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# Global properties of pair diffusion models


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**Abstract.** The paper deals with global properties of pair diffusion models with non-smooth data arising in semiconductor technology. The corresponding model equations are continuity equations for mobile and immobile species coupled with a nonlinear Poisson equation. The continuity equations for the mobile species are nonlinear parabolic PDEs containing drift, diffusion and reaction terms. The corresponding equations for the immobile species are ODEs involving reaction terms only. Starting with energy estimates obtained by methods of convex analysis we establish global upper and lower bounds for solutions of the initial boundary value problem. We use Moser iteration for the diffusing species, the non-diffusing species are treated separately. Finally, we study the asymptotic behaviour of solutions.

## 1 Introduction

The computer simulation of the manufacturing process of semiconductor devices has experienced considerable progress over the last years. One of the main process steps is the redistribution of dopants connected with or followed after the doping which determines the electrical device characteristics of the final device structure. In order to simulate this process different models have been applied. Nowadays so called pair diffusion models [2, 6, 14, 20] are prefered. Such models involve interactions between different kinds of point defects.

**Pair diffusion models.** We consider species $\mathrm{X}_i$, $i = 1, \ldots, m$, which exist in different charge states $\mathrm{X}_{ik}$, $k = 1, \ldots, k_i$ (for instance, $\mathrm{X}_i$ stands for A, I, V, AI, AV in Fig. 1, and A stands for arsenic, boron, or phosphorus). We denote by $q_{ik}$, $u_{ik}$, $\overline{u}_{ik}$, $b_{ik}$ the charge number, the density, a suitably chosen reference density and the chemical activity of the $ik$-th species, and assume that $q_{ik} = q_{i,k-1} + 1$ for $k = 2, \ldots, k_i$, $\overline{u}_{ik} \geq c > 0$, $b_{ik} = u_{ik}/\overline{u}_{ik}$. In heterostructures which we want to include in our considerations the reference densities depend on $x$, and they may jump when crossing interfaces between different materials. The densities $u_{ik}$ may jump, too, but the chemical activities $b_{ik}$ remain sufficiently smooth (more precisely, $b_{ik} \in H^1(\Omega)$ holds). Besides of the species $\mathrm{X}_i$ electrons e and holes h have to be taken into account. We assume that the kinetics of these carriers is very fast. Then their densities are given by the statistical ansatz

$$n = \overline{n}\, \mathrm{e}^{\psi}\,,\ p = \overline{p}\, \mathrm{e}^{-\psi}\,, \quad \overline{n}, \overline{p} > 0\,,$$

and the chemical potential of the electrons $\psi$ is sufficiently smooth and fulfills the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \psi) + \overline{n}\, \mathrm{e}^{\psi} - \overline{p}\, \mathrm{e}^{-\psi} = f + \sum_{i=1}^{m} \sum_{k=1}^{k_i} q_{ik}\, u_{ik} \tag{1.1}$$

also in heterostructures, $\varepsilon$ denotes the dielectric permittivity, $f$ represents a fixed background doping. For all the other species we have continuity equations of the form

$$\frac{\partial u_{ik}}{\partial t} + \nabla \cdot j_{ik} + R^{\mathrm{ion}}_{ik} + R_{ik} = 0\,,\ k = 1, \ldots, k_i\,,\ i = 1, \ldots, m\,, \tag{1.2}$$

$$j_{ik} = -D_{ik}\, \overline{u}_{ik}\, [\nabla b_{ik} + q_{ik}\, b_{ik}\, \nabla \psi] \tag{1.3}$$

where $D_{ik}$, $R_{ik}^{\text{ion}}$ and $R_{ik}$ denote the diffusivities as well as source terms generated by ionization reactions and by other reactions, respectively.

We consider ionization reactions of the form

$$\mathrm{X}_{ik} \rightleftharpoons \mathrm{X}_{i,k+1} + \mathrm{e}\,, \;\; \mathrm{X}_{ik} + \mathrm{h} \rightleftharpoons \mathrm{X}_{i,k+1}\,, \;\; k = 1, \ldots, k_i - 1\,.$$

According to the mass action law the corresponding reaction rates are given by

$$R_{ik}^1 = k_{ik}^1 \left[ b_{ik} - b_{i,k+1}\,\mathrm{e}^{\psi} \right]\,, \;\; R_{ik}^2 = k_{ik}^2 \left[ b_{ik}\,\mathrm{e}^{-\psi} - b_{i,k+1} \right]\,, \;\; k = 1, \ldots, k_i - 1\,,$$

with kinetic coefficients $k_{ik}^1$, $k_{ik}^2 > 0$. Setting $R_{ik}^1 = R_{ik}^2 = 0$ for $k = 0, k_i$ we obtain

$$R_{ik}^{\text{ion}} = R_{ik}^1 - R_{i,k-1}^1 + R_{ik}^2 - R_{i,k-1}^2\,, \;\; k = 1, \ldots, k_i\,, \quad \sum_{k=1}^{k_i} R_{ik}^{\text{ion}} = 0\,. \tag{1.4}$$

Now let us consider the situation that all ionization reactions are very fast. In other words, let $k_{ik}^1$, $k_{ik}^2 \to \infty$. If we require that the reaction rates remain bounded then the relations $b_{i,k+1} = b_{ik}\,\mathrm{e}^{-\psi}$, $k = 1, \ldots, k_i - 1$, must be fulfilled. This implies

$$\mathrm{e}^{q_{ik}\psi} b_{ik} = \mathrm{e}^{q_{i1}\psi} b_{i1}\,, \;\; k = 1, \ldots, k_i\,. \tag{1.5}$$

In order to eliminate the indefinite terms $R_{ik}^{\text{ion}}$ occuring in the continuity equations (1.2) we make use of the so called mass lumping. We introduce new quantities

$$u_i = \sum_{k=1}^{k_i} u_{ik}\,, \;\; j_i = \sum_{k=1}^{k_i} j_{ik}\,, \;\; R_i = \sum_{k=1}^{k_i} \left( R_{ik}^{\text{ion}} + R_{ik} \right) = \sum_{k=1}^{k_i} R_{ik} \tag{1.6}$$

where the last relation holds because of (1.4). Then for the lumped densities the continuity equations

$$\frac{\partial u_i}{\partial t} + \nabla \cdot j_i + R_i = 0\,, \;\; i = 1, \ldots, m\,, \tag{1.7}$$

are derived. In these equations as well as in the Poisson equation (1.1) all terms containing $u_{ik}$ must be rewritten using the new variables $u_i$ and $\psi$.

First, because of (1.6), (1.5) we obtain

$$\begin{aligned} u_i &= p_i(\psi)\,\mathrm{e}^{q_{i1}\psi}\, b_{i1}\,, & p_i(\psi) &= \textstyle\sum_{k=1}^{k_i} \overline{u}_{ik}\mathrm{e}^{-q_{ik}\psi}\,, \\ j_i &= -D_i(\psi)\, p_i(\psi)\, \nabla \frac{u_i}{p_i(\psi)}\,, & D_i(\psi) &= \frac{\sum_{k=1}^{k_i} D_{ik}\overline{u}_{ik}\mathrm{e}^{-q_{ik}\psi}}{p_i(\psi)}\,, \\ \sum_{k=1}^{k_i} q_{ik} u_{ik} &= Q_i(\psi)\, u_i\,, & Q_i(\psi) &= \frac{\sum_{k=1}^{k_i} q_{ik}\overline{u}_{ik}\mathrm{e}^{-q_{ik}\psi}}{p_i(\psi)}\,. \end{aligned} \tag{1.8}$$

In heterostructures the functions $p_i$, $D_i$, $Q_i$ depend explicitly on $x$, since the reference densities $\overline{u}_{ik}$ depend on $x$. In this paper we use the additional assumption that

$$\overline{u}_{ik}(x) = K_{ik}\,\overline{u}_{i1}(x) \text{ with } K_{ik} = \text{const} > 0\,, \;\; k = 1, \ldots, k_i\,.$$

Then the lumped charge numbers $Q_i$ do not explicitly depend on $x$,

$$Q_i(\psi) = \frac{\sum_{k=1}^{k_i} q_{ik} K_{ik}\mathrm{e}^{-q_{ik}\psi}}{\sum_{k=1}^{k_i} K_{ik}\mathrm{e}^{-q_{ik}\psi}}\,, \quad Q_i'(\psi) \le 0\,, \tag{1.9}$$

and it follows that

$$p_i(x,\psi) = p_{0i}(x)\,\mathrm{e}^{-P_i(\psi)}\,,\ \ p_{0i}(x) = \overline{u}_{i1}(x)\sum_{k=1}^{k_i} K_{ik} > 0\,,\ \ P_i(\psi) = \int_0^{\psi} Q_i(y)\,\mathrm{d}y\,. \tag{1.10}$$

We define electrochemical activities $a_i$ and chemical activities $b_i$ of the *lumped* species by $a_i = u_i/p_i(\psi)$ and $b_i = u_i/p_{0i}$. Then $b_i$ is sufficiently smooth, too, and

$$\frac{u_i}{p_i(\cdot,\psi)} = a_i = b_i\,\mathrm{e}^{P_i(\psi)}\,, \quad j_i = -D_i(\cdot,\psi)\,p_{0i}\,\left[\nabla b_i + b_i\,Q_i(\psi)\,\nabla\psi\right] \tag{1.11}$$

is obtained. As often done we assume that for a dopant (say $\mathrm{X}_i$) there exists only one charge state (then we set $\mathrm{X}_{i1} = \mathrm{X}_i$, $q_{i1} = q_i$, and so on), and that its diffusivity vanishes.

Next, the reaction terms $R_i$ in (1.7), (1.6) will be rewritten. We start with reactions describing the formation and disintegration of dopant-defect pairs. Let $i$, $j$, $l$ be fixed and consider reactions

$$\mathrm{X}_i + \mathrm{X}_{jk} + \alpha_n\,\mathrm{e} + \alpha_p\,\mathrm{h} \rightleftharpoons \mathrm{X}_{lk'} + \beta_n\,\mathrm{e} + \beta_p\,\mathrm{h}\,, \quad q_i + q_{jk} - \alpha_n + \alpha_p = q_{lk'} - \beta_n + \beta_p$$

for varying $k$, $k'$ and $\gamma = (\alpha_n, \alpha_p, \beta_n, \beta_p) \in \mathbb{Z}_+^4$. In the model described in Fig. 1 $\mathrm{X}_i$ stands for A, and $\mathrm{X}_{jk}$, $\mathrm{X}_{lk'}$ stand for different charge states of I, AI or V, AV. The corresponding rate formulas are

$$R_{kk'\gamma} = k_{kk'\gamma}\left[b_i b_{jk}\,\mathrm{e}^{\alpha_n\psi}\mathrm{e}^{-\alpha_p\psi} - b_{lk'}\,\mathrm{e}^{\beta_n\psi}\mathrm{e}^{-\beta_p\psi}\right]\,, \quad k_{kk'\gamma} > 0\,.$$

Using (1.5), (1.8) and (1.11) we easily obtain

$$R := \sum_{k,k',\gamma} R_{kk'\gamma} = k(\psi)\,\left[a_i\,a_j - a_l\right]\,, \quad k(\psi) = \sum_{k,k',\gamma} k_{kk'\gamma}\,\mathrm{e}^{-(-\alpha_n+\alpha_p+q_i+q_{jk})\psi}\,.$$

The contributions of these reactions to the corresponding continuity equations in (1.2) and (1.7) are

$$R_i = R\,,\ \ R_{jk} = \sum_{k',\gamma} R_{kk'\gamma}\,,\ \ R_{lk'} = -\sum_{k,\gamma} R_{kk'\gamma}\,,$$

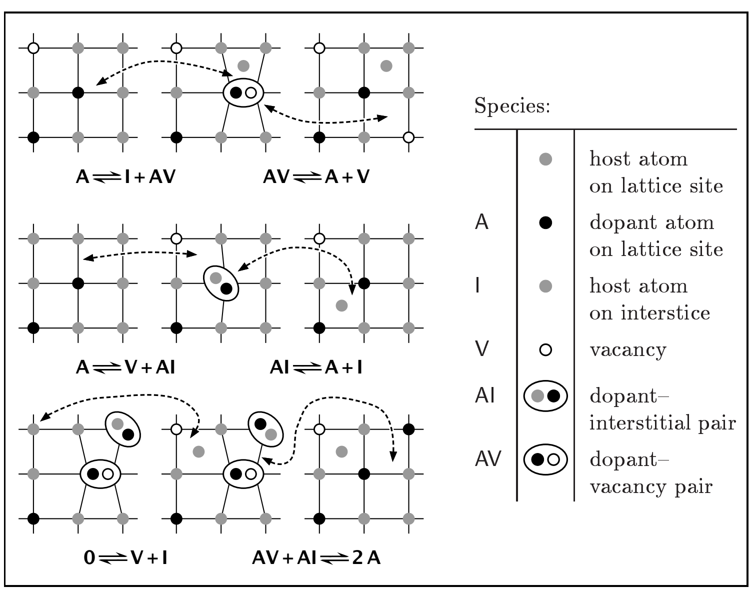


Figure 1: Species and reactions in a variant of pair diffusion models [2, 6].

$$R_i = R\,,\ R_j = \sum_k R_{jk} = R\,,\ R_l = \sum_{k'} R_{lk'} = -R\,.$$

Thus we find that all these reactions are reduced to the only reaction $X_i + X_j \rightleftharpoons X_l$ for the *lumped* species which is of mass action type, again. Reactions describing the generation and recombination of different kinds of defects can be treated analogously. Let $i$, $j$, $l$ and $\beta_i \in \mathbb{Z}_+$ be fixed and consider reactions

$$X_{jk} + X_{lk'} + \alpha_n\,e + \alpha_p\,h \rightleftharpoons \beta_i X_i + \beta_n\,e + \beta_p\,h\,, \quad q_{jk} + q_{lk'} - \alpha_n + \alpha_p = \beta_i q_i - \beta_n + \beta_p$$

for varying $k$, $k'$ and $\gamma = (\alpha_n, \alpha_p, \beta_n, \beta_p) \in \mathbb{Z}^4_+$. In the model of Fig. 1 $X_i$ stands for A, and $X_{jk}, X_{lk'}$ stand for charge states of I, V ($\beta_i = 0$), of I, AV or V, AI ($\beta_i = 1$), or of AI, AV ($\beta_i = 2$). The rate formulas are

$$R_{kk'\gamma} = k_{kk'\gamma}\left[b_{jk}b_{lk'}\,e^{\alpha_n\psi}e^{-\alpha_p\psi} - b_i^{\beta_i}\,e^{\beta_n\psi}e^{-\beta_p\psi}\right]\,, \quad k_{kk'\gamma} > 0\,.$$

Now we have

$$R := \sum_{k,k',\gamma} R_{kk'\gamma} = k(\psi)\,\left[a_j\,a_l - a_i^{\beta_i}\right]\,, \quad k(\psi) = \sum_{k,k',\gamma} k_{kk'\gamma}\,e^{-(-\alpha_n+\alpha_p+q_{jk}+q_{lk'})\psi}\,.$$

The contributions of these reactions to the corresponding continuity equations in (1.7) are

$$R_i = -\beta_i\,R\,,\ R_j = R\,,\ R_l = R\,.$$

Again, for the *lumped* species the mass action type reaction $X_j + X_l \rightleftharpoons \beta_i\,X_i$ is obtained. Finally, let us discuss a simple example that shows how boundary reactions can be included in the model. Let $j$ be fixed, and assume that $q_{jk^0_j} = 0$ for some $k^0_j$ and that on some part $\Gamma_1$ of the boundary $\Gamma$ we have the reaction

$$X_{jk^0_j} \rightleftharpoons 0\,,$$

$X_{jk^0_j}$ stands for uncharged I or V, for instance. The rate is $R = k^\Gamma\left[b_{jk^0_j} - 1\right]$, $k^\Gamma > 0$. Then the boundary condition

$$\nu\cdot j_{jk} = \begin{cases} 0 & \text{on } \Gamma, & k \neq k_{jk^0_j}\,, \\ 0 & \text{on } \Gamma\setminus\Gamma_1, & k = k_{jk^0_j}\,, \\ R & \text{on } \Gamma_1, & k = k_{jk^0_j} \end{cases}$$

must be added to the continuity equations (1.2). We set $k^\Gamma = 0$ on $\Gamma\setminus\Gamma_1$, and from (1.5), (1.8) and (1.11) we derive the boundary condition

$$\nu\cdot j_j = k^\Gamma\,[a_j - 1]\ \text{ on } \Gamma$$

for the continuity equations (1.7) which corresponds to a reaction of the form $X_j \rightleftharpoons 0$.

**Initial boundary value problem.** Motivated by the preceding discussion we investigate in this paper a rather general electro-reaction-diffusion system for $m$ species $X_i$. Unknown functions are the densities $u_i$ and the potential $\psi$, related functions are the chemical activities $b_i = u_i/p_{0i}$, the electrochemical activities $a_i = b_i e^{P_i(\psi)}$, and the electrochemical potentials $\zeta_i = \ln\,a_i$ (defined for $a_i > 0$). The initial boundary value problem which we are interested in reads as follows:

$$\left.\begin{aligned}
\frac{\partial u_i}{\partial t} + \nabla\cdot j_i + \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} (\alpha_i-\beta_i)\, R^\Omega_{\alpha\beta} &= 0 \quad \text{on } (0,\infty)\times\Omega\,,\\
\nu\cdot j_i - \sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma} (\alpha_i-\beta_i)\, R^\Gamma_{\alpha\beta} &= 0 \quad \text{on } (0,\infty)\times\Gamma\,,\ i=1,\dots,l\,;\\
\frac{\partial u_i}{\partial t} + \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} (\alpha_i-\beta_i)\, R^\Omega_{\alpha\beta} &= 0 \quad \text{on } (0,\infty)\times\Omega\,,\ i=l+1,\dots,m\,;\\
-\nabla\cdot(\varepsilon\nabla\psi) + e(\cdot,\psi) - \sum_{i=1}^m Q_i(\psi)u_i &= f \quad \text{on } (0,\infty)\times\Omega\,,\\
\nu\cdot(\varepsilon\nabla\psi) &= 0 \quad \text{on } (0,\infty)\times\Gamma\,;\\
u_i(0) &= U_i \quad \text{on } \Omega\,,\ i=1,\dots,m\,.
\end{aligned}\right\} \qquad (1.12)$$

The kinetic relations are assumed to be given by

$$j_i = -D_i(\cdot,b,\psi)p_{0i}\big[\nabla b_i + Q_i(\psi)\,b_i\nabla\psi\big]\,,\ i=1,\dots,l\,,$$

$$R^\Omega_{\alpha\beta}(x,b_1,\dots,b_m,\psi) = k^\Omega_{\alpha\beta}(x,b_1,\dots,b_m,\psi)\Big[\prod_{i=1}^m a_i^{\alpha_i} - \prod_{i=1}^m a_i^{\beta_i}\Big]\,,\ x\in\Omega\,,\ (\alpha,\beta)\in\mathcal{R}^\Omega\,,$$

$$R^\Gamma_{\alpha\beta}(x,b_1,\dots,b_l,\psi) = k^\Gamma_{\alpha\beta}(x,b_1,\dots,b_l,\psi)\Big[\prod_{i=1}^l a_i^{\alpha_i} - \prod_{i=1}^l a_i^{\beta_i}\Big]\,,\ x\in\Gamma\,,\ (\alpha,\beta)\in\mathcal{R}^\Gamma$$

where $\mathcal{R}^\Omega \subset \mathbb{Z}^m_+\times\mathbb{Z}^m_+$, $\mathcal{R}^\Gamma \subset \{(\alpha,\beta)\in\mathbb{Z}^m_+\times\mathbb{Z}^m_+\colon \alpha_i=\beta_i=0\,,\ i=l+1,\dots,m\}$, and the vector $(\alpha,\beta)=(\alpha_1,\dots,\alpha_m,\beta_1,\dots,\beta_m)$ represents the stoichiometric coefficients of a mass action type reaction of the form

$$\alpha_1X_1+\dots+\alpha_mX_m \rightleftharpoons \beta_1X_1+\dots+\beta_mX_m\,.$$

**Comments.** Basic assumptions on the data of this problem are formulated in the next section. Here let us only emphasize that we require $Q_i'(\psi)\le 0$ and $P_i'(\psi)=Q_i(\psi)$, cf. (1.9), (1.10). These properties guarantee that the relation between the electrochemical potentials $\zeta_i$ and densities $u_i$ has a potential in the sense of convex analysis, namely the free energy. Moreover, the special structure of the kinetic relations and natural assumptions on the kinetic coefficients imply that the free energy is a Lyapunov function for the evolution system (1.12). In [16] we established these results for a simplified version of (1.12) (for a homogeneous material and kinetic coefficients not depending on $b$). It is easy to see that the proofs given there carry over to the more general setting considered here. Therefore these results are summarized in Section 3 without detailed proofs. The main topic of this paper consists in deriving global estimates for solutions of (1.12). Assuming, that the source terms of the volume reactions and boundary reactions are of at most second and first order, respectively, global upper bounds are obtained in Section 4. Next, under the assumption that the initial densities fulfill the estimate $U_i\ge c_0>0$ a.e. on $\Omega$ we prove in Section 5 that $u_i(t)\ge c>0$ a.e. on $\Omega$ for all $t>0$. Finally, in Section 6 additional results concerning the asymptotic behaviour of solutions are given.

The existence of a solution of (1.12) for heterogeneous materials will be shown in a forthcoming paper. For homogeneous materials an existence and uniqueness result can be found in [18]. There $l=m$ is supposed, and all kinetic coefficients depend only on $\psi$. If each species has a constant charge number ($Q_i(\psi) = q_i$, $P_i(\psi) = q_i\,\psi$) then one gets a model of the form (1.1) – (1.3). Such model equations were studied in [8, 9, 10, 11] under the assumption that $l = m$ but for heterostructures. A pair diffusion model for uncharged species (then the Poisson equation is dropped) and for homogeneous materials is investigated in [15]. There $l < m$ is allowed.

**Notation.** Let us collect some notation used in the paper. The notation of function spaces corresponds to that in [17]. By $\mathbb{Z}^m_+$, $\mathbb{R}^m_+$, $L^p_+$ we denote the cones of non-negative elements. For the scalar product in $\mathbb{R}^m$ we use a centered dot. If $u \in \mathbb{R}^m$ then $u \geq 0$ ($u > 0$) means $u_i \geq 0\,\forall i$ ($u_i > 0\,\forall i$); $\sqrt{u}$ denotes the vector $\{\sqrt{u_i}\}_{i=1,\dots,m}$, and analogously $\ln u$, $\mathrm{e}^u$ are to be understood. For $u$, $v \in \mathbb{R}^m$ we set $uv = \{u_i v_i\}_{i=1,\dots,m}$, $u/v = \{u_i/v_i\}_{i=1,\dots,m}$. If $u \in \mathbb{R}^m_+$ and $\alpha \in \mathbb{Z}^m_+$ then $u^\alpha$ means the product $\prod_{i=1}^m u_i^{\alpha_i}$. 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 $\lim_{y\to\infty} d(y) = \infty$.

## 2 Formulation of the problem

We summarize the **basic assumptions (I)** which our considerations are based on.

i) $\Omega \subset \mathbb{R}^2$ is a bounded Lipschitzian domain, $U \in L^\infty_+(\Omega, \mathbb{R}^m)$, $f \in L^2(\Omega)$;

ii) $\varepsilon \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$,

$e\colon \Omega \times \mathbb{R} \to \mathbb{R}$ satisfies the Carathéodory conditions,

$|e(x,\psi)| \leq c\,\mathrm{e}^{c|\psi|}$ f.a.a. $x \in \Omega$, $\forall \psi \in \mathbb{R}$, $c > 0$,

$e(x,\psi) - e(x,\overline{\psi}) \geq e_0(x)\,(\psi - \overline{\psi})$ f.a.a. $x \in \Omega$, $\forall \psi, \overline{\psi} \in \mathbb{R}$ with $\psi \geq \overline{\psi}$,

$e_0 \in L^\infty_+(\Omega)$, $\|e_0\|_{L^1} > 0$,

$e(x,\cdot)$ is locally Lipschitz continuous uniformly with respect to $x$;

iii) $Q_i \in C^1(\mathbb{R})$, $|Q_i(\psi)| \leq c$, $Q_i'(\psi) \leq 0$,

$p_i(x,\psi) = p_{0i}(x)\,e^{-P_i(\psi)}$, $x \in \Omega$, $\psi \in \mathbb{R}$, $p_{0i} \in L^\infty_+(\Omega)$,

$\operatorname{ess\,inf}_{x\in\Omega} p_{0i}(x) \geq \epsilon_0 > 0$, $P_i(\psi) = \displaystyle\int_0^\psi Q_i(y)\,\mathrm{d}y$, $\psi \in \mathbb{R}$, $i = 1,\dots,m$;

iv) $\mathcal{R}^\Omega \subset \mathbb{Z}^m_+ \times \mathbb{Z}^m_+$, $\mathcal{R}^\Gamma \subset \big\{(\alpha,\beta) \in \mathbb{Z}^m_+ \times \mathbb{Z}^m_+ \colon \alpha_i = \beta_i = 0,\ i = l+1,\dots,m\big\}$,

for $\Sigma = \Omega$, $\Gamma$ and $(\alpha,\beta) \in \mathcal{R}^\Sigma$ we define $R^\Sigma_{\alpha\beta}\colon \Sigma \times \mathbb{R}^{m_\Sigma}_+ \times \mathbb{R} \to \mathbb{R}$ by

$R^\Sigma_{\alpha\beta}(x,b,\psi) := k^\Sigma_{\alpha\beta}(x,b,\psi)(a^\alpha - a^\beta)$, $a_i = b_i \mathrm{e}^{P_i(\psi)}$, $i = 1,\dots,m_\Sigma$,

$x \in \Sigma$, $b \in \mathbb{R}^{m_\Sigma}_+$, $\psi \in \mathbb{R}$, where $m_\Omega = m$, $m_\Gamma = l$,

$k^\Sigma_{\alpha\beta}\colon \Sigma \times \mathbb{R}^{m_\Sigma}_+ \times \mathbb{R} \to \mathbb{R}_+$ satisfies the Carathéodory conditions,

$k^\Sigma_{\alpha\beta}(x,b,\psi) \leq c_R$ f.a.a. $x \in \Sigma$, $\forall b \in \mathbb{R}^{m_\Sigma}_+$, $\forall \psi \in [-R,R]$, $R > 0$,

$k^\Sigma_{\alpha\beta}(x,b,\psi) \geq b^\Sigma_{\alpha\beta,R}(x)$ f.a.a. $x \in \Sigma$, $\forall b \in \mathbb{R}^{m_\Sigma}_+$, $\forall \psi \in [-R,R]$, $R > 0$,

$b^\Sigma_{\alpha\beta,R} \in L^\infty_+(\Sigma)$, $\|b^\Sigma_{\alpha\beta,R}\|_{L^1(\Sigma)} > 0$;

v) for $i=1,\dots,l:$ $D_i\colon \Omega\times\mathbb{R}^m_+\times\mathbb{R}\to\mathbb{R}_+$ satisfies the Carathéodory conditions,

$$D_i(x,b,\psi)\ge c>0 \text{ f.a.a. } x\in\Omega\,,\ \forall b\in\mathbb{R}^m_+\,,\ \forall\psi\in\mathbb{R}\,,$$

$$D_i(x,b,\psi)\le c_R \text{ f.a.a. } x\in\Omega\,,\ \forall b\in\mathbb{R}^m_+\,,\ \forall\psi\in[-R,R]\,,\ R>0\,;$$

vi) for $i=l+1,\dots,m:$ there is a reaction of the form

$$R^\Omega_{\alpha(i)\beta(i)}(x,b,\psi)=k^\Omega_{\alpha(i)\beta(i)}(x,b,\psi)\Big[\prod_{j=1}^{l}a_j^{\alpha(i)j}-a_i^2\Big]\,,\ x\in\Omega\,,\ b\in\mathbb{R}^m_+\,,\ \psi\in\mathbb{R}$$

with $\operatorname{ess\,inf}_{x\in\Omega} b^\Omega_{\alpha(i)\beta(i),R}(x)>0\,.$

A further assumption (II) ensuring the existence of a unique steady state is formulated in Section 3. An additional assumption (III) which we need for the proof of global upper bounds for the densities is introduced in Section 4. Adding the assumption (IV) in Section 5 we establish global lower bounds for the densities. All assumptions are formulated in such a way that pair diffusion models as discussed in Section 1 can be treated.

**Remark 2.1** The form of the reaction terms $R^\Sigma_{\alpha\beta}$, $(\alpha,\beta)\in\mathcal{R}^\Omega\cup\mathcal{R}^\Gamma$, involves that

$$(a^\alpha-a^\beta)\,(\alpha-\beta)\cdot\ln a\ge 0\quad\forall a\in\operatorname{int}\,\mathbb{R}^{m_\Sigma}_+ \tag{2.1}$$

what is important for obtaining energy estimates. Moreover, for $i=1,\dots,m_\Sigma$ we have

$$\begin{aligned}(a^\alpha-a^\beta)(\alpha_i-\beta_i)&\le\Big[\alpha_i\,a_i^{\alpha_i-1}\prod_{j\ne i}a_j^{\alpha_j}\Big]\,a_i\ \text{ if }\alpha_i>\beta_i\,,\\ (a^\alpha-a^\beta)(\alpha_i-\beta_i)&\le\Big[\beta_i\,a_i^{\beta_i-1}\prod_{j\ne i}a_j^{\beta_j}\Big]\,a_i\ \text{ if }\alpha_i<\beta_i\quad\forall a\in\mathbb{R}^{m_\Sigma}_+\end{aligned} \tag{2.2}$$

what we need for deriving lower estimates for the densities.

We use the function spaces

$$Y:=L^2(\Omega,\mathbb{R}^m)\,,\ X:=\{b\in Y\colon b_i\in H^1(\Omega)\,,\ i=1,\dots,l\}$$

and define the operators $B\colon Y\to Y$, $A\colon[X\times H^1(\Omega)]\cap[L^\infty_+(\Omega,\mathbb{R}^m)\times L^\infty(\Omega)]\to X^*$, $E\colon H^1(\Omega)\times Y\to(H^1(\Omega))^*$ by

$$\left.\begin{aligned}
(Bb,\overline{b})_Y&:=\int_\Omega\sum_{i=1}^m p_{0i}\,b_i\,\overline{b}_i\,\mathrm{d}x\,,\quad\overline{b}\in Y\,,\\
\langle A(b,\psi),\overline{b}\rangle_X&:=\int_\Omega\sum_{i=1}^l D_i(\cdot,b,\psi)\,p_{0i}\,[\nabla b_i+b_iQ_i(\psi)\nabla\psi]\cdot\nabla\overline{b}_i\\
&\quad+\int_\Omega\sum_{(\alpha,\beta)\in\mathcal{R}^\Omega}R^\Omega_{\alpha\beta}(\cdot,b_1,\dots,b_m,\psi)\sum_{i=1}^m(\alpha_i-\beta_i)\,\overline{b}_i\,\mathrm{d}x\\
&\quad+\int_\Gamma\sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma}R^\Gamma_{\alpha\beta}(\cdot,b_1,\dots,b_l,\psi)\,\sum_{i=1}^l(\alpha_i-\beta_i)\,\overline{b}_i\,\mathrm{d}\Gamma\,,\quad\overline{b}\in X\,,\\
\langle E(\psi,u),\overline{\psi}\rangle_{H^1}&:=\int_\Omega\Big\{\varepsilon\nabla\psi\cdot\nabla\overline{\psi}+\Big[e(\cdot,\psi)-\sum_{i=1}^m u_iQ_i(\psi)-f\Big]\,\overline{\psi}\Big\}\,\mathrm{d}x\,,\ \overline{\psi}\in H^1(\Omega)\,.
\end{aligned}\right\} \tag{2.3}$$

The precise formulation of the electro-reaction-diffusion system (1.12) reads as follows:

$$\left.\begin{array}{c} u'(t) + A(b(t),\psi(t)) = 0\,, \quad E(\psi(t),u(t)) = 0\,, \quad u(t) = Bb(t) \quad \text{f.a.a. } t>0\,, \\[2ex] u(0) = U\,, \\[2ex] u \in H^1_{\text{loc}}(\mathbb{R}_+, X^*)\,,\ b \in L^2_{\text{loc}}(\mathbb{R}_+, X) \cap L^\infty_{\text{loc}}(\mathbb{R}_+, L^\infty_+(\Omega,\mathbb{R}^m))\,, \\[2ex] \psi \in L^2_{\text{loc}}(\mathbb{R}_+, H^1(\Omega)) \cap L^\infty_{\text{loc}}(\mathbb{R}_+, L^\infty(\Omega))\,. \end{array}\right\} \qquad \text{(P)}$$

**Remark 2.2** Let $(u,b,\psi)$ be a solution of (P). Then $u$, $b$, $\psi$ have the following regularity properties. Because of $u \in H^1_{\text{loc}}(\mathbb{R}_+, X^*)$ and $b \in L^2_{\text{loc}}(\mathbb{R}_+, X)$ we have $b \in C(\mathbb{R}_+, Y)$ (cf. [12, Theorem 2.70]). Thus $u \in C(\mathbb{R}_+, Y)$, too. Moreover $u, b \in C_{w^*}(\mathbb{R}_+, L^\infty(\Omega,\mathbb{R}^m))$ and $\psi \in C(\mathbb{R}_+, H^1(\Omega))$. These properties imply that for all $t \in \mathbb{R}_+$

$$E(\psi(t),u(t)) = 0 \text{ in } (H^1(\Omega))^*\,,\ u(t) = p_0\, b(t) \text{ in } L^\infty(\Omega,\mathbb{R}^m)\,,\ u(t) \geq 0 \text{ a.e. on } \Omega\,. \qquad (2.4)$$

## 3 Global estimates for the free energy and their consequences

In this section results as in [16] are shortly presented. Additionally, further estimates are derived which we need in the next sections to get global estimates for the densities. With regard to methods and results of convex analysis we refer to [1, 3].

### 3.1 The nonlinear Poisson equation

**Lemma 3.1** *We assume* (I). *For any $u \in Y_+ = L^2_+(\Omega,\mathbb{R}^m)$ there exists a unique solution $\psi$ of $E(\psi,u) = 0$. Moreover, there are an exponent $q > 2$, a positive constant $c$ and a monotonously increasing function $d\colon \mathbb{R}_+ \to \mathbb{R}_+$ such that*

$$\|\psi - \overline{\psi}\|_{H^1} \leq c\,\|u - \overline{u}\|_Y \quad \forall u, \overline{u} \in Y_+\,,\ E(\psi,u) = E(\overline{\psi},\overline{u}) = 0\,,$$

$$\|\psi\|_{L^\infty} \leq c\Big\{1 + \sum_{i=1}^m \|u_i \ln u_i\|_{L^1} + d(\|\psi\|_{H^1})\Big\} \quad \forall u \in Y_+\,,\ E(\psi,u) = 0\,,$$

$$\|\psi\|_{W^{1,q}} \leq c\Big\{1 + \sum_{i=1}^m \|u_i\|_{L^{2q/(2+q)}} + d(\|\psi\|_{H^1})\Big\} \quad \forall u \in Y_+\,,\ E(\psi,u) = 0\,.$$

*Proof.* Up to the last inequality all assertions follow from [16, Lemma 1]. The last inequality is a consequence of Gröger's regularity result [13, Theorem 1] and of Trudinger's imbedding theorem (8.4). □

### 3.2 The energy functional

We define two functionals $\widetilde{F}_1, \widetilde{F}_2 : Y_+ \to \mathbb{R}$ by

$$\widetilde{F}_1(u) = \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla\psi|^2 + \int_0^\psi [e(\cdot,\psi) - e(\cdot,y)]\, \mathrm{d}y + \sum_{i=1}^m u_i(P_i(\psi) - Q_i(\psi)\psi)\Big\}\, \mathrm{d}x\,,\ u \in Y_+ \quad (3.1)$$

where $\psi \in H^1(\Omega) \cap L^\infty(\Omega)$ is the unique solution of the Poisson equation $E(\psi, u) = 0$,

$$\widetilde{F}_2(u) = \int_\Omega \sum_{i=1}^m \Big\{ u_i \Big[ \ln \frac{u_i}{p_{0i}} - 1 \Big] + p_{0i} \Big\} \,\mathrm{d}x \,, \quad u \in Y_+ \,. \tag{3.2}$$

and set $\widetilde{F} = \widetilde{F}_1 + \widetilde{F}_2$, $\widetilde{F}(u)$ can be interpreted as free energy of the state $u$. Let $u, \overline{u} \in Y_+$, and correspondingly $\psi, \overline{\psi} \in H^1(\Omega)$ with $E(\psi, u) = E(\overline{\psi}, \overline{u}) = 0$. We obtain

$$\begin{aligned} \widetilde{F}_1(u) - \widetilde{F}_1(\overline{u}) = \int_\Omega \Big\{ & \frac{\varepsilon}{2} |\nabla(\psi - \overline{\psi})|^2 + \int_{\overline{\psi}}^{\psi} [e(\cdot, \psi) - e(\cdot, y)] \,\mathrm{d}y \\ & + \sum_{i=1}^m P_i(\overline{\psi})(u_i - \overline{u}_i) + \sum_{i=1}^m u_i \int_{\overline{\psi}}^{\psi} [Q_i(y) - Q_i(\psi)] \,\mathrm{d}y \Big\} \,\mathrm{d}x \\ \geq & \,(P(\overline{\psi}), u - \overline{u})_Y + c \,\|\psi - \overline{\psi}\|_{H^1}^2 \geq (P(\overline{\psi}), u - \overline{u})_Y \,. \end{aligned} \tag{3.3}$$

From this relation it follows that $\widetilde{F}_1$ is convex and continuous on the convex set $Y_+$. We extend $\widetilde{F}_1$ to $Y$ by setting $\widetilde{F}_1(u) = +\infty$ for $u \in Y \setminus Y_+$. Then the extended functional $\widetilde{F}_1 : Y \to \overline{\mathbb{R}}$ is proper, convex, lower semi-continuous, and sub-differentiable in each point $u \in Y_+$, $P(\psi) \in \partial \widetilde{F}_1(u)$. Because of properties of its integrand the functional $\widetilde{F}_2$ is convex and continuous (see [10]) on $Y_+$. Again the extended functional $\widetilde{F}_2 : Y \to \overline{\mathbb{R}}$, $\widetilde{F}_2(u) = +\infty$ for $u \in Y \setminus Y_+$, is proper, convex and lower semi-continuous. For $u, \overline{u} \in Y_+$ with $\overline{u} \geq \delta > 0$ we obtain

$$\begin{aligned} \widetilde{F}_2(u) - \widetilde{F}_2(\overline{u}) &= \int_\Omega \sum_{i=1}^m \Big\{ \ln \frac{\overline{u}_i}{p_{0i}} (u_i - \overline{u}_i) + \int_{\overline{u}_i}^{u_i} (\ln y - \ln \overline{u}_i) \,\mathrm{d}y \Big\} \,\mathrm{d}x \\ &\geq (\ln \overline{u}/p_0, u - \overline{u})_Y + \|\sqrt{u} - \sqrt{\overline{u}}\|_Y^2 \geq (\ln \overline{u}/p_0, u - \overline{u})_Y \,. \end{aligned} \tag{3.4}$$

Thus, $\widetilde{F}_2$ is sub-differentiable in points $u \in Y_+$ with $u \geq \delta > 0$, and $\ln u/p_0 \in \partial \widetilde{F}_2(u)$. Finally, we extend both functionals to the space $X^*$ by

$$F_k = (\widetilde{F}_k^*|_X)^* : X^* \to \overline{\mathbb{R}} \,, \quad k = 1, 2 \,.$$

**Lemma 3.2** *The functional $F = F_1 + F_2 : X^* \to \overline{\mathbb{R}}$ is proper, convex and lower semi-continuous. For $u \in Y_+$ it can be evaluated according to* (3.1), (3.2). *The restriction $F|_{Y_+}$ is continuous. If $u \in Y_+$, $u/p_0 \in X$, $u \geq \delta > 0$ then*

$$\zeta = \ln \frac{u}{p_0} + P(\psi) = \ln \frac{u}{p(\psi)} \in \partial F(u)$$

*where $\psi$ is the solution of $E(\psi, u) = 0$.*

*Proof.* We denote the imbedding of $X$ into $Y$ by $I$, and correspondingly $I^* : Y \to X^*$. Then the definition of $F_k$ means

$$F_k = (\widetilde{F}_k^* \circ I)^* : X^* \to \overline{\mathbb{R}} \,, \quad F_k(u) = \sup_{w \in X} \big\{ \langle u, w \rangle_X - \widetilde{F}_k^*(Iw) \big\} \,, \ u \in X^* \,, \ k = 1, 2 \,.$$

1. If $u \in Y$ then $F_k(I^* u) = \sup_{w \in X} \big\{ (u, Iw)_Y - \widetilde{F}_k^*(Iw) \big\} \leq \widetilde{F}_k(u) \,, \ k = 1, 2.$

2. Let $u \in Y$, $v \in X$ and $Iv \in \partial \widetilde{F}_k(u)$. Then we have

$$\sup_{w \in X} \big\{ (u, Iw)_Y - \widetilde{F}_k^*(Iw) \big\} \geq (u, Iv)_Y - \widetilde{F}_k^*(Iv) = \widetilde{F}_k(u)$$

such that in this case it follows $F_k(I^*u) = \widetilde{F}_k(u)$, $k = 1, 2$. Moreover, $u \in \partial\widetilde{F}_k^*(Iv)$, or in other words,

$$\widetilde{F}_k^*(Iw) - \widetilde{F}_k^*(Iv) \geq (u, I(w-v))_Y = \langle I^*u, w-v\rangle_X \quad \forall w \in X\,.$$

Therefore we obtain $I^*u \in \partial(F_k^* \circ I)(v)$ and $v \in \partial F_k(I^*u)$, $k = 1, 2$.

3. If $u \in Y_+$ then $P(\psi) \in \partial\widetilde{F}_1(u)$ and $\psi \in H^1(\Omega)$. Since $P$ is Lipschitzian we have $P(\psi) \in X$ and from step 2 it follows that

$$F_1(I^*u) = \widetilde{F}_1(u)\,, \quad P(\psi) \in \partial F_1(I^*u)\,.$$

4. Let $u \in Y_+$, $u/p_0 \in X$ and $\delta \in \mathbb{R}$, $\delta > 0$. Then $\ln(u + \delta p_0)/p_0 \in X$ and $\ln(u + \delta p_0)/p_0 \in \partial\widetilde{F}_2(u + \delta p_0)$ hold. This results in

$$F_2(I^*(u + \delta p_0)) = \widetilde{F}_2(u + \delta p_0)\,, \quad \ln\frac{u + \delta p_0}{p_0} \in \partial F_2(I^*(u + \delta p_0))\,.$$

5. Let $u \in Y_+$ be given. Then there exists a sequence $u_n \in Y_+$ such that $u_n/p_0 \in X$, $u_u \to u$ in $Y$. Moreover, let $\delta > 0$ then $v_n := \ln(u_n + \delta p_0)/p_0 \in X$. By step 4 we find that $F_2(I^*(u_n + \delta p_0)) = \widetilde{F}_2(u_n + \delta p_0)$ and $v_n \in \partial F_2(I^*(u_n + \delta p_0))$. Thus we can estimate

$$\widetilde{F}_2(u_n + \delta p_0) \leq F_2(I^*u) - (Iv_n, u - (u_n + \delta p_0))_Y\,.$$

Let $v := \ln(u + \delta p_0)/p_0$. Using the estimate $|v_n - v| \leq c_\delta |u_n - u|$ we conclude that

$$|(Iv_n, u - (u_n + \delta p_0))_Y + (Iv, \delta p_0)_Y| \leq \int_\Omega \big\{c_\delta |u - u_n|^2 + |c_\delta + |v||\,|u - u_n|\big\}\,\mathrm{d}x \to 0 \ \text{ for } n \to \infty\,.$$

Because of the lower semi-continuity of $\widetilde{F}_2$ we derive

$$\widetilde{F}_2(u + \delta p_0) \leq F_2(I^*u) + \int_\Omega \delta\, p_0 \cdot \ln\frac{u + \delta p_0}{p_0}\,\mathrm{d}x\,.$$

Taking now the limit $\delta \to 0$ we obtain together with step 1 that $F_2(I^*u) = \widetilde{F}_2(u)$. $\square$

### 3.3 Invariants and steady states

We introduce the stoichiometric subspace $\mathcal{S}$ belonging to all reactions,

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

By integrating the continuity equations over $(0, t) \times \Omega$ one easily verifies the following invariance property.

**Lemma 3.3** *We assume* (I). *If* $(u, b, \psi)$ *is a solution of* (P) *then* $\int_\Omega \big\{u(t) - U\big\}\,dx \in \mathcal{S}$ *for all* $t \in \mathbb{R}_+$.

We ask for steady states belonging to the evolution problem (P) which satisfy such an invariance property, too. Therefore we have to solve the following problem.

$$\left.\begin{array}{c} A(b, \psi) = 0\,, \quad E(\psi, u) = 0\,, \quad u = Bb\,, \quad \displaystyle\int_\Omega \big\{u - U\big\}\,\mathrm{d}x \in \mathcal{S}\,, \\ u \in Y\,, \quad b \in X \cap L^\infty_+(\Omega, \mathbb{R}^m)\,, \quad \psi \in H^1(\Omega) \cap L^\infty(\Omega)\,. \end{array}\right\} \qquad \text{(S)}$$

We define the set $\mathcal{A} \subset \mathbb{R}^m$ by

$$\mathcal{A} = \Big\{a \in \mathbb{R}^m_+ : \ a^\alpha = a^\beta \ \forall(\alpha,\beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma , \ \int_\Omega \{u - U\} \,\mathrm{d}x \in \mathcal{S} ,$$
$$\text{where } u = ap(\psi) \text{ and } \psi \text{ is the solution of } E(\psi, u) = 0\Big\} .$$

If $(u, b, \psi)$ is a solution of (S) then $a = u/p(\psi) \in \mathcal{A}$. Vice versa, let $a \in \mathcal{A}$, let $u, \psi$ be chosen as in the definition of $\mathcal{A}$ and set $b = a\,\mathrm{e}^{-P(\psi)}$ then $(u, b, \psi)$ is a solution of (S).

As in [16], for our further investigations we additionally suppose that

$$\int_\Omega U \cdot \overline{\zeta} \,\mathrm{d}x > 0 \quad \forall \overline{\zeta} \in \mathcal{S}^\perp , \ \overline{\zeta} \geq 0 , \ \overline{\zeta} \neq 0 , \quad \mathcal{A} \cap \partial\mathbb{R}^m_+ = \emptyset . \tag{II}$$

**Theorem 3.1** *Let the assumptions* (I) *and* (II) *be fulfilled. Then there exists a unique solution* $(u^*, b^*, \psi^*)$ *of* (S). *This solution has the following properties:*

$$a^* = u^*/p(\psi^*) \in \mathbb{R}^m , \ a^* > 0 , \ \zeta^* = \ln a^* \in \mathcal{S}^\perp , \ u^* \geq c > 0 \ \textit{a.e. on } \Omega .$$

For the proof we refer to [16, Theorem 2].

## 3.4 Energy estimates

We define the set

$$M_D = \Big\{u \in L^\infty_+(\Omega, \mathbb{R}^m) : \sqrt{a} \in X \text{ where } a = u/p(\psi) \text{ and } E(\psi, u) = 0\Big\}$$

and some dissipation functional $D : M_D \to \mathbb{R}$ by

$$\begin{aligned} D(u) = \int_\Omega \Big\{ \sum_{i=1}^{l} 4\, D_i(\cdot, b, \psi) p_i(\cdot, \psi) |\nabla \sqrt{a_i}|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} 2\, k^\Omega_{\alpha\beta}(\cdot, b, \psi) |\sqrt{a}^{\,\alpha} - \sqrt{a}^{\,\beta}|^2 \Big\} \,\mathrm{d}x \\ + \int_\Gamma \sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma} 2\, k^\Gamma_{\alpha\beta}(\cdot, b_1, \ldots, b_l, \psi) |\sqrt{a}^{\,\alpha} - \sqrt{a}^{\,\beta}|^2 \,\mathrm{d}\Gamma , \ u \in M_D \end{aligned} \tag{3.5}$$

where $b = u/p_0$ and $\psi \in H^1(\Omega) \cap L^\infty(\Omega)$ is the unique solution of the Poisson equation $E(\psi, u) = 0$. Applying now the properties of the energy functional $F$ stated in Lemma 3.2 and the chain rule given in Lemma 8.2 the following theorem can be proved as in [16].

**Theorem 3.2** *Let the assumption* (I) *be fulfilled. Then along any solution* $(u, b, \psi)$ *of* (P) *the relation* $u(t) \in M_D$ *f.a.a.* $t \in \mathbb{R}_+$ *holds, and*

$$F(u(t_2)) + \int_{t_1}^{t_2} D(u(t))\, dt \leq F(u(t_1)) \leq F(U) , \quad 0 \leq t_1 \leq t_2 .$$

*Especially this means that the free energy* $F(u)$ *remains bounded from above by its initial value* $F(U)$ *and decreases monotonously. Moreover, there exists a constant* $c$ *depending only on the data such that*

$$\sum_{i=1}^{m} \|u_i \ln u_i\|_{L^\infty(\mathbb{R}_+, L^1(\Omega))} \leq c , \quad \|u\|_{L^\infty(\mathbb{R}_+, L^1(\Omega,\mathbb{R}^m))} \leq c , \quad \|b\|_{L^\infty(\mathbb{R}_+, L^1(\Omega,\mathbb{R}^m))} \leq c ,$$
$$\|\psi\|_{L^\infty(\mathbb{R}_+, H^1(\Omega))} \leq c , \quad \|\psi\|_{L^\infty(\mathbb{R}_+, L^\infty(\Omega))} , \ \|\psi\|_{L^\infty(\mathbb{R}_+, L^\infty(\Gamma))} \leq c$$

*for any solution of* (P).

**Remark 3.1** The last two estimates of Theorem 3.2 together with assumptions (I), iii)–vi) ensure that along solutions of (P)

$$
\begin{aligned}
&c_1 \le p_i(x,\psi(t,x)) \le c_2 \text{ f.a.a. } (t,x)\in\mathbb{R}_+\times\Sigma\,,\ \Sigma=\Omega,\Gamma\,,\ i=1,\dots,m\,,\\
&k^{\Sigma}_{\alpha\beta}(x,b_1(t,x),\dots,b_{m_\Sigma}(t,x),\psi(t,x)) \le c_2 \text{ f.a.a. } (t,x)\in\mathbb{R}_+\times\Sigma\,,\ (\alpha,\beta)\in\mathcal{R}^{\Sigma}\,,\ \Sigma=\Omega,\Gamma\,,\\
&D_i(x,b(t,x),\psi(t,x)) \le c_2 \text{ f.a.a. } (t,x)\in\mathbb{R}_+\times\Omega\,,\ i=1,\dots,l\,,\\
&D_i(x,b(t,x),\psi(t,x))\,p_{0i}(x) \ge \epsilon > 0 \text{ f.a.a. } (t,x)\in\mathbb{R}_+\times\Omega\,,\ i=1,\dots,l\,,\\
&2k^{\Omega}_{\alpha_{(j)}\beta_{(j)}}(x,b(t,x),\psi(t,x))\,\mathrm{e}^{2P_j(\psi(t,x))} \ge \widetilde{\epsilon} > 0 \text{ f.a.a. } (t,x)\in\mathbb{R}_+\times\Omega\,,\ j=l+1,\dots,m\,,
\end{aligned}
$$

with positive constants $c_1$, $c_2$, $\epsilon$, $\widetilde{\epsilon}$ depending only on the data.

**Theorem 3.3** *Let the assumptions* (I) *and* (II) *be fulfilled. Then along any solution* $(u,b,\psi)$ *of* (P) *the free energy* $F(u)$ *decays exponentially to its equilibrium value* $F(u^*)$,

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

*where* $\lambda$ *depends only on the data.*

For the proof see [16, Corollary 3]. From the preceding energy estimates we derive some further conclusions.

**Theorem 3.4** *We assume* (I) *and* (II). *Then there exists a constant* $c>0$ *depending only on the data such that for any solution* $(u,b,\psi)$ *of* (P)

$$\|u(t)-u^*\|_{L^1(\Omega,\mathbb{R}^m)}\,,\ \|b(t)-b^*\|_{L^1(\Omega,\mathbb{R}^m)}\,,\ \|\psi(t)-\psi^*\|_{H^1} \le c\,e^{-\frac{\lambda}{2}t} \quad \forall t\in\mathbb{R}_+ \tag{3.6}$$

*with* $\lambda$ *from Theorem* 3.3. *Moreover,*

$$\|b_i-b_i^*\|_{L^2(\mathbb{R}_+,L^2)} \le c\,, \quad i=1,\dots,l\,, \tag{3.7}$$

$$
\begin{aligned}
\|\psi-\psi^*\|_{L^2(\mathbb{R}_+,H^1)} &\le c\,,\\
\|b_i-b_i^*\|_{L^1(\mathbb{R}_+,L^1)} \le c\,,\ i=1,\dots,m\,,\ &\|b_i-b_i^*\|_{L^1(\mathbb{R}_+,L^1(\Gamma))} \le c\,,\ i=1,\dots,l\,.
\end{aligned} \tag{3.8}
$$

*Proof.* From Theorem 3.2, (3.5) we have $\|\psi\|_{L^\infty(\mathbb{R}_+,L^\infty)}$, $\|a\|_{L^\infty(\mathbb{R}_+,L^1(\Omega,\mathbb{R}^m))}$, $\|D(u)\|_{L^1(\mathbb{R}_+)} \le c$, $\|\sqrt{a/a^*}-1\|_{L^\infty(\mathbb{R}_+,L^2(\Omega,\mathbb{R}^m))} \le c$, $\|\nabla\sqrt{a_i/a_i^*}\|_{L^2(\mathbb{R}_+,L^2)} \le c$, $i=1,\dots,l$. From (3.3), (3.4), Lemma 3.3, and since $\zeta^*\in\mathcal{S}^\perp$ (cf. Theorem 3.1) we obtain that

$$
\begin{aligned}
F(u(t))-F(u^*) &\ge c\|\psi(t)-\psi^*\|^2_{H^1} + c\|\sqrt{u(t)}-\sqrt{u^*}\|^2_Y\\
&\ge c\|\psi(t)-\psi^*\|^2_{H^1} + c\|\sqrt{a(t)}-\sqrt{a^*}\|^2_Y \quad \forall t\in\mathbb{R}_+\,.
\end{aligned} \tag{3.9}
$$

Thus Theorem 3.3 ensures that

$$
\begin{aligned}
\|\psi(t)-\psi^*\|_{H^1},\ \|\sqrt{u(t)}-\sqrt{u^*}\|_{L^2(\Omega,\mathbb{R}^m)},\ \|\sqrt{a(t)/a^*}-1\|_{L^2(\Omega,\mathbb{R}^m)} \le c\,\mathrm{e}^{-\frac{\lambda}{2}t}\ \forall t\in\mathbb{R}_+\,,\\
\|\psi-\psi^*\|_{L^2(\mathbb{R}_+,H^1)}\,,\ \|\sqrt{a/a^*}-1\|_{L^2(\mathbb{R}_+,L^2(\Omega,\mathbb{R}^m)} \le c\,.
\end{aligned} \tag{3.10}
$$

Since $\|u_i-u_i^*\|_{L^1} \le \|\sqrt{u_i}-\sqrt{u_i^*}\|_{L^2}\|\sqrt{u_i}+\sqrt{u_i^*}\|_{L^2}$, from Theorem 3.2, Theorem 3.3 and (3.9) the remaining estimates of (3.6) are derived. The first two estimates in (3.8) result from (3.10), (3.6). Now let $i=1,\dots,l$. With the above results and (3.10) we have $\|\sqrt{a_i/a_i^*}-1\|_{L^2(\mathbb{R}_+,H^1)}\le c$, and interpolation between $L^2(\mathbb{R}_+,H^1)$ and $L^\infty(\mathbb{R}_+,L^2)$ yields $\|\sqrt{a_i/a_i^*}-1\|_{L^4(\mathbb{R}_+,L^4)}\le c$. Because of the estimate

$$|b_i-b_i^*|\le c(|a_i/a_i^*-1|+|\psi-\psi^*|)\le c(|\sqrt{a_i/a_i^*}-1|^2+|\sqrt{a_i/a_i^*}-1|+|\psi-\psi^*|) \tag{3.11}$$

we obtain that

$$\begin{aligned}&\|b_i-b_i^*\|^2_{L^2(\mathbb{R}_+,L^2)}\\ &\le c\Big\{\|\sqrt{a_i/a_i^*}-1\|^4_{L^4(\mathbb{R}_+,L^4)}+\|\sqrt{a_i/a_i^*}-1\|^2_{L^2(\mathbb{R}_+,L^2)}+\|\psi-\psi^*\|^2_{L^2(\mathbb{R}_+,H^1)}\Big\}\le c\,.\end{aligned}$$

The last estimate in (3.8) follows from (3.11), (8.1), (3.10) and

$$\int_{\mathbb{R}_+}\|b_i-b_i^*\|_{L^1(\Gamma)}\,\mathrm{d}s\le c\int_{\mathbb{R}_+}\Big\{\|\sqrt{a_i/a_i^*}-1\|^2_{H^1}+\|\sqrt{a_i/a_i^*}-1\|^{2/3}_{L^2}+\|\psi-\psi^*\|_{H^1}\Big\}\,\mathrm{d}s\le c\,. \quad \square$$

## 4 Global upper bounds for the densities

In this section we derive global upper bounds for the densities $u_i$ and chemical activities $b_i$. For this purpose we additionally suppose the following properties of the reaction system:

$$\left.\begin{aligned}&\max_{k=1,\dots,m}\{(a^\alpha-a^\beta)(\beta_k-\alpha_k)\}\le c\Big(\sum_{j=1}^m a_j^2+1\Big)\,,\quad \sum_{i=l+1}^m\alpha_i\cdot\sum_{i=l+1}^m\beta_i=0\\ &\forall a\in\mathbb{R}^m_+\,,\ \forall(\alpha,\beta)\in\mathcal{R}^\Omega\,,\\ &\max_{k=1,\dots,l}\{(a^\alpha-a^\beta)(\beta_k-\alpha_k)\}\le c\Big(\sum_{j=1}^l a_j+1\Big)\quad\forall a\in\mathbb{R}^m_+\,,\ \forall(\alpha,\beta)\in\mathcal{R}^\Gamma\,.\end{aligned}\right\} \tag{III}$$

We start with two preliminary estimates to achieve estimates for the $L^\infty(\mathbb{R}_+,L^2)$-norms and $L^\infty(\mathbb{R}_+,L^4)$-norms of the chemical activities. The final result then will be obtained by Moser iteration. Here we distinguish between diffusing and non-diffusing species. In our estimates we use the constants $\epsilon_0$, $\epsilon$, $\widetilde{\epsilon}$ which are defined in assumption (I), iii) and Remark 3.1.

**Lemma 4.1** *Let the assumptions* (I) – (III) *be fulfilled. Then there is a constant $c>0$ depending only on the data such that*

$$\|b_i(t)\|_{L^2}\le c\quad\forall t\in\mathbb{R}_+\,,\ i=1,\dots,m\,,$$

*for any solution $(u,b,\psi)$ of* (P)

*Proof.* 1. With the exponent $q$ from Lemma 3.1 we obtain from Lemma 3.1, Lemma 3.2 that

$$\|\psi(t)\|_{W^{1,q}}\le c\Big\{1+\sum_{j=1}^m\|u_j(t)\|_{L^{2q/(2+q)}}\Big\}\le c\Big\{1+\sum_{j=1}^m\|b_j(t)\|_{L^{2q/(2+q)}}\Big\}\quad\text{f.a.a. } t\in\mathbb{R}_+\,. \tag{4.1}$$

2. We use the test function $2\mathrm{e}^t\,b$ for (P) (more precisely, for the evolution equation in (P)). Taking into account the assumptions (I), vi) concerning the presence of reactions with quadratic

sink terms for the non-diffusing species, and (III) concerning the order of the source terms we can estimate

$$\int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} R^\Omega_{\alpha\beta}(\cdot,b,\psi)\,(\beta-\alpha)\cdot b\,\mathrm{d}x \le \int_\Omega \sum_{j=l+1}^{m} \Big\{c\sum_{i=1}^{l}(b_i^3+b_i^2b_j+b_ib_j^2+b_j^2+1)-\widetilde{\epsilon}\,b_j^3\Big\}\,\mathrm{d}x$$
$$\le c\sum_{i=1}^{l}\|b_i\|^3_{L^3}+c-\frac{\widetilde{\epsilon}}{2}\sum_{j=l+1}^{m}\|b_j\|^3_{L^3}\,.$$

The last estimate follows from Young's inequality.

3. Using the test function $2\mathrm{e}^t\,b$, the estimate from step 2, (8.1), (8.3) and Young's inequality we obtain for $t\in\mathbb{R}_+$

$$\sum_{i=1}^{m}\big(\epsilon_0\,\mathrm{e}^t\,\|b_i(t)\|^2_{L^2}-c\|U_i\|^2_{L^2}\big)$$
$$\le \int_0^t \mathrm{e}^s\Big\{\sum_{i=1}^{l}\big\{-2\epsilon\|b_i\|^2_{H^1}+c(\|b_i\|_{L^r}\|\psi\|_{W^{1,q}}\|b_i\|_{H^1}+\|b_i\|^3_{L^3}+\|b_i\|^2_{L^2(\Gamma)}+1)\big\}$$
$$+\sum_{j=l+1}^{m}\big\{-\widetilde{\epsilon}\|b_j\|^3_{L^3}+c\|b_j\|^2_{L^2}\big\}\Big\}\,\mathrm{d}s$$
$$\le \int_0^t \mathrm{e}^s\Big\{\sum_{i=1}^{l}\big\{-\epsilon\|b_i\|^2_{H^1}+\tilde{c}(\|b_i\|_{L^r}\|\psi\|_{W^{1,q}}\|b_i\|_{H^1}+\|b_i\|^4_{L^2}+1)\big\}-\sum_{j=l+1}^{m}\frac{\widetilde{\epsilon}}{2}\|b_j\|^3_{L^3}\Big\}\,\mathrm{d}s$$

where $r=2q/(q-2)$. With (4.1), (8.3), and Theorem 3.2 we estimate

$$\tilde{c}\|b_i\|_{L^r}\|\psi\|_{W^{1,q}}\|b_i\|_{H^1}\le c\|b_i\|^{2/r}_{L^2}\Big[1+\sum_{j=1}^{m}\|b_j\|^{2/r}_{L^2}\Big]\|b_i\|^{2(r-1)/r}_{H^1}\le\frac{\epsilon}{2}\|b_i\|^2_{H^1}+c\|b_i\|^2_{L^2}\sum_{j=1}^{m}\|b_j\|^2_{L^2}+c\,.$$

From both estimates we conclude that

$$\epsilon_0\,\mathrm{e}^t\sum_{j=1}^{m}\|b_j(t)\|^2_{L^2}\le\int_0^t\mathrm{e}^s\Big\{-\frac{\epsilon}{2}\sum_{i=1}^{l}\|b_i\|^2_{H^1}-\sum_{j=l+1}^{m}\frac{\widetilde{\epsilon}}{2}\|b_j\|^3_{L^3}$$
$$+c\sum_{j=1}^{m}\Big(\sum_{i=1}^{l}\|b_i\|^2_{L^2}+1\Big)\|b_j\|^2_{L^2}+c\Big\}\,\mathrm{d}s+c$$
$$\le\int_0^t\mathrm{e}^s\Big\{-\frac{\epsilon}{2}\sum_{i=1}^{l}\|b_i\|^2_{H^1}-\sum_{j=l+1}^{m}\frac{\widetilde{\epsilon}}{2}\|b_j\|^3_{L^3}$$
$$+\overline{c}\sum_{j=1}^{m}\Big(\sum_{i=1}^{l}\|b_i-b_i^*\|^2_{L^2}+1\Big)\|b_j\|^2_{L^2}+1\Big\}\,\mathrm{d}s+c\quad\forall t\in\mathbb{R}_+\,.$$

Because of (8.3) and Young's inequality

$$\overline{c}\|b_i\|^2_{L^2}\le c\|b_i\|_{L^1}\|b_i\|_{H^1}\le\frac{\epsilon}{2}\|b_i\|^2_{H^1}+c\|b_i\|^2_{L^1}\,,\quad i=1,\dots,l\,,$$

$$\overline{c}\|b_i\|^2_{L^2}\le c\|b_i\|^{1/2}_{L^1}\|b_i\|^{3/2}_{L^3}\le\frac{\widetilde{\epsilon}}{2}\|b_i\|^3_{L^3}+c\|b_i\|_{L^1}\,,\quad i=l+1,\dots,m\,,$$

and since $\|b\|_{L^\infty(\mathbb{R}_+,L^1(\Omega,\mathbb{R}^m))} \le c$ (see Theorem 3.2) we continue our estimate by

$$\mathrm{e}^t \sum_{j=1}^m \|b_j(t)\|_{L^2}^2 \le c\,\mathrm{e}^t + c\int_0^t \mathrm{e}^s \sum_{j=1}^m \sum_{i=1}^l \|b_i - b_i^*\|_{L^2}^2 \|b_j\|_{L^2}^2 \,\mathrm{d}s \quad \forall t \in \mathbb{R}_+ .$$

Since by Theorem 3.4, (3.7) the function $h := \sum_{i=1}^l \|b_i - b_i^*\|_{L^2}^2$ belongs to $L^1(\mathbb{R}_+)$ we can apply a special form of Gronwall's lemma (see [22, p. 14, 15]) to obtain

$$\mathrm{e}^t \sum_{j=1}^m \|b_j(t)\|_{L^2}^2 \le c\,\mathrm{e}^t + \int_0^t c\,\mathrm{e}^s h(s)\,\mathrm{e}^{\|h\|_{L^1(\mathbb{R}_+)}} \,\mathrm{d}s \le c\,\mathrm{e}^t\, \|h\|_{L^1(\mathbb{R}_+)} \mathrm{e}^{\|h\|_{L^1(\mathbb{R}_+)}} \le c\,\mathrm{e}^t \;\forall t \in \mathbb{R}_+ . \quad \square$$

**Corollary 4.1** *We assume* (I) – (III). *Let $q$ be defined as in Lemma* 3.1. *Then there is a constant $c_q > 0$ depending only on the data such that*

$$\|\psi\|_{L^\infty(\mathbb{R}_+,W^{1,q})} \le c_q$$

*for any solution $(u, b, \psi)$ of* (P).

*Proof.* Since $2q/(2+q) < 2$ the desired estimate results from (4.1) and Lemma 4.1. $\square$

We define

$$\kappa := c_q^{2r} + 1 \text{ where } r = 2q/(q-2)\,,\; q \text{ from Lemma 3.1.} \tag{4.2}$$

**Lemma 4.2** *We assume* (I) – (III). *Then there is a constant $c_{L^4} \ge 1$ depending only on the data such that*

$$\|b_i(t)\|_{L^4} \le c_{L^4} \quad \forall t \in \mathbb{R}_+\,,\; i = 1, \dots, m\,,$$

*for any solution $(u, b, \psi)$ of* (P).

*Proof.* We use the test function $4\mathrm{e}^t\,(b_1^3, \dots, b_m^3)$ for (P). Arguing similar as in step 2 of the proof of Lemma 4.1 we find that

$$\begin{aligned}\int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} R_{\alpha\beta}^\Omega \sum_{i=1}^m (\beta_i - \alpha_i) b_i^3 \,\mathrm{d}x &\le \int_\Omega \sum_{j=l+1}^m \Big\{ c \sum_{i=1}^l \big\{ (b_i^2+1)b_j^3 + (b_j^2+1)b_i^3 + b_i^5 \big\} - \widetilde{\epsilon}\, b_j^5 \Big\} \,\mathrm{d}x \\ &\le c\sum_{i=1}^l \|b_i\|_{L^5}^5 + c - \frac{\widetilde{\epsilon}}{2} \sum_{j=l+1}^m \|b_j\|_{L^5}^5 .\end{aligned}$$

Therefore, with $q$ from Lemma 3.1, $r = 2q/(q-2)$, we obtain for all $t \in \mathbb{R}_+$

$$\begin{aligned}\sum_{i=1}^m \big( \epsilon_0\,\mathrm{e}^t\, \|b_i(t)\|_{L^4}^4 - c\|U_i\|_{L^4}^4 \big) \le \int_0^t \mathrm{e}^s \Big\{ &\sum_{j=l+1}^m \big( -2\widetilde{\epsilon}\|b_j\|_{L^5}^5 + \|b_j\|_{L^4}^4 \big) \\ &+ \sum_{i=1}^l \big( -2\epsilon\|b_i^2\|_{H^1}^2 + c\big( \|\nabla\psi\|_{L^q} \|\nabla(b_i^2)\|_{L^2} \|b_i^2\|_{L^r} + \|b_i\|_{L^5}^5 + \|b_i\|_{L^4(\Gamma)}^4 + 1 \big)\big) \Big\} \,\mathrm{d}s .\end{aligned}$$

Next we apply the inequalities (8.1), (8.3) and the estimate $\|b_j\|_{L^4}^4 \le 2\widetilde{\epsilon}\|b_j\|_{L^5}^5 + c$. Moreover we use Corollary 4.1, (4.2), Young's inequality, and Lemma 4.1 to get

$$\epsilon_0\,\mathrm{e}^t \sum_{i=1}^m \|b_i(t)\|_{L^4}^4 \le \int_0^t \mathrm{e}^s \sum_{i=1}^l \Big\{ -\epsilon\|b_i^2\|_{H^1}^2 + c\big(\|\psi\|_{W^{1,q}}\|b_i^2\|_{L^1}^{1/r}\|b_i^2\|_{H^1}^{2-1/r}$$
$$+ \|b_i^2\|_{L^1}\|b_i^2\|_{H^1}^{3/2} + \|b_i^2\|_{L^1}^{1/2}\|b_i^2\|_{H^1}^{3/2} + 1\big)\Big\}\,\mathrm{d}s + c$$
$$\le c\int_0^t \mathrm{e}^s \sum_{i=1}^l \{\kappa\|b_i^2\|_{L^1}^2 + \|b_i^2\|_{L^1}^4 + \|b_i^2\|_{L^1}^2 + 1\}\,\mathrm{d}s + c \le c\,\mathrm{e}^t \quad \forall t \in \mathbb{R}_+\,. \quad \square$$

**Theorem 4.1** *Let the assumptions* (I) – (III) *be fulfilled. Then there exists a constant* $c > 0$ *depending only on the data such that*

$$\|b_i(t)\|_{L^\infty} \le c\,, \quad \|u_i(t)\|_{L^\infty} \le c \quad \forall t \in \mathbb{R}_+\,, \quad i = 1,\dots,m\,, \tag{4.3}$$

$$\|b_i\|_{L^\infty(\mathbb{R}_+, L^\infty(\Gamma))} \le c\,, \quad i = 1,\dots,l\,,$$

*for any solution* $(u, b, \psi)$ *of* (P).

*Proof.* The proof is based on Moser iteration and will be done in two steps. At first we establish global bounds for the diffusing species. Then, using these bounds we show the global bounds for the non-diffusing species. Let $K := \max\{1, \|b_1(0)\|_{L^\infty},\dots,\|b_m(0)\|_{L^\infty}\}$ and $z_i := (b_i - K)^+$, $i = 1,\dots,m$.

1. *Bounds for the diffusing species.* For $p \ge 8$ we use $p\mathrm{e}^t\,(z_1^{p-1},\dots,z_l^{p-1},0,\dots,0)$ as test function for (P) and set $w_i := z_i^{p/2}$. At first let us remark that

$$\sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} R^\Omega_{\alpha\beta}(\cdot,b,\psi)\,\sum_{i=1}^l(\beta_i-\alpha_i)z_i^{p-1} \le c\sum_{i=1}^l\sum_{j=1}^m(b_j^2+1)z_i^{p-1} \le c\sum_{i=1}^l\big(z_i^{p+1} + \sum_{j=l+1}^m z_i^{p-1}z_j^2\big) + c\,.$$

Lemma 4.2 ensures that $\|b_j\|_{L^\infty(\mathbb{R}_+,L^4)} \le c_{L^4}$, $j = l{+}1,\dots,m$. Thus we can estimate by Hölder's inequality

$$\int_\Omega z_i^{p-1}z_j^2\,\mathrm{d}x \le \|z_i\|_{L^{2(p-1)}}^{p-1}\|z_j\|_{L^4}^2 \le c_{L^4}^2\|w_i\|_{L^{4(p-1)/p}}^{2(p-1)/p}\,.$$

Therefore we obtain for all $t \in \mathbb{R}_+$

$$\epsilon_0\,\mathrm{e}^t\sum_{i=1}^l\|w_i(t)\|_{L^2}^2 \le \int_0^t \mathrm{e}^s\sum_{i=1}^l\Big\{ -2\epsilon\|w_i\|_{H^1}^2$$
$$+ cp\big(\|\nabla\psi\|_{L^q}\|\nabla w_i\|_{L^2}(\|w_i\|_{L^r}+1) + \|w_i\|_{L^{2(p+1)/p}}^{2(p+1)/p} + c_{L^4}^2\|w_i\|_{L^{4(p-1)/p}}^{2(p-1)/p} + \|w_i\|_{L^2(\Gamma)}^2 + 1\big)\Big\}\,\mathrm{d}s\,.$$

Next we apply for $r$, $\widetilde{p} := 2(p+1)/p$, and $\widetilde{p} := 4(p-1)/p$, respectively, Gagliardo–Nirenberg's inequality (8.3). The constants $c_{\widetilde{p},1}$ can be estimated by means of $\max\{c_{2,1}, c_{9/4,1}, 1\}^{1/2}$ and

$\max\{c_{7/2,1}, c_{4,1}, 1\}^{2/7}$, respectively,

$$
\begin{aligned}
&\epsilon_0\, \mathrm{e}^t \sum_{i=1}^{l} \|w_i(t)\|_{L^2}^2 \\
&\leq \int_0^t \mathrm{e}^s \sum_{i=1}^{l} \Big\{ -\epsilon\|w_i\|_{H^1}^2 + cp^{2r}(\|\psi\|_{W^{1,q}}^{2r}+1)(\|w_i\|_{L^1}^2+1) \\
&\quad + cp\big(\|w_i\|_{H^1}^{(p+2)/p}\|w_i\|_{L^1} + c_{L^4}^2\|w_i\|_{H^1}^{(3p-4)/2p}\|w_i\|_{L^1}^{1/2} + \|w_i\|_{H^1}^{3/2}\|w_i\|_{L^1}^{1/2} + 1\big)\Big\}\,\mathrm{d}s \\
&\leq \int_0^t \mathrm{e}^s \sum_{i=1}^{l} c\Big\{p^{2r}\kappa(\|w_i\|_{L^1}^2+1) + p^4\|w_i\|_{L^1}^{2p/(p-2)} + p^4 c_{L^4}^8\|w_i\|_{L^1}^{2p/(p+4)} + p^4\|w_i\|_{L^1}^2 + 1\Big\}\,\mathrm{d}s \\
&\leq cp^{2r}(\kappa + c_{L^4}^8)\,\mathrm{e}^t \sum_{i=1}^{l}\big(\sup_{s\in\mathbb{R}_+}\|z_i(s)\|_{L^{p/2}}^{p^2/(p-2)} + 1\big) \qquad \forall t\in\mathbb{R}_+\,.
\end{aligned}
$$

Thus we get the iteration formula

$$
\sum_{i=1}^{l}\|z_i(t)\|_{L^p}^p + 1 \leq p^{2r} c_M(\kappa + c_{L^4}^8)\Big(\sum_{i=1}^{l}\sup_{s\in\mathbb{R}^+}\|z_i(s)\|_{L^{p/2}}^{p/2} + 1\Big)^{2p/(p-2)} \qquad \forall t\in\mathbb{R}_+\,,\ p\geq 8
$$

where the constant $c_M > 1$ depends only on the data, $\kappa$, $r$ and $c_{L^4}$ are defined in (4.2) and Lemma 4.2. Now we set $p = 2^k$, $k\in\mathbb{N}$, $k\geq 3$. From the recursion formula

$$
\gamma_k \leq (2^{4r} c_M\,(\kappa + c_{L^4}^8)\,\gamma_2)^{c_\theta 2^k}\,, \quad \gamma_k := \sum_{i=1}^{l}\sup_{s\in\mathbb{R}_+}\|z_i(s)\|_{L^{2^k}}^{2^k} + 1\,, \quad c_\theta := \prod_{j=1}^{\infty}\frac{2^j}{2^j-1}
$$

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

$$
\sum_{i=1}^{l}\|z_i(t)\|_{L^\infty} \leq \sqrt{l}\,\Big(2^{4r} c_M\,(\kappa + c_{L^4}^8)\Big[\sum_{i=1}^{l}\sup_{s\in\mathbb{R}_+}\|z_i(s)\|_{L^4}^4 + 1\Big]\Big)^{c_\theta} \qquad \forall t\in\mathbb{R}_+\,.
$$

Applying Lemma 4.2 and (8.2) the desired estimates for $b_i$, $u_i$, $i = 1,\dots,l$, are verified.

2. *Bounds for the non-diffusing species.* We use the test function $p\mathrm{e}^t\,(0,\dots,0,z_{l+1}^{p-1},\dots,z_m^{p-1})$, $p\geq 2$. From assumptions (I), vi) and (III), from the estimates $b_j\geq z_j\geq 0$, $j = l+1,\dots,m$, and the $L^\infty(\mathbb{R}_+, L^\infty)$-estimates for $b_i$, $i = 1,\dots,l$, we find that a.e. in $\mathbb{R}_+\times\Omega$

$$
\begin{aligned}
&\sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} R^\Omega_{\alpha\beta}(\cdot,b,\psi)\sum_{j=l+1}^{m}(\beta_j - \alpha_j)\,z_j^{p-1} \\
&\leq c\sum_{i=1}^{l}\sum_{j=l+1}^{m}(b_i^2 + b_i + 1)z_j^{p-1} - \widetilde{\epsilon}\sum_{j=l+1}^{m} z_j^{p+1} \leq \widehat{c}\sum_{j=l+1}^{m} z_j^{p-1} - \widetilde{\epsilon}\sum_{j=l+1}^{m} z_j^{p+1} \leq (m-l)\frac{\widehat{c}^{(p+1)/2}}{\widetilde{\epsilon}^{(p-1)/2}}\,.
\end{aligned}
$$

The last estimate follows from Young's inequality. Therefore we obtain

$$
\epsilon_0\,\mathrm{e}^t\sum_{j=l+1}^{m}\|z_j(t)\|_{L^p}^p \leq p\int_0^t \mathrm{e}^s\int_\Omega (m-l)\frac{\widehat{c}^{(p+1)/2}}{\widetilde{\epsilon}^{(p-1)/2}}\,\mathrm{d}x\,\mathrm{d}s \leq \mathrm{e}^t\,p\,|\Omega|\,(m-l)\frac{\widehat{c}^{(p+1)/2}}{\widetilde{\epsilon}^{(p-1)/2}} \qquad \forall t\in\mathbb{R}_+\,.
$$

This yields

$$\|z_j(t)\|_{L^p} \le \left(p\,|\Omega|\,(m-l)\,\sqrt{\widetilde{\epsilon}\,\widehat{c}}/\epsilon_0\right)^{1/p}\,\sqrt{\widehat{c}/\widetilde{\epsilon}} \le c \quad \forall t \in \mathbb{R}_+\,,\ \forall p \ge 2\,,\ j = l+1,\dots,m\,.$$

Passing to the limit $p \to \infty$ we get

$$\|z_j(t)\|_{L^\infty} \le \sqrt{\widehat{c}/\widetilde{\epsilon}} \quad \forall t \in \mathbb{R}_+\,,\ j = l+1,\dots,m\,,$$

which leads to the desired $L^\infty$-estimate for $b_j$, $u_j$, $j = l+1,\dots,m$. $\square$

## 5 Global lower bounds for the densities

In this section we assume that for solutions of (P) global upper bounds for the chemical activities are known (see Section 4),

$$\|b_i\|_{L^\infty(\mathbb{R}_+,L^\infty)} \le c\,, \quad i = 1,\dots,m\,, \tag{III'}$$

and that the initial densities are strictly positive,

$$U_i \ge c > 0\,, \quad i = 1,\dots,m\,. \tag{IV}$$

We show that then the densities as well as chemical activities are bounded from below by a positive constant for all $t > 0$. We start with some results obtained without assumption (II) which lead to lower estimates depending on the length of the time interval such that $\ln b_i \in L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty)$, $i = 1,\dots,m$, is found. With this knowledge and now supposing the condition (II) we prove the global result. Let

$$K := \max\left\{\|[\ln b_1(0)]^-\|_{L^\infty},\dots,\|[\ln b_m(0)]^-\|_{L^\infty}\right\}\,. \tag{5.1}$$

**Lemma 5.1** *Let conditions* (I), (III'), (IV) *be fulfilled. Let $T > 0$ be fixed and suppose that*

$$\operatorname*{ess\,inf}_{x\in\Omega} b_i(t,x) \ge c_T > 0 \quad \forall t \in [0,T]\,,\ i = 1,\dots,l\,,$$

*for every solution $(u, b, \psi)$ of* (P). *Then the estimates*

$$\|(\ln b_j)^-(t)\|_{L^\infty} \le \gamma(c_T) \quad \forall t \in [0,T]\,,\ j = l+1,\dots,m\,,$$

*hold for any solution $(u, b, \psi)$ of* (P) *where the function $\gamma$ itself depends on the data and on the upper bounds of the densities, but not on $T$.*

*Proof.* Let $(u, b, \psi)$ be a solution of (P), let $j \in \{l+1,\dots,m\}$, $v_\delta := (\ln(b_j+\delta)+K)^-$, $K$ from (5.1), $\delta \in (0, \mathrm{e}^{-K})$. We use the test function $-p\,\mathrm{e}^t\,(0,\dots,0,v_\delta^{p-1}/(b_j+\delta),0,\dots,0)$, $p \ge 2$. Because of assumption (I), vi) there is a special reaction $R^\Omega_{\alpha_{(j)}\beta_{(j)}}$ which generates source terms in the $j$–th continuity equation containing electrochemical activities of diffusing species only. Since the activities of the diffusing species are supposed to be bounded from below by $c_T > 0$ there is a constant $\epsilon_r(c_T) > 0$ such that the estimate $2k^\Omega_{\alpha_{(j)}\beta_{(j)}}(\cdot,b,\psi)\prod_{i=1}^l a_i^{\alpha_{(j)i}} \ge \epsilon_r(c_T)$ a.e. in $[0,T]\times\Omega$ holds. Moreover, we apply Remark 3.1, (III'), and the inequality $v_\delta/(b_j+\delta) \ge v_\delta^2$ to get

$$-2\,k^\Omega_{\alpha_{(j)}\beta_{(j)}}(\cdot,b,\psi)\Big[\prod_{i=1}^l a_i^{\alpha_{(j)i}} - a_j^2\Big]\frac{v_\delta^{p-1}}{b_j+\delta} \le c\,\frac{a_j \mathrm{e}^{P_j(\psi)}\,b_j}{b_j+\delta}v_\delta^{p-1} - \epsilon_r(c_T)\,\frac{v_\delta^{p-1}}{b_j+\delta} \le c\,v_\delta^{p-1} - \epsilon_r(c_T)\,v_\delta^p\,.$$

Additionally using Remark 2.1 for all other reactions

$$R^{\Omega}_{\alpha\beta}(\alpha_j-\beta_j)\frac{v_\delta^{p-1}}{b_j+\delta}\le c\,\frac{a_j}{b_j+\delta}\,v_\delta^{p-1}\le c\,v_\delta^{p-1} \tag{5.2}$$

follows. Thus we find a constant $c_o>0$ such that

$$\sum_{(\alpha,\beta)\in\mathcal{R}^\Omega} R^{\Omega}_{\alpha\beta}(\cdot,b,\psi)\,(\alpha_j-\beta_j)\,\frac{v_\delta^{p-1}}{b_j+\delta}\le c_o\,v_\delta^{p-1}-\epsilon_r(c_T)\,v_\delta^p\le\frac{c_o^p}{\epsilon_r(c_T)^{p-1}}\,.$$

The last estimate follows from Young's inequality. Therefore we obtain

$$\epsilon_0\,\mathrm{e}^t\,\|v_\delta(t)\|^p_{L^p}\le p\int_0^t\mathrm{e}^s\int_\Omega\frac{c_o^p}{\epsilon_r(c_T)^{p-1}}\,\mathrm{d}x\,\mathrm{d}s\le\mathrm{e}^t\,p\,|\Omega|\,\frac{c_o^p}{\epsilon_r(c_T)^{p-1}}\quad\forall t\in[0,T]\,,\ \forall\delta\in(0,\mathrm{e}^{-K})\,.$$

Thus we arrive at

$$\|v_\delta(t)\|_{L^p}\le\big(p\,|\Omega|\,\epsilon_r(c_T)/\epsilon_0\big)^{1/p}\,\frac{c_o}{\epsilon_r(c_T)}\quad\forall t\in[0,T]\,,\ \forall\delta\in(0,\mathrm{e}^{-K})\,,\ \forall p\ge 2\,.$$

Passing to the limit $p\to\infty$ we get $\|v_\delta(t)\|_{L^\infty}\le c_o/\epsilon_r(c_T)$ for all $t\in[0,T]$, $\delta\in(0,\mathrm{e}^{-K})$. Therefore $b_j(t)>0$, $\lim_{\delta\to 0}v_\delta(t)=[\ln b_j+K]^-(t)$ a.e. in $\Omega$, and in the limit $\delta\to 0$ we have

$$\|(\ln b_j+K)^-(t)\|_{L^\infty}\le\frac{c_o}{\epsilon_r(c_T)}\quad\forall t\in[0,T]\,.\quad\square$$

**Lemma 5.2** *Let the conditions* (I), (III') *and* (IV) *be fulfilled. Then the recursion formula*

$$e^t\|(\ln(b_i+\delta)+K)^-(t)\|^p_{L^p}\le c\int_0^t e^s\,p^{2r}\kappa\big(\|(\ln(b_i+\delta)+K)^-(s)\|^p_{L^{p/2}}+1\big)\,ds$$
$$\forall t\in\mathbb{R}_+\,,\quad\forall\delta\in(0,e^{-K})\,,\quad\forall p\ge 2\,,\quad i=1,\dots,l\,,$$

*holds for any solution* $(u,b,\psi)$ *of* (P) *where* $\kappa$, $r$ *from* (4.2) *and* $c$ *depends only on the data.*

*Proof.* Let $(u,b,\psi)$ be a solution of (P), let $i\in\{1,\dots,l\}$, $v_\delta:=(\ln(b_i+\delta)+K)^-$, $\delta\in(0,\mathrm{e}^{-K})$. We use the test function $-p\,\mathrm{e}^t\,(0,\dots,0,v_\delta^{p-1}/(b_i+\delta),0,\dots,0)$, $p\ge 2$. Note that (5.2) is also valid for all reactions considered now. Applying the inequalities (8.1), (8.3) and Young's inequality the above test function leads to the estimates

$$\begin{aligned}
&\epsilon_0\,\mathrm{e}^t\|v_\delta(t)\|^p_{L^p}\\
&\le\int_0^t\mathrm{e}^s\Big\{\int_\Omega\Big[-pD_i(\cdot,b,\psi)p_{0i}[\nabla b_i+b_iQ_i(\psi)\nabla\psi]\frac{(p-1)v_\delta^{p-2}+v_\delta^{p-1}}{b_i+\delta}\nabla v_\delta+v_\delta^p\\
&\quad+p\sum_{(\alpha,\beta)\in\mathcal{R}^\Omega}R^{\Omega}_{\alpha\beta}(\alpha_i-\beta_i)\frac{v_\delta^{p-1}}{b_i+\delta}\Big]\,\mathrm{d}x+p\int_\Gamma\sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma}R^{\Gamma}_{\alpha\beta}(\alpha_i-\beta_i)\frac{v_\delta^{p-1}}{b_i+\delta}\,\mathrm{d}\Gamma\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^s\Big\{-2\epsilon\|\nabla v_\delta^{p/2}\|^2_{L^2}-\frac{\epsilon}{p}\|\nabla v_\delta^{(p+1)/2}\|^2_{L^2}+c\|v_\delta^{p/2}\|^2_{L^2}\\
&\quad+cp\|\psi\|_{W^{1,q}}\big(\|v_\delta^{p/2}\|_{L^r}+1\big)\|\nabla v_\delta^{p/2}\|_{L^2}+cp\big(\|v_\delta\|^{p-1}_{L^{p-1}}+\|v_\delta\|^{p-1}_{L^{p-1}(\Gamma)}\big)\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^s\Big\{-\epsilon\|v_\delta^{p/2}\|^2_{H^1}+cp\big(\|v_\delta^{p/2}\|^2_{L^2}+\|v_\delta^{p/2}\|_{L^2}\|v_\delta^{p/2}\|_{H^1}+1\big)\\
&\quad+cp^{2r}\,\kappa\,\big(\|v_\delta^{p/2}\|^2_{L^1}+1\big)\Big\}\,\mathrm{d}s\\
&\le\int_0^t\mathrm{e}^s cp^{2r}\,\kappa\,(\|v_\delta^{p/2}\|^2_{L^1}+1)\,\mathrm{d}s\qquad\forall t\in\mathbb{R}_+\,,\quad\forall\delta\in(0,\mathrm{e}^{-K})\,,\quad\forall p\ge 2\,.\quad\square
\end{aligned}$$

**Theorem 5.1** *Let the assumptions* (I), (III') *and* (IV) *be fulfilled. Then for every* $T \in \mathbb{R}_+$ *there exists a constant* $c(T) > 0$ *besides on* $T$ *depending only on the data such that*

$$\|(\ln b_i)^-(t)\|_{L^\infty} \le c(T) \quad \forall t \in [0,T]\,, \quad i = 1, \ldots, m\,,$$

*for any solution* $(u, b, \psi)$ *of* (P).

*Proof.* Let $T \in \mathbb{R}_+$ be arbitrarily given, and let $i \in \{1, \ldots, l\}$. We apply the recursion formula stated in Lemma 5.2 for $p = 2$ and continue as follows,

$$\begin{aligned} &\mathrm{e}^t \|(\ln(b_i + \delta) + K)^-(t)\|_{L^1}^2 \le c\,\mathrm{e}^t \,\|(\ln(b_i + \delta) + K)^-(t)\|_{L^2}^2 \\ &\le c \int_0^t \mathrm{e}^s \big(\|(\ln(b_i + \delta) + K)^-(s)\|_{L^1}^2 + 1\big)\,\mathrm{d}s \quad \forall t \in [0,T]\,, \quad \forall \delta \in (0, \mathrm{e}^{-K})\,. \end{aligned}$$

Then Gronwall's lemma yields that

$$\|(\ln(b_i + \delta) + K)^-(t)\|_{L^1}^2 \le c(T) \quad \forall t \in [0,T]\,, \quad \forall \delta \in (0, \mathrm{e}^{-K})\,. \tag{5.3}$$

Again applying the recursion formula we find similarly as in the proof of [5, Lemma 4.6] that

$$\|(\ln(b_i + \delta) + K)^-(t)\|_{L^\infty} \le c\kappa\big(\sup_{s \in [0,T]} \|(\ln(b_i + \delta) + K)^-(s)\|_{L^1} + 1\big)$$

which together with (5.3) leads to

$$\|(\ln(b_i + \delta) + K)^-(t)\|_{L^\infty} \le c(T) \quad \forall t \in [0,T]\,, \quad \forall \delta \in (0, \mathrm{e}^{-K})\,.$$

Passing to the limit $\delta \to 0$ and arguing as in Lemma 5.1 we obtain that

$$\|(\ln b_i + K)^-(t)\|_{L^\infty} \le c(T) \quad \forall t \in [0,T]\,.$$

Thus the assertion of the theorem is proved for $i = 1, \ldots, l$. The corresponding result for $i = l+1, \ldots, m$ now follows from Lemma 5.1. $\square$

**Lemma 5.3** *Let the assumptions* (I), (II), (III') *and* (IV) *be fulfilled. Then there exists a constant* $c > 0$ *depending only on the data such that*

$$\|(\ln b_i)^-(t)\|_{L^1} \le c \quad \forall t \in \mathbb{R}_+\,, \quad i = 1, \ldots, l\,,$$

*for any solution* $(u, b, \psi)$ *of* (P).

*Proof.* 1. Let $(u, b, \psi)$ and $(u^*, b^*, \psi^*)$ be a solution of (P) and the steady state of (P) (cf. Theorem 3.1), respectively. Let $i \in \{1, \ldots, l\}$ be fixed. Because of (III') and Theorem 5.1 we have $\ln b_i, \ln u_i \in L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty)$, $b_i^*/b_i \in L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty)$. Remark 2.2 implies $\ln b_i, \ln u_i \in C(\mathbb{R}_+, L^2)$. We define $\overline{z} := (1 - b_i^*/b_i)^-$, obviously $\overline{z} \in L^2_{\mathrm{loc}}(\mathbb{R}_+, H^1)$ (see Lemma 8.1).

2. We define the functional $\widetilde{\Theta}\colon L^2_-(\Omega) \to \mathbb{R}$,

$$\widetilde{\Theta}(w) := \int_\Omega u_i^*(x)\,\vartheta(w(x))\,\mathrm{d}x\,, \; w \in L^2_-(\Omega) := -L^2_+(\Omega)\,, \quad \vartheta(y) = -\ln(1 - y)\,, \; y \le 0$$

which is convex and continuous. The extended functional $\widetilde{\Theta}\colon L^2(\Omega) \to \overline{\mathbb{R}}$, $\widetilde{\Theta}(w) = +\infty$ if $w \in L^2(\Omega) \setminus L^2_-(\Omega)$, is proper, convex and lower semi-continuous. The functionals $\Theta =$

$\widetilde{\Theta}|_{H^1}\colon H^1(\Omega) \to \overline{\mathbb{R}}$, $G = \Theta^*\colon \left[H^1(\Omega)\right]^* \to \overline{\mathbb{R}}$ have the same properties. If $\overline{w} \in H^1(\Omega) \cap L^2_-(\Omega)$ then

$$\overline{u} := u_i^*/(1-\overline{w}) + h \in \partial\Theta(\overline{w}) \quad \forall h \in L^2_+(\Omega) \text{ with } h = 0 \text{ a.e. in } \Omega \setminus \{x\colon \overline{w}(x) = 0\}\,,$$

$$G(\overline{u}) = \langle \overline{u}, \overline{w}\rangle_{H^1} - \Theta(\overline{w})\,,$$

and especially for $\overline{w} = -\overline{z}(t)$, $h = [u_i(t) - u_i^*]^+$ we obtain

$$u_i(t) \in \partial\Theta(-\overline{z}(t))\,, \quad -\overline{z}(t) \in \partial G(u_i(t)) \quad \text{f.a.a. } t \in \mathbb{R}_+\,,$$

$$G(u_i(t)) = \int_\Omega \Big\{ u_i^* \left(\ln \frac{u_i}{u_i^*}\right)^-(t) - (u_i - u_i^*)^-(t) \Big\}\,\mathrm{d}x \quad \text{f.a.a. } t \in \mathbb{R}_+\,.$$

From Lemma 8.2 it follows, firstly, that the last equation holds for all $t \in \mathbb{R}_+$, and thus

$$G(u_i(t)) \geq c\,\|(\ln b_i)^-(t)\|_{L^1} - c_1 \quad \forall t \in \mathbb{R}_+\,,\ c, c_1 > 0\,. \tag{5.4}$$

Secondly, the chain rule yields

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

Let $z := (\ln b_i - \ln b_i^*)^-$. Since $\zeta_i^* = \text{const}$ (see Theorem 3.1) it follows $\nabla b_i^* + b_i^* Q_i(\psi^*)\nabla\psi^* = 0$,

$$\begin{aligned}\left[\nabla b_i + b_i Q_i(\psi)\nabla\psi\right]\nabla\overline{z} &= \left[\nabla b_i + b_i Q_i(\psi)\nabla\psi - \frac{b_i}{b_i^*}\nabla b_i^* - \frac{b_i}{b_i^*} b_i^* Q_i(\psi^*)\nabla\psi^*\right]\nabla\overline{z} \\ &= -b_i^*(\nabla z)^2 + b_i^*\left[Q_i(\psi)\nabla\psi - Q_i(\psi^*)\nabla\psi^*\right]\nabla z\,,\end{aligned}$$

and we derive

$$\begin{aligned} G(u_i(t)) \leq \int_0^t \Big\{ &-\epsilon \operatorname*{ess\,inf}_{x\in\Omega} b_i^*(x)\,\|\nabla z\|_{L^2}^2 + c\|\nabla(\psi - \psi^*)\|_{L^2}\|\nabla z\|_{L^2} \\ &+ c\|\psi - \psi^*\|_{H^1}\|\nabla\psi\|_{L^q}\|\nabla z\|_{L^2} \\ &+ \int_\Omega \sum_{(\alpha,\,\beta)\in\mathcal{R}^\Omega} k_{\alpha\beta}^\Omega \left[a^\alpha - a^\beta\right](\alpha_i - \beta_i)\,\overline{z}\,\mathrm{d}x \\ &+ \int_\Gamma \sum_{(\alpha,\,\beta)\in\mathcal{R}^\Gamma} k_{\alpha\beta}^\Gamma \left[a^\alpha - a^\beta\right](\alpha_i - \beta_i)\,\overline{z}\,\mathrm{d}\Gamma \Big\}\,\mathrm{d}s + G(U_i) \quad \forall t \in \mathbb{R}_+ \end{aligned} \tag{5.5}$$

where $\epsilon$ and $q$ are defined in Remark 3.1 and in Lemma 3.1, respectively, $r = 2q/(q-2)$. By assumption (IV) the initial value $G(U_i)$ is finite. From (III') and inequality (4.1) we find that $\|\nabla\psi\|_{L^\infty(\mathbb{R}_+,L^q)} \leq c$. In arguments $(s,x)$ with $\overline{z}(s,x) \neq 0$ we have

$$\left[a^\alpha - a^\beta\right](\alpha_i - \beta_i)\,\overline{z} = \left[a^\alpha - a^\beta\right](\alpha_i - \beta_i)\,\frac{1}{b_i}\,(b_i^* - b_i) \leq c\,|b_i^* - b_i| \quad \forall(\alpha,\beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma$$

because of (2.2) and (III'). Applying Theorem 3.4, (3.8) we continue estimate (5.5) by

$$G(u_i(t)) \leq c\big\{1 + \|\psi - \psi^*\|^2_{L^2(\mathbb{R}_+,H^1)} + \|b_i - b_i^*\|_{L^1(\mathbb{R}_+,L^1)} + \|b_i - b_i^*\|_{L^1(\mathbb{R}_+,L^1(\Gamma))}\big\} \leq c \quad \forall t \in \mathbb{R}_+\,.$$

Using (5.4) the assertion follows. $\square$

**Theorem 5.2** *Let the assumptions* (I), (II), (III') *and* (IV) *be fulfilled. Then there exist constants* $\overline{c}$, $c > 0$ *depending only on the data such that*

$$\|(\ln b_i)^-(t)\|_{L^\infty} \le \overline{c}\,, \quad \operatorname*{ess\,inf}_{x\in\Omega} b_i(t,x) \ge e^{-\overline{c}}\,, \quad \operatorname*{ess\,inf}_{x\in\Omega} u_i(t,x) \ge c \quad \forall t \in \mathbb{R}_+\,,\ i = 1,\dots,m\,,$$
$$\|(\ln b_i)^-\|_{L^\infty(\mathbb{R}_+,L^\infty(\Gamma))} \le \overline{c}\,,\ i = 1,\dots,l\,,$$

*for any solution* $(u,b,\psi)$ *of* (P).

*Proof.* 1. *Bounds for the diffusing species.* Let $i \in \{1,\dots,l\}$ and $K$ as in (5.1). Since $(\ln b_i + K)^- \in L^\infty_{\rm loc}(\mathbb{R}_+, L^\infty)$ (cf. Theorem 5.1) we can pass to the limit $\delta \to 0$ in the recursion formula of Lemma 5.2. We obtain

$$\mathrm{e}^t\|(\ln b_i + K)^-(t)\|^p_{L^p} \le c\int_0^t \mathrm{e}^s\, p^{2r}\kappa\big(\|(\ln b_i + K)^-(s)\|^p_{L^{p/2}} + 1\big)\,\mathrm{d}s \quad \forall t \in \mathbb{R}_+\,, \quad \forall p \ge 2\,,$$

and conclude as in the proof of Theorem 5.1 that

$$\|(\ln b_i + K)^-(t)\|_{L^\infty} \le c\kappa\big(\sup_{s\in\mathbb{R}_+}\|(\ln b_i + K)^-(s)\|_{L^1} + 1\big) \quad \forall t \in \mathbb{R}_+\,.$$

Using now the result of Lemma 5.3 we find that $\|(\ln b_i + K)^-(t)\|_{L^\infty} \le c$ for all $t \in \mathbb{R}_+$, $i = 1,\dots,l$, and therefore all the results for the diffusing species follow.

2. *Bounds for the non-diffusing species.* Let $j \in \{l+1,\dots,m\}$ and let $T \in \mathbb{R}_+$ be arbitrarily given. From Lemma 5.1 and the result of the first step of the present proof we find that

$$\|(\ln b_j)^-(t)\|_{L^\infty} \le \gamma(\mathrm{e}^{-\overline{c}}) \quad \forall t \in [0,T]\,.$$

Since the function $\gamma$ does not depend on $T$ we obtain the global result. □

**Corollary 5.1** *Under the assumptions* (I) – (IV) *there exists a constant* $c > 0$ *depending only on the data such that*

$$\operatorname*{ess\,inf}_{x\in\Omega} u_i(t,x) \ge c \quad \forall t \in \mathbb{R}_+\,,\ i = 1,\dots,m\,,$$

*for any solution* $(u,b,\psi)$ *of* (P).

## 6 Asymptotic behaviour

In addition to the results stated in Theorem 3.3, Theorem 3.4 we find the following asymptotic estimates concerning the densities $u_i$ and the potential $\psi$.

**Theorem 6.1** *We assume* (I) – (III). *Let* $p \in [1,+\infty)$. *Then there exist positive constants* $c$, $\widehat{c}$, $\lambda_p$, $\widehat{\lambda}$ *depending only on the data such that*

$$\|u(t) - u^*\|_{L^p(\Omega,\mathbb{R}^m)}\,,\ \|b(t) - b^*\|_{L^p(\Omega,\mathbb{R}^m)} \le c\,e^{-\lambda_p t} \quad \forall\, t \in \mathbb{R}_+\,,$$
$$\|\psi(t) - \psi^*\|_{W^{1,q}}\,,\ \|\psi(t) - \psi^*\|_{L^\infty} \le \widehat{c}\,e^{-\widehat{\lambda} t} \quad \forall\, t \in \mathbb{R}_+\,, \quad q \text{ as in Lemma } 3.1\,,$$

*for any solution* $(u,b,\psi)$ *of* (P).

*Proof.* Concerning the continuity properties of the functions $u$, $b$ and $\psi$ with respect to time we refer to Remark 2.2. We use the assertions (3.6) of Theorem 3.4, Theorem 4.1 and obtain for $p \in [1, +\infty)$, $i = 1, \ldots, m$,

$$\|u_i(t) - u_i^*\|_{L^p}^p \le \|u_i(t) - u_i^*\|_{L^1} \|u_i(t) - u_i^*\|_{L^\infty}^{p-1} \le c^p \, \mathrm{e}^{-\lambda t/2} \qquad \forall\, t \in \mathbb{R}_+ \,. \tag{6.1}$$

Because of $\|b_i(t) - b_i^*\|_{L^1} \le c\|u_i(t) - u_i^*\|_{L^1}$, $\|b_i(t) - b_i^*\|_{L^\infty} \le c\|u_i(t) - u_i^*\|_{L^\infty}$ and (6.1) we find the assertion of the theorem for $b_i$, $i = 1, \ldots, m$. Regularity results for elliptic equations [13, Theorem 1] applied to the solution $\overline{\psi} = \psi - \psi^*$ of

$$-\nabla \cdot (\varepsilon \nabla \overline{\psi}) + \overline{\psi} = h \text{ in } \Omega \,, \quad \nu \cdot (\varepsilon \nabla \overline{\psi}) = 0 \text{ on } \Gamma \,,$$

$$h = e(\psi^*) - e(\psi) + \sum_{i=1}^m \big(Q_i(\psi) u_i - Q_i(\psi^*) u_i^*\big) + \psi - \psi^*$$

supply that

$$\|\overline{\psi}\|_{L^\infty} \le c\|\overline{\psi}\|_{W^{1,q}} \le c\|h\|_{L^2} \,. \tag{6.2}$$

Since $\|\psi^*\|_{L^\infty}$, $\|\psi(t)\|_{L^\infty} \le c$, $t \in \mathbb{R}_+$, $Q_i \in C^1(\mathbb{R})$ and $e(x, \cdot)$ is locally Lipschitz continuous uniformly with respect to $x$ we obtain

$$\|h\|_{L^2} \le c\Big\{\|\psi - \psi^*\|_{H^1} + \sum_{i=1}^m \|u_i - u_i^*\|_{L^2}\Big\} \,.$$

Thus, from (6.2), Theorem 3.4 and (6.1) the last assertion follows. $\square$

## 7 Remarks

**1. Non-negativity.** Our formulation of (P) involved the requirement that $u$ is non-negative. This was mainly done by physical reasons since the kinetic coefficients $D_i$ and $k_{\alpha\beta}^\Sigma$ are defined in a natural way only for non-negative $b$. If we define the kinetic coefficients also for other $b \in \mathbb{R}^m$ in such a way that the assumptions (I) iv) and v) are fulfilled for all $b \in \mathbb{R}^m$ (e.g. by defining $D_i(x, b, \psi) := D_i(x, b^+, \psi)$, $k_{\alpha\beta}^\Sigma(x, b, \psi) := k_{\alpha\beta}^\Sigma(x, b^+, \psi)$ for $b \in \mathbb{R}^m \setminus \mathbb{R}_+^m$), and if we define the operator $A$ as in (2.3) on $[X \times H^1(\Omega)] \cap L^\infty(\Omega, \mathbb{R}^{m+1})$ we can consider the following modified formulation of (P):

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

**Lemma 7.1** *Let* $(u, b, \psi)$ *be a solution of* (P'). *Then* $u(t) \ge 0$, $b(t) \ge 0$ *a.e. on* $\Omega$ *for all* $t \in \mathbb{R}_+$, $b_i \ge 0$ *a.e. on* $\mathbb{R}_+ \times \Gamma$, $i = 1, \ldots, l$.

*Proof.* Let $(u, b, \psi)$ be a solution of (P'). Then for every $T > 0$ there exists a $c > 0$ such that $\|\psi(t)\|_{L^\infty}$, $\|\psi(t)\|_{L^\infty(\Gamma)}$, $\|b(t)\|_{L^\infty(\Omega, \mathbb{R}^m)}$, $\|b_i(t)\|_{L^\infty(\Gamma)} \le c$, $i = 1, \ldots, l$, f.a.a. $t \in [0, T]$. Again

[13, Theorem 1] ensures that $\|\psi(t)\|_{H^1}$, $\|\psi(t)\|_{W^{1,q}} \le c$ f.a.a. $t \in [0,T]$ for some $q > 2$. We test (P') with $-b^-$. First, we estimate

$$\int_\Omega D_i(\cdot,b,\psi)p_{0i}\left[\nabla b_i + b_i Q_i(\psi)\nabla\psi\right]\nabla b_i^-\,\mathrm{d}x \le -\epsilon\|\nabla b_i^-\|_{L^2}^2 + c\|b_i^-\|_{L^{2q/(q-2)}}\|\psi\|_{W^{1,q}}\|\nabla b_i^-\|_{L^2}$$
$$\le -\frac{\epsilon}{2}\|\nabla b_i^-\|_{L^2}^2 + c\|b_i^-\|_{L^2}^{(q-2)/q}\|b_i^-\|_{H^1}^{(q+2)/q} \le -\frac{\epsilon}{2}\|\nabla b_i^-\|_{L^2}^2 + c\|b_i^-\|_{L^2}^2 .$$

Next, we write

$$R^\Sigma_{\alpha\beta}(x,b,\psi)(\alpha_i-\beta_i)b_i^- = k^\Sigma_{\alpha\beta}(x,b_1,\dots,b_{m_\Sigma},\psi)\left[(a^+)^\alpha - (a^+)^\beta\right](\alpha_i-\beta_i)b_i^-$$
$$+ k^\Sigma_{\alpha\beta}(x,b_1,\dots,b_{m_\Sigma},\psi)\left[a^\alpha - a^\beta - (a^+)^\alpha + (a^+)^\beta\right](\alpha_i-\beta_i)b_i^- .$$

Because of (2.2) the first term is non-positive, and since $|a^\alpha - a^\beta - (a^+)^\alpha + (a^+)^\beta| \le c\|a^-\|_{\mathbb{R}^m}$ we find that

$$\int_\Omega \sum_{i=1}^m R^\Omega_{\alpha\beta}(x,b,\psi)(\alpha_i-\beta_i)b_i^-\,\mathrm{d}x \le c\sum_{i=1}^m \|b_i^-\|_{L^2}^2 ,$$

$$\int_\Gamma \sum_{i=1}^l R^\Gamma_{\alpha\beta}(x,b_1,\dots,b_l,\psi)(\alpha_i-\beta_i)b_i^-\,\mathrm{d}\Gamma \le c\sum_{i=1}^l \|b_i^-\|_{L^2(\Gamma)}^2 \le \sum_{i=1}^l \left\{\frac{\epsilon}{2}\|b_i^-\|_{H^1}^2 + c\|b_i^-\|_{L^2}^2\right\}.$$

Therefore, since $U \ge 0$ in summary

$$\sum_{i=1}^m \|b_i^-(t)\|_{L^2}^2 \le c\int_0^t \sum_{j=1}^m \|b_j^-(t)\|_{L^2}^2 \mathrm{d}s \quad \forall t \in [0,T]$$

follows, and Gronwall's lemma leads to the non-negativity of $b_i$ and $u_i$ on $\Omega$. The estimate for $b_i$, $i=1,\dots,l$, at the boundary follows from (8.2). □

**2. Uniqueness.** We prove a uniqueness result under the additional assumptions that

$$\left.\begin{array}{l} k^\Sigma_{\alpha\beta}(x,\cdot,\cdot) \text{ are locally Lipschitz continuous uniformly with respect to } x \\ \forall(\alpha,\beta)\in\mathcal{R}^\Sigma,\ \Sigma=\Omega,\Gamma; \\ D_i\colon \Omega\times\mathbb{R}\to\mathbb{R}_+,\ i=1,\dots,l, \text{ do not depend on } b, \\ D_i(x,\cdot) \text{ are locally Lipschitz continuous uniformly with respect to } x,\ i=1,\dots,l. \end{array}\right\} \quad \text{(V)}$$

**Lemma 7.2.** *Under the assumptions* (I) *and* (V) *there exists at most one solution of* (P).

*Proof.* Let $(u^j,b^j,\psi^j)$, $j=1,2$, be solutions of (P), let $T>0$, $S:=[0,T]$. Then there exists a constant $c$ such that

$$\|b_i^j(t)\|_{L^\infty},\ \|\psi^j(t)\|_{L^\infty},\ \|b_i^j(t)\|_{L^\infty(\Gamma)},\ \|\psi^j(t)\|_{L^\infty(\Gamma)},\ \|\psi^j(t)\|_{W^{1,q}} \le c \text{ f.a.a. } t\in S, \tag{7.1}$$

$j=1,2, i=1,\dots,m_\Sigma$, where $q>2$ (cf. Lemma 3.1). Let $\overline{b} := b^1-b^2$, $\overline{\psi} := \psi^1-\psi^2$. By Lemma 3.1 we obtain that

$$\|\overline{\psi}(t)\|_{H^1} \le c\|\overline{b}(t)\|_Y \text{ f.a.a. } t\in S. \tag{7.2}$$

Moreover, we apply Gröger's regularity result [13, Theorem 1] to the equation for $\overline{\psi}$ and estimate the $W^{-1,q}(\Omega\cup\Gamma)$–norm of the right hand side by the corresponding $L^2$-norm,

$$\|\overline{\psi}\|_{L^\infty} \le c\|\overline{\psi}\|_{W^{1,q}} \le c\|\psi^1-\psi^2+e(\psi^2)-e(\psi^1)+\textstyle\sum_{i=1}^m(Q_i(\psi^1)u_i^1 - Q_i(\psi^2)u_i^2)\|_{L^2} .$$

Properties of $e$ and $Q$ and the estimates in (7.1) and (7.2) ensure that

$$\|\overline{\psi}(t)\|_{L^\infty} \le c\|\overline{b}(t)\|_Y \text{ f.a.a. } t \in S\,. \tag{7.3}$$

We use $\overline{b} \in L^2(S,X)$ as test function for (P) and take into account that $R^\Sigma_{\alpha\beta}(x,\cdot,\cdot)$, $D_i(x,\cdot)$ are locally Lipschitz continuous uniformly with respect to $x$ and $Q_i$ are locally Lipschitz continuous. With $r := 2q/(q-2)$ and (8.1), (8.3), (7.2), (7.3) we get

$$\begin{aligned}
\frac{\epsilon_0}{2}\|\overline{b}(t)\|_Y^2 \le \int_0^t \Big\{ \sum_{i=1}^{l} \big\{ &-\epsilon\|\overline{b}_i\|_{H^1}^2 + c\big(\|\overline{b}_i\|_{L^r}\|\psi^1\|_{W^{1,q}} + \|\overline{\psi}\|_{L^\infty}(\|b_i^1\|_{H^1} + \|\psi^1\|_{H^1})\big)\|\overline{b}_i\|_{H^1} \\
&+ c\|\overline{\psi}\|_{H^1}\|\overline{b}_i\|_{H^1} + c\|\overline{b}_i\|^2_{L^2(\Gamma)}\big\} + c(\|\overline{b}\|_Y^2 + \|\overline{\psi}\|_{H^1}^2)\Big\}\,\mathrm{d}s \\
\le c\int_0^t \Big[\|\psi^1\|^r_{W^{1,q}} &+ \|\psi^1\|^2_{H^1} + \sum_{i=1}^{l}\|b_i^1\|^2_{H^1} + 1\Big]\|\overline{b}\|_Y^2\,\mathrm{d}s \quad \forall t \in S\,.
\end{aligned}$$

Since the function in the brackets belongs to $L^1(S)$ Gronwall's lemma yields $\overline{b} = 0$ on $S$. With (7.2) the assertion follows. □

**3. More general boundary conditions for the Poisson equation.** As mentioned in [16, Remark 3] also mixed boundary conditions for the Poisson equation can be considered such that the results of the present paper remain valid. For the treatment of such boundary conditions see also [10].

**4. Solvability.** Under the assumptions (I), (III) and the first assumption in (V) problem (P) has a solution. This will be proved in a forthcoming paper.

## 8 Appendix

Let $\Omega \subset \mathbb{R}^2$ be a bounded Lipschitzian domain. We apply Sobolev's imbedding theorems (see [17]) as well as some other imbedding results. By a modified application of the Hölder inequality from [17, p. 317, formula (5)] we derive

$$\|w\|^q_{L^q(\Gamma)} \le c_\Omega\, q\, \|w\|^{q-1}_{L^{2(q-1)}(\Omega)}\|w\|_{H^1(\Omega)} \quad \forall w \in H^1(\Omega)\,,\ 2 \le q < \infty\,. \tag{8.1}$$

By means of this trace inequality we get

$$\|w\|_{L^\infty(\Gamma)} \le \|w\|_{L^\infty(\Omega)} \quad \forall w \in H^1(\Omega) \cap L^\infty(\Omega)\,. \tag{8.2}$$

As a special version of the Gagliardo–Nirenberg inequality (see [4, 19]) we use the estimate

$$\|w\|_{L^q} \le c_{q,k}\,\|w\|^{k/q}_{L^k}\,\|w\|^{1-k/q}_{H^1} \quad \forall w \in H^1(\Omega)\,,\ 1 \le k < q < \infty\,. \tag{8.3}$$

Additionally, from Trudinger's imbedding theorem (see [21]) we get

$$\|\mathrm{e}^{|w|}\|_{L^q} \le d_q(\|w\|_{H^1}) \quad \forall w \in H^1(\Omega)\,,\ 1 \le q < \infty\,. \tag{8.4}$$

Moreover, we apply different rules of the calculus of weakly differentiable functions, especially the following chain rules.

**Lemma 8.1** *Let $f : \mathbb{R} \to \mathbb{R}$ be locally Lipschitz continuous, and let $u \in W^{1,1}_{\mathrm{loc}}(\Omega)$. Then $f \circ u \in W^{1,1}_{\mathrm{loc}}(\Omega)$, and*

$$\begin{aligned} \nabla f \circ u = 0\,,\ \nabla u = 0 \quad & \textit{a.e. on } \{x : u(x) \in A\}\,, \\ \nabla f \circ u = f'(u)\, \nabla u \quad & \textit{a.e. on } \{x : u(x) \notin A\} \end{aligned}$$

*where $A$ denotes the set of points in which $f$ is not differentiable.*

For the proof we refer to [7, pp. 127–129].

**Lemma 8.2** *Let $X$ be a Hilbert space, $X^*$ its dual, $S = [0, T]$. Let the functional $F : X^* \to \overline{\mathbb{R}}$ be proper, convex, lower semi-continuous. Suppose that $u \in H^1(S, X^*)$, $f \in L^2(S, X)$ and $f(t) \in \partial F(u(t))$ f.a.a. $t \in S$. Then the function $F \circ u : S \to \mathbb{R}$ is absolutely continuous, and*

$$\frac{\mathrm{d}\, F \circ u}{\mathrm{d}t}(t) = \Big\langle \frac{\mathrm{d}u}{\mathrm{d}t}(t), f(t) \Big\rangle_X \quad \textit{f.a.a. } t \in S\,.$$

*Proof.* We denote by $J : X \to X^*$ the duality map. Then we have $Jf \in L^2(S, X^*)$,

$$F(v) - F(u(t)) \geq \langle v - u(t), f(t) \rangle_X = (Jf(t), v - u(t))_{X^*} \quad \forall\, v \in X^*\,,\ \text{f.a.a. } t \in S\,,$$

and the assertions follow from [1, Lemma 3.3]. $\square$

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