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Electro-reaction-diffusion systems with nonlocal constraints

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Abstract. The paper deals with equations modelling the redistribution of charged particles by reactions, drift and diffusion processes. The corresponding model equations contain parabolic PDEs for the densities of mobile species, ODEs for the densities of immobile species, a possibly nonlinear, nonlocal Poisson equation and some nonlocal constraints. Based on applications to semiconductor technology these equations have to be investigated for non-smooth data and kinetic coefficients which depend on the state variables.
In two space dimensions we discuss the steady states of the system, we prove energy estimates, global a priori estimates and give a global existence result.

1 The model

We consider a widely general electro-reaction-diffusion system for m species X_i. Let z_0 denote the electrostatic potential, and additionally let the time functions $z_1, \ldots, z_k$ be internal parameters (e.g. electrochemical potentials of species, which have been eliminated by foregoing considerations). For examples of such model equations see §8. We write $z = (z_0, z_1, \ldots, z_k)$. Moreover, let $p_i(x, z)$ be suitable chosen reference densities such that

$$p_{0i}(x) := p_i(x, 0), \quad p_i(x, z) = p_{0i}(x)\mathrm{e}^{-P_i(z)}, \quad i = 1, \ldots, m,$$

where the functions P_i depend on z only. We call the quantities u_i, $b_i = u_i/p_{0i}$, $a_i = u_i/p_i(\cdot, z)$ the density, the chemical activity and the electrochemical activity of the i-th species. If $a_i > 0$ then $\zeta_i = \ln a_i$ corresponds to the electrochemical potential of the i-th species. All quantities are suitable scaled. We use the vectors $u = (u_1, \ldots, u_m)$, $b = (b_1, \ldots, b_m)$ and $a = (a_1, \ldots, a_m)$. Let $1 \le l \le m$. We assume that the species $X_1, \ldots, X_l$ are mobile which means that they underlie drift-diffusion processes. The second group of species $X_{l+1}, \ldots, X_m$ is assumed to be immobile, no drift-diffusion processes take place. The spatial and temporal variation of their densities is realised by reactions with mobile species and their transport processes. If the mobile and immobile species are charged they contribute to the charge density and influence the electrostatic potential z_0. The transport of the mobile species is based on the drift-diffusion flux densities

$$j_i = -D_i(\cdot, b, z)\, p_{0i}\big[\nabla b_i + Q_i(z)\, b_i \nabla z_0\big]\,,\ i = 1, \ldots, l,$$

with diffusion coefficients D_i depending on the spatial variable and on the state (b, z) and with charge numbers

$$Q_i(z) := \frac{\partial P_i}{\partial z_0}(z)\,,\ i = 1, \ldots, l. \tag{1}$$

The continuity equations for the mobile and immobile species contain source terms resulting from reversible mass action type reactions of the form

$$\alpha_1 X_1 + \cdots + \alpha_m X_m \rightleftharpoons \beta_1 X_1 + \cdots + \beta_m X_m\,,\ (\alpha, \beta) \in \mathcal{R},$$

where $\alpha,\,\beta\in\mathbf{Z}_+^m$ are the vectors of the corresponding stoichiometric coefficients and $\mathcal{R}$ is the (finite) set of all volume reactions under consideration. The respective reaction rates $R_{\alpha\beta}\,,\ (\alpha,\beta)\in\mathcal{R}$, write as

$$R_{\alpha\beta}(x,b,z)=k_{\alpha\beta}(x,b,z)\Big[\prod_{i=1}^m a_i^{\alpha_i}-\prod_{i=1}^m a_i^{\beta_i}\Big]\,,\ x\in\Omega\,,\ b\in\mathbf{R}_+^m\,,\ z\in\mathbf{R}^{k+1}\,,\ a_i=b_i\mathrm{e}^{P_i(z)}$$

with kinetic coefficients $k_{\alpha\beta}$ depending on the spatial variable and on the state (b,z). We consider the system

$$\left.\begin{aligned}
\frac{\partial u_i}{\partial t}+\nabla\cdot j_i+\sum_{(\alpha,\beta)\in\mathcal{R}}(\alpha_i-\beta_i)\,R_{\alpha\beta} &= 0 && \text{in } (0,\infty)\times\Omega,\\
\nu\cdot j_i &= 0 && \text{on } (0,\infty)\times\partial\Omega\,,\ i=1,\dots,l;\\
\frac{\partial u_i}{\partial t}+\sum_{(\alpha,\beta)\in\mathcal{R}}(\alpha_i-\beta_i)\,R_{\alpha\beta} &= 0 && \text{in } (0,\infty)\times\Omega\,,\ i=l+1,\dots,m;\\
u_i(0) &= U_i && \text{in } \Omega\,,\ i=1,\dots,m;\\
-\nabla\cdot(\varepsilon\nabla z_0)+\frac{\partial H}{\partial z_0}(\cdot,u,z) &= f_0 && \text{in } (0,\infty)\times\Omega,\\
z_0 &= 0 && \text{on } (0,\infty)\times\Gamma_D,\\
\nu\cdot(\varepsilon\nabla z_0)+\tau z_0 &= 0 && \text{on } (0,\infty)\times\Gamma_N;\\
\frac{1}{|\Omega|}\int_\Omega\frac{\partial H}{\partial z_j}(\cdot,u,z)\,\mathrm{d}x &= f_j && \text{on } (0,\infty)\,,\ j=1,\dots,k,
\end{aligned}\right\}\qquad(2)$$

where U_i are the initial densities, ε is the dielectric permittivity, τ a capacity, f_0 a fixed charge density, $f_j\in\mathbf{R}$, $j=1,\dots,k$, are time independent quantities and the function H is given by

$$H(x,u,z):=\begin{cases}h(x,z)-\sum_{i=1}^m u_iP_i(z) & \text{if } k>0\\ -\sum_{i=1}^m u_iq_iz_0,\ \ q_i\in\mathbf{R} & \text{if } k=0\end{cases}\qquad(3)$$

with a suitable function h (for examples see §8). Note that

$$\frac{\partial H}{\partial z_0}(\cdot,u,z)=\frac{\partial h}{\partial z_0}(\cdot,z)-\sum_{i=1}^m Q_i(z)u_i\qquad(4)$$

corresponds to an additional charge density depending on the state.

The continuity equations for $X_1,\dots,X_l$ are parabolic PDEs, for the species $X_{l+1},\dots,X_m$they are ODEs. If $l=m$ then all continuity equations are PDEs. Additionally, the system contains a nonlinear Poisson equation and k nonlocal constrains. If $k=0$ no nonlocal constraints are involved and the Poisson equation becomes linear.

Some notation. The notation of function spaces corresponds to that in [17]. By $\mathbf{R}_+^n$, $\mathbf{Z}_+^n$, L_+^p we denote the cones of non-negative elements. If $u\in\mathbf{R}^n$ then $u\geq 0$ ($u>0$) is to be understood as $u_i\geq 0\ \forall i$ ($u_i>0$ $\forall i$). If $u\in\mathbf{R}^n$ and $\alpha\in\mathbf{Z}_+^n$ then u^α denotes the product $\prod_{i=1}^n u_i^{\alpha_i}$. The scalar product in $\mathbf{R}^n$ is indicated by a centered dot. If $u,\,w\in\mathbf{R}^n$ then $uw=\{u_iw_i\}_{i=1,\dots,n}$, and u/w is defined analogously, e^u is to understand as $\{\mathrm{e}^{u_i}\}_{i=1,\dots,n}$. If $u\in\mathbf{R}_+^n$ then $\ln u=\{\ln u_i\}_{i=1,\dots,n}$. Positive constants which depend only on the data of our problem are denoted by c. Some further results which we use in our considerations are picked up in the appendix.

2 Assumptions

We define three classes of functions

$$\begin{aligned}
\mathcal{K}_1:=\Big\{&g\colon\mathbf{R}^{k+1}\to\mathbf{R}:\ \text{if } k=0 \text{ then } g(z)=-q\,z_0\,,\ q\in\mathbf{R};\\
&\text{if } k>0 \text{ then } g(z)=\widetilde{g}(z_0+z_1,z_2,\dots,z_k) \text{ with } \widetilde{g}\in C^1(\mathbf{R}^k)\,,\ \widetilde{g}(0)=0,\\
&\widetilde{g} \text{ is convex, there exists } c>0 \text{ with } \|\partial_w\widetilde{g}(w)\|_{\mathbf{R}^k}\leq c\quad\forall w\in\mathbf{R}^k,\\
&\text{for all } R>0 \text{ there exists } c_R>0 \text{ such that}\\
&\|\partial_w\widetilde{g}(w)-\partial_w\widetilde{g}(\overline{w})\|_{\mathbf{R}^k}\leq c_R\|w-\overline{w}\|_{\mathbf{R}^k}\ \forall w,\,\overline{w}\in[-R,R]^k\Big\},
\end{aligned}$$

$$\mathcal{K}_2 := \Big\{ g\colon \Omega\times\mathbf{R}^{k+1}\to\mathbf{R}:\ \text{if } k=0 \text{ then } g(x,z)=0;$$
$$\text{if } k>0 \text{ then } g(x,z)=\widetilde{g}(x,z_0+z_1,z_2,\dots,z_k) \text{ with}$$
$$\widetilde{g}\colon \Omega\times\mathbf{R}^{k}\to\mathbf{R} \text{ satisfies the Carathéodory-conditions},$$
$$\widetilde{g}(x,\cdot)\in C^1(\mathbf{R}^k) \text{ f.a.a. } x\in\Omega\,,\ \widetilde{g}(x,\cdot) \text{ convex f.a.a. } x\in\Omega,$$
$$\text{there exists } c>0 \text{ with } \|\partial_w\widetilde{g}(x,w)\|_{\mathbf{R}^k}\le c\mathrm{e}^{c\|w\|_{\mathbf{R}^k}} \text{ f.a.a. } x\in\Omega\,,\ \forall w\in\mathbf{R}^k,$$
$$\text{for all } R>0 \text{ there exists } c_R>0 \text{ such that}$$
$$\|\partial_w\widetilde{g}(x,w)-\partial_w\widetilde{g}(x,\overline{w})\|_{\mathbf{R}^k}\le c_R\|w-\overline{w}\|_{\mathbf{R}^k} \text{ f.a.a. } x\in\Omega\,,\ \forall w,\,\overline{w}\in[-R,R]^k\Big\},$$
$$\mathcal{K}_{2,s} := \Big\{ g\in\mathcal{K}_2\colon \widetilde{g}(x,0)=0 \text{ f.a.a. } x\in\Omega\,,\ \text{if } k>0 \text{ then there exists } c_0>0 \text{ with}$$
$$\widetilde{g}(x,\overline{w})-\widetilde{g}(x,w)-\partial_w\widetilde{g}(x,w)\cdot(\overline{w}-w)\ge c_0\|\overline{w}-w\|^2_{\mathbf{R}^k} \text{ f.a.a. } x\in\Omega\,,\ \forall w,\,\overline{w}\in\mathbf{R}^k\Big\}.$$

For our investigations of (2) we suppose up to the end of the paper the **Assumptions (I)**:

i) $\Omega\subset\mathbf{R}^2$ is a bounded Lipschitzian domain, $\Gamma:=\partial\Omega$, Γ_D, Γ_N are disjoint open subsets of Γ, $\Gamma=\overline{\Gamma_D}\cup\overline{\Gamma_N}$, $\overline{\Gamma_D}\cap\overline{\Gamma_N}$ consists of finitely many points;

ii) $k,m,l\in\mathbf{N}$, $1\le l\le m$, $U=(U_1,\dots,U_m)\in L^\infty_+(\Omega,\mathbf{R}^m), \varepsilon\in L^\infty(\Omega)$, $\varepsilon\ge c>0$, $\tau\in L^\infty_+(\Gamma_N)$ with $\operatorname{mes}\Gamma_D+\|\tau\|_{L^1(\Gamma_N)}>0, f_0\in L^2(\Omega)$, if $k>0$ then $f_j\in\mathbf{R}$, $j=1,\dots k$;

iii) $p_{0i}\in L^\infty_+(\Omega)$ with $\operatorname*{ess\,inf}_{x\in\Omega} p_{0i}(x)\ge\epsilon_0>0$, $-P_i\in\mathcal{K}_1$, $h\in\mathcal{K}_{2,s}$,
let $p_i\colon\Omega\times\mathbf{R}^{k+1}\to(0,\infty)$, $p_i(x,z):=p_{0i}(x)\,\mathrm{e}^{-P_i(z)}$, $x\in\Omega$, $z\in\mathbf{R}^{k+1}$,
$Q_i(z):=\dfrac{\partial P_i}{\partial z_0}(z)$, $z\in\mathbf{R}^{k+1}$, $i=1,\dots,m$,
$H\colon\Omega\times\mathbf{R}^m_+\times\mathbf{R}^{k+1}\to\mathbf{R}$, $H(x,u,z):=h(x,z)-\sum_{i=1}^m u_iP_i(z)$;

iv) $\mathcal{R}\subset\mathbf{Z}^m_+\times\mathbf{Z}^m_+$, for $(\alpha,\beta)\in\mathcal{R}$ we define $R_{\alpha\beta}\colon\Omega\times\mathbf{R}^m_+\times\mathbf{R}^{k+1}\to\mathbf{R}$ as
$R_{\alpha\beta}(x,b,z):=k_{\alpha\beta}(x,b,z)(a^\alpha-a^\beta)$, $a_i=b_i\,\mathrm{e}^{P_i(z)}$, $i=1,\dots,m$,
$x\in\Omega$, $b\in\mathbf{R}^m_+$, $z\in\mathbf{R}^{k+1}$,
$k_{\alpha\beta}\colon\Omega\times\mathbf{R}^m_+\times\mathbf{R}^{k+1}\to\mathbf{R}_+$ satisfies the Carathéodory-conditions,
$k_{\alpha\beta}(x,\cdot,\cdot)$ is locally Lipschitz-continuous uniformly with respect to x,
for all $R>0$ there are $c_R>0$, $b_{\alpha\beta,R}\in L^\infty_+(\Omega)$ with $\|b_{\alpha\beta,R}\|_{L^1(\Omega)}>0$ such that
$b_{\alpha\beta,R}(x)\le k_{\alpha\beta}(x,b,z)\le c_R$ f.a.a. $x\in\Omega$, $\forall b\in\mathbf{R}^m_+$, $\forall z\in[-R,R]^{k+1}$;

v) for $i=1,\dots,l$:
$D_i\colon\Omega\times\mathbf{R}^m_+\times\mathbf{R}^{k+1}\to\mathbf{R}_+$ satisfies the Carathéodory-conditions,
$D_i(x,b,z)\ge c>0$ f.a.a. $x\in\Omega$, $\forall b\in\mathbf{R}^m_+$, $\forall z\in\mathbf{R}^{k+1}$,
for all $R>0$ there exists $c_R>0$ such that
$D_i(x,b,z)\le c_R$ f.a.a. $x\in\Omega$, $\forall b\in\mathbf{R}^m_+$, $\forall z\in[-R,R]^{k+1}$;

vi) for $i=l+1,\dots,m$: there exists a reaction of the form
$$R_{\alpha_{(i)}\beta_{(i)}}(x,b,z)=k_{\alpha_{(i)}\beta_{(i)}}(x,b,z)\Big[\prod_{j=1}^l a_j^{\alpha_{(i)j}}-a_i^2\Big],\ x\in\Omega,\ b\in\mathbf{R}^m_+,\ z\in\mathbf{R}^{k+1},$$
with $\operatorname*{ess\,inf}_{x\in\Omega} b_{\alpha_{(i)}\beta_{(i)},R}(x)>0$.

Assumption (I) vi) ensures the existence of a reaction which guarantees a sufficiently large contribution of the immobile species to the dissipation rate for the electro-reaction-diffusion system. Further assumptions needed for the proof of the existence of steady states, of the exponential decay of the free energy, of global a priori estimates resp. of the existence of solutions of $(\mathcal{P})$ will be formulated in §4 and §5 (see (II), (III) and (IV)).

Remark 2.1 For energy estimates we will use the structural property of the reaction terms $R_{\alpha\beta}$ that

$$(a^\alpha - a^\beta)\,(\alpha-\beta)\cdot \ln a \geq 0 \quad \forall a\in \text{ int }\mathbf{R}^m_+\,,\ \forall(\alpha,\beta)\in\mathcal{R}. \tag{5}$$

Remark 2.2 The assumptions (I) ensure some fundamental properties often used in the paper.
i) Assumption (I) ii) supplies a constant $c>0$ such that

$$\|\nabla z_0\|^2_{L^2} + \int_{\Gamma_N} \tau z_0^2 \,\mathrm{d}\Gamma \geq c\|z_0\|^2_{H^1} \quad \forall z_0\in H^1_0(\Omega\cup\Gamma_N). \tag{6}$$

ii) Since $-P_i\in\mathcal{K}_1$ the function P_i is Lipschitz continuous and $p_i(x,\cdot)$ is locally Lipschitz continuous (uniformly with respect to x), $i=1,\dots,m$. Moreover, if $k>0$ then $\ln p_i\in\mathcal{K}_2$.
iii) The functions $p_i(x,\cdot)$ are convex f.a.a. $x\in\Omega$. If $k>0$ the corresponding functions $\widetilde{p}_i(x,\cdot)$ (see the definition of $\mathcal{K}_2$) are convex f.a.a. $x\in\Omega$, too.
iv) Let Z denote the space $Z:=H^1_0(\Omega\cup\Gamma_N)\times\mathbf{R}^k$. The properties $h\in\mathcal{K}_{2,s}$ and $-P_i\in\mathcal{K}_1$ ensure the convexity of $H(x,u,\cdot)$ and the monotonicity of $\frac{\partial H}{\partial z}(x,u,\cdot)$ for $u\in\mathbf{R}^m_+$, and a.a. $x\in\Omega$. If $z,\,\overline{z}\in Z$ then

$$\|\overline{z}_0-z_0\|^2_{H^1} + \int_\Omega\Big\{h(\cdot,\overline{z})-h(\cdot,z)-\sum_{j=0}^k\frac{\partial h}{\partial z_j}(\cdot,z)(\overline{z}_j-z_j)\Big\}\mathrm{d}x \geq c\|\overline{z}-z\|^2_Z, \tag{7}$$

$$\|z_0\|^2_{H^1} + \int_\Omega h(\cdot,z)\,\mathrm{d}x \geq c\|z\|^2_Z - \widetilde{c}. \tag{8}$$

Moreover, there exists a $c>0$ not depending on u such that for all $z,\,\overline{z}\in Z$ and all $u\in L^\infty_+(\Omega)$

$$\|\overline{z}_0-z_0\|^2_{H^1} + \int_\Omega\Big\{H(\cdot,u,\overline{z})-H(\cdot,u,z)-\sum_{j=0}^k\frac{\partial H}{\partial z_j}(\cdot,u,z)(\overline{z}_j-z_j)\Big\}\,\mathrm{d}x \geq c\|\overline{z}-z\|^2_Z, \tag{9}$$

$$\|\overline{z}_0-z_0\|^2_{H^1} + \int_\Omega\Big\{\sum_{j=0}^k\Big(\frac{\partial H}{\partial z_j}(\cdot,u,\overline{z})-\frac{\partial H}{\partial z_j}(\cdot,u,z)\Big)(\overline{z}_j-z_j)\Big\}\,\mathrm{d}x \geq c\|\overline{z}-z\|^2_Z. \tag{10}$$

v) For functions g belonging to the class $\mathcal{K}_1$ there is an estimate

$$|g(\overline{z})-g(z)-\partial_z g(z)\cdot(\overline{z}-z)| \leq c(R)\,\|\overline{z}-z\|^2_{\mathbf{R}^{k+1}} \quad \forall z,\,\overline{z}\in[-R,R]^{k+1}.$$

If $g\in\mathcal{K}_2$ we can estimate

$$|g(x,\overline{z})-g(x,z)-\partial_z g(x,z)\cdot(\overline{z}-z)| \leq c(R)\|\overline{z}-z\|^2_{\mathbf{R}^{k+1}} \text{ f.a.a. } x\in\Omega\,,\ \forall z,\,\overline{z}\in[-R,R]^{k+1}.$$

3 Weak formulation

We use the function spaces

$$Y:=L^2(\Omega,\mathbf{R}^m)\,,\ X:=\{b\in Y\colon b_i\in H^1(\Omega)\,,\ i=1,\dots,l\}\,,\ Z=H^1_0(\Omega\cup\Gamma_N)\times\mathbf{R}^k$$

and define the operators $\mathcal{B}\colon Y \to Y$, $\mathcal{A}$, $\mathcal{R}\colon [X\times Z]\cap[L^\infty_+(\Omega,\mathbf{R}^m)\times L^\infty(\Omega)\times\mathbf{R}^k] \to X^*$ and $\mathcal{E}\colon Z\times Y\to Z^*$,

$$\mathcal{B}b := p_0\, b,\quad p_0=(p_{01},\dots,p_{0m}),$$

$$\langle\mathcal{A}(b,z),\overline{b}\rangle_X := \int_\Omega \sum_{i=1}^{l} D_i(\cdot,b,z)p_{0i}(\nabla b_i + b_iQ_i(z)\nabla z_0)\cdot\nabla\overline{b}_i\,\mathrm{d}x,\quad \overline{b}\in X,$$

$$\langle\mathcal{R}(b,z),\overline{b}\rangle_X := \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta}(\cdot,b,z)\sum_{i=1}^{m}(\beta_i-\alpha_i)\,\overline{b}_i\,\mathrm{d}x,\quad \overline{b}\in X,$$

$$\langle\mathcal{E}(z,u),\overline{z}\rangle_Z := \int_\Omega\Big\{\varepsilon\nabla z_0\cdot\nabla\overline{z}_0 + \sum_{j=0}^{k}\big[\frac{\partial H}{\partial z_j}(\cdot,u,z)-f_j\big]\,\overline{z}_j\Big\}\,\mathrm{d}x + \int_{\Gamma_N}\tau z_0\overline{z}_0\,\mathrm{d}\Gamma,\quad \overline{z}\in Z.$$

Then the weak formulation of the electro-reaction-diffusion system (2) reads as

$$\left.\begin{array}{c} u'(t)+\mathcal{A}(b(t),z(t)) = \mathcal{R}(b(t),z(t)),\quad \mathcal{E}(z(t),u(t))=0,\quad u(t)=\mathcal{B}b(t)\quad \text{f.a.a. } t>0,\\ u(0)=U,\quad u\in H^1_{\mathrm{loc}}(\mathbf{R}_+,X^*)\cap L^2_{\mathrm{loc}}(\mathbf{R}_+,Y),\\ b\in L^2_{\mathrm{loc}}(\mathbf{R}_+,X)\cap L^\infty_{\mathrm{loc}}(\mathbf{R}_+,L^\infty_+(\Omega,\mathbf{R}^m)),\quad z\in L^2_{\mathrm{loc}}(\mathbf{R}_+,Z)\cap L^\infty_{\mathrm{loc}}(\mathbf{R}_+,L^\infty(\Omega)\times\mathbf{R}^k).\end{array}\right\}\ (\mathcal{P})$$

Remark 3.1 In difference to former papers (see [9, 10, 11]) the formulation $(\mathcal{P})$ allows that initial densities are zero on sets of positive measure and that some of the species are immobile. Moreover, now the kinetic coefficients depend on the state, too. A special case of $(\mathcal{P})$ is treated in the papers [12, 13, 16, 18].
Note that the Poisson equation and the nonlocal constraints are put together in a generalized Poisson equation.

Remark 3.2 If (u,b,z) is a solution of $(\mathcal{P})$ then it has the following regularity properties: $u,\ b\in C(\mathbf{R}_+,Y)$, $u,b\in C(\mathbf{R}_+,(L^\infty(\Omega,\mathbf{R}^m),w*))$. Moreover, by Lemma 4.3 below $z\in C(\mathbf{R}_+,Z)$. These properties ensure

$$\mathcal{E}(z(t),u(t))=0 \text{ in } Z^*,\quad u(t)=p_0\,b(t) \text{ in } L^\infty(\Omega,\mathbf{R}^m),\quad u(t)\ge 0 \text{ a.e. on } \Omega\quad \forall t\in\mathbf{R}_+. \tag{11}$$

4 Energy estimates

4.1 The generalized Poisson equation

Lemma 4.1 *For $u\in Y_+$ the operator $\mathcal{E}(\cdot,u)\colon Z\to Z^*$ is strongly monotone (uniformly with respect to u). Moreover, $\mathcal{E}(\cdot,u)$ is hemi-continuous for all $u\in Y_+$.*

Proof. 1. Let $u\in Y_+$, z, $\widetilde{z}\in Z$ and $\overline{z}=z-\widetilde{z}$. Because of (6) and (10) we obtain

$$\langle\mathcal{E}(z,u)-\mathcal{E}(\widetilde{z},u),\overline{z}\rangle_Z = \int_\Omega\varepsilon|\nabla\overline{z}_0|^2\,\mathrm{d}x + \int_{\Gamma_N}\tau\overline{z}_0^2\,\mathrm{d}\Gamma$$
$$+\int_\Omega\sum_{j=0}^{k}\Big(\frac{\partial H}{\partial z_j}(\cdot,u,z)-\frac{\partial H}{\partial z_j}(\cdot,u,\widetilde{z})\Big)\overline{z}_j\,\mathrm{d}x \ge c\|\overline{z}\|_Z^2,\ c>0.$$

2. We have to show that for all z, $\widehat{z}$, $\overline{z}\in Z$, $u\in Y_+$ the map $t\mapsto\langle\mathcal{E}(z+t\widehat{z},u),\overline{z}\rangle_Z$ is continuous on $[0,1]$. Let $t_0\in[0,1]$, $t_n\to t_0$, $t_n\in[0,1]$. Then

$$|\langle\mathcal{E}(z+t_n\widehat{z},u)-\mathcal{E}(z+t_0\widehat{z},u),\overline{z}\rangle_Z|$$
$$\le c|t_n-t_0|\|\widehat{z}_0\|_{H^1}\|\overline{z}_0\|_{H^1} + \Big|\int_\Omega\sum_{j=0}^{k}\Big(\frac{\partial H}{\partial z_j}(\cdot,u,z+t_n\widehat{z})-\frac{\partial H}{\partial z_j}(\cdot,u,z+t_0\widehat{z})\Big)\overline{z}_j\,\mathrm{d}x\Big|.$$

For $k=0$ the last term vanishes. Let now $k>0$. Because of $H(x,u,\cdot)\in C^1(\mathbf{R}^{k+1})$ f.a.a. $x\in\Omega$ and all $u\in Y_+$ the integrand in the last term converges to zero a.e. on Ω. Since $\ln p_i$, $h\in\mathcal{K}_2$ and $t_n\in[0,1]$ we find

$$\Big|\frac{\partial H}{\partial z_j}(\cdot,u,z+t_n\widehat{z})\overline{z}_j\Big| \le c\mathrm{e}^{c(\|z\|_{\mathbf{R}^{k+1}}+\|\widehat{z}\|_{\mathbf{R}^{k+1}})}|\overline{z}_j|\,\|u\|_{\mathbf{R}^m},$$

and Trudinger's imbedding result (68) supplies an integrable majorant. Then Lebesgue's theorem ensures the hemi-continuity of $\mathcal{E}(\cdot, u)$. □

Lemma 4.2 *For $z \in Z$ the operator $\mathcal{E}(z,\cdot)\colon Y \to Z^*$ is Lipschitz continuous (uniformly with respect to z).*

P r o o f. Let $u,\, \widetilde{u} \in Y$, $\overline{z} \in Z$. Since $-P_i \in \mathcal{K}_1$, $i = 1, \dots, m$, we obtain

$$\begin{aligned}\langle \mathcal{E}(z,u) - \mathcal{E}(z,\widetilde{u}), \overline{z}\rangle_Z &= \int_\Omega \sum_{j=0}^k \Big[\frac{\partial H}{\partial z_j}(\cdot,u,z) - \frac{\partial H}{\partial z_j}(\cdot,\widetilde{u},z)\Big]\overline{z}_j \,\mathrm{d}x \\ &= -\int_\Omega \sum_{i=1}^m (u_i - \widetilde{u}_i) \sum_{j=0}^k \frac{\partial P_i}{\partial z_j}(z)\overline{z}_j \,\mathrm{d}x \le c\|u-\widetilde{u}\|_Y \|\overline{z}\|_Z.\end{aligned}$$
□

Lemma 4.3 *For any $u \in Y$ there exists a unique solution $z \in Z$ of $\mathcal{E}(z,u^+) = 0$. Moreover there are an exponent $q > 2$, constants $c > 0$ and a monotonously increasing function $d\colon \mathbf{R}_+ \to \mathbf{R}_+$ such that*

$$\|z - \overline{z}\|_Z \le c\,\|u - \overline{u}\|_Y \quad \forall u, \overline{u} \in Y\,,\ \mathcal{E}(z,u^+) = \mathcal{E}(\overline{z},\overline{u}^+) = 0, \tag{12}$$

$$\|z_0\|_{L^\infty} \le c\Big\{1 + \sum_{i=1}^m \|u_i^+ \ln u_i^+\|_{L^1} + d(\|z\|_Z)\Big\} \quad \forall u \in Y\,,\ \mathcal{E}(z,u^+) = 0,$$

$$\|z_0\|_{W^{1,q}} \le c\Big\{1 + \sum_{i=1}^m \|u_i\|_{L^{2q/(2+q)}} + d(\|z\|_Z)\Big\} \quad \forall u \in Y\,,\ \mathcal{E}(z,u^+) = 0.$$

Finally, let $S = [0,T]$, $T > 0$. Then for every $u \in L^2(S,Y)$ there exists a unique $z \in L^2(S,Z)$ such that $\mathcal{E}(z(t),u^+(t)) = 0$ f.a.a. $t \in S$. If $u \in C(S,Y)$ then $z \in C(S,Z)$ follows and the last equation is fulfilled for all $t \in S$.

P r o o f. It suffices to prove the results for $u,\, \overline{u} \in Y_+$. Let $u \in Y_+$, according to Lemma 4.1 there is a unique solution of $\mathcal{E}(z,u) = 0$. For (z,u) and $(\overline{z},\overline{u})$ with $\mathcal{E}(z,u) = \mathcal{E}(\overline{z},\overline{u}) = 0$ Lemma 4.2 and Lemma 4.1 ensure

$$c\|z-\overline{z}\|_Z^2 \le \langle \mathcal{E}(z,u) - \mathcal{E}(\overline{z},u), z - \overline{z}\rangle_Z = \langle \mathcal{E}(\overline{z},\overline{u}) - \mathcal{E}(\overline{z},u), z-\overline{z}\rangle_Z \le c\|u-\overline{u}\|_Y\|z-\overline{z}\|_Z,$$

and the inequality (12) follows immediately. If $\mathcal{E}(z,u) = 0$ then, in particular

$$\int_\Omega \varepsilon \nabla z_0 \cdot \nabla \overline{z}_0 \,\mathrm{d}x + \int_{\Gamma_N} \tau z_0 \overline{z}_0 \,\mathrm{d}\Gamma = \int_\Omega \big[f_0 - \frac{\partial H}{\partial z_0}(\cdot,u,z)\big]\overline{z}_0 \,\mathrm{d}x \quad \forall \overline{z}_0 \in H_0^1(\Omega \cup \Gamma_N).$$

We apply [15, Theorem 1] and [14, Theorem 1] to that equation and obtain the estimates

$$\|z_0\|_{L^\infty} \le c\big(\|\frac{\partial H}{\partial z_0}(\cdot,u,z)\|_{L^\Psi} + 1\big), \quad \Psi(s) = (1+s)\ln(1+s) - s \text{ for } s \ge 0,$$

$$\|z_0\|_{W^{1,q}} \le c\big(\|\frac{\partial H}{\partial z_0}(\cdot,u,z)\|_{(W^{1,q/(q-1)})^*} + 1\big) \quad \text{for some } q > 2.$$

Using relation (4), Trudinger's imbedding result (68) and the fact that $-P_i \in \mathcal{K}_1$ and $h \in \mathcal{K}_2$ the relevant L^Ψ-norm can be estimated by

$$\|\sum_{i=1}^m \frac{\partial P_i}{\partial z_0}(z)u_i - \frac{\partial h}{\partial z_0}(\cdot,z)\|_{L^\Psi} \le c\,\Big(\sum_{i=1}^m \|u_i \ln u_i\|_{L^1} + d(\|z\|_Z) + 1\Big).$$

Again applying (68) and Sobolev's imbedding result we get

$$\|\sum_{i=1}^m \frac{\partial P_i}{\partial z_0}(z)u_i - \frac{\partial h}{\partial z_0}(\cdot,z)\|_{(W^{1,q/(q-1)})^*} \le c\Big(\sum_{i=1}^m \|u_i\|_{L^{2q/(2+q)}} + d(\|z\|_Z) + 1\Big).$$

The last claims of the lemma follow from the pointwise existence result and (12). □

Later on we will use another formulation of the generalized Poisson equation where we set $u = ap(\cdot, z)$ where $a \in \mathbf{R}^m_+$. Having in mind the identity $-\frac{\partial}{\partial z_j}\big(u_i\, P_i(z)\big) = a_i\, \frac{\partial p_i}{\partial z_j}(\cdot, z)$ we define $\widetilde{\mathcal{E}} : Z \times \mathbf{R}^m \to Z^*$ by

$$\begin{aligned}\langle \widetilde{\mathcal{E}}(z, a), \overline{z}\rangle_Z = &\int_\Omega \varepsilon \nabla z_0 \cdot \nabla \overline{z}_0 \,\mathrm{d}x + \int_{\Gamma_N} \tau z_0 \overline{z}_0 \,\mathrm{d}\Gamma \\ &+ \int_\Omega \sum_{j=0}^{k} \Big[\frac{\partial h}{\partial z_j}(\cdot, z) + \sum_{i=1}^{m} a_i \frac{\partial p_i}{\partial z_j}(\cdot, z) - f_j\Big]\, \overline{z}_j \,\mathrm{d}x, \quad \overline{z} \in Z.\end{aligned} \tag{13}$$

Lemma 4.4 *For any $a \in \mathbf{R}^m_+$ there exists a unique solution $z \in Z$ of $\widetilde{\mathcal{E}}(z, a) = 0$. Moreover, for every $R > 0$ there is a constant $c(R) > 0$ such that*

$$\|z\|_Z\,,\ \|z_0\|_{L^\infty} \le c(R) \quad \forall a \in R^m_+\,,\ \|a\|_{\mathbf{R}^m} \le R\,,\ \widetilde{\mathcal{E}}(z, a) = 0,$$

$$\|z - \overline{z}\|_Z \le c(R)\, \|a - \overline{a}\|_{\mathbf{R}^m} \quad \forall a,\, \overline{a} \in \mathbf{R}^m_+\,,\ \|a\|_{\mathbf{R}^m},\, \|\overline{a}\|_{\mathbf{R}^m} \le R\,,\ \widetilde{\mathcal{E}}(z, a) = \widetilde{\mathcal{E}}(\overline{z}, \overline{a}) = 0.$$

P r o o f. Since $h \in \mathcal{K}_{2,s}$ and $\ln p_i \in \mathcal{K}_2$ the operator $\widetilde{\mathcal{E}}(\cdot, a)$ is strongly monotone (uniformly with respect to a). Moreover, $\widetilde{\mathcal{E}}(\cdot, a)$ is hemi-continuous which is proven as in Lemma 4.1. Thus the existence and uniqueness result follows. Since $\langle \widetilde{\mathcal{E}}(z, a), z\rangle_Z = 0,\ \frac{\partial h}{\partial z_j}(\cdot, 0),\ \frac{\partial p_i}{\partial z_j}(\cdot, 0),\ f_j \in L^2(\Omega)$ the estimate

$$\begin{aligned}c\|z\|_Z^2 &\le \langle \widetilde{\mathcal{E}}(z, a) - \widetilde{\mathcal{E}}(0, a), z\rangle_Z \le \Big| \int_\Omega \sum_{j=0}^{k} \Big[\frac{\partial h}{\partial z_j}(\cdot, 0) + \sum_{i=1}^{m} a_i \frac{\partial p_i}{\partial z_j}(\cdot, 0) - f_j\Big]\, z_j \,\mathrm{d}x\Big| \\ &\le c(1 + \|a\|_{\mathbf{R}^m})\|z\|_Z\end{aligned}$$

ensures the assertion for $\|z\|_Z$. The result for the L^∞-norm of z_0 follows as in Lemma 4.3. Let $\widetilde{\mathcal{E}}(z, a) = \widetilde{\mathcal{E}}(\overline{z}, \overline{a}) = 0$. The monotonicity of $H(x, \overline{u}, \cdot)$ f.a.a. $x \in \Omega$ and the property that $|(\partial p_i/\partial z_j)(x, z)| \le c(R)$ a.e. in Ω for $\|a\|_{\mathbf{R}^m} \le R$ lead to

$$\begin{aligned}\|z - \overline{z}\|_Z^2 &\le \int_\Omega \sum_{j=0}^{k} \Big(\frac{\partial H}{\partial z_j}(\cdot, \overline{u}, \overline{z}) - \frac{\partial H}{\partial z_j}(\cdot, u, z)\Big)(z_j - \overline{z}_j) \,\mathrm{d}x \\ &\le \int_\Omega \sum_{j=0}^{k} \Big(\frac{\partial H}{\partial z_j}(\cdot, \overline{u}, z) - \frac{\partial H}{\partial z_j}(\cdot, u, z)\Big)(z_j - \overline{z}_j) \,\mathrm{d}x \\ &= \int_\Omega \sum_{j=0}^{k} \sum_{i=1}^{m} \frac{\partial p_i}{\partial z_j}(\cdot, z)(\overline{a}_i - a_i) \,\mathrm{d}x \le c(R)\|a - \overline{a}\|_{\mathbf{R}^m} \|z - \overline{z}\|_Z.\end{aligned}$$

□

4.2 The energy functional

We define the functionals $\widetilde{\mathcal{F}}_1, \widetilde{\mathcal{F}}_2 : Y_+ \to \mathbf{R}$ by

$$\widetilde{\mathcal{F}}_1(u) := \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla z_0|^2 - H(\cdot, u, z) + \sum_{j=0}^{k} \frac{\partial H}{\partial z_j}(\cdot, u, z) z_j\Big\} \,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2} z_0^2 \,\mathrm{d}\Gamma, \tag{14}$$

$$\widetilde{\mathcal{F}}_2(u) := \int_\Omega \sum_{i=1}^{m} \Big\{u_i \Big[\ln \frac{u_i}{p_{0i}} - 1\Big] + p_{0i}\Big\} \,\mathrm{d}x\,,\ u \in Y_+, \tag{15}$$

where $z \in Z$ is the solution of $\mathcal{E}(z, u) = 0$. The value $\widetilde{\mathcal{F}}_1(u) + \widetilde{\mathcal{F}}_2(u)$ can be interpreted as free energy of the state u. Because of (9) (with $\overline{z} = 0$) there exist $c,\ \widetilde{c} > 0$ such that

$$\widetilde{\mathcal{F}}_1(u) + \widetilde{\mathcal{F}}_2(u) \ge c\,\Big(\|z\|_Z^2 + \sum_{i=1}^{m} \|u_i \ln u_i\|_{L^1}\Big) - \widetilde{c}\,,\ u \in Y_+. \tag{16}$$

Let $u, \overline{u} \in Y_+$ and $\mathcal{E}(z,u) = \mathcal{E}(\overline{z},\overline{u}) = 0$. Using (9) we can estimate

$$\begin{aligned} \widetilde{\mathcal{F}}_1(u) - \widetilde{\mathcal{F}}_1(\overline{u}) &= \int_\Omega \frac{\varepsilon}{2}(|\nabla z_0|^2 - |\nabla \overline{z}_0|^2)\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2}(z_0^2 - \overline{z}_0^2)\,\mathrm{d}\Gamma \\ &\quad + \int_\Omega \Big\{ H(\cdot,\overline{u},\overline{z}) - H(\cdot,u,z) + \sum_{j=0}^{k} \Big[\frac{\partial H}{\partial z_j}(\cdot,u,z) z_j - \frac{\partial H}{\partial z_j}(\cdot,\overline{u},\overline{z})\overline{z}_j \Big] \Big\}\,\mathrm{d}x \\ &= \int_\Omega \frac{\varepsilon}{2} |\nabla(z_0 - \overline{z}_0)|^2\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2}(z_0 - \overline{z}_0)^2\,\mathrm{d}\Gamma \\ &\quad + \int_\Omega \Big\{ H(\cdot,\overline{u},\overline{z}) - H(\cdot,u,\overline{z}) \\ &\qquad + H(\cdot,u,\overline{z}) - H(\cdot,u,z) - \sum_{j=0}^{k} \frac{\partial H}{\partial z_j}(\cdot,u,z)(\overline{z}_j - z_j) \Big\}\,\mathrm{d}x \\ &\geq (P(\overline{z}), u - \overline{u})_Y + c\,\|z - \overline{z}\|_Z^2 \geq (P(\overline{z}), u - \overline{u})_Y. \end{aligned} \tag{17}$$

Thus $\widetilde{\mathcal{F}}_1$ is convex and continuous on the convex set Y_+. By setting $\widetilde{\mathcal{F}}_1(u) = +\infty$ for $u \in Y \setminus Y_+$ we extend $\widetilde{\mathcal{F}}_1$ to Y. The extended functional $\widetilde{\mathcal{F}}_1 : Y \to \overline{\mathbf{R}}$ is proper, convex, lower semi-continuous and subdifferentiable in all points $u \in Y_+$, and $P(z) \in \partial\widetilde{\mathcal{F}}_1(u)$. The properties of the integrand in $\widetilde{\mathcal{F}}_2$ ensure that the functional $\widetilde{\mathcal{F}}_2$ is convex (see [3]) and continuous on Y_+ The extended functional $\widetilde{\mathcal{F}}_2 : Y \to \overline{\mathbf{R}}$, $\widetilde{\mathcal{F}}_2(u) = +\infty$ for $u \in Y \setminus Y_+$, is proper, convex and lower semi-continuous, too. Because of the inequality $(\sqrt{x} - \sqrt{y})^2 \leq x(\ln(x/y) - 1) + y$ we obtain for $u, \overline{u} \in Y_+$ with $\overline{u} \geq \delta > 0$ the estimate

$$\begin{aligned} \widetilde{\mathcal{F}}_2(u) - \widetilde{\mathcal{F}}_2(\overline{u}) &= \int_\Omega \sum_{i=1}^{m} \Big\{ \ln \frac{\overline{u}_i}{p_{0i}}\,(u_i - \overline{u}_i) + \int_{\overline{u}_i}^{u_i} (\ln s - \ln \overline{u}_i)\,\mathrm{d}s \Big\}\,\mathrm{d}x \\ &\geq \Big(\ln \frac{\overline{u}}{p_0}\,, u - \overline{u} \Big)_Y + \|\sqrt{u} - \sqrt{\overline{u}}\|_Y^2 \geq \Big(\ln \frac{\overline{u}}{p_0}\,, u - \overline{u} \Big)_Y \,\mathrm{d}x. \end{aligned} \tag{18}$$

Thus, in $u \in Y_+$ with $u \geq \delta > 0$ the functional $\widetilde{\mathcal{F}}_2$ is subdifferentiable and $\ln \frac{u}{p_0} \in \partial\widetilde{\mathcal{F}}_2(u)$. Now we extend the functionals $\widetilde{\mathcal{F}}_i$, $i = 1, 2$, to the space X^* and define

$$\mathcal{F}_k = (\widetilde{\mathcal{F}}_k^*|_X)^* : X^* \to \overline{\mathbf{R}}\,,\ k = 1, 2, \tag{19}$$

where the star denotes the conjugation (see [3]). We can summarize the properties of the free energy functional as follows (details of the proof can be found in [8, Lemma 8.12]).

Lemma 4.5 *The functional $\mathcal{F} = \mathcal{F}_1 + \mathcal{F}_2$ is proper, convex and lower semi-continuous. For $u \in Y_+$ the equality $\mathcal{F}(u) = \widetilde{\mathcal{F}}_1(u) + \widetilde{\mathcal{F}}_2(u)$ holds where $\widetilde{\mathcal{F}}_1(u)$ and $\widetilde{\mathcal{F}}_2(u)$ are calculated according to* (14), (15)*. The restriction $\mathcal{F}|_{Y_+}$ is continuous. If $u \in Y_+$ then $P(z) \in \partial\mathcal{F}_1(u)$. If additionally $\frac{u}{p_0} \in X$ and $u \geq \delta > 0$ then*

$$\ln \frac{u}{p_0} \in \partial\mathcal{F}_2(u), \quad \zeta = P(z) + \ln \frac{u}{p_0} = \ln \frac{u}{p(\cdot, z)} \in \partial\mathcal{F}(u)$$

where z is the solution of $\mathcal{E}(z, u) = 0$.

Next we consider the conjugate functional $\mathcal{F}^* : X \to \overline{\mathbf{R}}$ of $\mathcal{F}$. In arguments ζ, where $\mathcal{F}^*$ is subdifferentiable and $u \in \partial\mathcal{F}^*(\zeta)$ (and consequently $\zeta \in \partial\mathcal{F}(u)$), we have

$$\mathcal{F}^*(\zeta) = \langle u, \zeta \rangle_X - \mathcal{F}(u), \quad \zeta \in \partial\mathcal{F}(u). \tag{20}$$

Now let $\zeta \in \mathbf{R}^m$, let $z \in (H_0^1(\Omega \cup \Gamma_N) \cap L^\infty(\Omega)) \times \mathbf{R}^k$ be the solution of $\widetilde{\mathcal{E}}(z, \mathrm{e}^\zeta) = 0$ and let $u = p(\cdot, z)\,\mathrm{e}^\zeta$. Then $u \in Y$, $u/p_0 \in X$, $u \geq \delta > 0$, $\zeta \in \partial\mathcal{F}(u)$ and $u \in \partial\mathcal{F}^*(\zeta)$. Using (20) and $\langle \widetilde{\mathcal{E}}(z, \mathrm{e}^\zeta), z\rangle_Z = 0$ we get

$$\begin{aligned}\mathcal{F}^*(\zeta) &= \langle u, \zeta\rangle_X - \mathcal{F}_2(u) + \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla z_0|^2 + H(\cdot, u, z) - \sum_{j=0}^k f_j z_j\Big\}\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2} z_0^2\,\mathrm{d}\Gamma \\ &= \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla z_0|^2 + h(\cdot, z) + \sum_{i=1}^m p_{0i}\big[\mathrm{e}^{\zeta_i - P_i(z)} - 1\big] - \sum_{j=0}^k f_j z_j\Big\}\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2} z_0^2\,\mathrm{d}\Gamma\,,\ \zeta \in \mathbf{R}^m.\end{aligned}$$

In the last step we used the relation $u_i\zeta_i - u_i \ln\frac{u_i}{p_{0i}} + u_i - p_{0i} - u_i\,P_i(z) = u_i - p_{0i} = p_{0i}[\mathrm{e}^{\zeta_i - P_i(z)} - 1]$. We define the restriction of $\mathcal{F}^*$ to $\mathbf{R}^m$,

$$\mathcal{G} = \mathcal{F}^*|_{\mathbf{R}^m} : \mathbf{R}^m \to \mathbf{R}. \tag{21}$$

Because of (6) and (8) we establish for $\mathcal{G}(\zeta)$ the estimate

$$\mathcal{G}(\zeta) \geq c\Big\{\|z\|_Z^2 + \|[\zeta - P(z)]^+\|_Y^2\Big\} - \widetilde{c},\ \zeta \in \mathbf{R}^m\,,\ c, \widetilde{c} > 0. \tag{22}$$

Applying the identity

$$\begin{aligned}&p_i(\cdot, \overline{z})\,\mathrm{e}^{\overline{\zeta}_i}[\ln p_i(\cdot, z) - \ln p_i(\cdot, \overline{z})] + p_{0i}[\mathrm{e}^{\zeta_i - P_i(z)} - \mathrm{e}^{\overline{\zeta}_i - P_i(\overline{z})}] \\ =&p_i(\cdot, \overline{z})\,\mathrm{e}^{\overline{\zeta}_i}(\zeta_i - \overline{\zeta}_i) + p_{0i}\big[\mathrm{e}^{\zeta_i - P_i(z)} - \mathrm{e}^{\overline{\zeta}_i - P_i(\overline{z})} - \mathrm{e}^{\overline{\zeta}_i - P_i(\overline{z})}[\zeta_i - P_i(z) - \overline{\zeta}_i + P_i(\overline{z})]\big]\end{aligned}$$

and $\langle \mathcal{E}(\overline{z}, p(\cdot, \overline{z})\mathrm{e}^{\overline{\zeta}}), z - \overline{z}\rangle_Z = 0$ we obtain for $\zeta, \overline{\zeta} \in \mathbf{R}^m$ and the corresponding z, $\overline{z}$, that

$$\mathcal{G}(\zeta) - \mathcal{G}(\overline{\zeta}) = \int_\Omega \sum_{i=1}^m p_i(\cdot, \overline{z}))\,\mathrm{e}^{\overline{\zeta}_i}(\zeta_i - \overline{\zeta}_i)\,\mathrm{d}x + \omega(\zeta, \overline{\zeta}), \tag{23}$$

$$\begin{aligned}\omega(\zeta, \overline{\zeta}) = &\int_\Omega \frac{\varepsilon}{2}|\nabla(z_0 - \overline{z}_0)|^2\,\mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2}(z_0 - \overline{z}_0)^2\,\mathrm{d}\Gamma \\ &+ \int_\Omega \Big\{H(\cdot, p(\cdot, \overline{z})\mathrm{e}^{\overline{\zeta}}, z) - H(\cdot, p(\cdot, \overline{z})\mathrm{e}^{\overline{\zeta}}, \overline{z}) - \sum_{j=0}^k \frac{\partial H}{\partial z_j}(\cdot, p(\cdot, \overline{z})\mathrm{e}^{\overline{\zeta}}, \overline{z})(z_j - \overline{z}_j) \\ &\quad + \sum_{i=1}^m p_{0i}\big(\mathrm{e}^{\zeta_i - P_i(z)} - \mathrm{e}^{\overline{\zeta}_i - P_i(\overline{z})} - \mathrm{e}^{\overline{\zeta}_i - P_i(\overline{z})}(\zeta_i - P_i(z) - \overline{\zeta}_i + P_i(\overline{z}))\big)\Big\}\mathrm{d}x.\end{aligned}$$

The convexity of $H(x, u, \cdot)$ and of the e-function ensure that $\omega(\zeta, \overline{\zeta}) \geq 0$ for all ζ, $\overline{\zeta} \in \mathbf{R}^m$. Lemma 4.4, the strong convexity of the e-function on compact intervals and estimate (9) lead to the stronger result that for all $R > 0$ there is a constant $c_1(R) > 0$ such that we have for all $\zeta, \overline{\zeta} \in \mathbf{R}^m$ with $\|\zeta\|_{\mathbf{R}^m}, \|\overline{\zeta}\|_{\mathbf{R}^m} \leq R$

$$\omega(\zeta, \overline{\zeta}) \geq c_1(R)\big\{\|z - \overline{z}\|_Z^2 + \|\zeta - \overline{\zeta} - (P(z) - P(\overline{z}))\|_{L^2}^2\big\}. \tag{24}$$

Moreover, because of the local Lipschitz continuity of $\partial_z(\ln p_i)$, $\partial_z h$ and of the e-function and because of Lemma 4.4 for all $R > 0$ there is a constant $c_2(R) > 0$ such that

$$\omega(\zeta, \overline{\zeta}) \leq c_2(R)\,\|\zeta - \overline{\zeta}\|_{\mathbf{R}^m}^2 \quad \forall \zeta, \overline{\zeta} \in \mathbf{R}^m \text{ with } \|\zeta\|_{\mathbf{R}^m}, \|\overline{\zeta}\|_{\mathbf{R}^m} \leq R. \tag{25}$$

The previous estimates ensure the following properties of the function $\mathcal{G}$.

Lemma 4.6 *The function $\mathcal{G} = \mathcal{F}^*|_{\mathbf{R}^m} : \mathbf{R}^m \to \mathbf{R}$ is strictly convex, continuous and Fréchet differentiable,*

$$\partial\mathcal{G}(\zeta) = \int_\Omega \mathrm{e}^\zeta\,p(\cdot, z)\,\mathrm{d}x, \quad \zeta \in \mathbf{R}^m, \quad \widetilde{\mathcal{E}}(z, \mathrm{e}^\zeta) = 0.$$

Next, we introduce the dissipation functional for problem ($\mathcal{P}$) or more precisely a lower estimate of the dissipation functional. We define the set

$$M_{\mathcal{D}} = \Big\{u \in L^\infty_+(\Omega, \mathbf{R}^m) : \sqrt{a} \in X, \text{ where } a = u/p(\cdot, z) \text{ and } \mathcal{E}(z, u) = 0\Big\} \tag{26}$$

and the functional $\mathcal{D} : M_{\mathcal{D}} \to \mathbf{R}$ by

$$\mathcal{D}(u) = 4 \int_\Omega \Big\{ \sum_{i=1}^{l} D_i(\cdot, b, z) p_i(\cdot, z) |\nabla \sqrt{a_i}|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\cdot, b, z) |\sqrt{a}^{\,\alpha} - \sqrt{a}^{\,\beta}|^2 \Big\} \,\mathrm{d}x, \tag{27}$$

$u \in M_{\mathcal{D}}$, where $b = u/p_0$, $a = u/p(\cdot, z)$ and $z \in (H^1(\Omega) \cap L^\infty(\Omega)) \times \mathbf{R}^k$ is the solution of $\mathcal{E}(z, u) = 0$.

Remark 4.7 i) We have $\mathcal{D}(u) \geq 0$ for all $u \in M_{\mathcal{D}}$.
ii) Let $u \in M_{\mathcal{D}}$ with $\mathcal{D}(u) = 0$ and let z be the solution of $\mathcal{E}(z, u) = 0$. Then according to the assumptions in (I) iv), v) and vi) the corresponding quantities $a = u/p(\cdot, z)$ fulfil $a \in \mathbf{R}^m_+$ and $a^\alpha = a^\beta$ for all $(\alpha, \beta) \in \mathcal{R}$.

4.3 Monotonicity and boundedness of the free energy

Theorem 4.8 *Let (u, b, z) be a solution of ($\mathcal{P}$), and set $a = u/p(\cdot, z)$. Then $\sqrt{a} \in L^2_{\text{loc}}(\mathbf{R}_+, X)$, $u(t) \in M_{\mathcal{D}}$* f.a.a. $t > 0$, *and for every $\lambda \in \mathbf{R}_+$ the following estimate holds*

$$\mathrm{e}^{\lambda t_2} \mathcal{F}(u(t_2)) - \mathrm{e}^{\lambda t_1} \mathcal{F}(u(t_1)) \leq \int_{t_1}^{t_2} \mathrm{e}^{\lambda t} \big\{ \lambda \mathcal{F}(u(t)) - \mathcal{D}(u(t)) \big\} \,\mathrm{d}t, \quad 0 \leq t_1 \leq t_2.$$

Proof. 1. The proof is based on ideas of the proof of [16, Theorem 1]. Let (u, b, z) be a solution of ($\mathcal{P}$), $\lambda \in \mathbf{R}_+$, $S = [t_1, t_2]$. Then $u \geq 0$, $u \in H^1(S, X^*)$, $z \in L^2(S, Z)$, $P(z) \in L^2(S, X)$ and $\nabla P(z) = Q(z) \nabla z_0$ (see Lemma 9.1). Moreover, let $u^\delta = u + \delta p_0$ and $b^\delta = b + \delta$ for $\delta > 0$. Then $u^\delta \in H^1(S, X^*)$, b^δ, $\ln b^\delta \in L^2(S, X)$ and $\nabla \ln(u^\delta_i / p_{0i}) = \nabla b_i / (b_i + \delta)$, $i = 1, \ldots, l$. Lemma 4.5 guarantees that

$$P(z(t)) \in \partial \mathcal{F}_1(u(t)), \quad \ln(u^\delta(t)/p_0) \in \partial \mathcal{F}_2(u^\delta(t)) \text{ f.a.a. } t \in S.$$

According to Lemma 9.2 the functions $t \mapsto \mathcal{F}_1(u(t))$ and $t \mapsto \mathcal{F}_2(u^\delta(t))$ are absolutely continuous on S, and

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}_1(u(t)) = \langle u'(t), P(z(t)) \rangle_X, \quad \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}_2(u^\delta(t)) = \Big\langle u'(t), \ln \frac{u^\delta(t)}{p_0} \Big\rangle_X \text{ f.a.a. } t \in S. \tag{28}$$

2. We set $\zeta^\delta = \ln(u^\delta / p(\cdot, z)) \in L^2(S, X)$ and $a^\delta = u^\delta / p(\cdot, z) = e^{\zeta^\delta}$. From (28) we derive the relation

$$\mathrm{e}^{\lambda t} \big[\mathcal{F}_1(u(t)) + \mathcal{F}_2(u^\delta(t)) \big] \Big|_{t_1}^{t_2} = \int_{t_1}^{t_2} \mathrm{e}^{\lambda t} \Big\{ \lambda \big[\mathcal{F}_1(u(t)) + \mathcal{F}_2(u^\delta(t)) \big] + \langle u'(t), \zeta^\delta(t) \rangle_X \Big\} \,\mathrm{d}t.$$

Using the evolution equation we find f.a.a. $t \in S$

$$\begin{aligned} \langle u'(t), \zeta^\delta(t) \rangle_X &= -\langle \mathcal{A}(b(t), z(t)) - \mathcal{R}(b(t), z(t)), \zeta^\delta(t) \rangle_X \\ &= -\langle \widehat{\mathcal{A}}(b(t), b^\delta(t), z(t)) - \widehat{\mathcal{R}}(b(t), b^\delta(t), z(t)), \zeta^\delta(t) \rangle_X + \theta^\delta(t) \end{aligned}$$

where $\widehat{\mathcal{R}}$, $\widehat{\mathcal{A}}$: $(X_+ \times X_+ \times Z) \cap L^\infty(\Omega, \mathbf{R}^{2m+k+1}) \to X^*$,

$$\begin{aligned} \langle \widehat{\mathcal{R}}(b, b^\delta, z), \bar{b} \rangle_X &:= \int_\Omega \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\cdot, b, z) \big((a^\delta)^\alpha - (a^\delta)^\beta \big) (\beta - \alpha) \cdot \bar{b} \,\mathrm{d}x, \quad \bar{b} \in X, \\ \langle \widehat{\mathcal{A}}(b, b^\delta, z), \bar{b} \rangle_X &:= \int_\Omega \sum_{i=1}^{l} D_i(\cdot, b, z) p_{0i} \big[\nabla b^\delta_i + b^\delta_i Q_i(z) \nabla z_0 \big] \cdot \nabla \bar{b}_i \,\mathrm{d}x, \quad \bar{b} \in X, \\ \theta^\delta &= \langle \widehat{\mathcal{A}}(b, b^\delta, z) - \widehat{\mathcal{A}}(b, b, z) - \widehat{\mathcal{R}}(b, b^\delta, z) + \widehat{\mathcal{R}}(b, b, z), \zeta^\delta \rangle_X. \end{aligned} \tag{29}$$

We have $\sqrt{a^\delta} \in L^2(S,X)$ and $\nabla\sqrt{a_i^\delta} = \frac{1}{2}\sqrt{a_i^\delta}\,\nabla\zeta_i^\delta$, $i = 1,\dots,l$. Because of the relations

$$p_{0i}\left[\nabla b_i^\delta + b_i^\delta Q_i(z)\nabla z_0\right]\cdot\nabla\zeta_i^\delta = p_i(\cdot,z)a_i^\delta|\nabla\zeta_i^\delta|^2 = 4p_i(\cdot,z)|\nabla\sqrt{a_i^\delta}|^2,$$
$$\left(\mathrm{e}^{\alpha\cdot\zeta^\delta} - \mathrm{e}^{\beta\cdot\zeta^\delta}\right)(\alpha-\beta)\cdot\zeta^\delta \geq 4|\sqrt{a^\delta}^{\,\alpha} - \sqrt{a^\delta}^{\,\beta}|^2, \quad (\alpha,\beta)\in\mathcal{R},$$

we obtain

$$\begin{aligned}
&4\int_{t_1}^{t_2}\int_\Omega \mathrm{e}^{\lambda t}\Big\{\sum_{i=1}^{l} D_i(\cdot,b,z)p_i(\cdot,z)|\nabla\sqrt{a_i^\delta}|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\cdot,b,z)|\sqrt{a^\delta}^{\,\alpha} - \sqrt{a^\delta}^{\,\beta}|^2\Big\}\,\mathrm{d}x\,\mathrm{d}t\\
&\leq \int_{t_1}^{t_2}\mathrm{e}^{\lambda t}\,\langle\widehat{\mathcal{A}}(b(t),b^\delta(t),z(t)) - \widehat{\mathcal{R}}(b(t),b^\delta(t),z(t)),\zeta^\delta(t)\rangle_X\,\mathrm{d}t = \Theta^\delta, \qquad (30)\\
&\Theta^\delta = \int_{t_1}^{t_2}\mathrm{e}^{\lambda t}\Big\{\lambda\big[\mathcal{F}_1(u(t)) + \mathcal{F}_2(u^\delta(t))\big] + \theta^\delta(t)\Big\}\,\mathrm{d}t - \mathrm{e}^{\lambda t}\big[\mathcal{F}_1(u(t)) + \mathcal{F}_2(u^\delta(t))\big]\,\Big|_{t_1}^{t_2}.
\end{aligned}$$

3. Now, let $\delta\to 0$. Since $\theta^\delta(t)\to 0$ f.a.a. $t\in S$ and because of the continuity of $\mathcal{F}_2|_{L^2_+(\Omega,\mathbf{R}^m)}$ we obtain

$$\Theta^\delta \to \Theta = \int_{t_1}^{t_2}\mathrm{e}^{\lambda t}\lambda\,\mathcal{F}(u(t))\,\mathrm{d}t - \mathrm{e}^{\lambda t}\,\mathcal{F}(u(t))\,\Big|_{t_1}^{t_2}.$$

Lebesgue's theorem ensures $\sqrt{a^\delta}\to\sqrt{a}$ in $L^2(S,Y)$, and therefore (at least for a subsequence) $\sqrt{a^\delta}\to\sqrt{a}$ a.e. on $S\times\Omega$. For $(\alpha,\beta)\in\mathcal{R}$ Fatou's lemma guarantees

$$\int_{t_1}^{t_2}\int_\Omega \mathrm{e}^{\lambda t}k_{\alpha\beta}(\cdot,b,z)|\sqrt{a}^{\,\alpha} - \sqrt{a}^{\,\beta}|^2\mathrm{d}x\,\mathrm{d}t \leq \liminf_{\delta\to 0}\int_{t_1}^{t_2}\int_\Omega \mathrm{e}^{\lambda t}k_{\alpha\beta}(\cdot,b,z)|\sqrt{a^\delta}^{\,\alpha} - \sqrt{a^\delta}^{\,\beta}|^2\mathrm{d}x\,\mathrm{d}t.$$

Let $i\in\{1,\dots,l\}$. Since $z\in L^\infty(S,L^\infty\times\mathbf{R}^k)$ and the sequence Θ^δ is bounded, (30) gives a constant $c>0$ such that $\|\nabla\sqrt{a_i^\delta}\|_{L^2(S,L^2)}\leq c$. Thus [19, Proposition 2.4] supplies

$$\nabla\sqrt{a_i}\in L^2(S,L^2), \quad \nabla\sqrt{a_i^\delta}\rightharpoonup\nabla\sqrt{a_i} \text{ in } L^2(S,L^2), \quad i=1,\dots,l.$$

The weak lower semi-continuity of continuous quadratic functionals leads to

$$\int_{t_1}^{t_2}\int_\Omega e^{\lambda t}D_i(\cdot,b,z)p_i(\cdot,z)|\nabla\sqrt{a_i}|^2\,\mathrm{d}x\,\mathrm{d}t \quad \leq \liminf_{\delta\to 0}\int_{t_1}^{t_2}\int_\Omega e^{\lambda t}D_i(\cdot,b,z)p_i(\cdot,z)|\nabla\sqrt{a_i^\delta}|^2\,\mathrm{d}x\,\mathrm{d}t.$$

Therefore $\sqrt{a}\in L^2(S,X)$, and in summary we obtain $\int_{t_1}^{t_2}e^{\lambda t}\mathcal{D}(u(t))\,\mathrm{d}t\leq\Theta$. □

Theorem 4.9 *Along any solution (u,b,z) of $(\mathcal{P})$ the free energy $\mathcal{F}(u)$ remains bounded by its initial value $\mathcal{F}(U)$ and it decays monotonously,*

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

Moreover, there is a constant $c>0$, depending only on the data such that

$$\|u_i\ln u_i\|_{L^\infty(\mathbf{R}_+,L^1(\Omega))}\leq c, \quad i=1,\dots,m, \quad \|u\|_{L^\infty(\mathbf{R}_+,L^1(\Omega,\mathbf{R}^m))}\leq c,$$
$$\|b\|_{L^\infty(\mathbf{R}_+,L^1(\Omega,\mathbf{R}^m))}\leq c, \quad \|z\|_{L^\infty(\mathbf{R}_+,Z)}\leq c, \quad \|z_0\|_{L^\infty(\mathbf{R}_+,L^\infty(\Omega))}\leq c$$

for any solution (u,b,z) of $(\mathcal{P})$.

P r o o f. The first assertions of the theorem are obtained by setting $\lambda=0$ in Theorem 4.8. The estimates of the norms are derived from (16) and Lemma 4.3. □

Remark 4.10 The last estimates from Theorem 4.9 together with the assumptions formulated in (I) iii)–vi) guarantee the existence of constants $c_a,\ c_b,\ \epsilon,\ \widetilde{\epsilon} > 0$ such that

$$\begin{aligned}
&c_a \le p_i(\cdot, z) \le c_b, \text{ a.e. in } \mathbf{R}_+ \times \Omega\,,\ i = 1, \dots, m,\\
&k_{\alpha\beta}(\cdot, b, z) \le c_b \text{ a.e. in } \mathbf{R}_+ \times \Omega\,,\ (\alpha, \beta) \in \mathcal{R},\\
&D_i(\cdot, b, z) \le c_b \text{ a.e. in } \mathbf{R}_+ \times \Omega, \quad i = 1, \dots, l,\\
&D_i(\cdot, b, z) p_{0i} \ge \epsilon \text{ a.e. in } \mathbf{R}_+ \times \Omega, \quad i = 1, \dots, l,\\
&2k_{\alpha_{(j)}\beta_{(j)}}(\cdot, b, z)\mathrm{e}^{2P_j(z)} \ge \widetilde{\epsilon} \text{ a.e. in } \mathbf{R}_+ \times \Omega, \quad j = l+1, \dots, m,
\end{aligned}$$

for any solution (u, b, z) of $(\mathcal{P})$.

4.4 Invariants and steady states

Let $\mathcal{S}$ denote the stoichiometric subspace belonging to the system of reactions in (2),

$$\mathcal{S} = \text{span}\{\alpha - \beta :\ (\alpha, \beta) \in \mathcal{R}\} \subset \mathbf{R}^m.$$

Integration of the continuity equations over $(0, t) \times \Omega$ leads to the following invariance property.

Lemma 4.11 *If (u, b, z) is a solution of $(\mathcal{P})$ then* $\displaystyle\int_\Omega \big\{u(t) - U\big\}\,\mathrm{d}x \in \mathcal{S} \quad \forall t \in \mathbf{R}_+.$

Therefore we are looking for steady states fulfilling such an invariance property, too. They are solutions of

$$\left.\begin{aligned}
\mathcal{A}(b, z) = \mathcal{R}(b, z), \quad \mathcal{E}(z, u) = 0, \quad u = \mathcal{B}b, \quad \int_\Omega \big\{u - U\big\}\,\mathrm{d}x \in \mathcal{S},\\
u \in Y, \quad b \in X \cap L^\infty_+(\Omega, \mathbf{R}^m), \quad z \in Z \cap (L^\infty(\Omega) \times \mathbf{R}^k).
\end{aligned}\right\} \qquad (\mathcal{SP})$$

Lemma 4.12 *If (u, b, z) is a solution of $(\mathcal{SP})$ then u belongs to $M_{\mathcal{D}}$ and $\mathcal{D}(u) = 0$.*

P r o o f. The proof uses ideas of the proof of Theorem 4.8. Let (u, b, z) be a solution of $(\mathcal{SP})$. For $\delta > 0$ we define $a = u/p(\cdot, z)$, $u^\delta = u + \delta p_0$, $b^\delta = b + \delta$, $a^\delta = u^\delta/p(\cdot, z)$ and $\zeta^\delta = \ln a^\delta$. Then $\zeta^\delta,\ \sqrt{a^\delta} \in X$ and for the operators $\widehat{\mathcal{A}}$, $\widehat{\mathcal{R}}$ defined in (29) we obtain $\langle \widehat{\mathcal{A}}(b, b^\delta, z) - \widehat{\mathcal{R}}(b, b^\delta, z), \zeta^\delta\rangle_X \to 0$ for $\delta \to 0$. Moreover, we get $\sqrt{a^\delta} \to \sqrt{a}$ in Y, and the estimate

$$\begin{aligned}
&4\int_\Omega \Big\{ \sum_{i=1}^{l} D_i(\cdot, b, z) p_i(\cdot, z) |\nabla \sqrt{a_i^\delta}|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}} k_{\alpha\beta}(\cdot, b, z) |\sqrt{a^\delta}^{\,\alpha} - \sqrt{a^\delta}^{\,\beta}|^2 \Big\}\,\mathrm{d}x\\
&\le \langle \widehat{\mathcal{A}}(b, b^\delta, z) - \widehat{\mathcal{R}}(b, b^\delta, z), \zeta^\delta\rangle_X
\end{aligned}$$

ensures that $\nabla\sqrt{a_i^\delta} \rightharpoonup \nabla\sqrt{a_i}$ in $L^2(\Omega)$, $i = 1, \dots, l$. Therefore $\sqrt{a} \in X$, $u \in M_{\mathcal{D}}$ and

$$0 \le \mathcal{D}(u) \le \liminf_{\delta\to 0} \langle \widehat{\mathcal{A}}(b, b^\delta, z) - \widehat{\mathcal{R}}(b, b^\delta, z), \zeta^\delta\rangle_X = 0. \qquad \square$$

Let

$$\begin{aligned}
\mathcal{N} \;=\; &\Big\{ a \in \mathbf{R}^m_+ :\ a^\alpha = a^\beta\ \forall (\alpha, \beta) \in \mathcal{R}\,,\ \int_\Omega \big\{u - U\big\}\,\mathrm{d}x \in \mathcal{S}\\
&\qquad \text{where } u = ap(\cdot, z) \text{ and } z \text{ is the solution of } \widetilde{\mathcal{E}}(z, a) = 0, \text{ see (13)}\Big\}.
\end{aligned}$$

Lemma 4.13 *If (u, b, z) is a solution of $(\mathcal{SP})$ then $a = u/p(\cdot, z)$ belongs to $\mathcal{N}$. Vice versa, if $a \in \mathcal{N}$ and $u,\ z,$ $b = \mathcal{B}^{-1}u$ are chosen as in the definition of $\mathcal{N}$ then (u, b, z) is a solution of $(\mathcal{SP})$.*

P r o o f. The first assertion follows from Lemma 4.12 and Remark 4.7. Because of Lemma 4.4, for $a \in \mathcal{N}$ we have $z \in Z \cap (L^\infty(\Omega) \times \mathbf{R}^k)$. Moreover, $b = a\mathrm{e}^{-P(z)} \in X \cap L^\infty(\Omega, \mathbf{R}^m)$, $u = ap(\cdot, z) \ge 0$, $\nabla b_i = -b_i \frac{\partial P_i}{\partial z_0}(z)\nabla z_0 = -b_i Q_i(z) \nabla z_0$, $i = 1, \dots, l$. Thus we get $\mathcal{A}(b, z) = \mathcal{R}(b, z) = 0$, $\mathcal{E}(z, u) = \widetilde{\mathcal{E}}(z, a) = 0$. $\square$

The investigation of solutions of $(\mathcal{SP})$ can be reduced to the discussion of a minimum problem for a functional $\mathcal{G}_0 : \mathbf{R}^m \to \overline{\mathbf{R}}$ defined by

$$\mathcal{G}_0(\zeta) = \mathcal{G}(\zeta) + I_{\mathcal{S}^\perp}(\zeta) - \int_\Omega U \cdot \zeta \,\mathrm{d}x, \quad \zeta \in \mathbf{R}^m,$$

where $\mathcal{G}$ is given in (21). Based on properties of $\mathcal{G}$ the function $\mathcal{G}_0$ is proper, convex and lower semi-continuous. Note that $\operatorname{dom}\mathcal{G}_0 = \mathcal{S}^\perp$. According to Lemma 4.6 the function $\mathcal{G}$ is continuous. Thus the Moreau-Rockafellar theorem (see [3]) ensures

$$\partial\mathcal{G}_0(\zeta) = \partial\mathcal{G}(\zeta) + \partial I_{\mathcal{S}^\perp}(\zeta) - \int_\Omega U \,\mathrm{d}x\,,\ \zeta \in \mathbf{R}^m. \tag{31}$$

Following the arguments in the proofs of [16, Lemma 9, 10] and using the estimate (22) we obtain the following assertions (for the complete proofs see [8, Lemma 8.21, 8.22]).

Lemma 4.14 1.) *If $a \in \mathcal{N} \cap \operatorname{int}\mathbf{R}^m_+$, then $\zeta = \ln a$ is a minimizer of $\mathcal{G}_0$. Vice versa, if $\zeta \in \mathbf{R}^m$ is a minimizer of $\mathcal{G}_0$ then $a = \mathrm{e}^\zeta \in \mathcal{N} \cap \operatorname{int}\mathbf{R}^m_+$.*

2.) *$\mathcal{N} \cap \operatorname{int}\mathbf{R}^m_+$ consists of at most one element; $\mathcal{N} \cap \operatorname{int}\mathbf{R}^m_+ \neq \emptyset$ if and only if*

$$\int_\Omega U \cdot \overline{\zeta}\,\mathrm{d}x > 0 \quad \forall \overline{\zeta} \in \mathcal{S}^\perp\,,\ \overline{\zeta} \geq 0\,,\ \overline{\zeta} \neq 0. \tag{II}$$

In summary we get the following results concerning the solutions of $(\mathcal{SP})$.

Theorem 4.15 *We assume* (I) *and* (II). *Then there exists a solution (u^*, b^*, z^*) of $(\mathcal{SP})$. It has the properties $a^* = u^*/p(\cdot, z^*) \in \mathbf{R}^m$, $a^* > 0$ and $\zeta^* = \ln a^* \in \mathcal{S}^\perp$. Moreover, there is a constant $c > 0$ such that $u^* \geq c$ a.e. on Ω. If additionally*

$$\mathcal{N} \cap \partial\mathbf{R}^m_+ = \emptyset \tag{III}$$

is fulfilled, then there is no other solution of $(\mathcal{SP})$.

4.5 Exponential decay of the free energy

Theorem 4.16 *We assume* (I) – (III). *Then, for every $R > 0$ there is a constant $c_R > 0$ such that*

$$\mathcal{F}(u) - \mathcal{F}(u^*) \leq c_R\,\mathcal{D}(u) \quad \forall u \in M_R = \Big\{u \in M_\mathcal{D} \colon \mathcal{F}(u) - \mathcal{F}(u^*) \leq R,\ \int_\Omega (u - U)\mathrm{d}x \in \mathcal{S}\Big\}.$$

P r o o f. 1. For $u \in M_R$ let z, a be defined via $\mathcal{E}(z, u) = 0$, $a = u/p(\cdot, z)$. According to Lemma 4.3 there is a $c(R) > 0$ such that $\|z\|_Z$, $\|z_0\|_{L^\infty} \leq c(R)$ for all $u \in M_R$. Since

$$\sqrt{a_i/a_{i^*}} - 1 = \sqrt{p_i(\cdot, z^*)/p_i(\cdot, z)}(\sqrt{u_i/u_{i^*}} - 1) + \sqrt{p_i(\cdot, z^*)/p_i(\cdot, z)} - 1$$

we find for $u \in M_R$ that

$$\|\sqrt{a/a^*} - 1\|_Y \leq c(R)\big(\|\sqrt{u/u^*} - 1\|_Y + \|z_0 - z_0^*\|_{L^2} + \sum_{j=1}^k |z_j - z_j^*|\big).$$

Setting $\widetilde{F}(u) = \mathcal{F}(u) - \mathcal{F}(u^*)$ and using the properties $\zeta^* = \ln a^* \in \mathcal{S}^\perp$ (cf.Theorem 4.15), $\int_\Omega (u - u^*)\,\mathrm{d}x \in \mathcal{S}$ (cf. Lemma 4.11), (17), (18) (used for $\overline{u} = u^*$), Lemma 4.3 and the inequality $x(\ln(x/y) - 1) + y \leq 1/y\,(x - y)^2$, we obtain for all $u \in M_R$ the estimates

$$\big\{\|\sqrt{u/u^*} - 1\|_Y^2 + \|z - z^*\|_Z^2\big\} \leq c\,\widetilde{F}(u), \tag{32}$$

$$c_1(R)\big\{\|\sqrt{a/a^*} - 1\|_Y^2 + \|z - z^*\|_Z^2\big\} \leq \widetilde{F}(u), \tag{33}$$

$$\widetilde{F}(u) \le c_2(R)\,\|u-u^*\|_Y^2, \tag{34}$$

$$\mathcal{D}(u) \ge c_3(R)\widetilde{D}(a),$$

$$\widetilde{D}(a) = \int_\Omega \Big\{ \sum_{i=1}^{l} \big|\nabla\sqrt{a_i/a_i^*}\big|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}} b_{\alpha\beta,c(R)} \big|\sqrt{a/a^*}^{\,\alpha} - \sqrt{a/a^*}^{\,\beta}\big|^2 \Big\}\,\mathrm{d}x$$

with positive constants $c_k(R)$. Next, we show: For every $R>0$ there is a $\widetilde{c}_R>0$ such that

$$\widetilde{F}(u) < \widetilde{c}_R\,\widetilde{D}(a) \quad \forall u\in M_R\setminus\{u^*\} \text{ (with } a \text{ corresponding to } u).$$

2. Suppose that assertion to be false. Then there would be an $R>0$ and sequences $\{c_n\}$ in $\mathbf{R}$, $\{u_n\}$ with $u_n \in M_R$ and corresponding a_n, z_n (determined by $\mathcal{E}(z_n,u_n)=0$, $a_n = u_n/p(\cdot,z_n)$) such that $c_n \to +\infty$ and

$$0 < c_n\,\widetilde{D}(a_n) \le \widetilde{F}(u_n) \le R. \tag{35}$$

Estimates (33) and (35) imply that $\|z_n\|_Z,\ \|\sqrt{a_n}\|_{L^2(\Omega,\mathbf{R}^m)} \le c(R)$ and $\widetilde{D}(a_n)\to 0$. Thus there is a $\widehat{z}\in Z$, such that (for subsequences) $z_{0n} \rightharpoonup \widehat{z}_0$ in H^1, $z_{0n}\to\widehat{z}_0$ in L^2, $z_{nj}\to\widehat{z}_j$ in $\mathbf{R}$, $j=1,\dots,k$. For $i=1,\dots,l$ there is a $\widehat{a}_i\in\mathbf{R}_+$ with $\sqrt{a_{ni}}\to\sqrt{\widehat{a}_i}$ in H^1 and L^p, $p<\infty$. For $i=l+1,\dots,m$ thanks to assumption (I) vi) there is a special reaction which ensures

$$\int_\Omega \Big| \prod_{j=1}^{l} \sqrt{a_{nj}/a_j^*}^{\,\alpha_{(i)\,j}} - a_{ni}/a_i^*\Big|^2\,\mathrm{d}x \to 0,$$

and we find at least $a_{ni} \to \widehat{a}_i \in \mathbf{R}_+$ in L^2. Fatou's lemma guarantees that $\widehat{a}^{\,\alpha} = \widehat{a}^{\,\beta}$ for all $(\alpha,\beta)\in\mathcal{R}$. Setting $\widehat{u}=\widehat{a}p(\cdot,\widehat{z})$ we obtain $u_n\to\widehat{u}$ in Y. $\int_\Omega (u_n-U)\,\mathrm{d}x\in\mathcal{S}$ leads to $\int(\widehat{u}-U)\,\mathrm{d}x\in\mathcal{S}$. The estimate $\|z_{n+k}-z_n\|_Z \le c\|u_{n+k}-u_n\|_Y$ (see Lemma 4.3) guarantees $z_n\to\widehat{z}$ in Z. Lemma 4.1 ensures that $\mathcal{E}(z_n,\widehat{u}) \rightharpoonup \mathcal{E}(\widehat{z},\widehat{u})$ in Z^*. Moreover, from $\mathcal{E}(z_n,u_n)=0$ and Lemma 4.2 we conclude that $\mathcal{E}(z_n,\widehat{u})\to 0$ in Z^*. Thus $\mathcal{E}(\widehat{z},\widehat{u}) = \widetilde{\mathcal{E}}(\widehat{z},\widehat{a}) = 0$ and we have verified that $\widehat{a}\in\mathcal{N}$. Assumption (III) supplies that $\widehat{a}=a^*$, $\widehat{u}=u^*$ and $z=z^*$. Since $u_u\to u^*$ in Y the inequality (34) leads to $\widetilde{F}(u_n)\to 0$.

3. We define

$$w_n = \sqrt{a_n/a^*}-1\,,\ \lambda_n = \sqrt{\widetilde{F}(u_n)}\,,\ v_n = \frac{w_n}{\lambda_n}\,,\ y_n = \frac{u_n-u^*}{\lambda_n}\,,\ \mu_n = \frac{z_n-z^*}{\lambda_n}.$$

In the formula for the dissipation rate

$$\widetilde{D}(a_n) = \int_\Omega \Big\{ \sum_{i=1}^{l} |\nabla w_{ni}|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}} b_{\alpha\beta,c(R)} \Big| \prod_{i=1}^{m}(1+w_{ni})^{\alpha_i} - \prod_{i=1}^{m}(1+w_{ni})^{\beta_i}\Big|^2 \Big\}\,\mathrm{d}x$$

we use the binomial expansion

$$\prod_{i=1}^{m}(1+w_{ni})^{\alpha_i} = 1 + \sum_{i=1}^{m}\alpha_i w_{ni} + \omega(w_n), \quad \frac{1}{\lambda_n}\,|\omega(w_n)| \le c\sum_{i=1}^{m}\big\{\lambda_n|v_{ni}|^2 + \lambda_n^{p_\alpha-1}|v_{ni}|^{p_\alpha}\big\}$$

where $p_\alpha = \max\{2,\sum_{i=1}^m \alpha_i\}$. The inequalities (33) and (35) ensure that $\|\mu_n\|_Z\,,\ \|v_n\|_{L^2(\Omega,\mathbf{R}^m)} \le c(R)$ and $\widetilde{D}(a_n)/\lambda_n^2 \to 0$. Therefore there is $\widehat{\mu}\in Z$ with $\mu_{n0}\rightharpoonup\widehat{\mu}_0$ in H^1, $\mu_{n0}\to\widehat{\mu}_0$ in L^2 and $\mu_{nj}\to\widehat{\mu}_j$ in $\mathbf{R}$, $j=1,\dots,k$. Moreover, for $i=1,\dots,l$ there are $\widehat{v}_i\in\mathbf{R}_+$ with $v_{ni}\to\widehat{v}_i$ in H^1 and in each L^p, and additionally $\lambda_n\|v_{ni}^2\|_{L^2}\to 0$. Based on assumption (I) vi), for $i=l+1,\dots,m$ the convergence

$$\int_\Omega \Big| \frac{1}{\lambda_n}\Big\{\prod_{j=1}^{l}(1+w_{nj})^{\alpha_{(i)\,j}} - 1\Big\} - 2v_{ni} - \lambda_n v_{ni}^2\Big|^2\,\mathrm{d}x \to 0$$

and the already proved convergences for w_j, v_j, $j = 1, \ldots, l$, guarantee the existence of quantities $\widehat{v}_i \in \mathbf{R}$, $i = l+1, \ldots, m$, such that $2v_{ni} + \lambda_n v_{ni}^2 \to 2\widehat{v}_i \in \mathbf{R}_+$ in L^2, $i = l+1, \ldots, m$. Because of $\lambda_n v_{ni} \geq -1$ we get

$$|v_{ni} - \widehat{v}_i| = \Big| \frac{(v_{ni} - \widehat{v}_i)(2 - \lambda_n v_{ni})}{2 - \lambda_n v_{ni}} \Big| \leq |(v_{ni} - \widehat{v}_i)(2 - \lambda_n v_{ni})| \leq |2v_{ni} + \lambda_n v_{ni}^2 - 2\widehat{v}_i| + \lambda_n |v_{ni}||\widehat{v}_i|$$

which leads to

$$\|v_{ni} - \widehat{v}_i\|_{L^2} \leq c\,(\|2v_{ni} + \lambda_n v_{ni}^2 - 2\widehat{v}_i\|_{L^2} + \lambda_n \|v_{ni}\|_{L^2}) \to 0.$$

Fatou's lemma yields $(\alpha - \beta) \cdot \widehat{v} = 0$ for all $(\alpha, \beta) \in \mathcal{R}$ which means $\widehat{v} \in \mathcal{S}^\perp$. Now, let $\widehat{y} = (\widehat{y}_1, \ldots, \widehat{y}_m)$ where

$$\widehat{y}_i = a_i^* p_i(\cdot, z^*)\big(2\widehat{v}_i - \partial_z P_i(z^*) \cdot \widehat{\mu}\big).$$

Using that $-P_i \in \mathcal{K}_1$ and conclusions from Remark 2.2, v) we derive (for details see [8, p. 114, 115])

$$\|y_n - \widehat{y}\|_Y \leq c(R)\Big\{\|v_n - \widehat{v}\|_Y + \|\mu_{n0} - \widehat{\mu}_0\|_{L^2} + \sum_{j=1}^{k} |\mu_{nj} - \widehat{\mu}_j| + \lambda_n \Big(\sum_{i=1}^{m} \|v_{ni}^2\|_{L^2} + 1\Big)\Big\} \to 0.$$

$\int_\Omega y_n\, dx \in \mathcal{S}$ implies $\int_\Omega \widehat{y}\, dx \in \mathcal{S}$, too. Since $\widehat{v} \in \mathcal{S}^\perp$ we obtain $(\widehat{v}, \widehat{y})_Y = 0$. Because of $\mathcal{E}(z_n, u_n) = \mathcal{E}(z^*, u^*) = 0$ and since $\mathcal{E}(\cdot, u)$ is monotone we find

$$\begin{aligned} 0 &\geq \frac{1}{\lambda_n^2} \langle \mathcal{E}(z^*, u_n) - \mathcal{E}(z_n, u_n), z_n - z^* \rangle_Z = \frac{1}{\lambda_n^2} \langle \mathcal{E}(z^*, u_n) - \mathcal{E}(z^*, u^*), z_n - z^* \rangle_Z \\ &= -\frac{1}{\lambda_n^2} \int_\Omega \sum_{i=1}^{m} \partial_z P_i(z^*) \cdot (z_n - z^*)(u_i - u_i^*)\, \mathrm{d}x = -\int_\Omega \sum_{i=1}^{m} \partial_z P_i(z^*) \cdot \mu_n y_{ni}\, \mathrm{d}x. \end{aligned}$$

Passing to the limit and taking $(\widehat{b}, \widehat{y})_Y = 0$ into account we arrive at

$$0 \geq -\int_\Omega \sum_{i=1}^{m} \frac{\partial P_i}{\partial z}(z^*) \cdot \widehat{\mu}\widehat{y}_i\, \mathrm{d}x = \int_\Omega \sum_{i=1}^{m} \Big\{2\widehat{v}_i - \frac{\partial P_i}{\partial z}(z^*) \cdot \widehat{\mu}\Big\}\widehat{y}_i\, \mathrm{d}x = \int_\Omega \sum_{i=1}^{m} \frac{1}{a_i^* p_i(\cdot, z^*)}\, |\widehat{y}_i|^2\, \mathrm{d}x.$$

Thus, $\widehat{y} = 0$, and (34) gives the contradiction $1 \leq c_2(R)\|y_n\|_Y^2 \to 0$. □

Theorem 4.17 *We suppose* (I) – (III)*. Then the free energy $\mathcal{F}(u)$ decays exponentially along solutions (u, b, z) of $(\mathcal{P})$ to its equilibrium value $\mathcal{F}(u^*)$, that is there is $\lambda > 0$, depending only on the data such that*

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

P r o o f. Theorem 4.9 and Lemma 4.11 ensure that $u(t) \in M_R$ f.a.a. $t > 0$ if $R = \max\{1, \mathcal{F}(U) - \mathcal{F}(u^*)\}$ is considered. We set $\lambda = 1/c_R$. Then Theorem 4.8 and Theorem 4.16 give the desired estimate. □

Corollary 4.18 *Let (u^*, b^*, z^*) be the (uniquely determined) steady state of $(\mathcal{P})$ and let (u, b, z) be any solution of $(\mathcal{P})$. Then there is a constant $c > 0$, depending only on the data such that with λ from Theorem 4.17 the estimates*

$$\|u(t) - u^*\|_{L^1(\Omega, \mathbf{R}^m)}\,,\ \|b(t) - b^*\|_{L^1(\Omega, \mathbf{R}^m)}\,,\ \|z(t) - z^*\|_Z \leq c\,\mathrm{e}^{-\lambda t/2} \quad \forall t \in \mathbf{R}_+ \tag{36}$$

are fulfilled. Moreover, the inequalities $\|b_i - b_i^*\|_{L^2(\mathbf{R}_+, L^2)} \leq c$, $i = 1, \ldots, l$, hold.

P r o o f. Let (u, b, z) be a solution of $(\mathcal{P})$. Theorem 4.9 guarantees that $\|z\|_{L^\infty(\mathbf{R}_+, Z)}$, $\|z_0\|_{L^\infty(\mathbf{R}_+, L^\infty)} \leq c$ and $\|a\|_{L^\infty(\mathbf{R}_+, L^1(\Omega, \mathbf{R}^m))}$, $\|\mathcal{D}(u)\|_{L^1(\mathbf{R}_+)} \leq c$, $\|\sqrt{a/a^*} - 1\|_{L^\infty(\mathbf{R}_+, Y)} \leq c$, $\|\nabla\sqrt{a_i/a_i^*}\|_{L^2(\mathbf{R}_+, L^2)} \leq c$, $i = 1, \ldots, l$. According to (32), (33) we have

$$\begin{aligned} F(u(t)) - F(u^*) &\geq c\|z(t) - z^*\|_Z^2 + c\|\sqrt{u(t)} - \sqrt{u^*}\|_Y^2 \\ &\geq c\|z(t) - z^*\|_Z^2 + c\|\sqrt{a(t)} - \sqrt{a^*}\|_Y^2 \quad \forall t \in \mathbf{R}_+. \end{aligned} \tag{37}$$

Therefore Theorem 4.17 ensures that

$$\begin{aligned}&\|z(t)-z^*\|_Z,\ \|\sqrt{u(t)}-\sqrt{u^*}\|_Y,\ \|\sqrt{a(t)/a^*}-1\|_Y\le c\,\mathrm{e}^{-\lambda t/2}\quad\forall t\in\mathbf{R}_+,\\&\|\sqrt{a/a^*}-1\|_{L^2(\mathbf{R}_+,Y)}\le c.\end{aligned}\tag{38}$$

With the inequality $\|u_i-u_i^*\|_{L^1}\le\|\sqrt{u_i}-\sqrt{u_i^*}\|_{L^2}\|\sqrt{u_i}+\sqrt{u_i^*}\|_{L^2}$, with Theorem 4.9, Theorem 4.17 and (38) we verify the remaining estimates in (36). Let now $i\in\{1,\dots,l\}$. Previous results and estimates (38) lead to $\|\sqrt{a_i/a_i^*}-1\|_{L^2(\mathbf{R}_+,H^1)}\le c$. Therefore interpolation between the spaces $L^2(\mathbf{R}_+,H^1)$ and $L^\infty(\mathbf{R}_+,L^2)$ yields $\|\sqrt{a_i/a_i^*}-1\|_{L^4(\mathbf{R}_+,L^4)}\le c$. Since z and z^* are bounded and the functions $p_i(x,\cdot)$ are locally Lipschitz continuous (see Remark 2.2, ii)), we can estimate

$$|b_i-b_i^*|\le c(|a_i/a_i^*-1|+\|z-z^*\|_{\mathbf{R}^{k+1}})\le c(|\sqrt{a_i/a_i^*}-1|^2+|\sqrt{a_i/a_i^*}-1|+\|z-z^*\|_{\mathbf{R}^{k+1}}).$$

Thus, for $i=1,\dots,l$, we verify

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

□

5 Global a priori estimates

Now we establish global upper bounds for the chemical activities b_i and densities u_i. For this reason we additionally assume that for the reaction system the properties

$$\max_{k=1,\dots,m}\big\{(a^\alpha-a^\beta)(\beta_k-\alpha_k)\big\}\le c\sum_{j=1}^m a_j^2+c,\ \sum_{i=l+1}^m\alpha_i\sum_{i=l+1}^m\beta_i=0\ \forall a\in\mathbf{R}_+^m,\ \forall(\alpha,\beta)\in\mathcal{R}\tag{IV}$$

are fulfilled. We start with estimates of the $L^\infty(\mathbf{R}_+,L^2)$-norm and the $L^\infty(\mathbf{R}_+,L^4)$-norm of the chemical activities b_i. Afterwards, the final result will be achieved by Moser iteration. Here mobile and immobile species must be handled in a different way. In the proof we use the constants ϵ_0, ϵ, $\widetilde{\epsilon}>0$ defined in (I), iii) and Remark 4.10.

Lemma 5.1 *We assume* (I) – (IV). *Let q be the exponent from Lemma* 4.3. *Then there are constants c, $c_q>0$ depending only on the data such that*

$$\|b_i(t)\|_{L^2}\le c\quad\forall t\in\mathbf{R}_+,\ i=1,\dots,m,\quad\|z_0\|_{L^\infty(\mathbf{R}_+,W^{1,q})}\le c_q$$

for any solution (u,b,z) of ($\mathcal{P}$).

Proof. 1. From Lemma 4.3 and Theorem 4.9 we get

$$\|z_0(t)\|_{W^{1,q}}\le c\Big(1+\sum_{i=1}^m\|u_i(t)\|_{L^{2q/(2+q)}}\Big)\le c\Big(1+\sum_{i=1}^m\|b_i(t)\|_{L^{2q/(2+q)}}\Big)\text{ f.a.a. }t\in\mathbf{R}_+.\tag{39}$$

2. We use the test function $2\mathrm{e}^t\,b$ for the evolution equation in ($\mathcal{P}$). According to the assumptions (I), vi) and (IV) we can estimate the occuring reaction terms as follows

$$\begin{aligned}\sum_{(\alpha,\beta)\in\mathcal{R}}R_{\alpha\beta}(\cdot,b,z)\,(\beta-\alpha)\cdot b&\le\sum_{j=l+1}^m\Big\{c\sum_{i=1}^l(b_i^3+b_i^2b_j+b_ib_j^2+b_j^2+1)-\widetilde{\epsilon}\,b_j^3\Big\}\\&\le c\sum_{i=1}^l|b_i|^3+c-\frac{\widetilde{\epsilon}}{2}\sum_{j=l+1}^m|b_j|^3.\end{aligned}$$

3. Using this estimate, inequality (66) and Young's inequality it results that for all $t \in \mathbf{R}_+$

$$\begin{aligned}
&\sum_{i=1}^{m} \big(\epsilon_0 \,\mathrm{e}^t \,\|b_i(t)\|_{L^2}^2 - c\|U_i\|_{L^2}^2\big) \\
&\leq \int_0^t \mathrm{e}^s \Big\{ \sum_{i=1}^{l} \big\{ -2\epsilon\|b_i\|_{H^1}^2 + c(\|b_i\|_{L^r}\|z_0\|_{W^{1,q}}\|b_i\|_{H^1} + \|b_i\|_{L^3}^3 + 1)\big\} \\
&\qquad\qquad + \sum_{j=l+1}^{m} \big\{ -\widetilde{\epsilon}\|b_j\|_{L^3}^3 + c\|b_j\|_{L^2}^2 \big\}\Big\}\,\mathrm{d}s \\
&\leq \int_0^t \mathrm{e}^s \Big\{ \sum_{i=1}^{l} \big\{\widetilde{c}(\|b_i\|_{L^r}\|z_0\|_{W^{1,q}}\|b_i\|_{H^1} + \|b_i\|_{L^2}^4 + 1) - \epsilon\|b_i\|_{H^1}^2\big\} - \sum_{j=l+1}^{m} \frac{\widetilde{\epsilon}}{2}\|b_j\|_{L^3}^3 \Big\}\mathrm{d}s
\end{aligned} \tag{40}$$

where $r = 2q/(q-2)$. We make use of the estimate (39), of Theorem 4.9, of the estimate $\|b_j\|_{L^{2q/(2+q)}} \leq \|b_j\|_{L^1}^{(r-2)/r}\|b_j\|_{L^2}^{2/r} \leq c\|b_j\|_{L^2}^{2/r}$, of Gagliardo-Nirenberg's inequality (66) and obtain

$$\begin{aligned}
&\widetilde{c}\|b_i\|_{L^r}\|z_0\|_{W^{1,q}}\|b_i\|_{H^1} \leq c\|b_i\|_{L^r}\Big(1 + \sum_{j=1}^{m}\|b_j\|_{L^{2q/(2+q)}}\Big)\|b_i\|_{H^1} \\
&\leq c\|b_i\|_{L^2}^{2/r}(1 + \sum_{j=1}^{m}\|b_j\|_{L^2}^{2/r})\|b_i\|_{H^1}^{2(r-1)/r} \leq \frac{\epsilon}{2}\|b_i\|_{H^1}^2 + c\|b_i\|_{L^2}^2\sum_{j=1}^{m}\|b_j\|_{L^2}^2 + c.
\end{aligned} \tag{41}$$

This together with (40) leads to

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

Gagliardo-Nirenberg's inequality (66) and Young's inequality guarantee

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

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

Since $\|b\|_{L^\infty(\mathbf{R}_+, L^1(\Omega, \mathbf{R}^m))} \leq c$ (see Theorem 4.9) we can proceed by

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

According to Corollary 4.18 the function $\eta := \sum_{i=1}^{l}\|b_i - b_i^*\|_{L^2(\Omega)}^2$ has a finite $L^1(\mathbf{R}_+)$-norm. Therefore we can apply Gronwall's lemma and obtain that for all $t \in \mathbf{R}_+$

$$\mathrm{e}^t \sum_{j=1}^{m}\|b_j(t)\|_{L^2}^2 \leq c\mathrm{e}^t + \int_0^t c\,\mathrm{e}^s\eta(s)\,\mathrm{e}^{\|\eta\|_{L^1(\mathbf{R}_+)}}\,\mathrm{d}s \leq c\,\mathrm{e}^t\,(1 + \|\eta\|_{L^1(\mathbf{R}_+)}\mathrm{e}^{\|\eta\|_{L^1(\mathbf{R}_+)}}) \leq c\,\mathrm{e}^t.$$

4. Since $2q/(2+q) < 2$ the estimate for $\|z_0\|_{L^\infty(\mathbf{R}_+,W^{1,q})}$ is a direct consequence of (39) and the first estimate in Lemma 5.1. □

We define

$$\kappa := c_q^{2r} + 1 \quad \text{where } r = 2q/(q-2), \quad q \text{ from Lemma 4.3}, \ c_q \text{ from Lemma 5.1.} \tag{42}$$

Lemma 5.2 *We assume* (I) – (IV). *Then there exists a constant* $c_{L^4} \geq 1$*, depending only on the data such that*

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

for any solution (u, b, z) *of* $(\mathcal{P})$*.*

P r o o f. We use the test function $4\mathrm{e}^t\,(b_1^3, \dots, b_m^3)$. First we estimate the reaction terms

$$\sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta}(\cdot, b, z) \sum_{i=1}^m (\beta_i - \alpha_i) b_i^3 \leq \sum_{j=l+1}^m \Big\{ c \sum_{i=1}^l \big\{ (b_i^2+1) b_j^3 + (b_j^2+1) b_i^3 + b_i^5 \big\} - \widetilde{\epsilon}\, b_j^5 \Big\}$$
$$\leq c \sum_{i=1}^l |b_i|^5 + c - \frac{\widetilde{\epsilon}}{2} \sum_{j=l+1}^m |b_j|^5.$$

With q from Lemma 4.3 and $r = 2q/(q-2)$ we obtain for all $t \in \mathbf{R}_+$

$$\sum_{i=1}^m \big(\epsilon_0\, \mathrm{e}^t\, \|b_i(t)\|_{L^4}^4 - c\|U_i\|_{L^4}^4 \big) \leq \int_0^t \mathrm{e}^s \Big\{ \sum_{j=l+1}^m \big(-2\widetilde{\epsilon}\|b_j\|_{L^5}^5 + \|b_j\|_{L^4}^4 \big)$$
$$+ \sum_{i=1}^l \big(-2\epsilon\|b_i^2\|_{H^1}^2 + c\big(\|\nabla z_0\|_{L^q} \|\nabla(b_i^2)\|_{L^2} \|b_i^2\|_{L^r} + \|b_i\|_{L^5}^5 + 1 \big) \big) \Big\}\, \mathrm{d}s.$$

Next we apply the estimate $\|b_j\|_{L^4}^4 \leq 2\widetilde{\epsilon}\|b_j\|_{L^5}^5 + c$, $j = l+1, \dots, m$, and the inequality (66). Moreover, we use Lemma 5.1, (42) and Young's inequality to get

$$\epsilon_0\, \mathrm{e}^t \sum_{i=1}^m \|b_i(t)\|_{L^4}^4 \leq \int_0^t \mathrm{e}^s \sum_{i=1}^l \Big\{ -\epsilon\|b_i^2\|_{H^1}^2 + c\big(\|z_0\|_{W^{1,q}} \|b_i^2\|_{L^1}^{1/r} \|b_i^2\|_{H^1}^{2-1/r}$$
$$+ \|b_i^2\|_{L^1} \|b_i^2\|_{H^1}^{3/2} + 1 \big) \Big\}\, \mathrm{d}s + c$$
$$\leq c \int_0^t \mathrm{e}^s \sum_{i=1}^l \big\{ \kappa \|b_i^2\|_{L^1}^2 + \|b_i^2\|_{L^1}^4 + 1 \big\}\, \mathrm{d}s + c \leq c\, \mathrm{e}^t \quad \forall t \in \mathbf{R}_+.$$

□

Theorem 5.3 *We assume* (I) – (IV). *Then there exists a constant* $c > 0$ *depending only on the data such that*

$$\|b_i(t)\|_{L^\infty} \leq c, \quad \|u_i(t)\|_{L^\infty} \leq c \quad \forall t \in \mathbf{R}_+, \quad i = 1, \dots, m, \tag{43}$$

for any solution (u, b, z) *of* $(\mathcal{P})$*.*

P r o o f. The main idea in the proof is a Moser iteration. First we verify the global bounds for the mobile species. Then, using these bounds we prove the assertion for the immobile species. Let $v_i := (b_i - K)^+$, $i = 1, \dots, m$, where $K := \max\{1, \|U_1/p_{01}\|_{L^\infty}, \dots, \|U_m/p_{0m}\|_{L^\infty}\}$.

1. *Bounds for the mobile species.* For $p \geq 8$ we use $p\mathrm{e}^t\,(v_1^{p-1}, \dots, v_l^{p-1}, 0, \dots, 0)$ as test function for the evolution equation and denote $w_i := v_i^{p/2}$. According to assumption (IV) we get

$$\sum_{(\alpha,\beta)\in\mathcal{R}} R_{\alpha\beta}(\cdot, b, z) \sum_{i=1}^l (\beta_i - \alpha_i) v_i^{p-1} \leq c \sum_{i=1}^l \sum_{j=1}^m (b_j^2+1) v_i^{p-1} \leq c \sum_{i=1}^l \big(v_i^{p+1} + \sum_{j=l+1}^m v_i^{p-1} v_j^2 \big) + c.$$

Lemma 5.2 and Hölder's inequality ensure

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

Thus we obtain

$$\epsilon_0\,\mathrm{e}^t \sum_{i=1}^{l} \|w_i(t)\|^2_{L^2} \le \int_0^t \mathrm{e}^s \sum_{i=1}^{l} \Big\{ -2\epsilon\|w_i\|^2_{H^1} + cp\|\nabla z_0\|_{L^q}\|\nabla w_i\|_{L^2}(\|w_i\|_{L^r}+1) + cp\big(\|w_i\|^{2(p+1)/p}_{L^{2(p+1)/p}} + c^2_{L^4}\|w_i\|^{2(p-1)/p}_{L^{4(p-1)/p}} + 1\big)\Big\}\,\mathrm{d}s \quad \forall t\in\mathbf{R}_+.$$

Now we apply for r, $\widetilde{p} := 2(p+1)/p$ and $\widetilde{p} := 4(p-1)/p$ the inequality (66)

$$\begin{aligned}\epsilon_0\mathrm{e}^t \sum_{i=1}^{l} \|w_i(t)\|^2_{L^2} &\le \int_0^t \mathrm{e}^s \sum_{i=1}^{l} \Big\{ -\epsilon\|w_i\|^2_{H^1} + cp^{2r}(\|z_0\|^{2r}_{W^{1,q}}+1)(\|w_i\|^2_{L^1}+1) \\ &\qquad + cp\big(\|w_i\|^{(p+2)/p}_{H^1}\|w_i\|_{L^1} + c^2_{L^4}\|w_i\|^{(3p-4)/2p}_{H^1}\|w_i\|^{1/2}_{L^1}+1\big)\Big\}\,\mathrm{d}s \\ &\le \int_0^t \mathrm{e}^s \sum_{i=1}^{l} c\Big\{p^{2r}\kappa(\|w_i\|^2_{L^1}+1) + p^4\|w_i\|^{2p/(p-2)}_{L^1} + p^4 c^8_{L^4}\|w_i\|^{2p/(p+4)}_{L^1} + 1\Big\}\,\mathrm{d}s \\ &\le cp^{2r}(\kappa + c^8_{L^4})\,\mathrm{e}^t \sum_{i=1}^{l}\big(\sup_{s\in\mathbf{R}_+}\|v_i(s)\|^{p^2/(p-2)}_{L^{p/2}}+1\big) \qquad \forall t\in\mathbf{R}_+.\end{aligned}$$

Thus it results the iteration formula

$$\sum_{i=1}^{l} \|v_i(t)\|^p_{L^p} + 1 \le p^{2r} c_M(\kappa + c^8_{L^4})\Big(\sum_{i=1}^{l}\sup_{s\in\mathbf{R}^+}\|v_i(s)\|^{p/2}_{L^{p/2}}+1\Big)^{2p/(p-2)} \quad \forall t\in\mathbf{R}_+,\ p\ge 8,$$

where $c_M > 1$ depends only on the data; κ, r and c_{L^4} are defined in (42) and Lemma 5.2. Next, we set $p = 2^n$, $n\in\mathbf{N}$, $n\ge 3$. The recursion formula ensures

$$\gamma_n \le (2^{4r} c_M\,(\kappa + c^8_{L^4})\,\gamma_2)^{c_\theta 2^n}, \quad \gamma_n := \sum_{i=1}^{l}\sup_{s\in\mathbf{R}_+}\|v_i(s)\|^{2^n}_{L^{2^n}} + 1, \quad c_\theta := \prod_{j=1}^{\infty}\frac{2^j}{2^j-1}.$$

Passing to the limit $n\to\infty$ we establish

$$\sum_{i=1}^{l}\|v_i(t)\|_{L^\infty} \le \sqrt{l}\,\Big(2^{4r}c_M\,(\kappa + c^8_{L^4})\Big(\sum_{i=1}^{l}\sup_{s\in\mathbf{R}_+}\|v_i(s)\|^4_{L^4}+1\Big)\Big)^{c_\theta} \quad \forall t\in\mathbf{R}_+,$$

and Lemma 5.2 leads to the desired estimates for b_i, u_i, $i=1,\dots,l$.

2. *Bounds for the immobile species.* We use $p\mathrm{e}^t\,(0,\dots,0,v_{l+1}^{p-1},\dots,v_m^{p-1})$, $p\ge 2$, as test function. Applying the assumptions (I), vi) and (IV), the inequalities $b_j \ge v_j \ge 0$ and the $L^\infty(\mathbf{R}_+, L^\infty)$-bounds for b_i, $i=1,\dots,l$, we obtain that a.e. in Ω

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

Thus we find

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

This ensures the estimate

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

Passing to the limit $p \to \infty$ we obtain $\|v_j(t)\|_{L^\infty} \le \sqrt{\widehat{c}/\widetilde{\epsilon}}$ for all $t \in \mathbf{R}_+$, $j = l+1, \ldots, m$, which leads to the desired L^∞-estimates for b_j, u_j, $j = l+1, \ldots, m$. □

6 Existence result

6.1 First regularized problem ($\mathcal{P}_N$)

To prove the existence of a solution of ($\mathcal{P}$) we investigate two regularized problems which are considered on an arbitrary given interval $S = [0, T]$. We start with a problem ($\mathcal{P}_N$) defined as follows. Let $N \in \mathbf{R}$, $N > 0$ be given and let $\rho_N \colon \mathbf{R}^{m+k+1} \to [0, 1]$ be a fixed Lipschitz continuous function satisfying

$$\rho_N(b, z) := \begin{cases} 0 & \text{if} \quad |(b, z)|_\infty \ge N, \\ 1 & \text{if} \quad |(b, z)|_\infty \le N/2 \end{cases}, \qquad |(b, z)|_\infty := \max\{|b_1|, \ldots, |b_m|, |z_0|, \ldots, |z_k|\}.$$

We introduce the functions $r_i \colon \Omega \times \mathbf{R}_+^m \times \mathbf{R}^{k+1} \to \mathbf{R}$, $i = 1, \ldots, m$, by

$$r_i(x, b, z) := \rho_N(b, z) \sum_{(\alpha,\, \beta) \in \mathcal{R}} R_{\alpha\beta}(x, b, z)(\beta_i - \alpha_i).$$

These functions r_i are Carathéodory functions. Moreover, the functions $r_i(x, \cdot, \cdot)$ are Lipschitz continuous (uniformly with respect to x). Further essential properties of these functions are

$$\sum_{i=1}^{m} r_i(x, b, z) \big(\ln b_i + P_i(z)\big) \le 0 \text{ f.a.a. } x \in \Omega\,,\ \forall (b, z) \in \mathbf{R}_+^m \times \mathbf{R} \times \mathbf{R}^k\,,\ b > 0, \tag{44}$$

$$|r_i(x, b, z)| \le c(N) \quad \text{f.a.a. } x \in \Omega\,,\ \forall (b, z) \in \mathbf{R}_+^m \times \mathbf{R} \times \mathbf{R}^k\,,\ i = 1, \ldots, m. \tag{45}$$

We define an operator $\mathcal{R}_N \colon X_+ \times Z \to X^*$ by

$$\langle \mathcal{R}_N(b, z), \overline{b} \rangle_X := \int_\Omega \sum_{i=1}^{m} r_i(\cdot, b, z)\, \overline{b}_i\, \mathrm{d}x, \quad \overline{b} \in X,$$

and formulate our first regularized problem as follows

$$\left.\begin{array}{c} u'(t) + \mathcal{A}(b(t), z(t)) = \mathcal{R}_N(b(t), z(t)), \quad \mathcal{E}(z(t), u(t)) = 0, \quad u(t) = \mathcal{B}b(t) \quad \text{f.a.a. } t \in S, \\ u(0) = U, \quad u \in H^1(S, X^*) \cap L^2(S, Y), \\ b \in L^2(S, X) \cap L^\infty(S, L_+^\infty(\Omega, \mathbf{R}^m)), \quad z \in L^2(S, Z) \cap L^\infty(S, L^\infty(\Omega) \times \mathbf{R}^k). \end{array}\right\} (\mathcal{P}_N)$$

6.2 Energy estimates for solutions of ($\mathcal{P}_N$)

We use the energy functional $\mathcal{F}$ from §4 and define the functional $\mathcal{D}_N \colon M_\mathcal{D} \to \mathbf{R}$,

$$\mathcal{D}_N(u) = \int_\Omega \sum_{i=1}^{l} 4\, D_i(\cdot, b, z) p_i(\cdot, z) |\nabla \sqrt{a_i}|^2\, \mathrm{d}x, \quad u \in M_\mathcal{D} \text{ (cf. (26))}. \tag{46}$$

Note that $\mathcal{D}_N$ is a lower estimate of the dissipation functional corresponding to problem ($\mathcal{P}_N$). Similar to the proof of Theorem 4.8 we can verify the following lemma (for the complete proof see [8, Lemma 8.32]).

Lemma 6.1 *Along any solution (u,b,z) of ($\mathcal{P}_N$) the free energy $\mathcal{F}(u)$ remains bounded by its initial value $\mathcal{F}(U)$ and decays monotonously,*

$$\mathcal{F}(u(t_2)) + \int_{t_1}^{t_2} \mathcal{D}_N(u(t))\,\mathrm{d}t \le \mathcal{F}(u(t_1)) \le \mathcal{F}(U), \quad 0 \le t_1 \le t_2 \le T.$$

Moreover, there exist positive constants, which do not depend on N and T such that for any solution of ($\mathcal{P}_N$)

$$\begin{aligned} &\|u_i \ln u_i\|_{L^\infty(S,L^1(\Omega))} \le c, \quad i=1,\dots,m, \quad \|u\|_{L^\infty(S,L^1(\Omega,\mathbf{R}^m))} \le c,\\ &\|z\|_{L^\infty(S,Z)} \le c, \quad \|z_0\|_{L^\infty(S,L^\infty(\Omega))}\,,\ \|z_j\|_{L^\infty(S)} \le c_{47}\,,\ j=1,\dots,k. \end{aligned} \tag{47}$$

Remark 6.2 The bounds for z obtained in (47) coincide with those of Theorem 4.9. Therefore Remark 4.10 remains valid for solutions of ($\mathcal{P}_N$) and we will now use the constants ϵ and $\widetilde{\epsilon}$ from Remark 4.10 again. Moreover, inequality (39) with q from Lemma 4.3 remains true.

6.3 A priori estimates for solutions of ($\mathcal{P}_N$)

As for solutions of ($\mathcal{P}$) the proof of a priori bounds for solutions of ($\mathcal{P}_N$) consists of three steps, namely to prove estimates for b_i, $i=1,\dots,m$, in $L^\infty(S,L^2(\Omega))$, $L^\infty(S,L^4(\Omega))$ and in $L^\infty(S,L^\infty(\Omega))$. In our proof the constants will depend on T, but not on N.

Theorem 6.3 *We assume* (I) *and* (IV). *Then there exist constants $c_{48} > 0$, $c_{49} \ge 1$ and $c_{50} > 0$ not depending on N such that*

$$\|b_i(t)\|_{L^2} \le c_{48} \quad \forall t \in S\,,\ i=1,\dots,m, \tag{48}$$

$$\|b_i(t)\|_{L^4} \le c_{49} \quad \forall t \in S\,,\ i=1,\dots,m, \tag{49}$$

$$\|b_i(t)\|_{L^\infty} \le c_{50} \quad \forall t \in S, \quad i=1,\dots,m, \tag{50}$$

for any solution (u,b,z) of ($\mathcal{P}_N$).

P r o o f. 1. We use the test function $2b$. According to (I) iv), vi) and (IV) we get with $\widetilde{\epsilon}$ from Remark 4.10

$$\sum_{i=1}^m r_i(\cdot,b,z)\,b_i \le \rho_N(b,z) \sum_{j=l+1}^m \Big\{ c\sum_{i=1}^l (b_i^3 + b_i^2 b_j + b_i b_j^2 + b_j^2 + 1) - \widetilde{\epsilon}\, b_j^3 \Big\} \le c\sum_{i=1}^l |b_i|^3 + c.$$

Therefore, similar to the arguments in the proof of Lemma 5.1 we obtain for $t \in S$

$$\sum_{i=1}^m \big(\epsilon_0 \|b_i(t)\|_{L^2}^2 - c\|U_i\|_{L^2}^2\big) \le \int_0^t \sum_{i=1}^l \big\{ \overline{c}(\|b_i\|_{L^r}\|z_0\|_{W^{1,q}}\|b_i\|_{H^1} + \|b_i\|_{L^2}^4 + 1) - \epsilon\|b_i\|_{H^1}^2 \big\}\,\mathrm{d}s$$

with $r = 2q/(q-2)$ and ϵ_0 and ϵ from (I) iii) and from Remark 4.10. We apply the estimate (41) and verify that

$$\sum_{j=1}^m \|b_j(t)\|_{L^2}^2 \le c\int_0^t \sum_{j=1}^m \sum_{i=1}^l \|b_i\|_{L^2}^2 \|b_j\|_{L^2}^2\,\mathrm{d}s + c \quad \forall t \in S. \tag{51}$$

First, let $i \in \{1,\dots,l\}$ be fixed. Lemma 6.1 and (46) ensure that $\|\nabla\sqrt{a_i}\|_{L^2(S,L^2)} \le c$, $\|u_i\|_{L^\infty(S,L^1)} \le c$, $\|z_0\|_{L^\infty(S,L^\infty)} \le c$, $\|z_j\|_{L^\infty(S)} \le c$, $j=1,\dots,k$, and therefore $\|\sqrt{a_i}\|_{L^2(S,H^1)} \le c$, $\|\sqrt{a_i}\|_{L^\infty(S,L^2)} \le c$. Interpolation yields $\|\sqrt{a_i}\|_{L^4(S,L^4)} \le c$, and thus $\|b_i\|_{L^2(S,L^2)} \le c$. Therefore we can apply Gronwall's Lemma in (51) and obtain that $\|b_i(t)\|_{L^2} \le c$, $i=1,\dots,m$, for all $t \in S$. Hence, for q from Lemma 4.3 there is a $\widehat{c}_q > 0$ not depending on N such that $\|z_0\|_{L^\infty(S,W^{1,q})} \le \widehat{c}_q$ for all solutions (u,b,z) of ($\mathcal{P}_N$). We denote

$$\widehat{\kappa} := \widehat{c}_q^{\,2r} + 1 \text{ with } r = 2q/(q-2)\,,\ q \text{ from Lemma 4.3.} \tag{52}$$

2. Next, we use the test function $4(b_1^3,\dots,b_m^3)$ for $(\mathcal{P}_N)$ and estimate the reaction terms by

$$\sum_{i=1}^m r_i(\cdot,b,z)\,b_i^3 \le \rho_N(b,z)\sum_{j=l+1}^m \Big\{c\sum_{i=1}^l \big\{(b_i^2+1)b_j^3+(b_j^2+1)b_i^3+b_i^5\big\}-\widetilde{\epsilon}b_j^5\Big\} \le c\sum_{i=1}^l |b_i|^5+c.$$

Similar to the proof of Lemma 5.2 by applying (66), (52) and Young's inequality as well as (48) we find

$$\begin{aligned}\sum_{i=1}^m \epsilon_0\|b_i(t)\|_{L^4}^4 &\le \int_0^t\sum_{i=1}^l\big\{-\tfrac{\epsilon}{2}\|b_i^2\|_{H^1}^2+c\big(\widehat{c}_q\|b_i^2\|_{L^1}^{1/r}\|b_i^2\|_{H^1}^{2-1/r}+\|b_i^2\|_{L^1}\|b_i^2\|_{H^1}^{3/2}+1\big)\big\}\,\mathrm{d}s\\ &\le c\int_0^t\sum_{i=1}^l\big\{\widehat{\kappa}\|b_i^2\|_{L^1}^2+\|b_i^2\|_{L^1}^4+\|b_i^2\|_{L^1}^2+1\big\}\,\mathrm{d}s\le c\quad \forall t\in S.\end{aligned}$$

3. The proof of the L^∞-bounds again is done in two steps, namely for the mobile and the immobile species, respectively. We employ some techniques of the proof of Theorem 5.3 and refer to the notation v_i, w_i and c_θ introduced there.
Bounds for the mobile species. We use $p\mathrm{e}^t\,(v_1^{p-1},\dots,v_l^{p-1},0,\dots,0)$, $p\ge 8$, as test function for $(\mathcal{P}_N)$ and estimate the regularized reaction terms by

$$\sum_{i=1}^l r_i(\cdot,b,z)\,v_i^{p-1}\le c\sum_{i=1}^l\sum_{j=1}^m(b_j^2+1)v_i^{p-1}\le c\sum_{i=1}^l\big(v_i^{p+1}+\sum_{j=l+1}^m v_i^{p-1}v_j^2\big)+c$$

a.e. on Ω. Estimate (49) and Hölder's inequality supply $\int_\Omega v_i^{p-1}v_j^2\,\mathrm{d}x\le\|v_i\|_{L^{2(p-1)}}^{p-1}\|v_j\|_{L^4}^2\le c_{49}^2\|w_i\|_{L^{4(p-1)/p}}^{2(p-1)/p}$. Following step 1 of the proof of Theorem 5.3 we arrive at

$$\epsilon_0\mathrm{e}^t\sum_{i=1}^l\|w_i(t)\|_{L^2}^2\le\, cp^{2r}(\widehat{\kappa}+c_{49}^8)\mathrm{e}^t\,\sum_{i=1}^l(\sup_{s\in S}\|v_i(s)\|_{L^{p/2}}^{p^2/(p-2)}+1)\quad\forall t\in S$$

which leads to

$$\sum_{i=1}^l\|v_i(t)\|_{L^\infty}\le\sqrt{l}\,\big(2^{4r}(\widehat{\kappa}+c_{49}^8)\,\overline{c}\big(\sum_{i=1}^l\sup_{s\in S}\|v_i(s)\|_{L^4}^4+1\big)\big)^{c_\theta}\quad\forall t\in S,$$

and with estimate (49) we obtain the desired L^∞-estimates for b_i, $i=1,\dots,l$.
Bounds for the immobile species. We use $p\mathrm{e}^t\,(0,\dots,0,v_{l+1}^{p-1},\dots,v_m^{p-1})$, $p\ge 2$, as test function for $(\mathcal{P}_N)$. Because of (I) vi) and (IV) the regularized reaction terms can be estimated by

$$\begin{aligned}\sum_{j=l+1}^m r_j(\cdot,b,z)\,v_j^{p-1}&\le\rho(b,z)(c\sum_{i=1}^l\sum_{j=l+1}^m(b_i^2+b_i+1)v_j^{p-1}-\widetilde{\epsilon}\sum_{j=l+1}^m v_j^{p+1})\\ &\le\rho(b,z)(\widehat{c}\sum_{j=l+1}^m v_j^{p-1}-\widetilde{\epsilon}\sum_{j=l+1}^m v_j^{p+1})\le\rho(b,z)(m-l)\frac{\widehat{c}^{(p+1)/2}}{\widetilde{\epsilon}^{(p-1)/2}}\le(m-l)\frac{\widehat{c}^{(p+1)/2}}{\widetilde{\epsilon}^{(p-1)/2}}\end{aligned}$$

a.e. in Ω. Now we can argue as in the second step of the proof of Theorem 5.3. □

6.4 Second regularized problem $(\mathcal{P}_M)$

The existence of solutions of problem $(\mathcal{P}_N)$ for fixed N is shown by a second regularization $(\mathcal{P}_M)$. For this purpose we take $M\ge M^*:=\max\big\{N+1,\max_{i=1,\dots,m}\|U_i/p_{0i}\|_{L^\infty}\big\}$ and use the projection

$$\sigma_M(y):=\begin{cases}-M & \text{for}\quad y<-M,\\ \;\;y & \text{for}\quad y\in[-M,M],\\ \;\;M & \text{for}\quad y>M,\end{cases}\qquad y\in\mathbf{R}.$$

Moreover we introduce the regularizations of D_i, $i = 1, \dots, l$,

$$D_{iM}(x, b, z) := D_i(x, b^+, \sigma_M(z_0), \sigma_M(z_1), \dots, \sigma_M(z_k)), \quad x \in \Omega\,,\ b \in \mathbf{R}^m\,,\ z \in \mathbf{R}^{k+1},$$

and define the operator $\mathcal{A}_M \colon X \times Z \to X^*$ by

$$\langle \mathcal{A}_M(b, z), \overline{b} \rangle_X := \int_\Omega \sum_{i=1}^{l} D_{iM}(\cdot, b, z) p_{0i} \big(\nabla b_i + [\sigma_M(b_i)]^+ Q_i(z) \nabla z_0 \big) \cdot \nabla \overline{b}_i \, \mathrm{d}x, \quad \overline{b} \in X.$$

We consider the regularized problem

$$\left. \begin{aligned} u'(t) + \mathcal{A}_M(b(t), z(t)) = \mathcal{R}_N(b^+(t), z(t)) \quad \text{f.a.a. } t \in S, \\ \mathcal{E}(z(t), u^+(t)) = 0, \quad u(t) = \mathcal{B} b(t) \quad \text{f.a.a. } t \in S, \\ u(0) = U, \quad u \in H^1(S, X^*) \cap L^2(S, Y)\,,\ b \in L^2(S, X)\,,\ z \in L^2(S, Z). \end{aligned} \right\} \qquad (\mathcal{P}_M)$$

Note that solutions (u, b, z) of ($\mathcal{P}_M$) possess the regularity properties $u,\ b \in C(S, Y)$ and $z \in C(S, Z)$.

6.5 Existence result for ($\mathcal{P}_M$)

First we give an equivalent formulation of ($\mathcal{P}_M$). We write b in the form $b = (v, w)$ where $v = (b_1, \dots, b_l)$, $w = (b_{l+1}, \dots, b_m)$ and introduce the spaces

$$\begin{aligned} &Y^l = L^2(\Omega, \mathbf{R}^l)\,,\ Y^{m-l} = L^2(\Omega, \mathbf{R}^{m-l})\,,\ X^l = H^1(\Omega, \mathbf{R}^l)\,,\ X^{l*} := (X^l)^*, \\ &W^l := \{ v \in L^2(S, X^l) \colon (\mathcal{B}_v v)' \in L^2(S, X^{l*}) \} \subset C(S, Y^l) \end{aligned}$$

and the operators $B_v \colon L^2(S, Y^l) \to L^2(S, Y^l)$, $B_w \colon L^2(S, Y^{m-l}) \to L^2(S, Y^{m-l})$,

$$\langle (\mathcal{B}_v v)(t), \overline{v} \rangle_{Y^l} := \int_\Omega \sum_{i=1}^{l} p_{0i}\, v_i(t)\, \overline{v}_i \, \mathrm{d}x, \quad \overline{v} \in Y^l,$$

$$\langle (\mathcal{B}_w w)(t), \overline{w} \rangle_{Y^{m-l}} := \int_\Omega \sum_{i=1}^{m-l} p_{0(l+i)}\, w_i(t)\, \overline{w}_i \, \mathrm{d}x, \quad \overline{w} \in Y^{m-l}, \quad t \in S.$$

Additionally, we define operators $\mathcal{A}_v \colon L^2(S, X^l) \times L^2(S, X^l) \times L^2(S, Y^{m-l}) \times L^2(S, Z) \to L^2(S, X^{l*})$, $\mathcal{A}_v^0$, $\mathcal{R}_v \colon L^2(S, X^l) \times L^2(S, Y^{m-l}) \times L^2(S, Z) \to L^2(S, X^{l*})$ and $\mathcal{R}_w \colon L^2(S, X^l) \times L^2(S, Y^{m-l}) \times L^2(S, Z) \to L^2(S, Y^{m-l})$ by

$$\langle \mathcal{A}_v(v; \widehat{v}, w, z), \overline{v} \rangle_{L^2(S, X^l)} := \int_S \int_\Omega \sum_{i=1}^{l} (D_{iM}(\cdot, \widehat{v}, w, z)\, p_{0i}\, \nabla v_i \cdot \nabla \overline{v}_i + v_i \overline{v}_i) \, \mathrm{d}x \, \mathrm{d}s,$$

$$\langle \mathcal{A}_v^0(v, w, z), \overline{v} \rangle_{L^2(S, X^l)} := \int_S \int_\Omega \sum_{i=1}^{l} (D_{iM}(\cdot, v, w, z)\, p_{0i}\, [\sigma_M(v_i)]^+ Q_i(z) \nabla z_0 \cdot \nabla \overline{v}_i - v_i \overline{v}_i) \, \mathrm{d}x \, \mathrm{d}s,$$

$$\langle \mathcal{R}_v(v, w, z), \overline{v} \rangle_{L^2(S, X^l)} := \int_S \langle \mathcal{R}_N(v^+, w^+, z), (\overline{v}, 0) \rangle_X \, \mathrm{d}s, \quad \overline{v} \in L^2(S, X^l),$$

$$\langle \mathcal{R}_w(v, w, z), \overline{w} \rangle_{L^2(S, Y^{m-l})} := \int_S \langle \mathcal{R}_N(v^+, w^+, z), (0, \overline{w}) \rangle_X \, \mathrm{d}s, \quad \overline{w} \in L^2(S, Y^{m-l}).$$

For every given $v \in L^2(S, Y^l)$ and $w \in L^2(S, Y^{m-l})$ the vector $(\mathcal{B}_v v, \mathcal{B}_w w)$ lies in $L^2(S, Y)$. Therefore, according to Lemma 4.3 there is a unique solution $z \in L^2(S, Z) \cap (L^\infty(S, L^\infty \times \mathbf{R}^k))$ of

$$\mathcal{E}(z(t), (\mathcal{B}_v v)^+(t), (\mathcal{B}_w w)^+(t)) = 0 \quad \text{f.a.a. } t \in S.$$

Let $\mathcal{T}_z\colon L^2(S,Y^l)\times L^2(S,Y^{m-l})\to L^2(S,Z)$ denote the corresponding solution operator such that $z=\mathcal{T}_z(v,w)$. Then problem $(\mathcal{P}_M)$ can be formulated equivalently as follows:

$$\begin{aligned}&(\mathcal{B}_v v)'+\mathcal{A}_v(v;v,w,\mathcal{T}_z(v,w))=\mathcal{R}_v(v,w,\mathcal{T}_z(v,w))-\mathcal{A}_v^0(v,w,\mathcal{T}_z(v,w)),\\&(\mathcal{B}_v v)(0)=(U_1,\dots,U_l),\quad v\in W^l,\end{aligned}\tag{53}$$

$$(\mathcal{B}_w w)'=\mathcal{R}_w(v,w,\mathcal{T}_z(v,w)),\quad (\mathcal{B}_w w)(0)=(U_{l+1},\dots,U_m),\quad \mathcal{B}_w w\in H^1(S,Y^{m-l}).\tag{54}$$

The existence result for $(\mathcal{P}_M)$ is shown by proving that the system (53), (54) can be solved. We remark that thanks to Lemma 4.3 the solution operator $\mathcal{T}_z\colon L^2(S,Y)\to Z$ of our generalized Poisson equation possesses in principle the same essential structural properties as the solution operator of the nonlinear Poisson equation in [13, Subsection 3.5], only the range differs. In our operators $\mathcal{A}_v^0,\ \mathcal{A}_v,\ \mathcal{R}_v,\ \mathcal{R}_w$ the dependences of the quantities $D_{Mi},\ \rho_N,\ k_{\alpha\beta}$ and Q_i on z are nearly of the same quality as in the operators in [13]. Therefore we can follow the principle ideas and estimates of the different steps of the existence proof in [13, Subsection 3.5]. For a complete proof of the existence of solutions of $(\mathcal{P}_M)$ see [8, Subsection 8.6.5]. Here we give only a short summary of the proof and refer to the corresponding lemmas in [13].

At the beginning we fix some $\widehat{v}\in W^l$ and solve the initial value problem

$$(\mathcal{B}_w w)'=\mathcal{R}_w(\widehat{v},w,\mathcal{T}_z(\widehat{v},w)),\quad (\mathcal{B}_w w)(0)=U_w,\quad \mathcal{B}_w w\in H^1(S,Y^{m-l}).$$

As in [13, Lemma 3.8] one proves that this problem has a unique solution $w=\mathcal{T}_w\widehat{v}$ with a solution operator $\mathcal{T}_w\colon W^l\to H^1(S,Y^{m-l})$. Next we solve the problem

$$\begin{aligned}(\mathcal{B}_v v)'+\mathcal{A}_v(v;\widehat{v},\mathcal{T}_w\widehat{v},\mathcal{T}_z(\widehat{v},\mathcal{T}_w\widehat{v}))&=\mathcal{R}_v(\widehat{v},\mathcal{T}_w\widehat{v},\mathcal{T}_z(\widehat{v},\mathcal{T}_w\widehat{v}))-\mathcal{A}_v^0(\widehat{v},\mathcal{T}_w\widehat{v},\mathcal{T}_z(\widehat{v},\mathcal{T}_w\widehat{v})),\\(\mathcal{B}_v v)(0)&=U_v,\quad v\in W^l.\end{aligned}$$

According to Lemma 9.3 there is a unique solution $v=\mathcal{Q}\widehat{v}$ of this problem. The operator $\mathcal{Q}\colon W^l\to W^l$ is completely continuous (see [13, Lemma 3.10]). By means of Schauder's Fixed Point Theorem similar to [13, Lemma 3.11] we can prove the existence of a fixed point $v\in W^l$ of the mapping $\mathcal{Q}$.

Theorem 6.4 *There is a solution (u,b,z) of problem $(\mathcal{P}_M)$.*

P r o o f. Since the mapping $\mathcal{Q}$ has a fixed point there is a solution v of the problem

$$\begin{aligned}(\mathcal{B}_v v)'+\mathcal{A}_v(v;v,\mathcal{T}_w v,\mathcal{T}_z(v,\mathcal{T}_w v))&=\mathcal{R}_v(v,\mathcal{T}_w v,\mathcal{T}_z(v,\mathcal{T}_w v))-\mathcal{A}_v^0(v,\mathcal{T}_w v,\mathcal{T}_z(v,\mathcal{T}_w v)),\\(\mathcal{B}_v v)(0)&=(U_1,\dots,U_l),\quad v\in W^l.\end{aligned}$$

We define $w:=\mathcal{T}_w v\in H^1(S,Y^{m-l})$. Then the pair (v,w) satisfies the system (53), (54) which is an equivalent formulation of problem $(\mathcal{P}_M)$. ☐

6.6 Energy estimates for solutions of $(\mathcal{P}_M)$

Lemma 6.5 *If (u,b,z) is a solution of $(\mathcal{P}_M)$ then $b(t)\ge 0$, $u(t)\ge 0$ a.e. on Ω for all $t\in S$.*

P r o o f. Let (u,b,z) be a solution of $(\mathcal{P}_M)$. We use the test function $-b^-$ for the evolution equation and take into account that

$$(\nabla b_i+[\sigma_M(b_i)]^+Q_i(z)\nabla z_0)\cdot\nabla b_i^-\le 0,\quad i=1,\dots,l,\quad -r_i(\cdot,b,z)\,b_i^-\le 0,\quad i=1,\dots,m.$$

Then we find that $\|b^-(t)\|_Y^2\le 0$ for all $t\in S$ which proves the lemma. ☐

We use a regularized energy functional $\mathcal{F}_M$ which is adapted to the regularizations done in problem $(\mathcal{P}_M)$. Let

$$l_M(y):=\begin{cases}\ln y & \text{if}\quad 0<y\le M,\\ \ln M-1+\frac{y}{M} & \text{if}\quad y>M.\end{cases}$$

We define the functional $\widetilde{\mathcal{F}}_{M2} : Y \to \mathbf{R}$ as

$$\widetilde{\mathcal{F}}_{M2}(u) := \begin{cases} \displaystyle\int_\Omega \sum_{i=1}^m \int_{p_{0i}}^{u_i} l_M(y/p_{0i})\,\mathrm{d}y\,\mathrm{d}x & \text{if} \quad u \in Y_+, \\ +\infty & \text{if} \quad u \in Y \setminus Y_+, \end{cases} \tag{55}$$

and introduce

$$\mathcal{F}_{M2} = (\widetilde{\mathcal{F}}^*_{M2}|_X)^* : X^* \to \overline{\mathbf{R}}, \quad \mathcal{F}_M = \mathcal{F}_1 + \mathcal{F}_{M2} : X^* \to \overline{\mathbf{R}} \quad \text{with } \mathcal{F}_1 \text{ from (14).}$$

Since the function l_M has the same fundamental properties as the function $\ln$ which appears in the definition of the functional $\mathcal{F}_2$ we obtain similar to the proof of Lemma 4.5 the following result.

Lemma 6.6 *The functional $\mathcal{F}_M = \mathcal{F}_1 + \mathcal{F}_{M2} : X^* \to \overline{\mathbf{R}}$ is proper, convex and lower semi-continuous. For $u \in Y_+$ it can be evaluated according to* (14), (55). *The restriction $\mathcal{F}_M|_{Y_+}$ is continuous. If $u \in Y_+$ and z is the solution of $\mathcal{E}(z,u) = 0$ then $P(z) \in \partial\mathcal{F}_1(u)$. If $u \in Y$, $u \geq \delta > 0$ and $u/p_0 \in X$ then $l_M(u/p_0) \in \partial\mathcal{F}_{M2}(u)$. Here $l_M(b)$ means the vector $\{l_M(b_i)\}_{i=1,\dots,m}$.*

Note that also the regularized free energy $\mathcal{F}_M$ has the important property that

$$\mathcal{F}_M(u) \geq c\left\{\|z\|_Z^2 + \sum_{i=1}^m \|u_i \ln u_i\|_{L^1} - c_1\right\} \quad \forall u \in Y_+. \tag{56}$$

Lemma 6.7 *Along any solution (u,b,z) of problem $(\mathcal{P}_M)$ the regularized free energy $\mathcal{F}_M$ remains bounded by its initial value $\mathcal{F}_M(U) = \mathcal{F}(U)$ and decays monotonously,*

$$\mathcal{F}_M(u(t_2)) \leq \mathcal{F}_M(u(t_1)) \leq \mathcal{F}(U), \quad 0 \leq t_1 \leq t_2.$$

Moreover, there are positive constants c, c_{57}, c_{58} which do not depend on M such that

$$\|z_0\|_{L^\infty(S,H^1(\Omega))} \leq c, \quad \|u_i \ln u_i\|_{L^\infty(S,L^1(\Omega))},\ \|u_i\|_{L^\infty(S,L^1(\Omega))} \leq c\,,\ i = 1,\dots,m,$$

$$\|b_i \ln b_i\|_{L^\infty(S,L^1(\Omega))} \leq c_{57}\,,\ i = 1,\dots,m, \tag{57}$$

$$\|z_0\|_{L^\infty(S,L^\infty(\Omega))},\ \|z_j\|_{L^\infty(S)} \leq c_{58}\,,\ j = 1,\dots,k, \tag{58}$$

for any solution (u,b,z) of $(\mathcal{P}_M)$.

Proof. 1. We use the techniques of the proof of Theorem 4.8 and define $u^\delta = u + \delta p_0$, $b^\delta = b + \delta$ for $\delta \in (0,1)$. Then $u^\delta \in H^1(S,X^*)$, $l_M(b^\delta) \in L^2(S,X)$ and $\nabla l_M(b_i^\delta) = \nabla b_i/\sigma_M(b_i^\delta)\,,\ i = 1,\dots,l$. Lemma 6.6 guarantees the relation $l_M(b^\delta(t)) \in \partial\mathcal{F}_{M2}(u^\delta(t))$ f.a.a. $t \in S$ and according to Lemma 9.2 the function $t \mapsto \mathcal{F}_{M2}(u^\delta(t))$ is absolutely continuous on S and

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}_{M2}(u^\delta(t)) = \big\langle u'(t), l_M(u^\delta(t))\big\rangle_X \text{ f.a.a. } t \in S.$$

We define $\zeta_M^\delta = P(z) + l_M(b^\delta)$, $\zeta^\delta = P(z) + \ln(b^\delta) \in L^2(S,X)$ and get

$$\big[\mathcal{F}_1(u(t)) + \mathcal{F}_{M2}(u^\delta(t))\big]\Big|_{t_1}^{t_2} = \int_{t_1}^{t_2} \langle u'(t), \zeta_M^\delta(t)\rangle_X\,\mathrm{d}t.$$

Using the evolution equation we can write a.e. on S

$$\langle u', \zeta_M^\delta\rangle_X = \langle \mathcal{R}_N(b,z) - \mathcal{A}_M(b,z), \zeta_M^\delta\rangle_X = \langle \widehat{\mathcal{R}}_N(b,b^\delta,z), \zeta^\delta\rangle_X - \langle \widehat{\mathcal{A}}_M(b,b^\delta,z), \zeta_M^\delta\rangle_X + h^\delta$$

with

$$h^\delta = \langle \widehat{\mathcal{A}}_M(b,b^\delta,z) - \widehat{\mathcal{A}}_M(b,b,z), \zeta_M^\delta\rangle_X + \langle \widehat{\mathcal{R}}_N(b,b,z) - \widehat{\mathcal{R}}_N(b,b^\delta,z), \zeta_M^\delta\rangle_X$$
$$+ \langle \widehat{\mathcal{R}}_N(b,b^\delta,z), \zeta_M^\delta - \zeta^\delta\rangle_X,$$

where the operator $\widehat{\mathcal{R}}_N$ is defined similar to the operator $\widehat{\mathcal{R}}$ given in (29) but here additionally the factor $\rho_N(b,z)$ is involved in the integrand and $\widehat{\mathcal{A}}_M : (X \times X \times Z) \to X^*$ is given by

$$\langle \widehat{\mathcal{A}}_M(b, b^\delta, z), \overline{b}\rangle_X := \int_\Omega \sum_{i=1}^{l} D_{iM}(\cdot, b, z) p_{0i} \big[\nabla b_i^\delta + [\sigma_M(b_i^\delta)]^+ Q_i(z)\nabla z_0\big] \cdot \nabla \overline{b}_i \,\mathrm{d}x,\ \ \overline{b} \in X.$$

Because of $\langle \widehat{\mathcal{R}}_N(b, b^\delta, z), \zeta^\delta\rangle_X \le 0$ and $\langle \widehat{\mathcal{A}}_M(b, b^\delta, z), \zeta_M^\delta\rangle_X \ge 0$ we find the inequality

$$\big[\mathcal{F}_1(u(t)) + \mathcal{F}_{M2}(u^\delta(t))\big]\,\big|_{t_1}^{t_2} \le \int_{t_1}^{t_2} h^\delta(t)\,\mathrm{d}t. \tag{59}$$

For small δ due to the choice of M we have that $\rho_N(b(x), z(x)) = 0$ if $\zeta_{Mi}^\delta(x) \ne \zeta_i^\delta(x)$, and thus the last term in h^δ vanishes identically.
3. Next, we let $\delta \to 0$. Since $\mathcal{F}_{M2}|_{Y_+}$ is continuous we obtain $\mathcal{F}_{M2}(u^\delta(t_k)) \to \mathcal{F}_{M2}(u(t_k))$, $k = 1, 2$. Moreover, the definition of $\widehat{\mathcal{A}}_M$ and Lebesgue's Theorem ensure that the time integral of the first term in h^δ tends to zero for $\delta \to 0$. A corresponding convergence is valid for the second term (here the uniform Lipschitz continuity of $r_i(x,\cdot,\cdot)$ is used). Thus we get $\int_{t_1}^{t_2} h^\delta(t)\,\mathrm{d}t \to 0$ for $\delta \to 0$, which leads together with (59) to $\mathcal{F}_M(u(t_2)) \le \mathcal{F}_M(u(t_1))$. Since $M \ge \max_{i=1,\ldots,m} \|U_i/p_{0i}\|_{L^\infty}$ we obtain $\mathcal{F}_M(U) = \mathcal{F}(U)$. Now all other assertions follow from (56) and Lemma 4.3. □

6.7 Further estimates for solutions of ($\mathcal{P}_M$)

Theorem 6.8 *There is a constant $c_{60} > 0$, not depending on M such that*

$$\|b_i\|_{L^\infty(S,L^\infty)} \le c_{60}, \quad i = 1, \ldots, m, \tag{60}$$

for all solutions (u, b, z) of ($\mathcal{P}_M$).

P r o o f. 1. The constants in the proof may depend on N (and T). As in the corresponding proofs for ($\mathcal{P}$) and ($\mathcal{P}_N$) the present proof is done in three steps namely estimating the norms of b_i in $L^2(\Omega)$, $L^4(\Omega)$ and $L^\infty(\Omega)$. Using the test function $(0,\ldots,0,u_{l+1},\ldots,u_m)$ and the property (45) of r_i we find that $\|u_i(t)\|_{L^2} \le c$ for all $t \in S$, $i = l+1,\ldots,m$. And therefore $\|u_i(t)\|_{L^{r'}} \le c$ for all $t \in S$, $i = l+1,\ldots,m$, where $r' = 2q/(2+q)$ with $q > 2$ from Lemma 4.3. Thus, for solutions (u, b, z) of ($\mathcal{P}_M$) we obtain

$$\|z_0(t)\|_{W^{1,q}} \le c\Big(1 + \sum_{i=1}^{m} \|u_i(t)\|_{L^{r'}}\Big) \le c\Big(1 + \sum_{i=1}^{l} \|b_i(t)\|_{L^{r'}}\Big) \quad \forall t \in S. \tag{61}$$

2. Let $r = 2q/(q-2)$. We test the evolution equation in ($\mathcal{P}_M$) with $2(b_1,\ldots,b_l,0,\ldots,0)$, estimate $[\sigma_M(b_i)]^+$ by b_i, use (45), the inequalities (61), (66), Young's inequality and Lemma 6.7. Then we get

$$\begin{aligned}\sum_{i=1}^{l} \big(\epsilon_0\|b_i(t)\|_{L^2}^2 - c\|U_i\|_{L^2}^2\big) &\le \int_0^t \sum_{i=1}^{l} \big\{c(\|b_i\|_{L^r}\|z_0\|_{W^{1,q}}\|b_i\|_{H^1} + \|b_i\|_{L^2}^2 + 1) - 2\epsilon\|b_i\|_{H^1}^2\big\}\,\mathrm{d}s \\ &\le \int_0^t \sum_{i=1}^{l} \Big\{\overline{c}\|b_i\|_{L^r}\|b_i\|_{H^1} \sum_{j=1}^{l} \|b_j\|_{L^{r'}} + c - \epsilon\|b_i\|_{H^1}^2\Big\}\,\mathrm{d}s \quad \forall t \in S.\end{aligned}$$

We handle the integrand as follows. We use (67) for $p = 2$ and Lemma 6.7

$$\begin{aligned}\overline{c}\sum_{i=1}^{l} \|b_i\|_{L^r}\|b_i\|_{H^1}\sum_{j=1}^{l} \|b_j\|_{L^{r'}} &\le \sum_{i=1}^{l} \Big(\tfrac{\epsilon}{2}\|b_i\|_{H^1}^2 + c\|b_i\|_{L^2}^2 \sum_{j=1}^{l} \|b_j\|_{L^2}^2\Big) \le \sum_{i=1}^{l} \big(\tfrac{\epsilon}{2}\|b_i\|_{H^1}^2 + c\|b_i\|_{L^2}^4\big) \\ &\le \sum_{i=1}^{l} \Big(\tfrac{\epsilon}{2}\|b_i\|_{H^1}^2 + \big(\tfrac{\sqrt{\epsilon}}{2c_{57}}\|b_i \ln b_i\|_{L^1}\|b_i\|_{H^1} + c\|b_i\|_{L^1}\big)^2\Big) \le \sum_{i=1}^{l} \epsilon\|b_i\|_{H^1}^2 + c.\end{aligned}$$

In summary we thus obtain positive constants $c,\ \widetilde{\kappa}$ not depending on M such that

$$\|b_i(t)\|_{L^2} \le c\,,\ i = 1,\dots,m\,,\ \|z_0(t)\|_{W^{1,q}}^{2r} + 1 \le \widetilde{\kappa} \quad \forall t \in S. \tag{62}$$

3. We follow the ideas in the second and last step of the proof of Theorem 6.3, estimate $[\sigma_M(b_i)]^+$ by b_i , take the constants $q,\ r$ from Lemma 4.3 and $\widetilde{\kappa}$ from (62) instead of $\widehat{\kappa}$. Thus we find for all solutions (u, b, z) of $(\mathcal{P}_M)$

$$\begin{aligned}
&\|b_i(t)\|_{L^4} \le \widetilde{c} \quad \forall t \in S,\ i = 1,\dots,m,\\
&\sum_{i=1}^{l} \|(b_i - K)^+(t)\|_{L^\infty} \le \sqrt{l}\left(2^{4r}(\widetilde{\kappa} + \widetilde{c}^8)\, cT \left(\sum_{i=1}^{l} \sup_{s\in S} \|(b_i - K)^+(s)\|_{L^4}^4 + 1\right)\right)^{c_\theta} \quad \forall t \in S,\\
&\|(b_i - K)^+(t)\|_{L^\infty} \le c \quad \forall t \in S,\ i = l+1,\dots,m,
\end{aligned}$$

(with K and c_θ from the proof of Theorem 5.3), which leads to the desired L^∞-bounds for b. □

6.8 Existence proof for problem ($\mathcal{P}_N$)

Theorem 6.9 *We suppose* (I). *Then there exists at least one solution of* ($\mathcal{P}_N$).

Proof. We choose

$$\overline{M} = \max\left\{c_{58}, c_{60}, N+1, \max_{i=1,\dots,m} \|U_i/p_{0i}\|_{L^\infty}\right\}$$

(see Lemma 6.7, Theorem 6.8). According to Theorem 6.4 there exists at least one solution (u, b, z) of ($\mathcal{P}_{\overline{M}}$). This solution fulfils $u \ge 0$ (see Lemma 6.5). Because of Lemma 6.7 and Theorem 6.8 all solutions of ($\mathcal{P}_{\overline{M}}$) are bounded, $\|z_0\|_{L^\infty(S,L^\infty(\Omega))}$, $\|z_j\|_{L^\infty(S)} \le \overline{M}$, $j = 1,\dots,k$, $\|b_i\|_{L^\infty(S,L^\infty)} \le \overline{M}$, $i = 1,\dots,m$. Thus the solutions (u, b, z) of ($\mathcal{P}_{\overline{M}}$) are solutions of ($\mathcal{P}_N$), too. □

6.9 Existence proof for problem ($\mathcal{P}$)

Theorem 6.10 *We assume* (I) *and* (IV). *Then there exists at least one solution of* ($\mathcal{P}$).

Proof. It suffices to prove the existence of a solution of ($\mathcal{P}$) on any finite time interval $S := [0, T]$. Such problems are denoted by ($\mathcal{P}_S$). We choose $\overline{N} := 2\max\{c_{47}, c_{50}\}$ (cf. Lemma 6.1, Theorem 6.3). According to Theorem 6.9 there is a solution (u, b, z) of ($\mathcal{P}_{\overline{N}}$). The choice of $\overline{N}$ guarantees that the operators $\mathcal{R}_{\overline{N}}$ and $\mathcal{R}$ coincide on this solution. Thus (u, b, z) is a solution of ($\mathcal{P}_S$), too. □

7 Asymptotic behaviour

In addition to the results formulated in Theorem 5.3, Theorem 4.17 and Corollary 4.18 the following assertions concerning the asymptotic behaviour of solutions of ($\mathcal{P}$) can be verified.

Theorem 7.1 *We suppose* (I) – (IV). *Let* $p \in [1, \infty)$. *Then there are constants* $c,\ \widehat{c},\ \lambda_p,\ \widehat{\lambda} > 0$, *depending only on the data such that*

$$\begin{aligned}
&\|u_i(t) - u_i^*\|_{L^p},\ \|b_i(t) - b_i^*\|_{L^p} \le c\, \mathrm{e}^{-\lambda_p t} \quad \forall t \in \mathbf{R}_+, \quad i = 1,\dots,m, \quad p \in [1,\infty),\\
&\|z_0(t) - z_0^*\|_{W^{1,q}},\ \|z_0(t) - z_0^*\|_{L^\infty} \le \widehat{c}\, \mathrm{e}^{-\widehat{\lambda} t} \quad \forall t \in \mathbf{R}_+, \quad q \text{ as in Lemma 4.3,}
\end{aligned}$$

for any solution (u, b, z) *of* ($\mathcal{P}$).

Proof. Using the estimates in (36) and Theorem 5.3 we obtain for $p \in [1, +\infty)$, $i = 1,\dots,m$,

$$\|u_i(t) - u_i^*\|_{L^p}^p \le \|u_i(t) - u_i^*\|_{L^1} \|u_i(t) - u_i^*\|_{L^\infty}^{p-1} \le c^p\, \mathrm{e}^{-\lambda t/2} \qquad \forall t \in \mathbf{R}_+. \tag{63}$$

Because of $\|b_i(t) - b_i^*\|_{L^1} \le c\|u_i(t) - u_i^*\|_{L^1}$ and $\|b_i(t) - b_i^*\|_{L^\infty} \le c\|u_i(t) - u_i^*\|_{L^\infty}$ for all $t \in \mathbf{R}_+$ this inequality supplies the assertion of the theorem for b_i, $i = 1, \dots, m$. The regularity result for elliptic equations with mixed boundary conditions [14, Theorem 1] applied to the solution $\phi(t) = z_0(t) - z_0^* \in H_0^1(\Omega \cup \Gamma_N)$ of

$$\int_\Omega \varepsilon \nabla\phi(t) \cdot \nabla\overline{z}_0 \,\mathrm{d}x + \int_{\Gamma_N} \tau\phi(t)\overline{z}_0 \,\mathrm{d}\Gamma = \int_\Omega \eta(t)\overline{z}_0 \,\mathrm{d}x \quad \forall \overline{z}_0 \in H_0^1(\Omega \cup \Gamma_N),$$
$$\eta(t) = \frac{\partial H}{\partial z_0}(\cdot, u^*, z^*) - \frac{\partial H}{\partial z_0}(\cdot, u(t), z(t))$$

guarantees that

$$\|z_0(t) - z_0^*\|_{L^\infty} \le c\|z_0(t) - z_0^*\|_{W^{1,q}} \le c\|\eta(t)\|_{L^2}. \tag{64}$$

Because of $\|z_0^*\|_{L^\infty}$, $\|z_0(t)\|_{L^\infty}$, $|z_j^*|$, $|z_j(t)| \le c$, $j = 1, \dots, k$, $t \in \mathbf{R}_+$, and since $h \in \mathcal{K}_2$, $-P_i \in \mathcal{K}_1$, the term $\eta(t)$ can be estimated by

$$\begin{aligned} |\eta(t)| &\le c\Big\{\Big|\frac{\partial h}{\partial z_0}(\cdot, z^*) - \frac{\partial h}{\partial z_0}(\cdot, z(t))\Big| + \sum_{i=1}^m \Big|\frac{\partial P_i}{\partial z_0}(z(t))u_i(t) - \frac{\partial P_i}{\partial z_0}(z^*)u_i^*\Big|\Big\} \\ &\le c\sum_{i=1}^m \Big\{|u_i(t) - u_i^*| + (u_i^* + 1)\sum_{j=0}^k |z_j(t) - z_j^*|\Big\} \end{aligned}$$

which ensures that $\|\eta(t)\|_{L^2} \le c\big\{\|z(t) - z^*\|_Z + \sum_{i=1}^m \|u_i(t) - u_i^*\|_{L^2}\big\}$. Therefore inequality (64), Corollary 4.18 and (63) lead to the last assertion. □

8 Comments

1. Examples. We consider a (reduced) pair diffusion model for the redistribution of dopants and defects in heterogeneous semiconductor structures. Such a model is physically motivated in [6] and mathematically prepared in [12] and fits to the form (2). The relevant species are dopants A and (possibly charged) interstitials I, vacancies V, dopant-interstitial-pairs AI and dopant-vacancy-pairs AV. They underly reaction-drift-diffusion processes and for the (lumped) species the following continuity equations are fulfilled:

$$\begin{aligned} u_I' &+ \nabla \cdot j_I &&= R_1 + R_3^A + R_5^A, \\ u_V' &+ \nabla \cdot j_V &&= R_1 + R_2^A + R_6^A, \\ u_{AI}' &+ \nabla \cdot j_{AI} &&= R_2^A - R_4^A - R_5^A, \\ u_{AV}' &+ \nabla \cdot j_{AV} &&= R_3^A - R_4^A - R_6^A, \\ u_A' & &&= -R_2^A - R_3^A + 2R_4^A + R_6^A \end{aligned} \tag{65}$$

with reaction terms

$$\begin{aligned} R_1 &= k_1(\cdot, v_0, \zeta_n)\,(1 - a_I a_V), & R_2^A &= k_2^A(\cdot, v_0, \zeta_n)\,(a_A - a_V a_{AI}), \\ R_3^A &= k_3^A(\cdot, v_0, \zeta_n)\,(a_A - a_I a_{AV}), & R_4^A &= k_4^A(\cdot, v_0, \zeta_n)\,(a_{AI} a_{AV} - a_A^2), \\ R_5^A &= k_5^A(\cdot, v_0, \zeta_n)\,(a_{AI} - a_I a_A), & R_6^A &= k_6^A(\cdot, v_0, \zeta_n)\,(a_{AV} - a_V a_A) \end{aligned}$$

and flux densities j_K, $K = I, V, AI, AV$,

$$j_K = -D_K(\cdot, v_0, \zeta_n)\, u_K \nabla(\ln a_k) = -D_K(\cdot, v_0, \zeta_n)\, p_{0K}\big(\nabla b_K + Q_K(v_0, \zeta_n) b_K \nabla v_0\big)$$

where

$$a_K = \frac{u_K}{p_K(\cdot, v_0, \zeta_n)}, \quad b_K = \frac{u_K}{p_{0K}},$$
$$p_K(x, v_0, \zeta_n) = \overline{u}_K(x) \sum_{j \in J_K} C_{K,j}\, \mathrm{e}^{-q_{K,j}(v_0+\zeta_n)}, \quad p_{0K}(x) = p_K(x, 0, 0),$$
$$P_K(v_0, \zeta_n) = \ln \frac{p_{0K}}{p_K(\cdot, v_0, \zeta_n)}, \quad Q_K(v_0, \zeta_n) = \frac{\partial P_K}{\partial v_0}(v_0, \zeta_n),$$
$$D_K(x, v_0, \zeta_n) = \frac{\overline{u}_K(x) \sum_{j \in J_K} D_{K,j}(x)\, C_{K,j}\, \mathrm{e}^{-q_{K,j}(v_0+\zeta_n)}}{p_K(x, v_0, \zeta_n)}$$

with suitable constants $C_{K,j}$, $q_{K,j}$ and functions $\overline{u}_K$, $D_{K,j}$. Here v_0 is the electrostatic potential and ζ_n is an additional unknown function $t \mapsto \zeta_n(t) \in \mathbf{R}$ (electrochemical potential of the electrons). The continuity equations (65) are coupled with the nonlinear Poisson equation and the global charge conservation

$$-\nabla \cdot (\varepsilon \nabla v_0) + \frac{\partial H}{\partial v_0}(\cdot, u, v_0, \zeta_n) = f_0, \quad \int_\Omega \frac{\partial H}{\partial \zeta_n}(\cdot, u, v_0, \zeta_n)\, \mathrm{d}x = f_1\, |\Omega|$$

where

$$H(x, u, v_0, \zeta_n) = h(x, v_0, \zeta_n) - \sum_{K=I,V,AI,AV,A} P_K(v_0, \zeta_n) u_K,$$
$$h(x, v_0, \zeta_n) = \overline{u}_n(x)(\mathrm{e}^{v_0+\zeta_n} - 1) + \overline{u}_p(x)(\mathrm{e}^{-(v_0+\zeta_n)} - 1)$$

with suitable positive functions $\overline{u}_n$, $\overline{u}_p$. The kinetic coefficients k_1, k_i^A, $i = 2, \ldots, 6$, D_K, $K = I, V, AI, AV$, and the functions P_K, $Q_K = \partial P_K / \partial v_0$ here depend on the sum $v_0 + \zeta_n$.

Now we additionally include in our model another dopant B and the corresponding dopant-defect-pairs BI and BV with the related reactions R_2^B to B_6^B. Moreover we introduce pairs of dopants AB and consider pairing reactions $AI + BV \rightleftharpoons AB$ and $AV + BI \rightleftharpoons AB$ with reaction rates

$$R_7 = k_7(\cdot, v_0, \zeta_n)\, (a_{AI} a_{BV} - a_{AB}), \quad R_8 = k_8(\cdot, v_0, \zeta_n)\, (a_{AV} a_{BI} - a_{AB}).$$

The resulting model equations contain nine continuity equations and 13 reactions and are of the form (2), too. Next, we reduce that model under the assumption that the kinetic processes of the point defects are very fast (D_I, D_V, $k_1 \to \infty$) and that the reactions R_i^L are very fast ($k_i^L \to \infty$, $L = A, B$, $i = 2, \ldots, 6$). Since the expressions for the flux densities j_I, j_V and the reaction rates of the fast reactions must remain bounded these assumptions lead to

$$\nabla \zeta_I = \nabla \ln a_I = 0, \quad a_V = \mathrm{e}^{-\zeta_I}, \quad a_{LI} = a_L \mathrm{e}^{\zeta_I}, \quad a_{LV} = a_L \mathrm{e}^{-\zeta_I}, \quad L = A, B,$$

where ζ_I only depends on time. Then the resulting model equations contain three continuity equations for the lumped concentrations $\widetilde{u}_L = u_L + u_{LI} + u_{LV}$, $L = A, B$, and for $\widetilde{u}_{AB} = u_{AB}$, namely

$$\begin{aligned} \widetilde{u}'_L \ + \nabla \cdot \widetilde{j}_L \ &= -(k_7 + k_8)\, (a_A a_B - a_{AB}), \quad L = A, B, \\ \widetilde{u}'_{AB} + \nabla \cdot \widetilde{j}_{AB} &= \quad (k_7 + k_8)\, (a_A a_B - a_{AB}) \end{aligned}$$

where

$$\widetilde{j}_L = -\Big\{ D_{LI}\, p_{0LI}\, \mathrm{e}^{\zeta_I - P_{LI}} + D_{LV}\, p_{0LV}\, \mathrm{e}^{-\zeta_I - P_{LV}} \Big\} a_L \nabla \ln a_L, \quad L = A, B,$$
$$\widetilde{j}_{AB} = -D_{AB}\, p_{0AB}\, \mathrm{e}^{-P_{AB}}\, a_{AB}\, \nabla \ln a_{AB}.$$

Moreover, that reduced model contains a nonlinear Poisson equation and two nonlocal constraints, namely the global charge conservation and the global conservation of the defect difference

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla v_0) = f_0 - \frac{\partial h}{\partial v_0}(\cdot, v_0, \zeta_n) + p_{0I} \mathrm{e}^{-P_I + \zeta_I} Q_I + p_{0V} \mathrm{e}^{-P_V - \zeta_I} Q_V + p_{0AB} \mathrm{e}^{-P_{AB}} Q_{AB} a_{AB} \\ + \sum_{L=A,B} \Big\{ p_{0LI} \mathrm{e}^{-P_{LI} + \zeta_I} Q_{LI} + p_{0LV} \mathrm{e}^{-P_{LV} - \zeta_I} Q_{LV} + p_{0L} \mathrm{e}^{-P_L} Q_L \Big\} a_L, \end{aligned}$$

$$\int_\Omega \Big\{ \frac{\partial h}{\partial \zeta_n}(\cdot, v_0, \zeta_n) - p_{0I}\mathrm{e}^{-P_I+\zeta_I}Q_I - p_{0V}\mathrm{e}^{-P_V-\zeta_I}Q_V - p_{0AB}\mathrm{e}^{-P_{AB}}Q_{AB}a_{AB}$$

$$- \sum_{L=A,B}\Big\{p_{0LI}\mathrm{e}^{-P_{LI}+\zeta_I}Q_{LI} + p_{0LV}\mathrm{e}^{-P_{LV}-\zeta_I}Q_{LV} + p_{0L}\mathrm{e}^{-P_L}Q_L\Big\}a_L\Big\}\,\mathrm{d}x = f_1\,|\Omega|,$$

$$\int_\Omega \Big\{p_{0I}\mathrm{e}^{-P_I+\zeta_I} + \sum_{L=A,B} p_{0LI}\mathrm{e}^{-P_{LI}+\zeta_I}a_L - p_{0V}\mathrm{e}^{-P_V-\zeta_I} - \sum_{L=A,B} p_{0LV}\mathrm{e}^{-P_{LV}-\zeta_I}a_L\Big\}\,\mathrm{d}x = f_2\,|\Omega|.$$

We assume that

$$p_{0LI}(x) = c_{LI}p_{0L}(x), \quad p_{0LV}(x) = c_{LV}p_{0L}(x) \quad \text{with } c_{LI},\ c_{LV} \text{ positive constants },\ L = A, B.$$

We use the vector $\widetilde{z} = (\widetilde{z}_0, \widetilde{z}_1, \widetilde{z}_2) = (v_0, \zeta_n, \zeta_I)$ and the functions

$$\widetilde{p}_{AB}(\cdot, \widetilde{z}) = p_{AB}(\cdot, \widetilde{z}_0, \widetilde{z}_1), \quad \widetilde{p}_{0AB} = p_{0AB},$$

$$\widetilde{p}_L(\cdot, \widetilde{z}) = p_{0L}\Big\{\mathrm{e}^{-P_L(\widetilde{z}_0,\widetilde{z}_1)} + c_{LI}\mathrm{e}^{\widetilde{z}_2 - P_{LI}(\widetilde{z}_0,\widetilde{z}_1)} + c_{LV}\mathrm{e}^{-\widetilde{z}_2 - P_{LV}(\widetilde{z}_0,\widetilde{z}_1)}\Big\},$$

$$\widetilde{p}_{0L} = \widetilde{p}_L(\cdot, 0),\ L = A, B, \quad \widetilde{P}_L(\widetilde{z}) = \ln \widetilde{p}_{0L} - \ln \widetilde{p}_L(\cdot, \widetilde{z}), \quad L = A, B, AB,$$

and define

$$\widetilde{h}(\cdot, \widetilde{z}) = h(\cdot, \widetilde{z}_0, \widetilde{z}_1) + p_{0I}\mathrm{e}^{-P_I(\widetilde{z}_0,\widetilde{z}_1)+\widetilde{z}_2} + p_{0V}\mathrm{e}^{-P_V(\widetilde{z}_0,\widetilde{z}_1)-\widetilde{z}_2} - p_{0I} - p_{0V},$$

$$\widetilde{H}(x, \widetilde{u}, \widetilde{z}) = \widetilde{h}(x, \widetilde{z}) - \sum_{L=A,B,AB} \widetilde{P}_L(\widetilde{z})\widetilde{u}_L.$$

In this notation the nonlinear Poisson equation, the global charge conservation and the global conservation of the defect difference read as

$$-\nabla\cdot(\varepsilon\nabla\widetilde{z}_0) + \frac{\partial\widetilde{H}}{\partial\widetilde{z}_0}(\cdot, \widetilde{u}, \widetilde{z}) = f_0, \qquad \int_\Omega \frac{\partial\widetilde{H}}{\partial\widetilde{z}_j}(\cdot, \widetilde{u}, \widetilde{z})\,\mathrm{d}x = f_j\,|\Omega|, \quad j = 1, 2,$$

and also that reduced model turns out to be a special case of the electro-reaction-diffusion system (2).

2. Uniqueness. If additionally to the assumptions (I) – (III) the diffusivities D_i do not depend on b and the functions $D_i(x, \cdot)$ are locally Lipschitz continuous uniformly with respect to x, $i = 1, \ldots, l$, then uniqueness of the solution of ($\mathcal{P}$) can be proved by means of the techniques of [12, Lemma 7.2].

3. Global lower bounds. If we additionally to (I) – (IV) suppose that the initial values are strictly positive,

$$U_i \ge c > 0 \text{ a.e. on } \Omega, \quad i = 1, \ldots, m,$$

we can obtain lower bounds for the solutions of ($\mathcal{P}$), $u_i(t),\ b_i(t) \ge C > 0$ a.e. on Ω for all $t \in \mathbf{R}_+$, $i = 1, \ldots, m$, (see [8, section 8.7]). Note, that here the asymptotic behaviour is exploited to find global lower bounds for the solutions.

4. Boundary reactions. All results of the paper remain true if one additionally takes into account boundary reactions of at most first order between the mobile species. Then, for the mobile species $X_1,\ldots,X_l$ the boundary conditions in the continuity equations in (2) are substituted by

$$\nu\cdot j_i = \sum_{(\alpha,\beta)\in\mathcal{R}^\Gamma} (\alpha_i - \beta_i)k^\Gamma_{\alpha\beta}(b_1, \ldots, b_l, z)\Big[\prod_{i=1}^l a_i^{\alpha_i} - \prod_{i=1}^l a_i^{\beta_i}\Big], \quad i = 1, \ldots, l.$$

This case is investigated in [8, Chap. 8].

9 Appendix

We suppose that $\Omega \subset \mathbf{R}^2$ is a bounded Lipschitzian domain. We use Sobolev's imbedding results and trace inequalities (see [17]) and some other imbedding results, especially we apply the Gagliardo-Nirenberg inequality

$$\|w\|_{L^p} \le c_p \, \|w\|_{L^1}^{1/p} \|w\|_{H^1}^{1-1/p} \quad \forall w \in H^1(\Omega)\,,\ 1<p<\infty \tag{66}$$

(see [4, 20]). As an extended version of this inequality one obtains that for any $\delta > 0$ and any $p \in (1,\infty)$ there exists a $c_{\delta,p} > 0$ such that

$$\|w\|_{L^p}^p \le \delta \, \|w \ln |w|\|_{L^1} \, \|w\|_{H^1}^{p-1} + c_{\delta,p} \, \|w\|_{L^1} \quad \forall w \in H^1(\Omega). \tag{67}$$

This inequality is verified in [1] for bounded smooth domains and $p = 3$. But (67) is true for bounded Lipschitzian domains and $p \in (1,\infty)$ since (66) is valid in this situation, too. Trudinger's imbedding theorem says

$$\|e^{|w|}\|_{L^p} \le d_p(\|w\|_{H^1}) \quad \forall w \in H^1(\Omega)\,,\ 1 \le p < \infty \tag{68}$$

(see [21]). And especially, weak convergence $w_j \rightharpoonup w$ in $H^1(\Omega)$ leads to strong convergence $\mathrm{e}^{w_j} \to \mathrm{e}^{w}$ in $L^2(\Omega)$. Moreover, we make use of two chain rules from the calculus of weakly differentiable functions.

Lemma 9.1 *Let $f : \mathbf{R} \to \mathbf{R}$ be locally Lipschitz continuous, let $u \in W^{1,1}_{\mathrm{loc}}(\Omega)$. Then $f \circ u \in W^{1,1}_{\mathrm{loc}}(\Omega)$, and*

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

where N denotes the set of points where f is not differentiable.

For the proof see [7, p. 127–129].

Lemma 9.2 *Let X be a Hilbert space, X^* its dual, $S = [0,T]$. Let the Functional $F : X^* \to \overline{\mathbf{R}}$ be proper, convex and semi-continuous. Assume 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 $F \circ u : S \to \mathbf{R}$ is absolutely continuous, and*

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

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

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

and the assertion results from [2, Lemma 3.3]. □

Let $p_0 \in L^\infty(\Omega)$, $\operatorname{ess\,inf}_{x\in\Omega} p_0(x) \ge c > 0$. We define $B : L^2(\Omega) \longrightarrow L^2(\Omega)$ by $Bw := p_0\, w$, $w \in L^2(\Omega)$. Let $S = [0,T]$ be a compact interval. The extended operator $B :\ L^2(S, L^2(\Omega)) \longrightarrow L^2(S, L^2(\Omega))$ is defined by $(Bw)(t) := B(w(t))$ f.a.a. $t \in S$. The following existence result can be proved as in [5, Chap. IV].

Lemma 9.3 *Let $A :\ L^2(S, H^1(\Omega)) \to L^2(S, H^1(\Omega)^*)$ be the operator*

$$\langle Aw, \overline{w} \rangle_{L^2(S,H^1)} := \int_0^T \int_\Omega \Big\{ a \nabla w \cdot \nabla \overline{w} + d w\, \overline{w} \Big\}\, \mathrm{d}x\, \mathrm{d}s, \quad w,\ \overline{w} \in L^2(S, H^1(\Omega)),$$

where $a,\ d \in L^\infty(S \times \Omega)$ with $a(t,x),\ d(t,x) \ge c > 0$ f.a.a. $(t,x) \in S \times \Omega$. Then for every $f \in L^2(S, H^1(\Omega)^*)$ and every $U \in L^2(\Omega)$ there exists a unique solution of

$$(Bw)' + Aw = f,\ (Bw)(0) = U,\ w \in L^2(S, H^1),\ (Bw)' \in L^2(S, H^{1*}).$$

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