) - v_0^*\|_{L^\infty} \le c$, $t \in \mathbb{R}_+$, we estimate

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

Under our assumptions we find

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

which together with the estimates (5.14) and (5.16) proves the second assertion. □

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 by the nondegeneracy requirement (5.9).

Theorem 5.7. *We assume* (2.1)–(2.5), (2.6) *and* (5.9). *Then there is a unique solution of* (P). *For this solution global estimates as in* (4.11) *and* (5.16) *are satisfied. Moreover the results on the asymptotic behaviour as in Theorem 5.4 and Theorem 5.6 are valid.*

6 Electro–diffusion systems with weakly nonlinear volume and boundary source terms

6.1 Formulation of the problem ($\mathrm{P_G}$)

In this section we are looking for a general existence result for a system of continuity equations with bounded Lipschitz continuous right hand sides and boundary terms coupled with the (possibly nonlinear, nonlocal) Poisson equation considered on arbitrarily fixed time intervals S. The purpose of such a result is that the solvability of more general equations of the form (1.5), (1.8) (for example with reactions of higher order) could be proved by means of our result if it is possible to regularize the reaction and boundary terms in a suitable way and to derive a priori estimates for this regularized problem which are independent of the regularization level.

We investigate such problems under the general assumptions (2.1)–(2.4) and replace the assumptions (2.5) and (2.6) by the following ones:

$$\left.\begin{array}{ll} \multicolumn{2}{l}{\text{For } \Sigma=\Omega,\Gamma,\ i=1,\dots,m, \text{ we have}} \\ \text{i)} & g_i^\Sigma\colon \Sigma\times\mathbb{R}^{m+1}\times\mathbb{R}\to\mathbb{R} \text{ satisfies the Carathéodory conditions,} \\ \text{ii)} & |g_i^\Sigma(x,y,z)-g_i^\Sigma(x,\overline{y},\overline{z})| \le L_\Sigma \max\left(\max_{i=0,\dots,m}|y_i-\overline{y}_i|, |z-\overline{z}|\right) \\ & \text{f.a.a. } x\in\Sigma,\ \forall (y,z),\ (\overline{y},\overline{z})\in\mathbb{R}^{m+2}, \\ \text{iii)} & \sum_{i=1}^m g_i^\Sigma(x,y,z)(y_i+q_iy_0)\ge 0 \ \text{ f.a.a. } x\in\Sigma,\ \forall (y,z)\in\mathbb{R}^{m+2}, \\ \text{iv)} & |g_i^\Sigma(x,y,z)|\le c^\Sigma \ \text{ f.a.a. } x\in\Sigma,\ \forall (y,z)\in\mathbb{R}^{m+2}, \\ \text{v)} & g_i^\Sigma(x,y,z)\le c^\Sigma \mathrm{e}^{y_i} \ \text{ f.a.a. } x\in\Sigma,\ \forall (y,z)\in\mathbb{R}^{m+2} \text{ with } y_i\le 0. \end{array}\right\} \tag{6.1}$$

We consider the problem

$$\left.\begin{array}{c} u'(t)+A_G(v(t),v(t))=0,\ u(t)=Ev(t) \text{ f.a.a. } t\in S,\ u(0)=U, \\ u\in H^1(S,X^*),\ v\in L^2(S,X)\cap L^\infty(S,L^\infty(\Omega,\mathbb{R}^{m+1})) \end{array}\right\} \tag{$\mathrm{P_G}$}$$

where E is defined as in Subsection 2.2 and the operator $A_G\colon W\times X\longrightarrow X^*$ now contains modified volume and boundary terms g_i^Ω, g_i^Γ and is given by

$$\begin{aligned} \langle A_G(w,v),\overline{v}\rangle := &\int_\Omega \sum_{i=1}^m \left\{D_i\overline{u}_i\mathrm{e}^{w_i}\nabla\zeta_i\cdot\nabla\overline{\zeta}_i \ + g_i^\Omega(\cdot,w,\pi(w_0))\,\overline{\zeta}_i\right\}\mathrm{d}x \\ &+\int_\Gamma\sum_{i=1}^m g_i^\Gamma(\cdot,w,\pi(w_0))\,\overline{\zeta}_i\,\mathrm{d}\Gamma,\quad \overline{v}\in X, \end{aligned}$$

where $\zeta_i=v_i+q_iv_0,\ \overline{\zeta}_i=\overline{v}_i+q_i\overline{v}_0,\ i=1,\dots,m$.

6.2 The regularized problem ($\mathrm{P_M}$)

To prove existence for ($\mathrm{P_G}$) we investigate a regularized problem ($\mathrm{P_M}$) which arises from ($\mathrm{P_G}$) by cutting the nonlinearities in front of the diffusion terms and in the statistics and adding some regularizing term vanishing under the cutting level. We show the solvability of ($\mathrm{P_M}$) and find a priori estimates not depending on the cutting level M. Thus a solution of ($\mathrm{P_M}$) is a solution of ($\mathrm{P_G}$) if one had taken the cutting level sufficiently large. We fix $M \geq M^* \geq 1$ with

$$\overline{u}_i \mathrm{e}^{-M^*} \leq U_i \leq \overline{u}_i \mathrm{e}^{M^*}, \quad i = 1, \dots, m. \tag{6.2}$$

We denote by P_M the projection from $\mathbb{R}$ onto $[-M, M]$,

$$P_M(y) := \begin{cases} -M & \text{if } \; y < -M, \\ y & \text{if } \; y \in [-M, M], \\ M & \text{if } \; y > M, \end{cases}$$

and define operators $\mathcal{E}_M \colon X \times X \longrightarrow X^*$, $E_M \colon X \longrightarrow X^*$ and $A_M \colon X \times X \longrightarrow X^*$ by

$$\langle \mathcal{E}_M(w,v), \overline{v} \rangle := \langle E_0 v_0, \overline{v}_0 \rangle + \int_\Omega \sum_{i=1}^m \overline{u}_i \mathrm{e}^{P_M w_i}\, \overline{v}_i \,\mathrm{d}x, \quad \overline{v} \in X, \quad E_M v := \mathcal{E}_M(v,v),$$

$$\begin{aligned} \langle A_M(w,v), \overline{v} \rangle := \int_\Omega \sum_{i=1}^m \Big\{ & D_i \overline{u}_i \mathrm{e}^{P_M w_i} \nabla \zeta_i \cdot \nabla \overline{\zeta}_i + C_M (\zeta_i - P_M w_i - P_M(q_i w_0))\, \overline{\zeta}_i \\ & + g_i^\Omega(\cdot, w, \pi(w_0))\, \overline{\zeta}_i \Big\} \,\mathrm{d}x + \int_\Gamma \sum_{i=1}^m g_i^\Gamma(\cdot, w, \pi(w_0))\, \overline{\zeta}_i \,\mathrm{d}\Gamma, \quad \overline{v} \in X \end{aligned}$$

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

$$C_M := 2 \max \{ L_\Omega (m+1) + 2 c_{1.19}{}^2 \, L_\Gamma{}^2 (m+1)^2 \delta_M{}^{-1}, \delta_M \},$$

$c_{1.19}$ comes from the trace inequality (1.19), and $\delta_M > 0$ is fixed such that

$$\delta_M \leq D_i \overline{u}_i \mathrm{e}^{-M} \text{ f.a.a. } x \in \Omega, \; i = 1, \dots, m.$$

We are looking for solutions of the regularized problem

$$\left. \begin{aligned} u'(t) + A_M(v(t), v(t)) = 0, \; u(t) = E_M v(t) \text{ f.a.a. } t \in S, \; u(0) = U, \\ u \in H^1(S, X^*), \; v \in L^2(S, X). \end{aligned} \right\} \tag{$\mathrm{P_M}$}$$

6.3 A priori estimates for solutions of ($\mathrm{P_M}$)

First, let us note that assertions like in Remark 2.8 and Remark 2.9 are valid. Especially it holds $u_i(t) = \overline{u}_i \mathrm{e}^{P_M v_i(t)}$ in $L^\infty(\Omega)$ for all $t \in \mathbb{R}_+$. Energy estimates as in Section 3.3 can be obtained, too. We define regularized energy functionals $\Phi_M \colon X \longrightarrow \mathbb{R}$,

$$\Phi_M(v) := \int_\Omega \Big\{ \tfrac{\varepsilon}{2} |\nabla v_0|^2 + \int_0^{v_0} e_0(y) \,\mathrm{d}y + \sum_{i=1}^m \overline{u}_i \int_0^{v_i} \mathrm{e}^{P_M y} \,\mathrm{d}y \Big\} \,\mathrm{d}x + \int_{\Gamma_N} \tfrac{\tau}{2} \left(v_0 - \pi(v_0)\right)^2 \mathrm{d}\Gamma,$$

and $F_M := \Phi_M^*$. It holds $\partial \Phi_M(v) = E_M v$. Thus, if $u = E_M v$, $v \in X$, then

$$\begin{aligned} F_M(u) = & \langle E_M v, v \rangle - \Phi_M(v) \\ = & \int_\Omega \Big\{ \tfrac{\varepsilon}{2} |\nabla v_0|^2 + \phi_0(v_0) + \sum_{i=1}^m \big(u_i (\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i \big) \Big\} \,\mathrm{d}x + \int_{\Gamma_N} \tfrac{\tau}{2} (v_0 - \pi(v_0))^2 \,\mathrm{d}\Gamma. \end{aligned}$$

Let (u,v) be a solution of $(\mathrm{P_M})$ with M fulfilling (6.2). Then $v(t)\in\partial F_M(u(t))$ for a.a. $t\in S$. Because of $(\zeta_i-P_Mv_i-P_M(q_iv_0))\zeta_i\ge 0$ and the property (6.1), iii) of g_i^Σ we have $\langle A_M(v,v),v\rangle\ge 0$ and we can conclude by the Brézis formula (see [6]) that

$$F_M(u(t))+\int_0^t\langle A_M(v,v),v\rangle\,\mathrm{d}s\le F_M(U)=F(U)\le c\quad\forall t\in S$$

independently of M. Note, that by Lemma 3.2 and (6.2) the values for $F(U)$ and $F_M(U)$ coincide. With (2.7), (2.8) we find by the definition of F_M that the norms $\|v_0(t)\|_{H^1}$ and $\|u_i(t)\ln u_i(t)\|_{L^1}$ for $t\in S$ are bounded independently of M. Thus $\|u_0(t)\ln|u_0(t)|\|_{L^1}\le c$ for $t\in S$ and the relations (3.1) and (3.2) guarantee independently of M the estimates

$$\begin{aligned}&\|v_0(t)\|_{L^\infty},\ \|v_0(t)\|_{L^\infty(\Gamma)},\ |\pi(v_0(t))|\le c_{6.3},\\&\|v_0(t)\|_{W^{1,q}}\le c\Big(\sum_{i=1}^m\|u_i(t)\|_{L^{2q/(2+q)}}+1\Big)\ \forall t\in S.\end{aligned}\tag{6.3}$$

Lemma 6.1. *We suppose the assumptions* (2.1)–(2.4) *and* (6.1) *to be fulfilled. Let* $M\ge\max\{c_{6.3}\max_{i=1,\dots,m}|q_i|,M^*\}$. *Then there exists a constant* $c>0$ *not depending on* M *such that*

$$\|u_i(t)\|_{L^2}\le c\quad\forall t\in S,\ i=1,\dots,m,$$

for any solution (u,v) *of* $(\mathrm{P_M})$.

Proof. The proof is based on the ideas of Lemma 4.1. Since we have for any solution (u,v) of $(\mathrm{P_M})$ and for $K\ge\max\{1,\|U_1/\overline{u}_1\|_{L^\infty},\dots,\|U_m/\overline{u}_m\|_{L^\infty}\}$ that

$$(\zeta_i-P_Mv_i-P_M(q_iv_0))\Big(\frac{u_i}{\overline{u}_i}-K\Big)^+=(v_i-P_Mv_i))\Big(\frac{u_i}{\overline{u}_i}-K\Big)^+\ge 0$$

we can omit this term in our estimates. Additionally, taking into account that now $u_i=\overline{u}_i\mathrm{e}^{P_Mv_i}$ and that by assumption (6.1), iv) all volume and boundary source terms may be estimated by c^Σ times the test function. According to relation (6.3) $\|\nabla v_0\|_{L^q}$ can be estimated in exactly the same way as in Lemma 4.1. □

Lemma 6.2. *We suppose the assumptions* (2.1)–(2.4) *and* (6.1) *to be fulfilled. Let* $M\ge\max\{c_{6.3}\max_{i=1,\dots,m}|q_i|,M^*\}$. *Then there exists a constant* $c_{6.4}>0$ *depending on the data, but not on* M, *such that*

$$\|u_i(t)/\overline{u}_i\|_{L^\infty}\le c_{6.4}\quad\forall t\in S,\ i=1,\dots,m,\tag{6.4}$$

for any solution (u,v) *of* $(\mathrm{P_M})$.

Proof. Having in mind the remarks in the proof of Lemma 6.1 concerning the regularized terms and the boundedness of the source terms g_i^Σ (cf. (6.1), iv)) the proof is the same as in Theorem 4.2. □

Lemma 6.3. *We suppose the assumptions* (2.1)–(2.4) *and* (6.1) *to be fulfilled. Let* $M\ge\max\{c_{6.3}\max_{i=1,\dots,m}|q_i|,\ln(c_{6.4}+1),M^*\}$. *Then there exists an increasing function* $d_{6.5}$ *depending on the data, but not on* M, *such that*

$$\|\ln(u_i(t)/\overline{u}_i)\|_{L^\infty}\le d_{6.5}(T)\quad\forall t\in S,\ i=1,\dots,m,\tag{6.5}$$

for any solution (u,v) *of* $(\mathrm{P_M})$.

Proof. We apply the techniques of the proofs of Theorem 4.3, Lemma 4.2 and Lemma 4.3. Again we set $z = (\ln(u_i/\overline{u}_i) + K)^-$ with K from Lemma 4.2. Due to the choice of M for any solution of $(\mathrm{P_M})$ it holds $q_i v_0 = P_M(q_i v_0)$ and $v_i \le P_M v_i$ (see (6.3) and (6.4)). Therefore it follows that

$$-(\zeta_i - P_M v_i - P_M(q_i\, v_0))\frac{\overline{u}_i}{u_i} z^{p-1} \ge 0$$

and this term can be omitted in the estimates. If $z > 0$ then it holds $\mathrm{e}^{v_i} \le \mathrm{e}^{P_M v_i} = u_i/\overline{u}_i$ and $v_i \le 0$. Therefore we obtain from (6.1), v) the relation

$$g_i^\Sigma \frac{\overline{u}_i}{u_i}\, z^{p-1} \le c^\Sigma\, \mathrm{e}^{v_i}\, \frac{\overline{u}_i}{u_i}\, z^{p-1} \le c^\Sigma\, z^{p-1}, \quad \Sigma = \Omega, \Gamma.$$

Thus the estimates of Lemma 4.2 remain true, and we can continue to argue as in the proofs of Theorem 4.3 and Lemma 4.3. □

6.4 Solvability of $(\mathrm{P_M})$

For fixed M, we use a time discretization scheme to show the existence of a solution of $(\mathrm{P_M})$. For $n \in \mathbb{N}$ let $h_n := T/n$ and $S_n^j :=](j-1)h_n, jh_n]$. If V is any Banach space we denote by $C_n(S, V)$ the space of all functions $u\colon]0,T] \longrightarrow V$ which are constant on each of the intervals S_n^j. The value of $u \in C_n(S, V)$ on S_n^j is denoted by u^j. We define the operators

$$\begin{aligned}
&\Delta_n : C_n(S, X^*) \longrightarrow C_n(S, X^*),\; K_n : C_n(S, X^*) \longrightarrow C(S, X^*),\\
&(\Delta_n u)^j := \frac{1}{h_n}(u^j - u^{j-1}),\\
&(K_n v)(t) := \frac{1}{h_n}\Big((t_n^j - t)u^{j-1} + (t - t_n^{j-1})u^j\Big) \quad \forall t \in S_n^j
\end{aligned}$$

where $u^0 := U$ is the initial value of problem $(\mathrm{P_G})$. Obviously, $(K_n u)' = \Delta_n u$. For $n \in \mathbb{N}$ we investigate the problem

$$\left.\begin{aligned}
\Delta_n u_n(t) + A_M(v_n(t), v_n(t)) = 0,\; u_n(t) = E_M v_n(t)\; \forall t \in (0,T],\\
v_n \in C_n(S, X).
\end{aligned}\right\} \qquad (\mathrm{P_{Mn}})$$

Remark 6.1. As in Remark 2.8 for solutions of $(\mathrm{P_{Mn}})$ it holds that

$$u_{n0}(t) = \sum_{i=1}^m q_i u_{ni}(t)|_H \;\text{ in } H^* \quad \forall t \in S. \tag{6.6}$$

Lemma 6.4. *We assume* (2.1)–(2.4) *and* (6.1). *Then for every $n \in \mathbb{N}$ there exists at least one solution of* $(\mathrm{P_{Mn}})$. *Furthermore*

$$\sup_{n\in\mathbb{N}} \Big\{ \|v_n\|_{L^2(S,X)} + \|K_n u_n\|_{C(S,Y)} + \|K_n u_n\|_{H^1(S,X^*)} \Big\} < \infty. \tag{6.7}$$

Proof. 1. We show that for given $u^{j-1} \in X^*$, $h_n \in \mathbb{R}_+$, there exists a solution $(u^j, v^j) \in X^* \times X$ of the problem

$$u^j + h_n A_M(v^j, v^j) = u^{j-1}, \quad u^j = E_M v^j. \tag{6.8}$$

Let $B : X \to X^*$ be defined by $B(v) := E_M v + h_n\, A_M(v,v)$. Using the decomposition $B(v) = \mathcal{B}(v,v)$ with

$$\mathcal{B}(w,v) := \mathcal{E}_M(w,v) + h_n\, A_M(w,v),\ \ (w,v) \in X \times X,$$

we easily find that B is a coercive operator of variational type (cf. [48]). By [48, p. 182] the problem (6.8) has at least one solution.

2. Next, we prove estimates for the solutions (u_n, v_n) of $(\mathrm{P_{Mn}})$. Since for $t > 0$ it holds $u_n(t) = E_M v_n(t) \in \partial\Phi_M(v_n(t))$ we have $v_n(t) \in \partial F_M(u_n(t))$ and

$$\langle u_n(t) - \widetilde{u}, v_n(t)\rangle \geq F_M(u_n(t)) - F_M(\widetilde{u}) \quad \forall \widetilde{u} \in X^* \quad \forall t \in (0,T].$$

Therefore, for $l = 1, \ldots, n$,

$$\begin{aligned} F_M(u_n^l) - F_M(U) &= \sum_{j=1}^{l} F_M(u_n^j) - F_M(u_n^{j-1}) \leq \sum_{j=1}^{l} \langle u_n^j - u_n^{j-1}, v_n^j\rangle \\ &= -\, h_n \sum_{j=1}^{l} \langle A_M(v_n^j, v_n^j), v_n^j\rangle \leq -h_n \sum_{j=1}^{l} \big(c_M \sum_{i=1}^{m} \|\zeta_{ni}^j\|_{H^1}^2 - C_M\big). \end{aligned}$$

Because of the definition of F_M, (2.7) and (2.8) we obtain that

$$\sup_{n\in\mathbb{N}} \|v_{n0}\|_{L^\infty(S,H^1)},\ \sup_{n\in\mathbb{N}} \|\zeta_n\|_{L^2(S,(H^1)^m)},\ \sup_{n\in\mathbb{N}} \|v_n\|_{L^2(S,X)} < \infty.$$

Thus, from $\Delta_n u_n = -A_M(v_n, v_n)$ we get

$$\sup_{n\in\mathbb{N}} \|\Delta_n u_n\|_{L^2(S,X^*)} < \infty.$$

The equation $u_n = E_M v_n$ forces that $u_{ni} = \overline{u}_i \mathrm{e}^{P_M v_{ni}}$ in $L^\infty(S, L^2)$, $i = 1, \ldots, m$. Having in mind (6.6) we state $u_{n0} = \sum_{i=1}^{m} q_i u_{ni}$ in $L^\infty(S, L^2)$ and we find that $K_n u_n \in C(S,Y)$ and

$$\sup_{n\in\mathbb{N}} \|K_n u_n\|_{C(S,Y)} < \infty.$$

Since $\|K_n u_n\|_{L^2(S,X^*)} \leq c\,\|K_n u_n\|_{L^2(S,Y)} \leq c\,\|K_n u_n\|_{C(S,Y)}$ and $\Delta_n u_n = (K_n u_n)'$ we obtain

$$\sup_{n\in\mathbb{N}} \|K_n u_n\|_{H^1(S,X^*)} < \infty$$

which completes the proof. □

Lemma 6.5. *We assume* (2.1)–(2.4) *and* (6.1). *Then there exists at least one solution of* $(\mathrm{P_M})$.

Proof. 1. Let, for $n \in \mathbb{N}$, (u_n, v_n) be a solution of $(\mathrm{P_{Mn}})$. Because of (6.7) there exist $v \in L^2(S,X)$, $u \in H^1(S,X^*) \cap L^2(S,Y)$ such that, at least for subsequences, $v_n \rightharpoonup v$ in $L^2(S,X)$, $K_n u_n \rightharpoonup u$ in $H^1(S,X^*)$, $L^2(S,Y)$. In particular, $K_n u_n \rightharpoonup u$, $\Delta_n u_n \rightharpoonup u'$ in $L^2(S,X^*)$. If $t \in S$, $\overline{v} \in X$ are fixed the mapping

$$w \mapsto \langle w(t), \overline{v}\rangle_X \quad \text{for } w \in H^1(S,X^*)$$

defines a continuous linear functional on $H^1(S,X^*)$. Therefore

$$K_n u_n(t) \rightharpoonup u(t) \text{ in } X^* \quad \forall t \in S. \tag{6.9}$$

We find that
$$\|u_n - K_n u_n\|^2_{L^2(S,X^*)} \le h_n^2 \|\Delta_n u_n\|^2_{L^2(S,X^*)} \to 0.$$
Thus, without loss of generality, we may assume that
$$(K_n u_n - u_n)(t) \to 0 \text{ in } X^*, \quad u_n(t) \rightharpoonup u(t) \text{ in } X^* \quad \text{f.a.a. } t \in S.$$
Since $\|K_n u_n(t)\|_Y$, $\|u_n(t)\|_Y \le c$ for all $t \in S$ (see (6.7)) we conclude that
$$K_n u_n(t) \rightharpoonup u(t) \text{ in } Y \ \forall t \in S, \quad u_n(t) \rightharpoonup u(t) \text{ in } Y \quad \text{f.a.a. } t \in S. \tag{6.10}$$
Because of $K_n u_n(0) = U$ we have $u(0) = U$.

2. From $u_{ni} = \overline{u}_i \, \mathrm{e}^{P_M v_{ni}}$ we find by (6.7) that the sequences $(u_{ni}/\overline{u}_i)_{n\in\mathbb{N}}$, $i = 1,\dots,m$, are bounded in $L^2\left(S, H^1\right)$. From (6.10) we have that
$$u_{ni}(t)/\overline{u}_i \rightharpoonup u_i(t)/\overline{u}_i \text{ in } L^2 \text{ f.a.a. } t \in S,\ i = 1,\dots,m. \tag{6.11}$$
Thus, applying Lebesgue's theorem
$$u_{ni}/\overline{u}_i \rightharpoonup u_i/\overline{u}_i \text{ in } L^2(S,L^2), \quad i = 1,\dots,m. \tag{6.12}$$
Now we use the inequality (6.40) in [46, p. 529]:

For all $\epsilon > 0$ there is an $N_\epsilon > 0$ such that
$$\|w\|^2_{L^2} \le \sum_{j=1}^{N_\epsilon} (w,\psi_j)^2_{L^2} + \epsilon \|w\|^2_{H^1} \quad \forall w \in H^1(\Omega) \quad (\{\psi_j\}_{j\in\mathbb{N}} \text{ ON-base in } L^2).$$

We integrate this inequality for $w := u_{ni}/\overline{u}_i - u_{li}/\overline{u}_i$ over $[0,T]$. Using (6.11), the boundedness of $u_n(t)$ in Y for $t \in S$, $n \in \mathbb{N}$, Lebesgue's theorem and the boundedness of $u_{ni}/\overline{u}_i$ in $L^2\left(S, H^1\right)$, we find that $\{u_{ni}/\overline{u}_i\}$ is a Cauchy sequence in $L^2(S,L^2)$. By (6.12) we get
$$u_{ni}/\overline{u}_i \to u_i/\overline{u}_i, \quad u_{ni} \to u_i \text{ in } L^2(S,L^2), \quad i = 1,\dots,m. \tag{6.13}$$
Together with $K_n u_n - u_n \to 0$ in $L^2\left(S, X^*\right)$ this leads to
$$(K_n u_n)_i \to u_i \text{ in } L^2(S,(H^1)^*), \quad i = 1,\dots,m. \tag{6.14}$$

3. Because of (6.6) and (6.13) we obtain from $u_{n0} \rightharpoonup u_0$ in $L^2\left(S, H^*\right)$ and $\sum_{i=1}^m q_i u_{ni} \to \sum_{i=1}^m q_i u_i$ in $L^2(S,(H^1)^*)$ that
$$u_{n0} \to u_0 = \sum_{i=1}^m q_i u_i|_H \ \text{ in } L^2(S,H^*),\ u_n \to u,\ K_n u_n \to u \text{ in } L^2\left(S, X^*\right).$$

4. Let $\tilde u \in Y$ with $F_M(\tilde u) < +\infty$ and S_1 be any subinterval of S. Since for $t \in (0,T]$, $u_n(t) = E_M v_n(t)$ we have $v_n(t) \in \partial F_M(u_n(t))$. Using $v_n \rightharpoonup v$ in $L^2\left(S, X\right)$, $u_n \to u$ in $L^2\left(S, X^*\right)$ and the lower semicontinuity of F_M on X^* we conclude that
$$\begin{aligned}\int_{S_1} \langle \tilde u - u(t), v(t)\rangle \,\mathrm{d}t &= \lim_{n\to\infty} \int_{S_1} \langle \tilde u - u_n(t), v_n(t)\rangle \,\mathrm{d}t \\ &\le \limsup_{n\to\infty} \int_{S_1} \{F_M(\tilde u) - F_M(u_n(t))\} \,\mathrm{d}t \\ &\le \int_{S_1} \{F_M(\tilde u) - F_M(u(t))\} \,\mathrm{d}t.\end{aligned}$$

Because S_1 was an arbitrary subinterval we obtain

$$\langle \tilde{u} - u(t), v(t)\rangle \le F_M(\tilde{u}) - F_M(u(t)) \quad \text{f.a.a. } t \in S$$

which means $v(t) \in \partial F_M(u(t))$ f.a.a. $t \in S$. Thus $u(t) \in \partial\Phi_M(v(t)) = E_M v(t)$ f.a.a. $t \in S$ and

$$F_M(u(t)) - F_M(U) = \int_0^t \langle u'(s), v(s)\rangle \,\mathrm{d}s \quad \forall t \in S. \tag{6.15}$$

5. By the Lipschitz continuity of E_0^{-1} and by $u_n \to u$ in $L^2(S, X^*)$ we find

$$\|v_{n0} - E_0^{-1}u_0\|^2_{L^2(S,H^1)} = \|E_0^{-1}u_{n0} - E_0^{-1}u_0\|^2_{L^2(S,H^1)} \le c\|u_{n0} - u_0\|^2_{L^2(S,H^*)} \to 0.$$

On the other hand, we have $v_n \rightharpoonup v$ in $L^2(S, X)$ which implies $E_0^{-1}u_0 = v_0$ and $v_{n0} \to v_0$ in $L^2(S, H^1)$, $v_0 \in L^2(S, H)$.

6. In what follows f_n denotes terms with $\lim_{n\to\infty} f_n = 0$. Since $v_n \rightharpoonup v$ in $L^2(S, X)$, $\Delta_n u_n \rightharpoonup u'$ in $H^1(S, X^*)$ we obtain from ($\mathrm{P_{Mn}}$) and (6.15)

$$\begin{aligned} 0 =& \int_S \langle \Delta_n u_n + A_M(v_n, v_n), v_n - v\rangle \,\mathrm{d}s \\ =& f_n + \int_S \langle \Delta_n u_n, v_n\rangle - \langle u', v\rangle + \langle A_M(v_n, v_n) - A_M(v, v), v_n - v\rangle \,\mathrm{d}s \\ =& f_n + F_M(u_n(T)) - F_M(u(T)) + \int_S \langle A_M(v_n, v_n) - A_M(v, v), v_n - v\rangle \,\mathrm{d}s. \end{aligned} \tag{6.16}$$

We split the terms with A_M in two parts and estimate each part separately. Firstly,

$$\begin{aligned} &\langle A_M(v_n, v_n) - A_M(v_n, v), v_n - v\rangle \\ &\quad = \sum_{i=1}^m \int_\Omega \Big\{ D_i \overline{u}_i \mathrm{e}^{P_M v_n} |\nabla(\zeta_{ni} - \zeta_i)|^2 + C_M(\zeta_{ni} - \zeta_i)^2 \Big\} \,\mathrm{d}x \\ &\quad \ge \sum_{i=1}^m \Big\{ \delta_M \|\nabla(\zeta_{ni} - \zeta_i)\|^2_{L^2} + C_M\|\zeta_{ni} - \zeta_i\|^2_{L^2} \Big\}. \end{aligned} \tag{6.17}$$

Secondly,

$$\begin{aligned} &\int_S \langle A_M(v_n, v) - A_M(v, v), v_n - v\rangle \,\mathrm{d}s = \\ &\int_S \Big(\int_\Omega \sum_{i=1}^m \Big\{ D_i(u_{ni} - u_i)\nabla\zeta_i \nabla(\zeta_{ni} - \zeta_i) + (g_i^\Omega(\cdot, v_n, \pi(v_{n0})) - g_i^\Omega(\cdot, v, \pi(v_0)))(\zeta_{ni} - \zeta_i) \\ &\qquad - C_M(P_M v_{ni} - P_M v_i + P_M(q_i v_{n0}) - P_M(q_i v_0))(\zeta_{ni} - \zeta_i) \Big\} \,\mathrm{d}x \\ &\quad + \int_\Gamma \sum_{i=1}^m (g_i^\Gamma(\cdot, v_n, \pi(v_{n0})) - g_i^\Gamma(\cdot, v, \pi(v_0)))(\zeta_{ni} - \zeta_i) \,\mathrm{d}\Gamma \Big) \,\mathrm{d}s. \end{aligned}$$

By (6.13) and $v_n \rightharpoonup v$ in $L^2(S, X)$ we conclude that $P_M v_{ni} \to P_M v_i$, $P_M(q_i v_{n0}) \to P_M(q_i v_0)$ in $L^2(S, L^2)$, $\zeta_{ni} \rightharpoonup \zeta_i$ in $L^2(S, H^1)$, $(u_{ni} - u_i)\nabla\zeta_i \to 0$ in $L^2(S, L^2)$, $i = 1, \dots, m$. Thus we find that the gradient terms as well as the terms with C_M tend to zero if $n \to \infty$. Moreover, since by assumption (6.1), ii) the functions $g_i^\Sigma(x, \cdot, \cdot)$ are uniformly Lipschitz continuous and

$|v_{ni} - v_i| \leq |\zeta_{ni} - \zeta_i| + |q_i||v_{n0} - v_0|$, $|\pi(v_{n0}) - \pi(v_0)| \leq c_\pi \|v_{n0} - v_0\|_{H^1}$, we obtain by the boundedness of $\|\zeta_{ni} - \zeta_i\|_{L^2(S,H^1)}$ and $v_{n0} \to v_0$ in $L^2(S, H^1)$ that

$$\int_S \langle A_M(v_n, v) - A_M(v,v), v_n - v\rangle \,\mathrm{d}s \geq f_n -$$
$$\int_S \sum_{i=1}^m \Big\{ L_\Omega(m+1)\|\zeta_{ni} - \zeta_i\|_{L^2}^2 + \tfrac{2}{\delta_M} c_{1.19}^2 L_\Gamma^2 (m+1)^2 \|\zeta_{ni} - \zeta_i\|_{L^2}^2 + \tfrac{\delta_M}{2}\|\zeta_{ni} - \zeta_i\|_{H^1}^2 \Big\} \,\mathrm{d}s.$$

Because of the choice of C_M from (6.17) and the last inequality we get

$$\int_S \langle A_M(v_n, v_n) - A_M(v,v), v_n - v\rangle \,\mathrm{d}s \geq f_n + \tfrac{\delta_M}{2} \sum_{i=1}^m \|\zeta_{ni} - \zeta_i\|_{L^2(S,H^1)}^2. \tag{6.18}$$

Inserting this in (6.16) we obtain

$$F_M(u(T)) - F_M(u_n(T)) \geq f_n + \tfrac{\delta_M}{2} \sum_{i=1}^m \|\zeta_{ni} - \zeta_i\|_{L^2(S,H^1)}^2.$$

Since F_M is weakly lower semicontinuous on X^*, $K_n u_n(t) \rightharpoonup u(t)$ in X^* for all $t \in S$ (see (6.9)) and $K_n u_n(T) = u_n(T)$, $n \in \mathbb{N}$, we find

$$\liminf_{n\to\infty} F_M(u_n(T)) \geq F_M(u(T)).$$

Thus, passing to the limit we obtain

$$\limsup_{n\to\infty} \sum_{i=1}^m \|\zeta_{ni} - \zeta_i\|_{L^2(S,H^1)}^2 \leq 0.$$

This means $\zeta_{ni} \to \zeta_i$ in $L^2(S,H^1)$, $i = 1, \dots, m$. Combining this result with $v_{n0} \to v_0$ in $L^2(S,H)$ we get $v_n \to v$ in $L^2(S,X)$.

7. The last convergence result implies immediately that $A_M(v_n, v_n) \to A_M(v,v)$ in $L^2(S,X^*)$. From the first step we know that $A_M(v_n,v_n) = -\Delta_n u_n \rightharpoonup -u'$ in $L^2(S,X^*)$. Thus $u' + A_M(v,v) = 0$ a.e. on $\mathbb{R}_+$, the validity of $u = E_M v$ a.e. on $\mathbb{R}_+$ was stated in step 4, and so the proof is complete. □

6.5 Existence and uniqueness result

Theorem 6.1. *We assume* (2.1)–(2.4) *and* (6.1). *Then there exists a unique solution of* ($\mathrm{P_G}$).

Proof. Let (u,v) be a solution of ($\mathrm{P_M}$) (see Lemma 6.5) with M satisfying

$$M \geq \max\{c_{6.3} \max_{i=1,\dots,m} |q_i|, \ln(c_{6.4}+1), d_{6.5}(T), M^*\}$$

(see (6.3), Lemma 6.2, Lemma 6.3, (6.2)). Then we have $v_i = P_M v_i$, $q_i v_0 = P_M(q_i v_0)$ a.e. on $S \times \Omega$, $i = 1, \dots, m$, and therefore (u,v) is a solution of ($\mathrm{P_G}$), too. Uniqueness can be proved as in Theorem 3.1 now using the uniform Lipschitz continuity of $g_i^\Sigma(x,\cdot,\cdot)$, $\Sigma = \Omega, \Gamma$, $i = 1, \dots, m$. □

7 Relations between the basic model and the reduced model

7.1 Preliminaries

In this section we investigate relations between the basic model (1.5), (1.8) introduced in Subsection 1.1 (where the kinetic coefficients in (1.14) are finite, but very large) and the reduced model (1.5**), (1.8**) derived in Subsection 1.2 (under the assumption that these kinetic coefficients tend to infinity). For this purpose all quantities, spaces and operators for the reduced model are marked by a '$\sim$' whereas all quantities belonging to the basic model have the same notation used in the previous sections. The common weak formulation of both problems has been given in Subsection 2.2. In Table 1 we summarize once more, how relevant quantities have to be chosen in order to get the basic model and the reduced model, respectively. As in the previous sections we suppose that for the data of the basic model (P) at least the assumptions (2.1)–(2.5) are fulfilled. From this one easily obtains corresponding properties for the data of the reduced problem ($\widetilde{\mathrm{P}}$) what is summarized in the following lemma.

Lemma 7.1. *The assumptions* (2.1)–(2.5) *for* (P) *ensure the validity of the corresponding properties* (2.1)–(2.5) *for* ($\widetilde{\mathrm{P}}$). *If for* (P) *additionally* (2.6) *is fulfilled this property is carried over to the reduced problem.*

	basic problem (P)	reduced problem ($\widetilde{\mathrm{P}}$)
number of species	m	$\widetilde{m} = m - 2$
densities	$u_0 = \sum_{i=1}^{m} q_i u_i$	$\widetilde{u}_0 = \sum_{i=1}^{\widetilde{m}} q_i \widetilde{u}_i$
	$u_i,\ i = 1, \dots, m$	$\widetilde{u}_i,\ i = 1, \dots, \widetilde{m}$
potentials	$v_0,\ v_i,\ i = 1, \dots, m$	$\widetilde{v}_0,\ \widetilde{v}_i,\ i = 1, \dots, \widetilde{m}$
Hilbert spaces	$H = H_0^1(\Omega \cup \Gamma_N)$	$\widetilde{H} = H_0^1(\Omega \cup \Gamma_N) + \mathbb{R}$
	$X = H \times H^1(\Omega, \mathbb{R}^m)$	$\widetilde{X} = \widetilde{H} \times H^1(\Omega, \mathbb{R}^{\widetilde{m}})$
continuity equations	$\mathcal{R}^\Sigma \subset \mathbb{Z}_+^m \times \mathbb{Z}_+^m$	$\widetilde{\mathcal{R}}^\Sigma \subset \mathbb{Z}_+^{\widetilde{m}} \times \mathbb{Z}_+^{\widetilde{m}}$ as in (1.4**)
	$R_{\alpha\beta}$ as in (1.4)	$\widetilde{R}_{\widetilde{\alpha}\widetilde{\beta}}$ as in (1.4**)
Poisson equation	$e_0(v_0) = \sum_{i=1}^{m} q_i U_i$	$\widetilde{e}_0(\widetilde{v}_0) = \sum_{i=1}^{m} q_i U_i + \overline{u}_{m-1}\, \mathrm{e}^{\widetilde{v}_0} - \overline{u}_m\, \mathrm{e}^{-\widetilde{v}_0}$
	$\pi(v_0) = 0$	$\widetilde{\pi}(\widetilde{v}_0) = \begin{cases} \lvert\Gamma_D\rvert^{-1} \int_{\Gamma_D} \widetilde{v}_0 \,\mathrm{d}\Gamma, & \lvert\Gamma_D\rvert \neq 0 \\ \lVert\tau\rVert_{L^1(\Gamma_N)}^{-1} \int_{\Gamma_N} \tau\, \widetilde{v}_0 \,\mathrm{d}\Gamma, & \lvert\Gamma_D\rvert = 0 \end{cases}$
initial values	$U_0 = \sum_{i=1}^{m} q_i U_i$	$\widetilde{U}_0 = \sum_{i=1}^{\widetilde{m}} q_i \widetilde{U}_i$
	$U_i,\ i = 1, \dots, m$	$\widetilde{U}_i = U_i,\ i = 1, \dots, \widetilde{m}$

Table 1: Overview on relevant quantities for the basic and the reduced model, respectively.

Remark 7.1. The result concerning the validity of (2.6) for $(\widetilde{\mathrm{P}})$ can be improved as follows. Assume that for (P) the reaction terms have the more general property

$$\max_{i=1,\dots,m-2}\Big\{(\mathrm{e}^{\alpha\cdot\zeta}-\mathrm{e}^{\beta\cdot\zeta})(\beta_i-\alpha_i)\Big\}\le c\,\mathrm{e}^{c(|\zeta_{m-1}|+|\zeta_m|)}\Big(\sum_{j=1}^{m-2}\mathrm{e}^{n_\Sigma\,\zeta_j}+1\Big)$$
$$\forall\zeta\in\mathbb{R}^m,\ \forall(\alpha,\beta)\in\mathcal{R}^\Sigma,\ \Sigma=\Omega,\Gamma,\ \text{with } n_\Omega=2,\ n_\Gamma=1,\ c>0$$

then for $(\widetilde{\mathrm{P}})$ the assumption (2.6) is fulfilled. Thus, for models including some special higher order reactions (of higher order with respect to *electrons* and *holes*) existence results can be obtained by the methods of this paper if the corresponding reduced form of the model is used.

Let us remember that the reduction of the model equations was carried out under the assumptions that for the basic model the relations (1.11) are fulfilled, that $q_{m-1}=-1$, $q_m=1$ and that the special reaction (1.13) is present. These assumptions imply

$$(0,\dots,0,1,1)\in\mathcal{S},\ q=(q_1,\dots,q_{m-2},-1,1)\in\mathcal{S}^\perp \tag{7.1}$$

and we shall suppose the properties (7.1) to be fulfilled in this section, too. By (7.1) we easily find that

$$\begin{aligned}&\text{if } \kappa=(\kappa_1,\dots,\kappa_m)\in\mathcal{S}^\perp \text{ then } \kappa_{m-1}=-\kappa_m,\\ &\kappa=\kappa_m\,q+\widehat{\kappa} \text{ with } \widehat{\kappa}\in\mathcal{S}^\perp,\ \widehat{\kappa}_{m-1}=\widehat{\kappa}_m=0.\end{aligned} \tag{7.2}$$

From the definition of $\widetilde{\mathcal{R}}^\Omega$, $\widetilde{\mathcal{R}}^\Gamma$ in (1.4**) we obtain

$$\widetilde{\mathcal{S}}=\Big\{\widetilde{\rho}\in\mathbb{R}^{\widetilde{m}}:\widetilde{\rho}_i=\rho_i,\ i=1,\dots,\widetilde{m},\ \rho\in\mathcal{S}\Big\},$$
$$\widetilde{\mathcal{S}}^\perp=\Big\{\widetilde{\kappa}\in\mathbb{R}^{\widetilde{m}}:(\widetilde{\kappa},0,0)\in\mathcal{S}^\perp\Big\}$$

and (7.2) ensures that

$$\kappa\in\mathcal{S}^\perp \text{ if and only if } \kappa=\kappa_m\,q+(\widetilde{\kappa},0,0) \text{ and } \widetilde{\kappa}\in\widetilde{\mathcal{S}}^\perp. \tag{7.3}$$

Finally, this implies that $\dim\widetilde{\mathcal{S}}^\perp=\dim\mathcal{S}^\perp-1$ and $\dim\widetilde{\mathcal{S}}=\dim\mathcal{S}-1$.

7.2 Reconstructed quantities

We do not expect that the kinetics of the reduced problem $(\widetilde{\mathrm{P}})$ and of the basic problem (P) coincide, but we shall show that some important properties are preserved nevertheless and that both problems are asymptotically equivalent in some sense. By (1.15), (1.16) and (1.17) we have a rule, how to compute from quantities related to the reduced model $(\widetilde{\mathrm{P}})$ new quantities related to the basic model (P). We will mark these reconstructed quantities with a '$\smile$'. Thus we define the vectors $\breve{u}=(\breve{u}_0,\dots,\breve{u}_m)$, $\breve{v}=(\breve{v}_0,\dots,\breve{v}_m)$ and $\breve{\zeta}=(\breve{\zeta}_1,\dots,\breve{\zeta}_m)$, $\breve{a}=(\breve{a}_1,\dots,\breve{a}_m)$ by

$i=0$	$i=1,\dots,m-2$	$i=m-1,m$
$\breve{u}_0=E_0\breve{v}_0$	$\breve{u}_i=\widetilde{u}_i$	$\breve{u}_i=\overline{u}_i\mathrm{e}^{-q_i\widetilde{v}_0}$
$\breve{v}_0=\widetilde{v}_0-\widetilde{\pi}(\widetilde{v}_0)$	$\breve{v}_i=\widetilde{v}_i$	$\breve{v}_i=-q_i\widetilde{v}_0$
	$\breve{\zeta}_i=\widetilde{\zeta}_i-q_i\widetilde{\pi}(\widetilde{v}_0)$	$\breve{\zeta}_i=-q_i\widetilde{\pi}(\widetilde{v}_0)$
	$\breve{a}_i=\widetilde{a}_i\mathrm{e}^{-q_i\widetilde{\pi}(\widetilde{v}_0)}$	$\breve{a}_i=\mathrm{e}^{-q_i\widetilde{\pi}(\widetilde{v}_0)}$

(7.4)

and obtain that the so defined quantities fulfill the relations

$$\breve{u}_i = \overline{u}_i \mathrm{e}^{\breve{v}_i} = \overline{u}_i \breve{a}_i \mathrm{e}^{-q_i \breve{v}_0}, \quad \breve{a}_i = \mathrm{e}^{\breve{\zeta}_i}, \quad \breve{\zeta}_i = \breve{v}_i + q_i \breve{v}_0, \quad i = 1, \dots, m. \tag{7.5}$$

We apply the formulas (7.4) not only to solutions $(\widetilde{u}, \widetilde{v})$ of $(\widetilde{\mathrm{P}})$ but also to the corresponding initial value $(\widetilde{U}, \widetilde{V}) = (\widetilde{u}(0), \widetilde{v}(0))$ and steady state $(\widetilde{u}^*, \widetilde{v}^*)$. These reconstructed quantities are denoted by $(\breve{U}, \breve{V})$ and $(\breve{u}^*, \breve{v}^*)$, respectively.

Lemma 7.2. *Let $\widetilde{v}_0 \in \widetilde{H}$, $\widetilde{u} \in \widetilde{H}^* \times L^2_+(\Omega, \mathbb{R}^{m-2})$ be given and let $\breve{v}_0$, $\breve{u}$ be defined as in (7.4). Then $\breve{v}_0 \in H$, $\breve{u} \in H^* \times L^2_+(\Omega, \mathbb{R}^m)$. Moreover, the following assertions are valid:*

i) *If $\widetilde{E}_0 \widetilde{v}_0 = \widetilde{u}_0$ then $F(\breve{u}) = \widetilde{F}(\widetilde{u})$.*

ii) *If $\widetilde{E}_0 \widetilde{v}_0 = \widetilde{u}_0$ and $\widetilde{u}_0 = \sum_{i=1}^{m-2} q_i \widetilde{u}_i$ in $L^2(\Omega)$ then $\breve{u}_0 = \sum_{i=1}^{m} q_i \breve{u}_i$ in $L^2(\Omega)$.*

iii) *If $\widetilde{E}_0 \widetilde{v}_0 = \widetilde{u}_0$ and $\widetilde{u} \in \widetilde{\mathcal{U}} + \widetilde{U}$ then $\breve{u} \in \mathcal{U} + U$.*

Proof. Essentially the proof is based on the definition of the spaces H, $\widetilde{H}$ and on properties of the functional $\widetilde{\pi}$ (see Table 1 and (2.3)).
i) Taking into account that $E_0 \breve{v}_0 = \breve{u}_0$, $\widetilde{E}_0 \widetilde{v}_0 = \widetilde{u}_0$, we obtain

$$F(\breve{u}) = \widetilde{F}(\widetilde{u}) - \int_\Omega \Big\{ \widetilde{\phi}_0(\widetilde{v}_0) - \sum_{i=m-1}^{m} \Big\{ \breve{u}_i \Big(\ln \frac{\breve{u}_i}{\overline{u}_i} - 1 \Big) + \overline{u}_i \Big\} \Big\} \, \mathrm{d}x = \widetilde{F}(\widetilde{u})$$

since (see Remark 2.3)

$$\widetilde{\phi}_0(\widetilde{v}_0) = - \sum_{i=m-1}^{m} \Big\{ q_i \overline{u}_i \mathrm{e}^{-q_i \widetilde{v}_0} \, \widetilde{v}_0 + \overline{u}_i (\mathrm{e}^{-q_i \widetilde{v}_0} - 1) \Big\} = \sum_{i=m-1}^{m} \Big\{ \breve{u}_i \Big(\ln \frac{\breve{u}_i}{\overline{u}_i} - 1 \Big) + \overline{u}_i \Big\}.$$

ii) For arbitrary $h \in H \subset \widetilde{H}$ we find that

$$\begin{aligned}
\langle \breve{u}_0, h \rangle_H &= \langle E_0 \breve{v}_0, h \rangle_H \\
&= \langle \widetilde{E}_0 \widetilde{v}_0, h \rangle_{\widetilde{H}} + \int_\Omega (e_0 - \widetilde{e}_0(\widetilde{v}_0)) \, h \, \mathrm{d}x \\
&= \langle \widetilde{u}_0, h \rangle_{\widetilde{H}} + \int_\Omega (e_0 - \widetilde{e}_0(\widetilde{v}_0)) \, h \, \mathrm{d}x \\
&= \int_\Omega \Big\{ \sum_{i=1}^{m-2} q_i \widetilde{u}_i + e_0 - \widetilde{e}_0(\widetilde{v}_0) \Big\} \, h \, \mathrm{d}x = \int_\Omega \sum_{i=1}^{m} q_i \breve{u}_i \, h \, \mathrm{d}x
\end{aligned}$$

and thus $\breve{u}_0 = \sum_{i=1}^m q_i \breve{u}_i$ in $L^2(\Omega)$.
iii) $\widetilde{u} - \widetilde{U} \in \widetilde{\mathcal{U}}$ means that

$$\widetilde{u}_0 - \widetilde{U}_0 = \sum_{i=1}^{m-2} q_i (\widetilde{u}_i - U_i) \text{ in } L^2(\Omega), \quad \sum_{i=1}^{m-2} \widetilde{\kappa}_i \langle \widetilde{u}_i - U_i, 1 \rangle_{H^1} = 0 \ \forall \widetilde{\kappa} \in \widetilde{\mathcal{S}}^\perp.$$

Since $\widetilde{U}_0 = \sum_{i=1}^{m-2} q_i U_i$, $U_0 = \sum_{i=1}^m q_i U_i$ (see Table 1) because of ii) we obtain

$$\breve{u}_0 - U_0 = \sum_{i=1}^{m} q_i (\breve{u}_i - U_i) \text{ in } L^2(\Omega)$$

and it remains to show that

$$\sum_{i=1}^{m} \kappa_i \langle \breve{u}_i - U_i, 1\rangle_{H^1} = 0 \ \forall \kappa \in \mathcal{S}^\perp.$$

First we set $\kappa = q$. Then

$$\sum_{i=1}^{m} q_i \langle \breve{u}_i - U_i, 1\rangle_{H^1} = \int_\Omega \sum_{i=1}^{m} q_i(\breve{u}_i - U_i)\,\mathrm{d}x = \int_\Omega \Big\{ \sum_{i=1}^{m-2} q_i \widetilde{u}_i - \widetilde{e}_0(\widetilde{v}_0) \Big\}\,\mathrm{d}x = \langle \widetilde{u}_0 - \widetilde{E}_0 \widetilde{v}_0, 1\rangle_{\widetilde{H}} = 0.$$

For arbitrary $\kappa \in \mathcal{S}^\perp$ by using the decomposition (7.3), $\kappa = (\widetilde{\kappa}, 0, 0) + \kappa_m q$, $\widetilde{\kappa} \in \widetilde{\mathcal{S}}^\perp$, we ensure that

$$\sum_{i=1}^{m} \kappa_i \langle \breve{u}_i - U_i, 1\rangle_{H^1} = \sum_{i=1}^{m-2} \widetilde{\kappa}_i \langle \widetilde{u}_i - U_i, 1\rangle_{H^1} + \kappa_m \sum_{i=1}^{m} q_i \langle \breve{u}_i - U_i, 1\rangle_{H^1} = 0. \quad \square$$

Lemma 7.3. *Let $(\widetilde{u}, \widetilde{v})$ be a solution and $(\widetilde{u}^*, \widetilde{v}^*)$ the steady state of $(\widetilde{\mathrm{P}})$. Let $(\breve{u}, \breve{v})$ and $(\breve{u}^*, \breve{v}^*)$ be defined by (7.4). Then*

$$\breve{v}_0 \in C(\mathbb{R}_+, H^1(\Omega)),\ \ \breve{u}, \breve{v} \in C(\mathbb{R}_+, L^2(\Omega, \mathbb{R}^{m+1})),\ \ \breve{u}(0) = \breve{U},\ \ \breve{v}(0) = \breve{V}.$$

Moreover, there is a constant c depending only on the data of (P) *such that for all $t \in \mathbb{R}_+$ the following relations are fulfilled:*

$$\begin{aligned}
&\|\breve{v}_0(t)\|_{H^1},\ \|\breve{v}_0(t)\|_{L^\infty} \le c,\\
&\sum_{i=0}^{m} \|\breve{u}_i(t)\|_{L^\infty} \le c\Big(\sum_{i=1}^{m-2} \|\widetilde{u}_i(t)\|_{L^\infty} + 1\Big),\\
&\sum_{i=1}^{m} \|\breve{v}_i(t)\|_{L^\infty} \le c\Big(\sum_{i=1}^{m-2} \|\widetilde{v}_i(t)\|_{L^\infty} + 1\Big),\\
&\|\breve{v}_0(t) - \breve{v}_0^*\|_{H^1} \le c\,\|\widetilde{v}_0(t) - \widetilde{v}_0^*\|_{H^1},\\
&\sum_{i=1}^{m} \|\breve{u}_i(t) - \breve{u}_i^*\|_{L^p} \le c\Big(\sum_{i=1}^{m-2} \|\widetilde{u}_i(t) - \widetilde{u}_i^*\|_{L^p} + \|\widetilde{v}_0(t) - \widetilde{v}_0^*\|_{L^p}\Big),\\
&\sum_{i=1}^{m} \|\breve{v}_i(t) - \breve{v}_i^*\|_{L^p} \le c \sum_{i=0}^{m-2} \|\widetilde{v}_i(t) - \widetilde{v}_i^*\|_{L^p}, \quad p \in [1, +\infty).
\end{aligned}$$

Proof. We know that $\widetilde{v}_0 \in C(\mathbb{R}_+, H^1(\Omega))$ (see Remark 2.9) and $\|\widetilde{v}_0(t)\|_{H^1}, \|\widetilde{v}_0(t)\|_{L^\infty} \le c$ for all $t \in \mathbb{R}_+$ (see Theorem 3.2, Corollary 3.1). Then because of (7.4) we obtain for $i = m-1, m$

$$\|\breve{u}_i(t_1) - \breve{u}_i(t_2)\|_{L^2} \le c\,\|\widetilde{v}_0(t_1) - \widetilde{v}_0(t_2)\|_{L^2},\ t_1, t_2 \in \mathbb{R}_+$$

and thus $\breve{u}_{m-1}, \breve{u}_m \in C(\mathbb{R}_+, L^2)$. Again taking into account Remark 2.9 and (7.4) all other assertions are easily verified. $\square$

The results of Lemma 7.2 and Lemma 7.3 show that further properties which can be derived for the '$\sim$'–quantities of the reduced problem $(\widetilde{\mathrm{P}})$ like the global estimates in (4.11) and (5.16) and the results on the asymptotic behaviour of Theorem 5.4 and Theorem 5.6 carry over to the '$\smile$'–quantities. For example, if $(\widetilde{\mathrm{P}})$ is solvable and for its solution $(\widetilde{u}, \widetilde{v})$ it holds for all $t \in \mathbb{R}_+$

$$\widetilde{F}(\widetilde{u}(t)) - \widetilde{F}(\widetilde{u}^*) \le \mathrm{e}^{-\lambda t}\,(\widetilde{F}(\widetilde{U}) - \widetilde{F}(\widetilde{u}^*)), \quad \sum_{i=1}^{m-2} \|\widetilde{u}_i(t) - \widetilde{u}_i^*\|_{L^1} + \|\widetilde{v}_0(t) - \widetilde{v}_0^*\|_{H^1} \le c\,\mathrm{e}^{-\lambda t/2}$$

then for the reconstructed quantities $(\breve{u}, \breve{v})$ we obtain

$$F(\breve{u}(t)) - F(\breve{u}^*) \le \mathrm{e}^{-\lambda t}(F(\breve{U}) - F(\breve{u}^*)), \quad \sum_{i=1}^{m} \|\breve{u}_i(t) - \breve{u}_i^*\|_{L^1} + \|\breve{v}_0(t) - \breve{v}_0^*\|_{H^1} \le c\,\mathrm{e}^{-\lambda t/2}.$$

7.3 Invariants, steady states and asymptotic behaviour

An immediate consequence of Lemma 7.2, iii) is the following result.

Theorem 7.1. *Let $(\tilde{u}, \tilde{v})$ be a solution of $(\widetilde{\mathrm{P}})$. Then*

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

This result means that up to the transformation (7.4) both problems (P) and $(\widetilde{\mathrm{P}})$ have the same invariants: If I_κ, $\kappa \in \mathcal{S}^\perp$, is given as in Remark 5.1 then

$$I_\kappa(u(t)) = I_\kappa(\breve{u}(t)) = I_\kappa(U) \quad \forall t \in \mathbb{R}_+$$

for any solution of (P) and $(\widetilde{\mathrm{P}})$, respectively. Next we show that again up to the transformation (7.4) both problems (P) and $(\widetilde{\mathrm{P}})$ have the same steady state.

Lemma 7.4. *Let $(\tilde{a}, \tilde{v}_0) \in \widetilde{\mathcal{M}}$ be given and let $(\breve{a}, \breve{v}_0)$ be defined according to (7.4). Then $(\breve{a}, \breve{v}_0) \in \mathcal{M}$. Moreover, if $\tilde{a} \in \operatorname{int} \mathbb{R}_+^{m-2}$ then $\breve{a} \in \operatorname{int} \mathbb{R}_+^m$, too.*

Proof. $(\tilde{a}, \tilde{v}_0) \in \widetilde{\mathcal{M}}$ means that $\tilde{a} \in \mathbb{R}_+^{m-2}$, $\tilde{v}_0 \in \widetilde{H}$,

$$\begin{aligned} &\prod_{i=1}^{m-2} \tilde{a}_i^{\tilde{\alpha}_i} - \prod_{i=1}^{m-2} \tilde{a}_i^{\tilde{\beta}_i} = 0 \quad \forall (\tilde{\alpha}, \tilde{\beta}) \in \widetilde{\mathcal{R}}^\Omega \cup \widetilde{\mathcal{R}}^\Gamma, \\ &\tilde{u} \in \widetilde{\mathcal{U}} + \widetilde{U} \text{ where } \tilde{u}_0 = \widetilde{E}_0 \tilde{v}_0,\ \tilde{u}_i = \overline{u}_i \tilde{a}_i \mathrm{e}^{-q_i \tilde{v}_0},\ i = 1, \ldots, m-2. \end{aligned} \tag{7.6}$$

Now define $(\breve{a}, \breve{v}_0)$ as well as $\breve{u}$ according to (7.4). Obviously, we have $\breve{a} \in \mathbb{R}_+^m$, $\breve{v}_0 \in H$. For arbitrary $(\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma$ we set $\tilde{\alpha} = (\alpha_1, \ldots, \alpha_{m-2})$, $\tilde{\beta} = (\beta_1, \ldots, \beta_{m-2})$. Then because of (1.4**) and (7.6)

$$\prod_{i=1}^{m} \breve{a}_i^{\alpha_i} - \prod_{i=1}^{m} \breve{a}_i^{\beta_i} = \mathrm{e}^{-q \cdot \alpha\, \widetilde{\pi}(\tilde{v}_0)} \Big[\prod_{i=1}^{m-2} \tilde{a}_i^{\tilde{\alpha}_i} - \prod_{i=1}^{m-2} \tilde{a}_i^{\tilde{\beta}_i} \Big] = 0$$

is obtained if $(\tilde{\alpha}, \tilde{\beta}) \neq (0,0)$. Otherwise this relation is trivially satisfied. Finally, we have

$$\breve{u}_0 = E_0 \breve{v}_0, \quad \breve{u}_i = \overline{u}_i \breve{a}_i \mathrm{e}^{-q_i \breve{v}_0},\ i = 1, \ldots, m,$$

and by (7.6) and Lemma 7.2, iii) we conclude that $\breve{u} \in \mathcal{U} + U$. Thus $(\breve{a}, \breve{v}_0) \in \mathcal{M}$. The last assertion of the lemma follows immediately from the construction of $\breve{a}$ from $\tilde{a}$ and $\tilde{v}_0$. □

Theorem 7.2. *There are unique steady states (u^*, v^*) of (P) and $(\tilde{u}^*, \tilde{v}^*)$ of $(\widetilde{\mathrm{P}})$ and it holds*

$$u^* = \breve{u}^*, v^* = \breve{v}^*.$$

Proof. The existence of the unique steady states for (P) and $(\widetilde{\mathrm{P}})$ (in the sense of (5.2)) follows with Lemma 7.1 from Theorem 5.1 applied to the corresponding problems. If $(\widetilde{u}^*, \widetilde{v}^*)$ is the steady state of $(\widetilde{\mathrm{P}})$ then the related quantities $(\widetilde{a}^*, \widetilde{v}_0^*)$ with $\widetilde{a}_i = \mathrm{e}^{\widetilde{v}_i^* + q_i \widetilde{v}_0^*}$, $i = 1, \dots, m-2$, belong to $\widetilde{\mathcal{M}}$ and $\widetilde{a}^* \in \operatorname{int} \mathbb{R}_+^{m-2}$ (see Remark 5.2). Because of Lemma 7.4 the pair $(\breve{a}^*, \breve{v}_0^*)$ lies in $\mathcal{M}$ and $\breve{a}^* \in \operatorname{int} \mathbb{R}_+^m$. Again using Remark 5.2 the pair $(\breve{u}^*, \breve{v}^*)$ with $\breve{u}_0^* = E_0 \breve{v}_0^*$, $\breve{u}_i^* = \overline{u}_i \breve{a}_i^* \mathrm{e}^{-q_i \breve{v}_0^*}$, $\breve{v}_i^* = \ln(\breve{u}_i^* / \overline{u}_i)$, $i = 1, \dots, m$, is a steady state of (P). The uniqueness of the steady state of (P) now ensures that $u^* = \breve{u}^*$, $v^* = \breve{v}^*$. □

Now we are able to prove the announced asymptotic equivalence of both the problems (P) and $(\widetilde{\mathrm{P}})$, at least under the additional assumption that (5.9) for problem (P) is fulfilled. From Lemma 7.4 one easily obtains the following assertion.

Lemma 7.5. *If the additional assumption* (5.9) *for problem* (P) *is fulfilled, then the property* (5.9) *is valid for the set* $\widetilde{\mathcal{M}}$ *corresponding to the reduced problem* $(\widetilde{\mathrm{P}})$, *too.*

Theorem 7.3. *Let the assumption* (5.9) *for* (P) *be fulfilled. If* (u, v) *and* $(\widetilde{u}, \widetilde{v})$ *are solutions of* (P) *and of* $(\widetilde{\mathrm{P}})$, *respectively, then the following estimates are satisfied:*

$$|F(u(t)) - F(\breve{u}(t))| \le c\,\mathrm{e}^{-\lambda t} \quad \forall t \in \mathbb{R}_+,$$
$$\sum_{i=1}^{m} \|u_i(t) - \breve{u}_i(t)\|_{L^1} + \|v_0(t) - \breve{v}_0(t)\|_{H^1} \le c\,\mathrm{e}^{-\lambda t/2} \quad \forall t \in \mathbb{R}_+$$

where the constants c, $\lambda > 0$ *depend only on the data. If additionally assumption* (2.6) *for* (P) *is fulfilled then there are unique globally bounded solutions* (u, v) *of* (P) *and* $(\widetilde{u}, \widetilde{v})$ *of* $(\widetilde{\mathrm{P}})$ *and for* $p \in [1, +\infty)$ *it holds*

$$\sum_{i=0}^{m} \Big(\|u_i(t) - \breve{u}_i(t)\|_{L^p} + \|v_i(t) - \breve{v}_i(t)\|_{L^p} \Big) \le c\,\mathrm{e}^{-\lambda_p t} \quad \forall t \in \mathbb{R}_+$$

where again the constants $\lambda_p > 0$, c *depend only on the data.*

Proof. Applying Theorem 5.4 to (P) and $(\widetilde{\mathrm{P}})$, respectively, we find

$$F(u(t)) - F(u^*)\,,\ \widetilde{F}(\widetilde{u}(t)) - \widetilde{F}(\widetilde{u}^*) \ \le c\,\mathrm{e}^{-\lambda t} \quad \forall t \in \mathbb{R}_+.$$

From Lemma 7.2, i) and Theorem 7.2 we conclude that

$$F(\breve{u}(t)) - F(\breve{u}^*) = F(\breve{u}(t)) - F(u^*) \ \le c\,\mathrm{e}^{-\lambda t} \quad \forall t \in \mathbb{R}_+$$

and by using the triangle inequality the first assertion is verified. The second one follows analogously from Corollary 5.2, Lemma 7.3 and Theorem 7.2. Under the additional assumption (2.6) the existence of unique solutions of (P) and $(\widetilde{\mathrm{P}})$ and their global boundedness are established in Theorem 5.7. Using now Theorem 5.6, Lemma 7.3 and Theorem 7.2 the last estimate is obtained. □

8 Examples

8.1 Example 1

First we are looking for a simple example of a class of model equations different variants of which have been applied in order to simulate technological processes in the fabrication of semiconductor devices and integrated circuits (see e.g. [14, 15, 28, 36, 37, 38, 43, 55]). Especially we will discuss the validity of our assumptions (5.9) and (2.6).

We consider a homogeneous semiconductor material with $m = 6$ species as outlined in Fig. 1, Table 2 and four volume reactions[1] as listed in the upper part of Table 3 and Table 4.

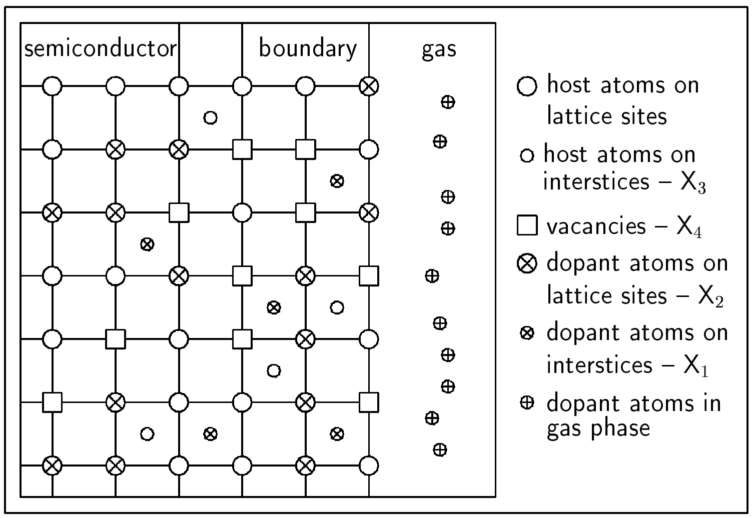

Fig. 1: Species considered in the example.

species	name of the species	charge number
X_1	dopant atoms on interstices	0
X_2	dopant atoms on lattice sites	-1
X_3	self-interstitial host atoms	0
X_4	vacancies in the host lattice	0
X_5	electrons	-1
X_6	holes	$+1$

Table 2: Species, their names and charges.

In the third column of Table 4 we have written the rate formulas as usual starting from the mass action law. The coefficients $\overline{k}_j$, $\widehat{k}_j$, $j = 1, \ldots, 4$, are assumed to be positive constants. We require that there exists a simultaneous equilibrium to all reactions under consideration with strictly positive densities. To ensure this some necessary and sufficient conditions (the so called

[1]In this section we use a more convenient numbering of the reactions.

Reaction	name of the reaction	reaction equation
R_1	Kick-out reaction	$X_1 \rightleftharpoons X_2 + X_3 + X_6$
R_2	Frank-Turnbull mechanism	$X_1 + X_4 \rightleftharpoons X_2 + X_6$
R_3	defect generation and recombination	$X_3 + X_4 \rightleftharpoons 0$
R_4	electron-hole generation and recombination	$X_5 + X_6 \rightleftharpoons 0$
R_5	infiltration of dopants to interstitial sites	$X_1 \rightleftharpoons 0$
R_6	surface recombination of self-interstitials	$X_3 \rightleftharpoons 0$
R_7	surface recombination of vacancies	$X_4 \rightleftharpoons 0$

Table 3: Volume and boundary reactions between the different species.

Reaction	$\alpha - \beta$	rate formulas	
R_1	$(1, -1, -1, 0, 0, -1)$	$\widehat{k}_1(u_1 - \overline{k}_1 u_2 u_3 u_6)$	$k_1(\mathrm{e}^{\zeta_1} - \mathrm{e}^{\zeta_2+\zeta_3+\zeta_6})$
R_2	$(1, -1, 0, 1, 0, -1)$	$\widehat{k}_2(u_1 u_4 - \overline{k}_2 u_2 u_6)$	$k_2(\mathrm{e}^{\zeta_1+\zeta_4} - \mathrm{e}^{\zeta_2+\zeta_6})$
R_3	$(0, 0, 1, 1, 0, 0)$	$\widehat{k}_3(u_3 u_4 - \overline{k}_3)$	$k_3(\mathrm{e}^{\zeta_3+\zeta_4} - 1)$
R_4	$(0, 0, 0, 0, 1, 1)$	$\widehat{k}_4(u_5 u_6 - \overline{k}_4)$	$k_4(\mathrm{e}^{\zeta_5+\zeta_6} - 1)$
R_5	$(1, 0, 0, 0, 0, 0)$	$\widehat{k}_5(u_1 - \overline{k}_5)$	$k_5(\mathrm{e}^{\zeta_1} - 1)$
R_6	$(0, 0, 1, 0, 0, 0)$	$\widehat{k}_6(u_3 - \overline{k}_6)$	$k_6(\mathrm{e}^{\zeta_3} - 1)$
R_7	$(0, 0, 0, 1, 0, 0)$	$\widehat{k}_7(u_4 - \overline{k}_7)$	$k_7(\mathrm{e}^{\zeta_4} - 1)$

Table 4: Reactions and their rate formulas.

Wegscheider conditions [59]) must be fulfilled. In our example ($R_j = 0$, $j = 1, \dots, 4$) there is only one condition, namely

$$\overline{k}_1 \, \overline{k}_3 = \overline{k}_2.$$

Then choosing arbitrary constants $\overline{u}_1$, $\overline{u}_4$, $\overline{u}_5 > 0$ and setting

$$\overline{u}_2 = \frac{1}{\overline{k}_2 \overline{k}_4} \overline{u}_1 \overline{u}_4 \overline{u}_5, \; \overline{u}_3 = \frac{\overline{k}_3}{\overline{u}_4}, \; \overline{u}_6 = \frac{\overline{k}_4}{\overline{u}_5} \tag{8.1}$$

we obtain that $\overline{u}_i = \text{const} > 0$, $i = 1, \dots, 6$, and $R_j = 0$, $j = 1, \dots, 4$. Choosing these $\overline{u}_i$ as reference densities, introducing the electrostatic potential[2] φ, the chemical potentials μ_i, as well as the electrochemical potentials ζ_i and activities a_i according to

$$\mu_i = \ln (u_i / \overline{u}_i), \quad \zeta_i = \mu_i + q_i \varphi, \quad a_i = \mathrm{e}^{\zeta_i}, \quad i = 1, \dots, 6,$$

and finally defining

$$k_1 = \widehat{k}_1 \, \overline{u}_1, \; k_2 = \widehat{k}_2 \, \overline{u}_1 \, \overline{u}_4, \; k_j = \widehat{k}_j \, \overline{k}_j, \; j = 3, 4,$$

[2]In our examples we do not make use of the transformation (1.7) and denote the potentials v_0, v_i before applying (1.7) by φ, μ_i.

we obtain the reaction rates as written in the last column of Table 4. On the other hand, we could firstly introduce electrochemical potentials

$$\zeta_i = \ln(u_i/\overline{u}_i) + q_i\varphi, \quad i = 1, \dots, 6,$$

and rate formulas as in the last column of Table 4 (see [33, 44]). Now the coefficients k_j, $j = 1, \dots, 4$, and $\overline{u}_i$, $i = 1, \dots, 6$, are given positive constants. Then we easily obtain rate formulas as written in the third column of Table 4. The equilibrium constants are

$$\overline{k}_1 = \frac{\overline{u}_1}{\overline{u}_2\overline{u}_3\overline{u}_6}, \ \overline{k}_2 = \frac{\overline{u}_1\overline{u}_4}{\overline{u}_2\overline{u}_6}, \ \overline{k}_3 = \overline{u}_3\overline{u}_4, \ \overline{k}_4 = \overline{u}_5\overline{u}_6, \tag{8.2}$$

and the Wegscheider condition is obviously fulfilled.

We denote by $q := (0, -1, 0, 0, -1, 1) \in \mathbb{R}^6$ the vector of charge numbers. Then (α, β) corresponding to the reactions R_1 to R_4 fulfill the relation (1.11). Moreover, in our example it holds $\alpha \cdot q = \beta \cdot q = 0$. Finally, the stoichiometric subspace belonging to this reaction system and its orthogonal complement are given by

$$\begin{aligned} &\mathcal{S} = \operatorname{span}\{(1,-1,-1,0,0,-1), (0,0,1,1,0,0), (0,0,0,0,1,1)\}, \\ &\mathcal{S}^\perp = \operatorname{span}\{q, (1,1,0,0,0,0), (0,1,-1,1,0,0)\}, \\ &\dim \mathcal{S} = \dim \mathcal{S}^\perp = 3. \end{aligned} \tag{8.3}$$

The system of continuity equations reads as

$$\left.\begin{aligned} \frac{\partial u_i}{\partial t} + \nabla \cdot j_i + R_i^\Omega &= 0 \quad \text{on } (0,\infty) \times \Omega, \\ j_i \cdot \nu &= 0 \quad \text{on } (0,\infty) \times \Gamma, \\ u_i(0) &= U_i \quad \text{on } \Omega, \ i = 1, \dots, 6, \end{aligned}\right\} \tag{8.4}$$

$$R^\Omega = (R_1 + R_2, -R_1 - R_2, -R_1 + R_3, R_2 + R_3, R_4, -R_1 - R_2 + R_4).$$

For the sake of simplicity we use homogeneous boundary data for the Poisson equation (1.6), thus (see footnote 2 on page 47)

$$\left.\begin{aligned} -\nabla \cdot (\varepsilon \nabla \varphi) &= f + \sum_{i=1}^{6} q_i u_i \quad \text{on } (0,\infty) \times \Omega, \\ \varphi &= 0 \qquad\qquad\quad \text{on } (0,\infty) \times \Gamma_D, \\ \nu \cdot (\varepsilon \nabla \varphi) + \tau\varphi &= 0 \qquad\qquad\quad \text{on } (0,\infty) \times \Gamma_N \end{aligned}\right\} \tag{8.5}$$

where $f = f^\Omega$ denotes a fixed background doping. For the data we assume that $U_i \in L^\infty(\Omega)$, $U_i \geq c > 0$, $i = 1, \dots, 6$, $f \in L^\infty(\Omega)$. Especially we are interested in the case that in addition

$$\int_\Omega \Big\{ f + \sum_{i=1}^{6} q_i U_i \Big\} \, \mathrm{d}x = \int_\Omega \Big\{ f - U_2 - U_5 + U_6 \Big\} \, \mathrm{d}x = 0. \tag{8.6}$$

Because of Remark 5.1 and (8.3), (8.6) we have three invariants the values of which are given by the initial state, namely

$$\begin{aligned} I_1(t) &= \int_\Omega (f - u_2(t) - u_5(t) + u_6(t)) \, \mathrm{d}x = 0, \\ I_2(t) &= \int_\Omega (u_1(t) + u_2(t)) \, \mathrm{d}x = \int_\Omega (U_1 + U_2) \, \mathrm{d}x, \\ I_3(t) &= \int_\Omega (u_2(t) - u_3(t) + u_4(t)) \, \mathrm{d}x = \int_\Omega (U_2 - U_3 + U_4) \, \mathrm{d}x, \quad t \geq 0. \end{aligned} \tag{8.7}$$

In applications to semiconductor technology precise initial data U_5, U_6 for electrons and holes, respectively, are hardly known. Mostly they are determined by one of the two following procedures.

Lemma 8.1. *Let $U_2 \in L^\infty(\Omega)$ and $f \in L^\infty(\Omega)$ be given. Then there exist unique U_5, U_6 such that*

$$U_5 U_6 = \overline{k}_4,\ f - U_2 - U_5 + U_6 = 0,\ U_5,\, U_6 \geq 0 \quad \text{a.e. on } \Omega. \tag{8.8}$$

Furthermore, $U_i \in L^\infty(\Omega)$, $U_i \geq c > 0$, $i = 5, 6$, and (8.6) is satisfied.

Proof. The unique solution of (8.8) is given by

$$U_5 = -\frac{U_2 - f}{2} + \sqrt{\Big[\frac{U_2 - f}{2}\Big]^2 + \overline{k}_4}\,, \quad U_6 = \frac{U_2 - f}{2} + \sqrt{\Big[\frac{U_2 - f}{2}\Big]^2 + \overline{k}_4}\,.$$

From this the other assertions follow. □

Lemma 8.2. *Let $U_2 \in L^\infty(\Omega)$ and $f \in L^\infty(\Omega)$ be given. Then there exist a unique weak solution $\varphi \in H_0^1(\Omega \cup \Gamma_N)$, $\zeta \in \mathbb{R}$ to*

$$\left.\begin{aligned} -\nabla\cdot(\varepsilon\,\nabla\varphi) + \overline{u}_5 \mathrm{e}^{\varphi+\zeta} - \overline{u}_6 \mathrm{e}^{-(\varphi+\zeta)} &= f - U_2 && \text{on } \Omega,\\ \varphi &= 0 && \text{on } \Gamma_D,\\ \nu\cdot(\varepsilon\,\nabla\varphi) + \tau\varphi &= 0 && \text{on } \Gamma_N,\\ \int_\Omega \Big\{\overline{u}_5 \mathrm{e}^{\varphi+\zeta} - \overline{u}_6 \mathrm{e}^{-(\varphi+\zeta)}\Big\}\,\mathrm{d}x &= \int_\Omega \Big\{f - U_2\Big\}\,\mathrm{d}x, && \end{aligned}\right\} \tag{8.9}$$

and for

$$U_5 = \overline{u}_5 \mathrm{e}^{\varphi+\zeta},\ U_6 = \overline{u}_6 \mathrm{e}^{-(\varphi+\zeta)}$$

it holds $U_i \in L^\infty(\Omega)$, $U_i \geq c > 0$, $i = 5, 6$, and (8.6) is satisfied.

Proof. Problem (8.9) is equivalent to the nonlinear nonlocal Poisson equation (8.15) below for $t = 0$, and since the corresponding operator $\widetilde{E}_0$ is strongly monotone and hemicontinuous all assertions are easily obtained. □

The situation in Lemma 8.1 means that U_5, U_6 are chosen such that $R_4 = 0$ and the local electroneutrality condition is fulfilled. In Lemma 8.2 it is assumed that the initial electrochemical potentials of electrons and holes are constant, that $R_4 = 0$ and the global electroneutrality condition (8.6) is satisfied.

Next we shall discuss properties of the set $\mathcal{M}$ (see (5.4)). In our new notation this set is characterized as follows

$$\mathcal{M} = \Big\{ (a,\varphi) \in \mathbb{R}^6_+ \times H^1_0(\Omega \cup \Gamma_N) :$$

$$a_1 = a_2 a_3 a_6,\ a_1 a_4 = a_2 a_6,\ a_3 a_4 = 1,\ a_5 a_6 = 1, \tag{8.10}$$

$$\left.\begin{aligned} &\int_\Omega (f - u_2 - u_5 + u_6)\,\mathrm{d}x = 0,\\ &\int_\Omega (u_1 + u_2)\,\mathrm{d}x = I_2(0),\\ &\int_\Omega (u_2 - u_3 + u_4)\,\mathrm{d}x = I_3(0), \end{aligned}\right\} \tag{8.11}$$

where $u_i = \overline{u}_i a_i \mathrm{e}^{-q_i\varphi}$ and φ is the unique weak solution to the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \varphi) + \overline{u}_2 a_2 \mathrm{e}^{\varphi} + \overline{u}_5 a_5 \mathrm{e}^{\varphi} - \overline{u}_6 a_6 \mathrm{e}^{-\varphi} = f \text{ on } \Omega \tag{8.12}$$

with boundary conditions as in (8.9)$\Big\}$.

Of course, this set depends on the choice of the initial values U_i. But it is easy to see that $\mathcal{M}$ does not depend on the concrete choice of U_5, U_6 so far as (8.6) is fulfilled.

Lemma 8.3. *Let $U_1, \dots, U_4 \in L^\infty(\Omega)$ be fixed and consider different initial values U_5^j, $U_6^j \in L^\infty(\Omega)$, $j = 1, 2$, satisfying*

$$\int_\Omega \Big\{ f - U_2 - U_5^j + U_6^j \Big\}\,\mathrm{d}x = 0.$$

Then for the corresponding sets $\mathcal{M}^j$ it holds $\mathcal{M}^1 = \mathcal{M}^2$.

Proof. The assertion follows from the obvious relation

$$\Big\{ \int_\Omega (U_i^1 - U_i^2)\,\mathrm{d}x \Big\}_{i=1,\dots,6} = \int_\Omega (U_5^1 - U_5^2)\,\mathrm{d}x\ (0,0,0,0,1,1) \in \mathcal{S}. \quad \square$$

Especially, initial values U_5, U_6 chosen as in Lemma 8.1 and Lemma 8.2, respectively, generate the same set $\mathcal{M}$.

Lemma 8.4. *Assumption* (5.9) *is fulfilled.*

Proof. Let $(a, \varphi) \in \mathcal{M}$. From (8.10) it follows that a_3, a_4, a_5, $a_6 > 0$, (8.11) yields

$$\int_\Omega (\overline{u}_1 a_1 + \overline{u}_2 a_2\, \mathrm{e}^{\varphi})\,\mathrm{d}x = \int_\Omega (U_1 + U_2)\,\mathrm{d}x > 0.$$

Therefore at least $a_1 > 0$ or $a_2 > 0$. Using the first (or the second) relation in (8.10) we conclude that a_1, $a_2 > 0$. $\square$

Now let us summarize the results of Theorem 5.1 and Remark 5.2 for the present example. There exists a unique steady state (in the sense of (5.2))

$$u_i^*,\ \varphi^*,\ \mu_i^*,\ i = 1, \dots, 6,$$

and it holds

$$\mathcal{M} = \{(a^*, \varphi^*)\},\ a_i^* = u_i^* / \overline{u}_i\, \mathrm{e}^{q_i \varphi^*},\ i = 1, \dots, 6.$$

Moreover, the energy estimates of Theorem 5.4 are valid in this example.

Lemma 8.5. *If* $f = \text{const}$ *then* $\varphi^* = 0$, $u_i^* = \text{const}$, $i = 1, \dots, 6$, *and* $f - u_2^* - u_5^* + u_6^* = 0$.

Proof. We ask for constant densities $u_i > 0$ such that

$$u_1 u_4 = \overline{k}_2 u_2 u_6, \ u_3 u_4 = \overline{k}_3, \ u_5 u_6 = \overline{k}_4$$

and (see (8.7))

$$f - u_2 - u_5 + u_6 = 0, \ u_1 + u_2 = c_2 = \frac{I_2(0)}{\operatorname{mes}\Omega} > 0, \ u_2 - u_3 + u_4 = c_3 = \frac{I_3(0)}{\operatorname{mes}\Omega}.$$

Then

$$\left.\begin{aligned} u_6 = \psi(u_2) &= \frac{u_2 - f}{2} + \sqrt{\left[\frac{u_2 - f}{2}\right]^2 + \overline{k}_4}, \ u_5 = \frac{\overline{k}_4}{u_6}, \\ u_4 &= \overline{k}_2 u_2 u_6 \frac{1}{c_2 - u_2}, \ u_3 = \frac{\overline{k}_3}{u_4}, \ u_1 = c_2 - u_2, \end{aligned}\right. \tag{8.13}$$

and we arrive at an equation for u_2, namely

$$\chi(u_2) = u_2 - \frac{\overline{k}_3}{\overline{k}_2} \frac{c_2 - u_2}{u_2 \psi(u_2)} + \overline{k}_2 \frac{u_2 \psi(u_2)}{c_2 - u_2} = c_3, \ 0 < u_2 < c_2.$$

Since $\chi \in C^1(0, c_2)$, $\chi'(u_2) > 0$ for all $u_2 \in (0, c_2)$ and $\lim_{u_2 \to 0} \chi(u_2) = -\infty$, $\lim_{u_2 \to c_2} \chi(u_2) = +\infty$, this equation has a unique solution $u_2 \in (0, c_2)$ for any $c_3 \in \mathbb{R}$ and the other densities u_i are found by (8.13). Now setting $a_i = u_i / \overline{u}_i$, $\varphi = 0$ we get $(a, \varphi) \in \mathcal{M}$, thus $a^* = a$, $\varphi^* = \varphi = 0$. □

Under the assumption of Lemma 8.5 the local electroneutrality condition is fulfilled in the steady state but this condition can be violated during the evolution process even if the initial state is chosen according to Lemma 8.1.

Finally we discuss the assumption (2.6) which would ensure global estimates and the existence result (see Theorem 5.7). In our example the kick-out reaction R_1 contains terms of third order which occur as source terms in the continuity equation for the species X_1 such that assumption (2.6) is violated. Thus global estimates and existence can not be proved by the methods used in this paper. But exploiting the concrete form of the reactions $R_1, \dots, R_4$ we can investigate this example in the framework of a more general class of electro–reaction–diffusion systems including some specific (cluster) reactions of higher order which we have studied in [27] (X_1 has to be interpreted as a cluster species and R_1 as a cluster reaction). Thus all assertions concerning global estimates and existence remain valid for our example, too. Let us note that omitting the reaction R_1 the remaining system would fulfil both assumptions (2.6) and (5.9) and all desired results could be obtained by means the methods of the present paper.

8.2 The reduced version of example 1

Now we discuss the situation for the reduced model[3] introduced in Subsection 1.2. According to (1.5**) here we have only continuity equations for the species X_1 to X_4

$$\left.\begin{aligned} \frac{\partial \widetilde{u}_i}{\partial t} + \nabla \cdot \widetilde{j}_i + \widetilde{R}_i^\Omega &= 0 \quad \text{on } (0, \infty) \times \Omega, \\ \widetilde{j}_i \cdot \nu &= 0 \quad \text{on } (0, \infty) \times \Gamma, \\ \widetilde{u}_i(0) &= U_i \quad \text{on } \Omega, \ i = 1, \dots, 4, \end{aligned}\right\} \tag{8.14}$$

[3] Using the notation of this section the transformation (1.17) reads as follows: $\widetilde{\varphi} = \varphi + \zeta$, $\widetilde{u}_i = u_i$, $\widetilde{\mu}_i = \mu_i$, $\widetilde{\zeta}_i = \zeta_i + q_i \zeta$, $i = 1, \dots, 4$, where $\zeta = \zeta_5$ denotes the electrochemical potential of the electrons.

$$\widetilde{R}^{\Omega} = (\widetilde{R}_1 + \widetilde{R}_2, -\widetilde{R}_1 - \widetilde{R}_2, -\widetilde{R}_1 + \widetilde{R}_3, \widetilde{R}_2 + \widetilde{R}_3),$$

coupled with the corresponding nonlinear nonlocal Poisson equation (1.8**)

$$\left.\begin{aligned}
-\nabla\cdot(\varepsilon\,\nabla\widetilde{\varphi}) + \overline{u}_5 e^{\widetilde{\varphi}} - \overline{u}_6 e^{-\widetilde{\varphi}} &= f - \widetilde{u}_2 && \text{on } (0,\infty)\times\Omega,\\
\widetilde{\varphi} &= \zeta && \text{on } (0,\infty)\times\Gamma_D,\\
\nu\cdot(\varepsilon\,\nabla\widetilde{\varphi}) + \tau\widetilde{\varphi} &= \tau\zeta && \text{on } (0,\infty)\times\Gamma_N,\\
\int_{\Omega}\Big\{\overline{u}_5 e^{\widetilde{\varphi}} - \overline{u}_6 e^{-\widetilde{\varphi}}\Big\}\,\mathrm{d}x &= \int_{\Omega}\Big\{f - \widetilde{u}_2\Big\}\,\mathrm{d}x && \text{on } (0,\infty).
\end{aligned}\right\} \tag{8.15}$$

The reaction terms $\widetilde{R}_i$ are obtained via (1.4**),

$$\widetilde{R}_1 = k_1(e^{\widetilde{\zeta}_1} - e^{\widetilde{\zeta}_2+\widetilde{\zeta}_3}), \quad \widetilde{R}_2 = k_2(e^{\widetilde{\zeta}_1+\widetilde{\zeta}_4} - e^{\widetilde{\zeta}_2}), \quad \widetilde{R}_3 = k_3(e^{\widetilde{\zeta}_3+\widetilde{\zeta}_4} - 1).$$

For the reduced stoichiometric subspace it holds

$$\begin{aligned}
&\widetilde{\mathcal{S}} = \mathrm{span}\{(1,-1,-1,0),(0,0,1,1)\}, \quad \widetilde{\mathcal{S}}^{\perp} = \mathrm{span}\{(1,1,0,0),(0,1,-1,1)\},\\
&\dim\widetilde{\mathcal{S}} = \dim\widetilde{\mathcal{S}}^{\perp} = 2.
\end{aligned}$$

Now the structure of $\widetilde{\mathcal{S}}^{\perp}$ ensures only two invariants, namely I_2 and I_3 (cf. (8.7)). The first invariant I_1 is guaranteed by the nonlocal constraint in (8.15).

Lemma 7.5 ensures the property (5.9) for the reduced model. Finally, the volume reactions $\widetilde{R}_1$, $\widetilde{R}_2$, $\widetilde{R}_3$ are of at most second order, such that assumption (2.6) is fulfilled for the reduced model (cf. Remark 7.1). Therefore all results of the paper can be applied to this version of our example. Similar examples we have studied in [23, 25] where the Poisson equation has been replaced by the local electroneutrality condition.

8.3 Example 1 with boundary reactions

Now we include into our model the boundary reactions $R_5, \dots, R_7$ as described in the lower part of Table 3 and Table 4. We assume that

$$\overline{k}_j = \text{const} > 0,\ \widehat{k}_j \in L^{\infty}_{+}(\Gamma),\ \|\widehat{k}_j\|_{L^1(\Gamma)} > 0,\ j = 5,\dots,7.$$

Here the Wegscheider conditions read as follows

$$\overline{k}_1\,\overline{k}_3 = \overline{k}_2, \quad \overline{k}_6\,\overline{k}_7 = \overline{k}_3. \tag{8.16}$$

As reference densities fulfilling all volume and boundary reactions we choose

$$\overline{u}_1 = \overline{k}_5,\ \overline{u}_4 = \overline{k}_7,\ \overline{u}_5 = \text{const} > 0,\ \overline{u}_2,\ \overline{u}_3,\ \overline{u}_6 \text{ as in (8.1).}$$

By setting

$$k_j = \widehat{k}_j\,\overline{k}_j,\ j = 5,\dots,7,$$

we obtain the reaction rates as written in the the last column of Table 4. The stoichiometric subspace belonging to this reaction system is given by

$$\begin{aligned}
&\mathcal{S} = \{\rho \in \mathbb{R}^6 : \rho\cdot q = 0\}, \quad \mathcal{S}^{\perp} = \mathrm{span}\{q\},\\
&\dim\mathcal{S} = 5,\ \dim\mathcal{S}^{\perp} = 1.
\end{aligned} \tag{8.17}$$

In the continuity equations (8.4) the boundary conditions have to be replaced by

$$j_i \cdot \nu - R_i^\Gamma = 0 \text{ on } (0,\infty) \times \Gamma, \quad i = 1,\dots,6, \text{ with } R^\Gamma = (R_5, 0, R_6, R_7, 0, 0)$$

whereas the Poisson equation (8.5) remains unchanged. For this model we have only the invariant I_1. In the definition of the set $\mathcal{M}$ in Subsection 8.1 the relations (8.10) must be replaced by

$$a_1 = a_2 a_3 a_6, \; a_1 a_4 = a_2 a_6, \; a_3 a_4 = 1, \; a_5 a_6 = 1, \; a_1 = a_3 = a_4 = 1.$$

If $(a,\varphi) \in \mathcal{M}$ then obviously $a_i > 0$, $i = 1,\dots,6$, which ensures the validity of (5.9). With regard to the validity of (2.6) we have the same situation as described at the end of Subsection 8.1.

Now we consider the reduced model. For the reduced stoichiometric subspace it holds

$$\widetilde{\mathcal{S}} = \mathbb{R}^4, \quad \widetilde{\mathcal{S}}^\perp = \{0\}, \quad \dim \widetilde{\mathcal{S}} = 4, \quad \dim \widetilde{\mathcal{S}}^\perp = 0. \tag{8.18}$$

Note that in this setting the stoichiometric structure gives no invariants and the invariant I_1 is a consequence of the corresponding reduced Poisson equation, again. Because of Lemma 7.5 the property (5.9) for $\widetilde{\mathcal{M}}$ is fulfilled and as in Subsection 8.2 the growth condition (2.6) is valid, too.

8.4 Example 1 in a heterostructure

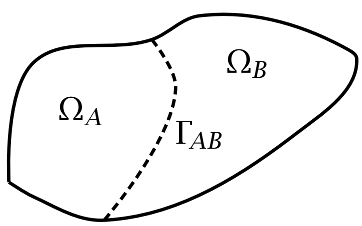

Fig. 2: Example of a heterostructure consisting of two materials A and B, $\Omega = \operatorname{int}(\overline{\Omega_A} \cup \overline{\Omega_B})$ where Ω_A, Ω_B are bounded open domains with $\Omega_A \cap \Omega_B = \emptyset$ and $\Gamma_{AB} = \overline{\Omega_A} \cap \overline{\Omega_B}$ has positive (surface) measure.

Now let us consider Example 1 in a heterostructure consisting of two different homogeneous materials as outlined in Fig. 2. The state equations in Ω_A and Ω_B, respectively, are

$$u_i = N_{i,C}\, e^{\mu_i - E_{i,C}} = N_{i,C}\, e^{\zeta_i - q_i\varphi - E_{i,C}}, \; i = 1,\dots,6, \; C = A, B,$$

with given constants $N_{i,C} > 0$ and $E_{i,C}$. Crossing the interface Γ_{AB} the electrochemical potentials should be continuous while the chemical and electrostatic potentials could jump (see [33]). We choose functions

$$\mu_{i,AB}(x) = \begin{cases} 0 & , x \in \Omega_A \\ \Delta\mu_i = \text{const} & , x \in \Omega_B \end{cases}, \quad \varphi_{AB}(x) = \begin{cases} 0 & , x \in \Omega_A \\ \Delta\varphi = \text{const} & , x \in \Omega_B \end{cases}$$

representing the discontinuities of the functions φ, μ_i and set

$$\mu_i = \widetilde{\mu}_i + \mu_{i,AB}, \; \varphi = \widetilde{\varphi} + \varphi_{AB}$$

such that the functions $\widetilde{\varphi}$, $\widetilde{\mu}_i$ remain continuous. The potential $\widetilde{\varphi}$ has to satisfy the Poisson equation with boundary conditions which are modified by the double layer potential φ_{AB}. Because of the continuity of ζ_i we get $\Delta\mu_i = -q_i \Delta\varphi$. Defining reference densities

$$\overline{u}_i(x) = \begin{cases} \overline{u}_{i,A} = N_{i,A}\, e^{-E_{i,A}} & , x \in \Omega_A \\ \overline{u}_{i,B} = N_{i,B}\, e^{-E_{i,B} - q_i\Delta\varphi} & , x \in \Omega_B \end{cases}$$

and omitting now the tilde we obtain state equations in our standard form,

$$u_i = \overline{u}_i\, \mathrm{e}^{\mu_i} = \overline{u}_i\, \mathrm{e}^{\zeta_i - q_i\varphi}.$$

It is obvious that $\overline{u}_i \in L^\infty(\Omega)$, $\overline{u}_i \geq c > 0$. Because of the jumps of $\overline{u}_i$ across the interface the densities u_i will have discontinuities, too. The ratio

$$s_i = \frac{\lim\limits_{x' \in \Omega_A,\, x' \to x} u_i(x')}{\lim\limits_{x' \in \Omega_B,\, x' \to x} u_i(x')} = \frac{\overline{u}_{i,A}}{\overline{u}_{i,B}}, \; x \in \Gamma_{AB}$$

is called the segregation coefficient of the species X_i at the interface. In general we have $s_i \neq 1$.

Next, the reaction rates are written as in the last column of Table 4 with kinetic coefficients k_j which are different in Ω_A and Ω_B, respectively. This gives formulas as in the third column of Table 4 but now the equilibrium 'constants' $\overline{k}_j$ in (8.2) will depend on x. Also the diffusivities D_i and the permittivity ε have different values in Ω_A and Ω_B, respectively. Thus we arrive at an example for our basic model in a heterostructure which can be further discussed as in Subsection 8.1. Especially, there exists a unique steady state but the assertion of Lemma 8.5 is wrong in general. Even in the case that $f = \text{const}$, near the interface boundary layers are formed where the space charge density does not vanish (cf. Fig. 6, too).

Now let us ask if there are steady states for a modified model where the local electroneutrality condition is used instead of the Poisson equation. For this purpose let us define the set

$$\mathcal{M}_{\mathrm{LEN}} = \Big\{ (a,\varphi) \in \mathbb{R}^6_+ \times L^\infty(\Omega) :$$

$$a_1 = a_2 a_3 a_6,\; a_1 a_4 = a_2 a_6,\; a_3 a_4 = 1,\; a_5 a_6 = 1, \tag{8.19}$$

$$\left.\begin{aligned} &\int_\Omega (u_1 + u_2)\,\mathrm{d}x = I_2(0), \\ &\int_\Omega (u_2 - u_3 + u_4)\,\mathrm{d}x = I_3(0), \end{aligned}\right\} \tag{8.20}$$

where $u_i = \overline{u}_i a_i \mathrm{e}^{-q_i\varphi}$ and

$$\overline{u}_2 a_2 \mathrm{e}^{\varphi} + \overline{u}_5 a_5 \mathrm{e}^{\varphi} - \overline{u}_6 a_6 \mathrm{e}^{-\varphi} = f \text{ a.e. on } \Omega \tag{8.21}$$

is fulfilled$\Big\}$.

As in Lemma 8.4 we find that $a_i > 0$, $i = 1, \ldots, 6$, if $(a,\varphi) \in \mathcal{M}_{\mathrm{LEN}}$. Furthermore, for given constants a_2, a_5, $a_6 > 0$ equation (8.21) has a unique solution $\varphi \in L^\infty(\Omega)$.

Lemma 8.6. *The set $\mathcal{M}_{\mathrm{LEN}}$ is not empty. If $(a^n, \varphi^n) \in \mathcal{M}_{\mathrm{LEN}}$, $n = 1, 2$, then*

$$a_1^1 = a_1^2,\; a_3^1 = a_3^2,\; a_4^1 = a_4^2,\; \varphi^1 - \varphi^2 = \ln\frac{a_2^2}{a_2^1} = \ln\frac{a_5^2}{a_5^1} = -\ln\frac{a_6^2}{a_6^1} = \text{const},$$

but the corresponding densities u_i and chemical potentials μ_i are uniquely determined,

$$u_i^1 = u_i^2,\; \mu_i^1 = \mu_i^2,\; i = 1, \ldots, 6.$$

Proof. Using the notation $\widetilde{a}_2 = a_2/a_5$ equation (8.21) is written as

$$\Big(1 + \frac{\overline{u}_5}{\overline{u}_2}\frac{1}{\widetilde{a}_2}\Big) u_2 - \overline{u}_6 \overline{u}_2 \widetilde{a}_2 \frac{1}{u_2} = f \text{ a.e. on } \Omega.$$

For any $\widetilde{a}_2 > 0$ the solution of this equation is given by

$$u_2(x) = \psi(x, \widetilde{a}_2),\ \psi(\cdot, \widetilde{a}_2) = \frac{1}{2}\frac{\widetilde{a}_2 f}{\widetilde{a}_2 + \overline{u}_5/\overline{u}_2} + \sqrt{\frac{1}{4}\Big[\frac{\widetilde{a}_2 f}{\widetilde{a}_2 + \overline{u}_5/\overline{u}_2}\Big]^2 + \frac{\overline{u}_6\overline{u}_2\widetilde{a}_2^2}{\widetilde{a}_2 + \overline{u}_5/\overline{u}_2}}$$

and thus

$$i_2 = \int_\Omega u_2 \,\mathrm{d}x = \Psi(\widetilde{a}_2),\ \Psi(\widetilde{a}_2) = \int_\Omega \psi(x, \widetilde{a}_2)\,\mathrm{d}x\,.$$

It is easy to check that $\Psi \in C^1(\mathbb{R}_+)$, $\Psi'(\widetilde{a}_2) > 0$ for all $\widetilde{a}_2 \in \mathbb{R}_+$ and $\Psi(0) = 0$. Because f.a.a. $x \in \Omega$ and for all $\widetilde{a}_2 \geq 0$

$$\psi(x, \widetilde{a}_2) \geq \frac{c\widetilde{a}_2}{\sqrt{c\widetilde{a}_2 + 1}} \min\Big\{\sqrt{\overline{k}_4(x)}, f(x)/2 + \sqrt{[f(x)/2]^2 + \overline{k}_4(x)}\Big\}, \quad c = \operatorname*{ess\,inf}_{x\in\Omega} \frac{\overline{u}_2(x)}{\overline{u}_5(x)},$$

we find that $\lim_{\widetilde{a}_2\to+\infty} \Psi(\widetilde{a}_2) = +\infty$ such that $\Psi^{-1} : \mathbb{R}_+ \to \mathbb{R}_+$ exists. From (8.19), (8.20) we derive an equation for i_2, namely

$$\chi(i_2) = i_2 - c_1 \frac{I_2(0) - i_2}{\Psi^{-1}(i_2)} + c_2 \frac{\Psi^{-1}(i_2)}{I_2(0) - i_2} = I_3(0),\ 0 < i_2 < I_2(0),$$

$$c_1 = \frac{\int_\Omega \overline{u}_3 \,\mathrm{d}x}{\int_\Omega \overline{u}_1 \,\mathrm{d}x}, \quad c_2 = \int_\Omega \overline{u}_4 \,\mathrm{d}x \int_\Omega \overline{u}_1 \,\mathrm{d}x.$$

Again we have $\chi \in C^1(0, I_2(0))$, $\chi'(i_2) > 0$ for all $i_2 \in (0, I_2(0))$ and $\lim_{i_2\to 0} \chi(i_2) = -\infty$, $\lim_{i_2\to I_2(0)} \chi(i_2) = +\infty$ such that $\chi^{-1} : \mathbb{R} \to (0, I_2(0))$ exists. Therefore we can state that (a, φ) belongs to $\mathcal{M}_{\mathrm{LEN}}$ if and only if

$$a_1 = \frac{1}{\int_\Omega \overline{u}_1 \,\mathrm{d}x}\Big[I_2(0) - \chi^{-1}(I_3(0))\Big],\ a_2 = \widetilde{a}_2\, a_5,\ \widetilde{a}_2 = \Psi^{-1}(\chi^{-1}(I_3(0))),$$

$$a_3 = \frac{a_1}{\widetilde{a}_2},\ a_4 = \frac{1}{a_3},\ a_5 > 0,\ a_6 = \frac{1}{a_5},\ \varphi = \ln\frac{\psi(\cdot, \widetilde{a}_2)}{\overline{u}_2\widetilde{a}_2} - \ln a_5.$$

From this statement all assertions of the lemma follow. We see that a_5 (or $\zeta_5 = \ln a_5$, the so called Fermi level of the electrons) is not fixed by the relations defining the set $\mathcal{M}_{\mathrm{LEN}}$. □

Finally, let us note that the densities and chemical potentials obtained from elements of $\mathcal{M}$ and $\mathcal{M}_{\mathrm{LEN}}$, respectively, will not coincide in general.

8.5 Example 2

Our second example is devoted to the diffusion of boron in strained Si/SiGe/Si heterostructures (see [34, 35, 39, 40]). We use the reduced version of a simplified model where we have only the species $X_2 = B$, X_5, X_6 (see Table 2) and only the reaction R_4 (see Table 3, Table 4). Mainly we are interested here in the presentation of some numerical results concerning the nonlocal nonlinear Poisson equation.

We start with state equations for the electrons and holes based on Boltzmann statistics ([13, 56]),

$$n = N_C \exp\Big[\frac{E_F - E_C + e\varphi}{kT}\Big], \quad p = N_V \exp\Big[-\frac{E_F + E_V + e\varphi}{kT}\Big]$$

where n, p denote the densities of electrons and holes, respectively, N_C, N_V are the effective densities of states in the conduction and valence band, E_C, E_V the corresponding energy band edges, E_F is the Fermi level, e the elementary charge, k the Boltzmann constant and T the absolute temperature. Introducing the bandgap E_g, the intrinsic carrier density n_i and the intrinsic Fermi level E_i,

$$E_g = E_C - E_V, \quad n_i = \sqrt{N_C N_V} \exp\Big[-\frac{E_g}{2kT}\Big], \quad E_i = \frac{E_c + E_v}{2} + kT \ln\sqrt{N_V/N_C}$$

the state equations can be written as

$$n = n_i \exp\Big[\frac{E_F - E_i + e\varphi}{kT}\Big], \quad p = n_i \exp\Big[-\frac{E_F - E_i + e\varphi}{kT}\Big].$$

The band energies E_C, E_V, E_g and E_i have different values in Si and SiGe (or more precisely, in $Si_{1-x}Ge_x$). We assume that E_i lies always in the middle of the bandgap and that ([34, 58])

$$\Delta E_C = E_{C,\mathrm{Si}} - E_{C,\mathrm{SiGe}} = 0, \qquad \Delta E_V = E_{V,\mathrm{Si}} - E_{V,\mathrm{SiGe}} = \Delta E_g,$$

$$\Delta E_g = E_{g,\mathrm{Si}} - E_{g,\mathrm{SiGe}} = 0.6585\,\mathrm{x}\, E_{g,\mathrm{Si}}, \qquad \Delta E_i = E_{i,\mathrm{Si}} - E_{i,\mathrm{SiGe}} = 0.5\,\Delta E_g.$$

Using $E_0 = E_{i,\mathrm{Si}}$ as reference value the state equation are finally written in the form[4]

$$n = \overline{n} \exp\Big[\frac{E_F - E_0 + e\varphi}{kT}\Big], \qquad p = \overline{p} \exp\Big[-\frac{E_F - E_0 + e\varphi}{kT}\Big],$$

$$\overline{n} = n_i \exp\Big[\frac{E_0 - E_i}{kT}\Big], \qquad \overline{p} = n_i \exp\Big[-\frac{E_0 - E_i}{kT}\Big].$$

For x = 0.2 and different values of T all necessary data are summarized in Table 5.

	800° C	950° C	1100° C
$n_{i,\mathrm{Si}}$ [cm^{-3}]	$1.925\,10^{18}$	$5.524\,10^{18}$	$1.292\,10^{19}$
$E_{g,\mathrm{Si}}$ [eV]	0.8513	0.7894	0.7261
$n_{i,\mathrm{SiGe}}$ [cm^{-3}]	$3.529\,10^{18}$	$9.046\,10^{18}$	$1.935\,10^{19}$
$E_{g,\mathrm{SiGe}}$ [eV]	0.7392	0.6854	0.6305
ΔE_i [eV]	0.0561	0.0520	0.0478
$n_{i,\mathrm{SiGe}}/n_{i,\mathrm{Si}}$	1.833	1.638	1.498
$\overline{n}_{\mathrm{SiGe}}/\overline{n}_{\mathrm{Si}}$	1.000	1.000	1.000
$\overline{p}_{\mathrm{SiGe}}/\overline{p}_{\mathrm{Si}}$	3.361	2.681	2.244
$\varepsilon_{rel,\mathrm{Si}}$	12.0		
$\varepsilon_{rel,\mathrm{SiGe}}$	12.8		

Table 5: Data for the materials Si and $Si_{0.8}Ge_{0.2}$.

[4]The scaling used in the previous sections reads as follows: $\zeta := (E_F - E_0)/kT$, $\varphi := e\varphi/kT$.

For an one dimensional situation the reduced model equations are (see (8.14), (8.15))

$$\begin{aligned}
\frac{\partial u}{\partial t} + \nabla \cdot j &= 0, & t > 0,\ x \in (0, L),\\
j &= 0, & t > 0,\ x = 0,\ L,\\
u(0) &= U, & x \in (0, L),\\
-\nabla \cdot (\varepsilon_{rel}\, \varepsilon_0\, \nabla\varphi) + e\, e_0\Big(\frac{E_F - E_0 + e\varphi}{kT}\Big) &= -e\, u, & t > 0,\ x \in (0, L),\\
\varphi &= 0, & t > 0,\ x = L,\\
\frac{\partial \varphi}{\partial x} &= 0, & t > 0,\ x = 0,\\
\int_0^L e\,\Big\{e_0\Big(\frac{E_F - E_0 + e\varphi}{kT}\Big) + u\Big\}\,\mathrm{d}x &= 0, & t > 0.
\end{aligned}$$

Here u denotes the density of boron, j the boron flux density, ε_0 is the permittivity in vacuum and $e_0(y) = \overline{n}\, \mathrm{e}^y - \overline{p}\, \mathrm{e}^{-y}$. The SiGe layer has a thickness of 30 nm and lies between $x = 0.07\,\mu$m and $x = 0.1\,\mu$m. The depth of the structure is assumed to be $L = 500\,\mu$m. Besides of the global charge conservation we have yet the invariant

$$\int_0^L u(t)\,\mathrm{d}x = \int_0^L U\,\mathrm{d}x, \quad t \geq 0.$$

First, we present some results concerning the reconstructed initial electron and hole densities (cf. Lemma 8.2, too). For the initial density of boron we assume a Gaussian distribution,

$$U = N_\square \frac{1}{\sqrt{2\pi}\sigma_p} \exp\left(-\frac{(x - R_p)^2}{2\,\sigma_p^2}\right), \quad N_\square = 3.5\,10^{13}\,\mathrm{cm}^{-2}, \quad R_p = 0.085\,\mu\mathrm{m}.$$

For different values of the standard deviation σ_p such boron profiles are plotted in Fig. 3. Corresponding energy band diagrams and reconstructed initial electron and hole densities are shown in Fig. 4a (for $T = 800^\circ$ C) and in Fig. 4b (for $T = 1100^\circ$ C).

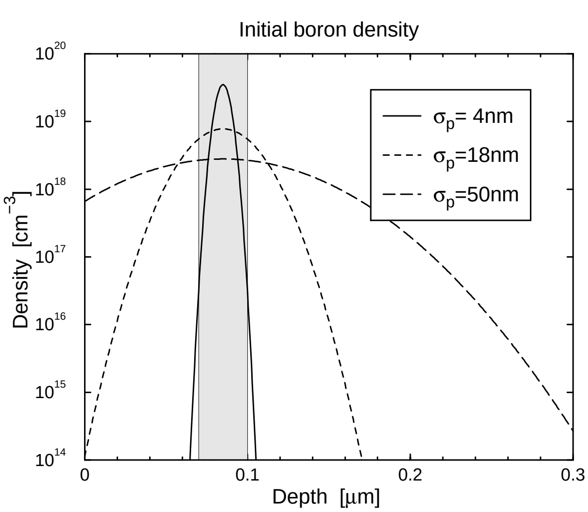

Fig. 3: Doping.

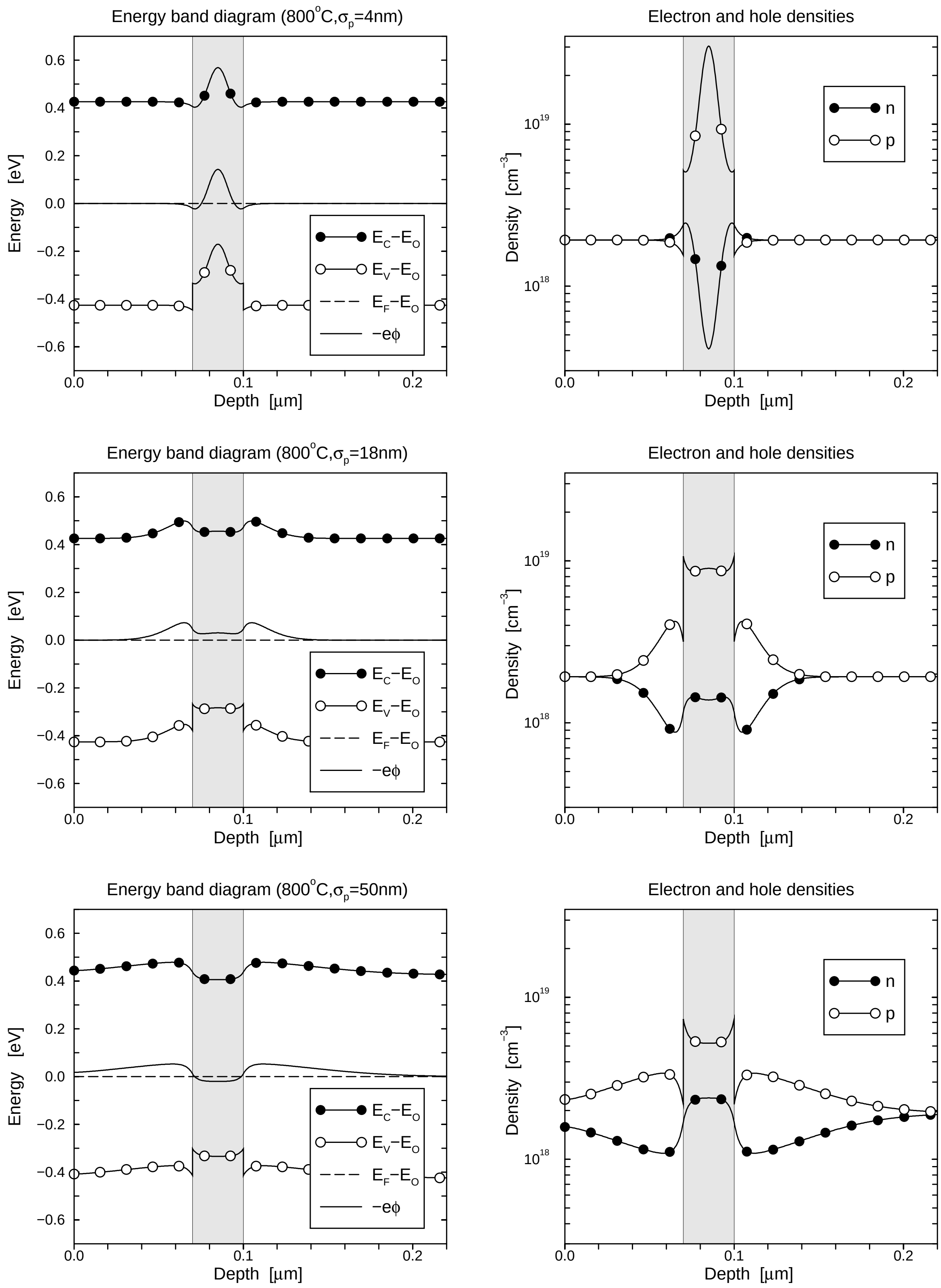

Fig. 4a: Initial state for $T = 800^\circ$ C. Variation of standard deviation.

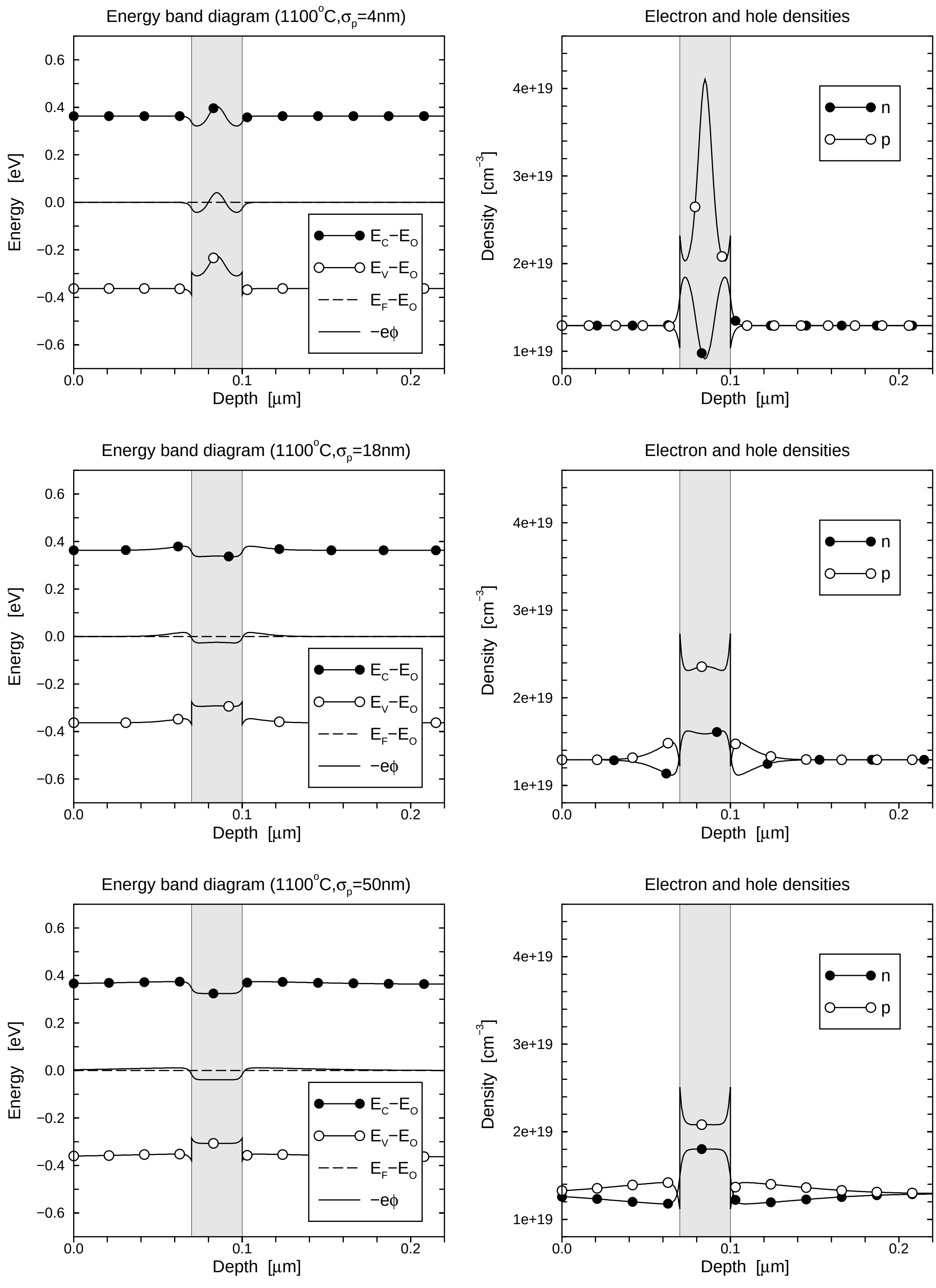

Fig. 4b: Initial state for $T = 1100^\circ$ C. Variation of standard deviation.

Since we have assumed that $\Delta E_C = 0$ the electron density remains continuous when crossing the interfaces but not the hole density. In Fig. 5 we have plotted the limit values of the hole density at the right interface taken from the left hand side and from the right hand side, respectively. This figure shows also corresponding results based on the local electroneutrality approximation (cf. Lemma 8.1, too).

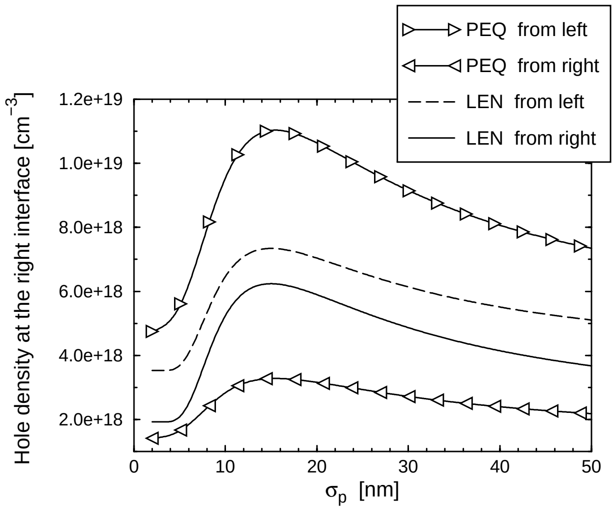

Fig. 5: Hole densities at the right interface from left and from right as function of the standard deviation ($T = 800^\circ$ C).

Finally, we have computed steady state solutions for different values of the boron segregation coefficient s. The equilibrium boron density u^* and the space charge density $-n^* + p^* - u^*$ are shown in Fig. 6. These results do not essentially depend on the standard deviation of the initial boron distribution.

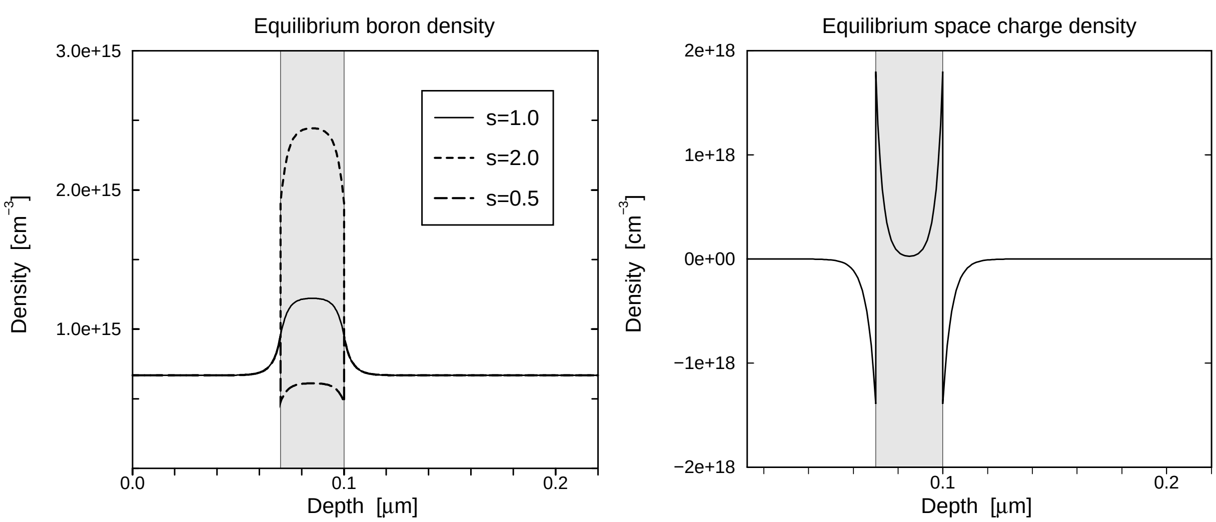

Fig. 6: Steady state for $T = 800^\circ$ C.

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