Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

Analysis of electronic models for solar cells including energy resolved defect densities

Annegret Glitzky

submitted: July 15, 2010

Weierstrass Institute
for Applied Analysis and Stochastics
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: annegret.glitzky@wias-berlin.de

No. 1524
Berlin 2010

2010 *Mathematics Subject Classification.* 35K57, 35R05, 35B45, 78A35.

Key words and phrases. Reaction-diffusion systems, drift-diffusion processes, energy resolved defect densities, motion of charged particles, existence, uniqueness, a priori estimates.

Edited by

Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)

Mohrenstraße 39

10117 Berlin

Germany

Fax: +49 30 2044975

E-Mail: preprint@wias-berlin.de

World Wide Web: http://www.wias-berlin.de/

Abstract

We introduce an electronic model for solar cells including energy resolved defect densities. The resulting drift-diffusion model corresponds to a generalized van Roosbroeck system with additional source terms coupled with ODEs containing space and energy as parameters for all defect densities. The system has to be considered in heterostructures and with mixed boundary conditions from device simulation. We give a weak formulation of the problem. If the boundary data and the sources are compatible with thermodynamic equilibrium the free energy along solutions decays monotonously. In other cases it may be increasing, but we estimate its growth. We establish boundedness and uniqueness results and prove the existence of a weak solution. This is done by considering a regularized problem, showing its solvability and the boundedness of its solutions independent of the regularization level.

1 Introduction and notation

In this paper we deal with the analysis of electronic models for solar cells which take into account energy resolved defect (trap) densities.

Gröger [13] investigated semiconductor models with varying densities of ionized impurities. But there the impurities are associated to fixed energy levels. Also in this context, we studied in [12] stationary energy models for semiconductor devices with incompletely ionized impurities. There, additionally to the continuity equations and the Poisson equation an energy balance equation is contained in the model, such that the equations are strongly coupled.

Our equations are based on models proposed by engineers working on solar cells (see e.g. [20, Sect. 4.2]). Let $\Omega \subset \mathbb{R}^d$ denote the solar cell domain. For the analysis we rescale the quantities, such that energies are counted in units of $k_B T$, where k_B is Boltzmann's constant and T is the temperature. In the new energy scale for $E \in E_G = [E_1, E_2]$ we take into account l different types of defects with given defect distributions $N_j(x, E)$, $j = 1, \dots, l$. To include also measure valued distributions of traps on the energy scale we use finite nonnegative measures $\mu_{2j+1} = \mu_{2j+2} = N_j \mathrm{d}E$ on $G := \Omega \times E_G$ proposing Young measure type properties such that $\mu_i(x, \cdot)$ are Radon measures on E_G a.e. on Ω and $x \mapsto \int_{E_G} g(E)\mu_i(x, \mathrm{d}E)$ is measurable for all continuous functions $g : E_G \to \mathbb{R}$.

This setting allows for $\mu_i(x, \cdot) = \sum_{k=1}^{K} \theta_k(x)\delta_{E_k(x)}(\cdot)$ such that the case of point-like distributed traps at single energies $E_{trap} \in E_G$ as discussed in [13] result as special case of our investigations, too.

We use the abbreviation

$$\langle\langle g \rangle\rangle_i := \int_{E_G} g(E)\mu_i(x, \mathrm{d}E).$$

Besides the densities of electrons u_1 and holes u_2 depending only on the spatial position x we have to balance the following densities: The probability that the defect states with defect distribution $N_j(x,E)$ are occupied by an electron can be interpreted as the density of defects occupied by electrons on $G=\Omega\times E_G$ with respect to the measure μ_{2j+1}. We denote it by u_{2j+1}, and $u_{2j+2}=1-u_{2j+1}$ corresponds to the density of non occupied defect states with respect to the measure μ_{2j+2}.

Moreover, we introduce

$$\lambda_1=-1,\quad \lambda_2=1,\quad \lambda_{2j+1}=\begin{cases}-1 & \text{for acceptor like traps}\\ 0 & \text{for donator like traps}\end{cases},\quad \lambda_{2j+2}=\lambda_{2j+1}+1,$$

$j=1,\dots,l$, the charge numbers of the different species.

The electronic model for bulk material proposed in [20] is a drift-diffusion model for the charge carriers coupled with ODEs for $u_{2j+1}(x,E)$, $(x,E)\in G$, $j=1,\dots,l$. The light, generating pairs of electrons and holes is treated as a given source term G_{phot}. The resulting drift-diffusion model corresponds to a generalized van Roosbroeck system with additional source terms coupled with ODEs for the defects. In scaled form, let z denote the electrostatic potential and let ζ_1, ζ_2 be the electrochemical potentials of electrons and holes. In our notation the model for bulk material proposed in [20, Sect. 4.2] can be written in the form

$$-\nabla\cdot(\varepsilon\nabla z)=f-u_1+u_2+\sum_{i=3}^{2l+2}\lambda_i\langle\langle u_i\rangle\rangle_i \quad \text{in } \mathbb{R}_+\times\Omega,$$

$$\frac{\partial}{\partial t}u_1-\nabla\cdot(D_1u_1\nabla\zeta_1)=G_{phot}-R-\sum_{j=1}^{l}\langle\langle R_j^n\rangle\rangle_{2j+1} \quad \text{in } \mathbb{R}_+\times\Omega,$$

$$\frac{\partial}{\partial t}u_2-\nabla\cdot(D_2u_2\nabla\zeta_2)=G_{phot}-R-\sum_{j=1}^{l}\langle\langle R_j^p\rangle\rangle_{2j+2} \quad \text{in } \mathbb{R}_+\times\Omega,$$

and the ODEs

$$\begin{aligned}&\frac{\partial}{\partial t}u_{2j+1}=R_j^n-R_j^p \quad \text{on } \mathbb{R}_+\times\operatorname{supp}\mu_{2j+1},\\ &\frac{\partial}{\partial t}u_{2j+2}=-\frac{\partial}{\partial t}u_{2j+1} \quad \text{on } \mathbb{R}_+\times\operatorname{supp}\mu_{2j+2},\quad j=1,\dots,l.\end{aligned}$$

The right-hand sides of the evolution equations are given by

$$\begin{aligned}R&=R(u_1,u_2)=r(u_1,u_2)(u_1u_2-\overline{k}),\\ R_j^n&=R_j^n(E,u_1,u_{2j+1},u_{2j+2})=r_j^n[u_1u_{2j+2}-(\overline{k}_j^n(E)+e_j^{n\,opt}(E))u_{2j+1}],\\ R_j^p&=R_j^p(E,u_2,u_{2j+1},u_{2j+2})=r_j^p[u_2u_{2j+1}-(\overline{k}_j^p(E)+e_j^{p\,opt}(E))u_{2j+2}],\end{aligned} \tag{1.1}$$

where the positive coefficients r, $\overline{k}$ are allowed to depend in a nonsmooth way on the spatial position and the positive coefficients r_j^n, r_j^p, $\overline{k}_j^n$, $\overline{k}_j^p$ and the nonnegative coefficients $e_j^{n\,opt}$, $e_j^{p\,opt}$, $j=1,\dots,l$, depend on (x,E). Moreover, the coefficients $\overline{k}$, $\overline{k}_j^n$, $\overline{k}_j^p$ fulfill

$$\overline{k}=\overline{k}_j^n\overline{k}_j^p \quad \mu_{2j+1}\text{-a.e. on } G,\quad j=1,\dots,l.$$

We introduce positive reference densities $\overline{u}_1$, $\overline{u}_2$ such that $\overline{u}_1\overline{u}_2 = \overline{k}$ and choose μ_{2j+1}-positive reference quantities $\overline{u}_{2j+1}$, $\overline{u}_{2j+2}$ with the property

$$\overline{u}_{2j+2} = \frac{\overline{u}_2}{\overline{k}^p_j}\overline{u}_{2j+1} = \frac{\overline{k}^n_j}{\overline{u}_1}\overline{u}_{2j+1} > 0 \quad \mu_{2j+1}\text{-a.e. on } G, \quad j = 1,\dots,l.$$

Note that the reference quantities $\overline{u}_1$, $\overline{u}_2$, $\overline{u}_{2j+1}$, $\overline{u}_{2j+2}$, $j = 1,\dots,l$, are taken in such a way that the reaction rates R, R^n_j and R^p_j in (1.1) are zero if the optical coefficients $e^{n\,opt}_j$, $e^{p\,opt}_j$ vanish (if no optical effects would occur).

For an analytical investigation we introduce the chemical activities $b_i = \frac{u_i}{\overline{u}_i}$, $i = 1,\dots,2l{+}2$, so that in the considered case of Boltzmann statistics the electrochemical potentials ζ_1, ζ_2 being the driving forces of the fluxes in the continuity equations for electrons and holes have the form $\zeta_i = \ln b_i + \lambda_i z$, $i = 1, 2$. Using the reaction coefficients

$$k_0 := r\overline{k}, \quad k^n_j := r^n_j\overline{k}^n_j\overline{u}_{2j+1}, \quad k^p_j := r^p_j\overline{k}^p_j\overline{u}_{2j+2}, \quad e^n_j := \frac{e^{n\,opt}_j}{\overline{k}^n_j}, \quad e^p_j := \frac{e^{p\,opt}_j}{\overline{k}^p_j}$$

the reaction rates in (1.1) take the form

$$\begin{aligned} R &= k_0(b_1b_2 - 1),\\ R^n_j &= k^n_j(b_1b_{2j+2} - (1 + e^n_j)b_{2j+1}),\\ R^p_j &= k^p_j(b_2b_{2j+1} - (1 + e^p_j)b_{2j+2}). \end{aligned}$$

The boundary $\partial\Omega$ of Ω splits up into a part Γ_D, representing the contacts of the device and a part Γ_N, where the device is insulated. We complete the model equations by boundary conditions for the Poisson equation and the continuity equations for electrons and holes

$$z = z^D, \;\; b_i = b^D_i \text{ on } \mathbb{R}_+ \times \Gamma_D, \quad \nu\cdot(\varepsilon\nabla z) = 0, \;\; \nu\cdot(D_iu_i\nabla\zeta_i) = 0 \text{ on } \mathbb{R}_+ \times \Gamma_N, \quad i = 1, 2,$$

and by initial conditions for the densities of all species

$$u_i(0) = U_i, \quad i = 1,\dots,2l + 2.$$

Remark 1.1 *The scaled quantities z, b_i, $\zeta_i = \ln b_i + \lambda_i z$, called in our mathematical model the electrostatic potential, chemical activity, and electrochemical potential, result from the original physical quantities φ – electrostatic potential, E_{F_n}, E_{F_p} – quasi Fermi energies of electrons and holes, q – electron charge, k_B – Boltzmann's constant, T – temperature by*

$$z = -\frac{q}{k_BT}\varphi, \quad \ln b_1 = \frac{E_{F_n} - q\varphi}{k_BT}, \quad \ln b_2 = \frac{-E_{F_p} + q\varphi}{k_BT}$$

(see e.g. [2, 20, 21]). Moreover, we use $\varepsilon = \frac{\varepsilon_0\varepsilon_r}{q^2}k_BT$, $D_1 = \mu_nk_BT$, $D_2 = \mu_pk_BT$, where ε_0, ε_r are the absolute and relative dielectric constant and μ_n, μ_p are the electron and hole mobilities.

Remark 1.2 *As already mentioned, our model is a generalization of the classical van Roosbroeck system [23] describing the motion of electrons and holes in a semiconductor* *device due to drift and diffusion within a self-consistent electrical field. Semiconductor device simulation is based on this model. First mathematical analysis for the transient system was done in [18], for more references see [6]. Recently [24] investigated existence and asymptotic behavior of solutions for the whole space situation. Global existence and uniqueness of weak solutions under physically realistic conditions in two space dimensions is achieved in [7]. In [15] the van Roosbroeck system is reformulated as an evolution equation for the potentials. In this setting a unique, local in time solution in Lebesgue spaces is available and leads to classical solutions to the drift-diffusion equations in the two-dimensional case.*

To handle the electronic model for solar cells including space and time resolved defect densities we profit from techniques approved for the van Roosbroeck system and combine them with new ideas.

The paper is organized as follows: In Section 2 we collect some notation, formulate our general assumptions and give a weak formulation (P) of the electronic model for solar cells including energy resolved defect densities. Section 3 contains analytical results and their proofs. Subsection 3.1 is devoted to the Poisson equation, in Subsection 3.2 we prove first properties of the solutions to (P), and Subsection 3.3 contains the uniqueness result. Energy estimates are presented in Subsection 3.4 and Subsection 3.5 deals with L^∞-estimates for the solution to (P). Section 4 is devoted to the existence proof for (P). For a regularized problem (P_M) introduced in Subsection 4.1 we show its solvability in Subsection 4.2. After establishing energy estimates (Subsection 4.3) and L^∞-estimates for solutions to (P_M) (Subsection 4.4) which are independent on the regularization level M, we prove in Subsection 4.5 the existence of a solution to (P). The Appendix collects analytical results from the literature being relevant in the treatment of our model equations.

2 Assumptions and weak formulation

2.1 Assumptions

Some notation. The notation of function spaces in the present paper corresponds to that in [16]. For a Banach space B we denote by B_+ the cone of non-negative elements and by B^* its dual space. We write u^+ (u^-) for the positive (negative) part of a function u. If $u \in \mathbb{R}^m$, $m = 2l + 2$, then $u \geq 0$ ($u > 0$) is to be understood as $u_i \geq 0\ \forall i$ ($u_i > 0\ \forall i$). If $u, w \in \mathbb{R}^m$ then $uw = \{u_i w_i\}_{i=1,\dots,m}$, and u/w is defined analogously, e^u is to understand as $\{\mathrm{e}^{u_i}\}_{i=1,\dots,m}$. If $u \in (0,\infty)^m$ then $\ln u = \{\ln u_i\}_{i=1,\dots,m}$. The abbreviation a.e. means $\mathcal{L}^d$-a.e., for the measures μ_i we write μ_i-a.e. The scalar product in $\mathbb{R}^d$ is indicated by a centered dot. Positive constants which depend only on the data of our problem are denoted by c.

Now we collect the general assumptions our analytical investigations are based on.

(A1) $\Omega \subset \mathbb{R}^2$ is a bounded Lipschitzian domain, Γ_D, Γ_N are disjoint open subsets of $\partial\Omega$, $\partial\Omega = \Gamma_D \cup \Gamma_N \cup (\overline{\Gamma_D} \cap \overline{\Gamma_N})$, mes $\Gamma_D > 0$, $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points ($\Omega \cup \Gamma_N$ is regular in the sense of Gröger [14]);

(A2) N_j generates Young like measures $\mu_{2j+1} = \mu_{2j+2} = N_j \mathrm{d}E$ on G, $j = 1, \dots, l$.
$\int_{E_G} \mu_i(x, \mathrm{d}E) \le \widehat{c}$ a.e. in Ω, $i = 3, \dots, 2l+2$;

(A3) $G_{phot} \in L^\infty(\mathbb{R}_+, L^\infty_+(\Omega))$, $\|G_{phot}(t)\|_{L^\infty} \le c$ f.a.a. $t \in \mathbb{R}_+$,
$k_0 : \Omega \times \mathbb{R}^2_+ \to \mathbb{R}_+$, $k_0(x, \cdot)$ Lipschitzian, uniformly w.r.t. $x \in \Omega$,
$k_0(\cdot, y)$ measurable for all $y \in \mathbb{R}^2_+$, $k_0(\cdot, 0) \in L^\infty(\Omega)$,
k^n_j, e^n_j, k^p_j, $e^p_j \in L^\infty_+(G; \mathrm{d}\mu_{2j+1})$, $j = 1, \dots, l$;

(A4) $\varepsilon \in L^\infty(\Omega)$, $\varepsilon \ge c > 0$, $f \in L^2(\Omega)$, $\overline{u}_i \in L^\infty(\Omega)$, $\overline{u}_i \ge \epsilon_0 > 0$ a.e. on Ω, $i = 1, 2$,
$\overline{u}_i \in L^\infty(G; \mathrm{d}\mu_i)$, $\overline{u}_i \ge \epsilon_0 > 0$ μ_i-a.e. on G, $i = 3, \dots, 2l+2$,
$b^D = (b^D_1, b^D_2, 0, \dots, 0)$, $\ln b^D_i$, $z^D \in W^{1,\infty}(\Omega)$, $u^D_i = \overline{u}_i b^D_i$, $i = 1, 2$;

(A5) $D_i \in L^\infty_+(\Omega)$, $D_i \overline{u}_i \ge \epsilon > 0$ a.e. on Ω, $i = 1, 2$;

(A6) $U_i \in L^\infty_+(\Omega)$, $i = 1, 2$, U_{2j+1}, $U_{2j+2} \in L^\infty(G; \mathrm{d}\mu_{2j+1})$,
$0 \le U_{2j+1}$, $U_{2j+2} \le 1$, $U_{2j+1} + U_{2j+2} = 1$ μ_{2j+1}-a.e. on G, $j = 1, \dots, l$.

Remark 2.1 *The assumptions in (A3) concerning k_0 allow it to include Shockley-Read-Hall as well as Auger generation/recombination processes. The assumptions (A2) - (A6) are well suited to cover the situation of model equations given in [20, Sect. 4.2] in the case of Boltzmann statistics for all species.*

2.2 Weak formulation

We introduce the function spaces

$$Y := L^2(\Omega)^2 \times \prod_{i=3}^{2l+2} L^2(G; d\mu_i) \qquad V := L^\infty(\Omega)^2 \times \prod_{i=3}^{2l+2} L^\infty(G; d\mu_i),$$
$$X := \{b \in Y : b_i \in H^1_0(\Omega \cup \Gamma_N),\ i = 1, 2\}, \qquad Z := H^1_0(\Omega \cup \Gamma_N)$$

and define the operators $\mathcal{B}\colon Y \to Y$, $\mathcal{A}\colon [(X + b^D) \cap V_+] \times (Z + z^D)] \to X^*$,
$\mathcal{R}\colon [X + b^D] \cap V_+ \to X^*$, and $\mathcal{P}\colon (Z + z^D) \times Y \to Z^*$ by

$$\mathcal{B}b := (\overline{u}_i\, b_i)_{i=1,\dots,2l+2},$$
$$\langle \mathcal{A}(b, z), \overline{b} \rangle_X := \int_\Omega \sum_{i=1}^{2} D_i \overline{u}_i (\nabla b_i + \lambda_i b_i \nabla z) \cdot \nabla \overline{b}_i \,\mathrm{d}x\,, \quad \overline{b} \in X,$$

$$\begin{aligned}\langle \mathcal{R}(b), \overline{b}\rangle_X :=& \sum_{j=1}^{l} \int_G k_j^n \big(b_1 b_{2j+2} - (1+e_j^n) b_{2j+1}\big)(\overline{b}_1 + \overline{b}_{2j+2} - \overline{b}_{2j+1}) \,\mathrm{d}\mu_{2j+1} \\ &+ \sum_{j=1}^{l} \int_G k_j^p \big(b_2 b_{2j+1} - (1+e_j^p) b_{2j+2}\big)(\overline{b}_2 + \overline{b}_{2j+1} - \overline{b}_{2j+2}) \,\mathrm{d}\mu_{2j+1} \\ &+ \int_\Omega \big\{k_0(b_1 b_2 - 1)(\overline{b}_1 + \overline{b}_2) - G_{phot}(\overline{b}_1 + \overline{b}_2)\big\} \,\mathrm{d}x, \quad \overline{b} \in X,\end{aligned}$$

$$\langle \mathcal{P}(z,u), \overline{z}\rangle_Z := \int_\Omega \Big\{\varepsilon \nabla z \cdot \nabla \overline{z} - \big[f + \sum_{i=1}^{2} \lambda_i u_i\big]\,\overline{z}\Big\} \,\mathrm{d}x - \sum_{i=3}^{2l+2} \int_G \lambda_i u_i \overline{z} \,\mathrm{d}\mu_i, \quad \overline{z} \in Z.$$

Then the weak formulation of the electronic model for solar cells with energy resolved defect densities reads as

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

3 Results

3.1 The Poisson equation

Lemma 3.1 *We assume* (A1), (A2), (A4). *For any $u \in Y$ there exists a unique solution $z \in Z + z^D$ to $\mathcal{P}(z,u) = 0$. Moreover there are constants $q > 2$ and $c > 0$ such that*

$$\|z - \widehat{z}\|_Z \le c\,\|u - \widehat{u}\|_Y \quad \forall u, \widehat{u} \in Y,\ \mathcal{P}(z,u) = \mathcal{P}(\widehat{z}, \widehat{u}) = 0, \tag{3.1}$$

$$\|z\|_{W^{1,q}} \le c\Big\{1 + \sum_{i=1}^{2} \|u_i\|_{L^{2q/(2+q)}} + \sum_{i=3}^{2l+2} \|u_i\|_{L^{2q/(2+q)}(G; d\mu_i)}\Big\} \quad \forall u \in Y,\ \mathcal{P}(z,u) = 0.$$

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

Proof. 1. We define the operator $\mathcal{P}_0 \colon Z \to Z^*$ and set for $u \in Y$ the quantity $g(u)$ as follows

$$\begin{aligned}\langle \mathcal{P}_0 y, \overline{y}\rangle_Z &= \int_\Omega \varepsilon \nabla y \cdot \nabla \overline{y} \,\mathrm{d}x, \quad \overline{y} \in Z, \\ \langle g(u), \overline{y}\rangle_Z &= \int_\Omega \Big\{\big(f + \sum_{i=1}^{2} \lambda_i u_i\big)\overline{y} - \varepsilon \nabla z^D \cdot \nabla \overline{y}\Big\} \,\mathrm{d}x + \sum_{i=3}^{2l+2} \lambda_i \int_\Omega \langle\langle u_i \rangle\rangle_i \overline{y} \,\mathrm{d}x, \quad \overline{y} \in Z.\end{aligned}$$

Clearly, $g(u) \in Z^*$, for the last summands we argue as follows: Because of (A2) we have

$$\begin{aligned}\int_\Omega \langle\langle u_i\rangle\rangle_i \overline{y}\,\mathrm{d}x = \int_G u_i \overline{y}\,\mathrm{d}\mu_i &\le \|u_i\|_{L^2(G;\mathrm{d}\mu_i)}\|\overline{y}\|_{L^2(G;\mathrm{d}\mu_i)} \\ &\le c\|u_i\|_{L^2(G;\mathrm{d}\mu_i)}\|\overline{y}\|_{L^2} \le c\|u_i\|_{L^2(G;\mathrm{d}\mu_i)}\|\overline{y}\|_Z, \quad \overline{y} \in Z.\end{aligned}$$

For $u \in Y$ the problem $\mathcal{P}(z,u) = 0$ may be written equivalently by $\mathcal{P}_0(z - z^D) = g(u)$. The operator $\mathcal{P}_0$ is Lipschitz continuous and strongly monotone. Therefore, for all right-hand sides $g(u) \in Z^*$ there is a unique solution to $\mathcal{P}_0(z - z^D) = g(u)$ and (3.1) follows immediately. As a direct consequence we obtain the result for the time dependent functions.

2. According to Gröger's regularity result for elliptic equations with mixed boundary conditions [14, Theorem 1] and (A4), (A1) we can fix a $q = q(\Omega, \varepsilon) > 2$ such that, if

$$\forall \overline{y} \in H_0^1(\Omega \cup \Gamma_N):\ \langle \mathcal{P}_0 y, \overline{y}\rangle_Z = \langle g, \overline{y}\rangle, \quad g \in W^{-1,q}(\Omega \cup \Gamma_N),\ y \in H_0^1(\Omega \cup \Gamma_N)$$

then $y \in W_0^{1,q}(\Omega \cup \Gamma_N)$. We set

$$r = \frac{2q}{q-2}, \quad r' = \frac{2q}{q+2}. \tag{3.2}$$

Note that $g(u) \in W^{-1,q}(\Omega \cup \Gamma_N)$. For the last summands we use again (A2):

$$\begin{aligned}\int_\Omega \langle\langle u_i\rangle\rangle_i \overline{y}\,\mathrm{d}x = \int_G u_i \overline{y}\,\mathrm{d}\mu_i &\le \|u_i\|_{L^{r'}(G;\mathrm{d}\mu_i)}\|\overline{y}\|_{L^r(G;\mathrm{d}\mu_i)} \\ &\le c\|u_i\|_{L^{r'}(G;\mathrm{d}\mu_i)}\|\overline{y}\|_{L^r} \le c\|u_i\|_{L^{r'}(G;\mathrm{d}\mu_i)}\|\overline{y}\|_{W^{1,q'}}.\end{aligned}$$

Gröger's regularity result for elliptic equation thus implies

$$\|z - z^D\|_{W_0^{1,q}} \le c\|g(u)\|_{W^{-1,q}} \le c\Big(1 + \sum_{i=1}^{2}\|u_i\|_{L^{r'}} + \sum_{i=3}^{2l+2}\|u_i\|_{L^{r'}(G;\mathrm{d}\mu_i)}\Big).$$

Especially, due to (A4) we can estimate

$$\|\nabla z\|_{L^q} \le \|z - z^D\|_{W_0^{1,q}} + \|\nabla z^D\|_{L^q} \le c\Big(1 + \sum_{i=1}^{2}\|u_i\|_{L^{r'}} + \sum_{i=3}^{2l+2}\|u_i\|_{L^{r'}(G;\mathrm{d}\mu_i)}\Big), \tag{3.3}$$

which finishes the proof. □

3.2 First properties of solutions to (P)

Remark 3.1 *If (u, b, z) is a solution to* (P) *then $u, b \in C(\mathbb{R}_+, Y)$. Thus, by Lemma 3.1 $z - z^D \in C(\mathbb{R}_+, Z)$. These properties ensure for all $t \in \mathbb{R}_+$*

$$\mathcal{P}(z(t), u(t)) = 0 \text{ in } Z^*, \quad u_i(t) = \overline{u}_i\, b_i(t) \text{ in } L^\infty(\Omega), \quad u_i(t) \ge 0 \text{ a.e. on } \Omega, \quad i = 1, 2;$$

$$u_i(t) = \overline{u}_i\, b_i(t) \text{ in } L^\infty(G; d\mu_i), \quad u_i(t) \ge 0\ \mu_i\text{-a.e. on } G \quad i = 3, \ldots, 2l+2.$$

Lemma 3.2 *We assume* (A1) – (A6)*. If* (u, b, z) *is a solution to* (P) *then*

$$\forall t \in \mathbb{R}_+ : \quad u_{2j+1}(t) + u_{2j+2}(t) = U_{2j+1} + U_{2j+2} = 1 \quad \mu_{2j+1}\text{-a.e. on } G,$$
$$0 \le u_{2j+1}(t),\, u_{2j+2}(t) \le 1 \quad \mu_{2j+1}\text{-a.e. on } G, \quad j = 1, \dots, l.$$

Proof. Let $B_s^G(y)$ denote the intersection of G and the ball centered at y with radius s. Let $\chi_{B_s^G(y)}$ be the characteristic function of $B_s^G(y)$, and let $i = 2j+1$, where $j \in \{1, \dots, l\}$ is arbitrarily chosen. Then we obtain for μ_i-a.a. $y = (x, E)$ in G by using for (P) the test function being $\mu_i(B_s^G(y))^{-1}\, \chi_{B_s^G(y)}$ in the ith and $(i+1)$th component and all other components being zero

$$\frac{1}{\mu_i(B_s^G(y))} \int_{B_s^G(y)} \big(u_i(t,z) + u_{i+1}(t,z)\big)\, \mathrm{d}\mu_i = \frac{1}{\mu_i(B_s^G(y))} \int_{B_s^G(y)} \big(U_i(z) + U_{i+1}(z)\big)\, \mathrm{d}\mu_i.$$

Taking the limit $s \downarrow 0$ gives the first desired result. Remark 3.1 guarantees us that $u_i,\, u_{i+1} \ge 0$ μ_i-a.e. on G. Together with the first invariance result we obtain that $u_i,\, u_{i+1} \le 1$, $b_i \le \overline{u}_i^{-1}$, $b_{i+1} \le \overline{u}_{i+1}^{-1}$ μ_i-a.e. on G. □

3.3 Uniqueness

Theorem 3.1 *Under the assumptions* (A1) – (A6) *there exists at most one solution to* (P).

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

$$\|u^k(t)\|_V,\ \|b^k(t)\|_V,\ \|\nabla z^k(t)\|_{L^q} \le c \text{ f.a.a. } t \in S\,,\ k = 1, 2,$$

where $q > 2$ (cf. (3.3)). Let $\widetilde{z} := z^1 - z^2$, $\widetilde{b} := b^1 - b^2$. Due to (3.1) we obtain

$$\|\widetilde{z}(t)\|_{H^1} \le c\|\widetilde{b}(t)\|_Y \quad \text{f.a.a. } t \in S. \tag{3.4}$$

We use $\widetilde{b} \in L^2(S, X)$ as test function for (P) and take into account that the reaction rates are uniformly locally Lipschitz continuous in the state variable. With the Gagliardo-Nirenberg inequality $\|\widetilde{b}_i\|_{L^r} \le \|\widetilde{b}_i\|_{L^2}^{2/r} \|\widetilde{b}_i\|_{H^1}^{1-2/r}$ for r from (3.2) and $i = 1, 2$, with inequality (3.4), and with Young's inequality we conclude as follows

$$\begin{aligned}
&\|\widetilde{b}(t)\|_Y^2 + \sum_{i=1}^{2} \int_0^t \|\widetilde{b}_i\|_{H^1}^2 \mathrm{d}s \\
&\quad \le c \int_0^t \Big\{ \sum_{i=1}^{2} \Big\{ \|\widetilde{b}_i\|_{L^r} \|\nabla z^1\|_{L^q} \|\nabla \widetilde{b}_i\|_{L^2} + \|\nabla \widetilde{z}\|_{L^2} \|\nabla \widetilde{b}_i\|_{L^2} \Big\} + \|\widetilde{b}\|_Y^2 \Big\} \mathrm{d}s \\
&\quad \le \int_0^t \Big\{ \sum_{i=1}^{2} \Big\{ \tfrac{1}{4} \|\widetilde{b}_i\|_{H^1}^2 + c\|\widetilde{b}_i\|_{L^2}^{2/r} \|\nabla z^1\|_{L^q} \|\widetilde{b}_i\|_{H^1}^{2-2/r} \Big\} + c\|\widetilde{b}\|_Y^2 \Big\} \mathrm{d}s \\
&\quad \le \int_0^t \Big\{ \sum_{i=1}^{2} \Big\{ \tfrac{1}{2} \|\widetilde{b}_i\|_{H^1}^2 + c\|\nabla z^1\|_{L^q}^r \|\widetilde{b}_i\|_{L^2}^2 \Big\} + c\|\widetilde{b}\|_Y^2 \Big\} \mathrm{d}s \\
&\quad \le \int_0^t \Big\{ \sum_{i=1}^{2} \tfrac{1}{2} \|\widetilde{b}_i\|_{H^1}^2 + c\|\widetilde{b}\|_Y^2 \Big\} \mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

Gronwall's lemma yields $\widetilde{b} = 0$ on S. With (3.4) the assertion follows. □

3.4 Energy estimates

We define the functionals $\widetilde{F}_1$, $\widetilde{F}_2 \colon Y_+ \to \mathbb{R}$,

$$\widetilde{F}_1(u) := \int_\Omega \frac{\varepsilon}{2} |\nabla(z - z^D)|^2 \,\mathrm{d}x,$$

$$\begin{aligned}\widetilde{F}_2(u) &:= \int_\Omega \sum_{i=1}^{2} \int_{u_i^D}^{u_i} \ln \frac{y}{u_i^D} \,\mathrm{d}y \,\mathrm{d}x + \sum_{i=3}^{2l+2} \int_G \int_{\overline{u}_i}^{u_i} \ln \frac{y}{\overline{u}_i} \,\mathrm{d}y \,\mathrm{d}\mu_i \\ &= \int_\Omega \sum_{i=1}^{2} \{u_i(\ln \frac{u_i}{u_i^D} - 1) + u_i^D\} \,\mathrm{d}x + \sum_{i=3}^{2l+2} \int_G \{u_i(\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i\} \,\mathrm{d}\mu_i,\end{aligned}$$

where z is the solution to $\mathcal{P}(z, u) = 0$ (see Lemma 3.1). The value $\widetilde{F}_1(u) + \widetilde{F}_2(u)$ can be interpreted as free energy of the state u. Because of (A4) we find the estimate

$$\widetilde{F}_1(u)+\widetilde{F}_2(u) \geq c\Big(\|z - z^D\|_Z^2 + \sum_{i=1}^{2} \|u_i \ln u_i\|_{L^1} + \sum_{i=3}^{2l+2} \|u_i \ln u_i\|_{L^1(G,\mathrm{d}\mu_i)}\Big) - \widetilde{c}, \quad u \in Y_+.$$

Let $u, \widetilde{u} \in Y_+$ and $\mathcal{P}(z, u) = \mathcal{P}(\widetilde{z}, \widetilde{u}) = 0$. Using that $\langle \mathcal{P}(z, u), \widetilde{z} - z^D\rangle_Z = 0$ and $\langle \mathcal{P}(\widetilde{z}, \widetilde{u}), \widetilde{z} - z^D\rangle_Z = 0$ we calculate

$$\begin{aligned}\widetilde{F}_1(u) - \widetilde{F}_1(\widetilde{u}) &= \int_\Omega \Big\{\frac{\varepsilon}{2}|z - \widetilde{z}|^2 + \sum_{i=1}^{2} \lambda_i(u_i - \widetilde{u}_i)(\widetilde{z}-z^D)\Big\} \,\mathrm{d}x + \sum_{i=3}^{2l+2} \lambda_i(u_i - \widetilde{u}_i)(\widetilde{z}-z^D) \,\mathrm{d}\mu_i \\ &\geq c\|\widetilde{z} - z^D\|_Z^2 + \langle \lambda(\widetilde{z} - z^D), u - \widetilde{u}\rangle_Y \geq \langle \lambda(\widetilde{z} - z^D), u - \widetilde{u}\rangle_Y.\end{aligned}$$

The functional $\widetilde{F}_1$ is convex and continuous on the convex set Y_+. Due to the properties of the integrand in $\widetilde{F}_2$ (see [4]) the same is true for $\widetilde{F}_2$. By setting $\widetilde{F}_k(u) = +\infty$ for $u \in Y \setminus Y_+$ we extend $\widetilde{F}_k$ to Y and obtain proper, convex and lower semicontinuous functionals $\widetilde{F}_k : Y \to \overline{\mathbb{R}}$, $k = 1, 2$. $\widetilde{F}_1$ is subdifferentiable in all $u \in Y_+$ and $\lambda(z - z^D) \in \partial\widetilde{F}_1(u)$ where $\mathcal{P}(u, z) = 0$. Since $x \ln \frac{x}{y} - x + y \geq 0$ for $x \geq 0$, $y > 0$ we find for $u, \widetilde{u} \in Y_+$ with $\widetilde{u} \geq \delta$ that

$$\begin{aligned}\widetilde{F}_2(u) - \widetilde{F}_2(\widetilde{u}) &= \sum_{i=1}^{2} \int_\Omega \big\{(u_i - \widetilde{u}_i) \ln \frac{\widetilde{b}_i}{b_i^D} + u_i \ln \frac{u_i}{\widetilde{u}_i} - u_i + \widetilde{u}_i\big\} \,\mathrm{d}x \\ &\quad + \sum_{i=3}^{2l+2} \int_G \big\{(u_i - \widetilde{u}_i) \ln \widetilde{b}_i + u_i \ln \frac{u_i}{\widetilde{u}_i} - u_i + \widetilde{u}_i\big\} \,\mathrm{d}\mu_i \qquad (3.5) \\ &\geq \sum_{i=1}^{2} \int_\Omega (u_i - \widetilde{u}_i) \ln \frac{\widetilde{b}_i}{b_i^D} \,\mathrm{d}x + \sum_{i=3}^{2l+2} \int_G (u_i - \widetilde{u}_i) \ln \widetilde{b}_i \,\mathrm{d}\mu_i.\end{aligned}$$

Therefore, in arguments $u \in Y_+$ with $u \geq \delta$ the functional $\widetilde{F}_2$ is subdifferentiable and $(\ln \frac{b_1}{b_1^D}, \ln \frac{b_2}{b_2^D}, \ln b_3, \ldots, \ln b_{2l+2}) \in \partial\widetilde{F}_2(u)$ where $u = \mathcal{B}b$.

Next, we extend $\widetilde{F}_k$, $k = 1, 2$, to the space X^* by the definition

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

Here the star denotes the conjugation (see [4]). Following the ideas of a precise derivation (for a slightly different situation) in [9, Lemma 8.12] we find that the free energy functional $F := F_1 + F_2$ is proper, convex and lower semicontinuous. For $u \in Y_+$ the relation $F(u) = \widetilde{F}_1(u) + \widetilde{F}_2(u)$ is fulfilled, $F|_{Y_+}$ is continuous. Moreover, if $u \in Y_+$, $u > \delta$ and $(\ln \frac{b_1}{b_1^D}, \ln \frac{b_2}{b_2^D}, \ln b_3, \ldots, \ln b_{2l+2}) \in X$, then

$$\lambda(z - z^D) + \big(\ln \frac{b_1}{b_1^D}, \ln \frac{b_2}{b_2^D}, \ln b_3, \ldots, \ln b_{2l+2}\big) \in \partial F(u), \quad \text{where } u = \mathcal{B}b.$$

Theorem 3.2 *We assume* (A1) – (A6)*. Let* (u, b, z) *be a solution to* (P) *and* $T \in \mathbb{R}_+$*. Then*

$$F(u(t)) \le (F(U) + c_0)e^{c_0 t} \quad \forall t \in [0, T],$$

where $c_0 > 0$ *is a constant independent of* U *and* T*. Moreover, if* $\ln b_i^D + \lambda_i z^D$*,* $i = 1, 2$*, are spatially constant, if* $G_{phot} = 0$*, and if* $b_1^D b_2^D = 1$*,* $1 + e_j^n = b_1^D$*,* $1 + e_j^p = b_2^D$*,* $j = 1, \ldots, l$*, then* c_0 *can be chosen as zero.*

Proof. 1. Let

$$0 < \delta < \min\big\{ \min_{i=1,2}\{\operatorname*{ess\,inf}_{\Omega} \frac{U_i}{\overline{u}_i}, \operatorname*{ess\,inf}_{\Omega} b_i^D\}, \min_{i=3,\ldots,2l+2}\{\operatorname*{ess\,inf}_{G,\mu_i} \frac{U_i}{\overline{u}_i}\}\big\} \tag{3.6}$$

and $b^\delta = \max\{b, \delta\}$. Analogously to $\widetilde{F}_2$ and F_2 we define functionals $\widetilde{F}_2^\delta \colon Y_+ \to \mathbb{R}$ and $F_2^\delta \colon X^* \to \overline{\mathbb{R}}$ by

$$\widetilde{F}_2^\delta(u) := \int_\Omega \sum_{i=1}^{2} \int_{u_i^D}^{u_i} \big(\ln \max\{\frac{y}{\overline{u}_i}, \delta\} - \ln b_i^D\big) \, \mathrm{d}y \, \mathrm{d}x + \sum_{i=3}^{2l+2} \int_G \int_{\overline{u}_i}^{u_i} \ln \max\{\frac{y}{\overline{u}_i}, \delta\} \, \mathrm{d}y \, \mathrm{d}\mu_i$$

and $F_2^\delta := (\widetilde{F}_2^{\delta\,*}|_X)^*$. One calculates for $u \in Y_+$ that

$$w^\delta := \big(\ln \frac{b_1^\delta}{b_1^D}, \ln \frac{b_2^\delta}{b_2^D}, \ln b_3^\delta, \ldots, \ln b_{2l+2}^\delta\big) \in \partial F_2^\delta(u).$$

Due to the choice of δ we have $F_2^\delta(U) = F_2(U)$. Let (u, b, z) be a solution to (P), $S = [0, T]$. Then u, $b \ge 0$, $u \in H^1(S, X^*)$, $z - z^D \in L^2(S, Z)$, $\ln b_i^\delta - \ln b_i^D \in L^2(S, H_0^1(\Omega \cup \Gamma_N))$, $i = 1, 2$, and $\ln b_i^\delta \in L^2(G, \mathrm{d}\mu_i)$, $i = 3, \ldots, 2l + 2$. Moreover, f.a.a. $t \in S$

$$\lambda(z(t) - z^D) \in \partial F_1(u(t)), \quad w^\delta(t) \in \partial F_2^\delta(u(t)).$$

By Lemma 5.1 in the Appendix we conclude that the mappings $t \mapsto F_1(u(t))$, $t \mapsto F_2^\delta(u(t))$ are absolutely continuous on S and

$$\frac{\mathrm{d}}{\mathrm{d}t} F_1(u(t)) = \langle u'(t), \lambda(z(t) - z^D)\rangle_X, \quad \frac{\mathrm{d}}{\mathrm{d}t} F_2^\delta(u(t)) = \langle u'(t), w^\delta(t)\rangle_X \quad \text{f.a.a. } t \in S$$

and we obtain with $\zeta^\delta = w^\delta + \lambda(z - z^D)$ that

$$F_1(u(t)) + F_2^\delta(u(t)) - F_1(U) - F_2(U) = \int_0^t \langle u'(s), \zeta^\delta(s)\rangle_X \, \mathrm{d}s. \tag{3.7}$$

2. In view of the evolution equation we find for the integrand in (3.7)

$$\begin{aligned}\langle u'(s), \zeta^\delta(s)\rangle_X &= -\langle \mathcal{A}(b(s), z(s)) + \mathcal{R}(b(s)), \zeta^\delta(s)\rangle_X \\ &= -\langle \mathcal{A}(b^\delta(s), z(s)) + \mathcal{R}(b^\delta(s)), \zeta^\delta(s)\rangle_X + \theta^\delta(s)\end{aligned}$$

where

$$\theta^\delta := \langle \mathcal{A}(b^\delta, z) - \mathcal{A}(b, z) + \mathcal{R}(b^\delta) - \mathcal{R}(b), \zeta^\delta\rangle_X \to 0 \quad \text{for } \delta \downarrow 0.$$

The convergence $F_2^\delta(u) \to F_2(u)$ for $\delta \downarrow 0$ if $u \in Y_+$ ensures that

$$\Theta^\delta := \int_0^t \theta^\delta(s)\,\mathrm{d}s - F_1(u(s))|_0^t - F_2^\delta(u(s))|_0^t \to -F(u(s))|_0^t \quad \text{for } \delta \downarrow 0.$$

Additionally, because of (A4), (A5) we have

$$\begin{aligned}\langle \mathcal{A}(b^\delta, z), \zeta^\delta\rangle_X &= \sum_{i=1}^2 \int_\Omega D_i\overline{u}_i(\nabla b_i^\delta + \lambda_i b_i^\delta \nabla z)\cdot\nabla(\ln b_i^\delta + \lambda_i z - \ln b_i^D - \lambda_i z^D)\,\mathrm{d}x \\ &= \sum_{i=1}^2 D_i\overline{u}_i b_i^\delta\Big\{|\nabla(\ln b_i^\delta + \lambda_i z)|^2 - \nabla(\ln b_i^\delta + \lambda_i z)\cdot\nabla(\ln b_i^D + \lambda_i z^D)\Big\}\,\mathrm{d}x \\ &\geq -c\sum_{i=1}^2 \|b_i^\delta\|_{L^1}\|\nabla(\ln b_i^D + \lambda_i z^D)\|_{L^\infty}^2.\end{aligned}$$

Concerning the reaction terms, using $(x-y)(\ln x - \ln y) \geq 0$ for $x, y > 0$, using (A3), (A4), Lemma 3.2 and a case by case analysis for iii) we obtain

i) $k_j^n\big(b_1^\delta b_{2j+2}^\delta - (1+e_j^n)b_{2j+1}^\delta\big)\ln\frac{b_1^\delta b_{2j+2}^\delta}{b_1^D b_{2j+1}^\delta} \geq -c(|b_1^\delta|+1)|\ln\frac{1+e_j^n}{b_1^D}|, \quad j = 1,\dots,l,$

ii) $k_j^p\big(b_2^\delta b_{2j+1}^\delta - (1+e_j^p)b_{2j+2}^\delta\big)\ln\frac{b_2^\delta b_{2j+1}^\delta}{b_2^D b_{2j+2}^\delta} \geq -c(|b_2^\delta|+1)|\ln\frac{1+e_j^p}{b_2^D}|, \quad j = 1,\dots,l,$

iii) $(b_1^\delta b_2^\delta - 1)\ln\frac{b_1^\delta b_2^\delta}{b_1^D b_2^D} \geq -c|\ln b_1^D b_2^D|,$

iv) $G_{phot}\big(\ln\frac{b_i^\delta}{b_i^D} + \lambda_i(z - z^D)\big) \leq |G_{phot}|\big(|b_i^\delta| + |\ln b_i^D| + |z - z^D|\big),\ i = 1, 2.$

Taking additionally into account the Lipschitz continuity of k_0 we find

$$\begin{aligned}&\langle \mathcal{R}(b^\delta), w^\delta + \lambda(z - z^D)\rangle_X \geq \\ &-c(1+\sum_{i=1}^2\|b_i^\delta\|_{L^1})\Big(\|\ln b_1^D b_2^D\|_{L^\infty} + \sum_{j=1}^l\Big\{\|\ln\tfrac{1+e_j^n}{b_1^D}\|_{L^\infty(G;\mathrm{d}\mu_{2j+1})} + \|\ln\tfrac{1+e_j^p}{b_2^D}\|_{L^\infty(G;\mathrm{d}\mu_{2j+2})}\Big\}\Big) \\ &-\|G_{phot}\|_{L^\infty}\Big\{\sum_{i=1}^2\big(\|b_i^\delta\|_{L^1} + \|\ln b_i^D\|_{L^1}\big) + \|z - z^D\|_{L^1}\Big\}.\end{aligned}$$

3. In summary, according to the previous discussions, the limit $\delta \downarrow 0$ in (3.7) leads to

$$\begin{aligned} & F(u(t)) - F(U) \\ & \le c \int_0^t \sum_{i=1}^2 (1+\|b_i\|_{L^1}) \Big(\|\nabla(b_i^D + \lambda_i z^D)\|_{L^\infty}^2 + \|\ln b_1^D b_2^D\|_{L^\infty} \\ & \qquad + \sum_{j=1}^l \Big\{ \|\ln \tfrac{1+e_j^n}{b_1^D}\|_{L^\infty(G,\mathrm{d}\mu_{2j+1})} + \|\ln \tfrac{1+e_j^p}{b_2^D}\|_{L^\infty(G,\mathrm{d}\mu_{2j+1})} \Big\} \Big) \,\mathrm{d}s \\ & \quad + \int_0^t \|G_{phot}\|_{L^\infty} \Big\{ \sum_{i=1}^2 \big(\|b_i\|_{L^1} + \|\ln b_i^D\|_{L^1} \big) + \|z - z^D\|_{L^1} \Big\} \,\mathrm{d}s. \end{aligned}$$

If $\ln b_i^D + \lambda_i z^D$, $i = 1, 2$, are spatially constant, if $G_{phot} = 0$, and if $b_1^D b_2^D = 1$, $1 + e_j^n = b_1^D$, $1 + e_j^p = b_2^D$, $j = 1, \ldots, l$, then the right-hand side of the previous estimate is zero. Therefore the last assertion of the theorem follows immediately.

In the more general case we proceed as follows: Using (A3), (A4) the last line in the previous estimate can be majorized by

$$c \int_0^t \Big(\sum_{i=1}^2 \|b_i\|_{L^1} + \|z - z^D\|_Z^2 + 1 \Big) \,\mathrm{d}s.$$

Additionally, since $\sum_{i=1}^2 \|b_i\|_{L^1} + \|z - z^D\|_Z^2 \le cF(u) + c$ for $u = \mathcal{B}b$, $\mathcal{P}(z, u) = 0$ and since (A3) and (A4) guarantee that the L^∞-norms on the right-hand side in the estimate for $F(u(t)) - F(U)$ are bounded, we can apply Gronwall's lemma to finish the proof. □

Remark 3.2 *Theorem 3.2 guarantees that the weak formulation (P) of the electronic model for a solar cell with energy resolved defect densities is thermodynamically correct. The free energy functional F is something like a Lyapunov function for the solution (u, b, z) to (P). Namely, under the special assumptions on the data that $G_{phot} = 0$ and $\ln b_i^D + \lambda_i z^D$, $i = 1, 2$, are spatially constant and $b_1^D b_2^D = 1$, $1 + e_j^n = b_1^D$, $1 + e_j^p = b_2^D$, $j = 1, \ldots, l$, (meaning the absence of external sources) the function $t \mapsto F(u(t))$ is monotonously decreasing. For the more general case of data which is of interest in the treatment of realistic solar cells, the free energy may be increasing, but its growth can be estimated by Theorem 3.2.*

3.5 L^∞-estimates of the solution

Lemma 3.2 provides global upper and lower bounds for u_i and b_i, $i = 3, \ldots, 2l + 2$. To achive upper bounds for densities and chemical activities of electrons and holes we proceed in two steps. We start with estimates of the $L^2(\mathbb{R}_+, L^2)$-norm of the chemical activities b_i, $i = 1, 2$. Then the final estimate results from Moser iteration arguments.

Lemma 3.3 *Let* (A1) – (A6) *be satisfied. Then there exists a monotonous function $d : \mathbb{R}_+ \to \mathbb{R}_+$ depending only on the data (but not on T) such that*

$$\sum_{i=1}^2 \|u_i(t)\|_{L^2} \le d(\|F(u)\|_{C(S)}) \quad \forall t \in S = [0, T]$$

for any solution (u, b, z) *to* (P).

Proof. We use the test function $\mathrm{e}^{2t}(v_1, v_2, 0, \dots, 0)$,

$$v_i := (b_i - K)^+, \quad \text{where } K \geq \widehat{K} := \max\Big(1, \|U/\overline{u}\|_V, \max_{i=1,2} \|b_i^D\|_{L^\infty}\Big) \tag{3.8}$$

will be fixed later. Due to the choice of $\widehat{K}$ we have $v_i(0) = 0$, $v_i|_{\Gamma_D} = 0$, $i = 1, 2$.

$$\begin{aligned}
&\frac{\mathrm{e}^{2t}}{2} \sum_{i=1}^{2} \int_\Omega \overline{u}_i v_i(t)^2 \, \mathrm{d}x \\
&= \int_0^t \mathrm{e}^{2s} \Big\{ \int_\Omega \Big\{ \sum_{i=1}^{2} \big(\overline{u}_i v_i^2 - D_i \overline{u}_i (\nabla v_i + \lambda_i b_i \nabla z) \cdot \nabla v_i\big) + G_{phot}(v_1 + v_2) \\
&\qquad\qquad + k_0(\cdot, b_1, b_2)(1 - b_1 b_2)(v_1 + v_2)\Big\} \, \mathrm{d}x \\
&\quad + \sum_{j=1}^{l} \int_G \Big\{ k_j^n((1 + e_j^n) b_{2j+1} - b_1 b_{2j+2}) v_1 + k_j^p((1 + e_j^p) b_{2j+2} - b_2 b_{2j+1}) v_2 \Big\} \, \mathrm{d}\mu_{2j+1} \Big\} \mathrm{d}s \\
&\leq \int_0^t \mathrm{e}^{2s} \sum_{i=1}^{2} \big\{ - \epsilon \|v_i\|_{H^1}^2 + c\|b_i\|_{L^r} \|\nabla z\|_{L^q} \|v_i\|_{H^1} + c\|v_i\|_{L^2}^2 + cK^2 \big\} \, \mathrm{d}s.
\end{aligned}$$

Here the exponent $q > 2$ is taken from Lemma 3.1. Concerning the reaction terms we refer to (A3) and Lemma 3.2. Additionally, we exploited that, due to (A2), $\|v_i\|_{L^2(G, \mathrm{d}\mu_{2j+1})} \leq c\|v_i\|_{L^2(\Omega)}$, $i = 1, 2$, $j = 1, \dots, l$. Now we use (3.3) and the three variants of the Gagliardo-Nirenberg estimate

$$\|v_i\|_{L^2}^2 \leq \|v_i\|_{L^1} \|v_i\|_{H^1}, \qquad \|v_i\|_{L^r} \leq \|v_i\|_{L^1}^{1/r} \|v_i\|_{H^1}^{1/r'}, \qquad \|v_i\|_{L^{r'}} \leq \|v_i\|_{L^1}^{1/r'} \|v_i\|_{H^1}^{1/r},$$

where r and r' are defined in (3.2). Then Young's inequality leads to

$$\begin{aligned}
\frac{e^{2t}}{2} \epsilon_0 \sum_{i=1}^{2} \|v_i(t)\|_{L^2}^2 \leq \int_0^t \mathrm{e}^{2s} \sum_{i=1}^{2} \Big\{ \big(- \frac{\epsilon}{2} + \widetilde{c} \sum_{j=1}^{2} \|v_j\|_{L^1} \big) \|v_i\|_{H^1}^2 \\
+ c(K) \big(\|v_i\|_{L^1}^2 + 1 \big) \Big\} \mathrm{d}s
\end{aligned} \tag{3.9}$$

for all $t \in S$ with a monotonously increasing function $c(K)$. For K fulfilling the inequality $\ln K > \max_{i=1,2} \|\ln b_i^D\|_{L^\infty} + 1$ we can estimate

$$\begin{aligned}
F(u) &\geq \sum_{i=1}^{2} \int_\Omega \big\{ u_i(\ln b_i - \ln b_i^D - 1) + \overline{u}_i b_i^D \big\} \, \mathrm{d}x \\
&\geq \sum_{i=1}^{2} \int_{\{x : v_i = (b_i - K)^+ > 0\}} u_i(\ln K - \max_{k=1,2} \|\ln b_k^D\|_{L^\infty} - 1) \, \mathrm{d}x \\
&\geq (\ln K - \max_{k=1,2} \|\ln b_k^D\|_{L^\infty} - 1) \epsilon_0 \sum_{i=1}^{2} \|v_i\|_{L^1}
\end{aligned}$$

with ϵ_0 from (A4). Fixing now $K \geq \widehat{K}$ as a monotonously increasing function of $\|F(u)\|_{C(S)}$ fulfilling

$$\widetilde{c}\sum_{i=1}^{2}\|v_i\|_{L^1} \leq \quad \frac{\widetilde{c}\|F(u)\|_{C(S)}}{\epsilon_0(\ln K - \max_{k=1,2}\|\ln b_k^D\|_{L^\infty} - 1)} < \frac{\epsilon}{2}$$

(see Theorem 3.2), the term in front of the H^1-norm in (3.9) is negative. We obtain

$$\mathrm{e}^{2t}\sum_{i=1}^{2}\|v_i(t)\|_{L^2}^2 \leq \mathrm{e}^{2t}\, c\, c(K)(\|F(u)\|_{C(S)}^2 + 1).$$

Together with $u_i \leq \overline{u}_i(v_i + K)$ this proves the lemma. □

Remark 3.3 *Applying Lemma 3.1, Lemma 3.3 and Lemma 3.2, we find that for solutions* (u, b, z) *to (P) for all* $t \in S$ *the norm* $\|z(t)\|_{W^{1,q}(\Omega)}$ *is bounded by a continuous function of* $\|F(u)\|_{C(S)}$ *depending on the data but not on* T*. The exponent* $q > 2$ *is guaranteed by Lemma 3.1.*

We use the abbreviation

$$\kappa = \Big(\|\nabla z\|_{L^\infty(S,L^q(\Omega))} + 1\Big)^{2r}. \tag{3.10}$$

Theorem 3.3 *Let* (A1) – (A6) *be satisfied. Then there exist constants* $c > 0$ *and a continuous function* d *of* $\|F(u)\|_{C(S)}$ *depending only on the data* (*but not on* T) *such that*

$$\sum_{i=1}^{2}\|u_i(t)\|_{L^\infty}, \sum_{i=1}^{2}\|b_i(t)\|_{L^\infty} \leq c\,\kappa\sum_{i=1}^{2}\Big(\sup_{s\in S}\|u_i(s)\|_{L^1} + 1\Big),$$
$$\|z(t)\|_{L^\infty} \leq d(\|F(u)\|_{C(S)}) \qquad \forall t \in S$$

for any solution (u, b, z) *to* (P).

Proof. 1. The proof uses Moser iteration techniques. Such techniques are e.g. applied in [7] to the classical van Roosbroeck system, in [10] to spin-polarized drift-diffusion systems and in [11] to problems from semiconductor technology. Let $v_i := (b_i - \widehat{K})^+$, $i = 1, 2$, with $\widehat{K}$ from (3.8). By the test functions $\beta\,\mathrm{e}^{\beta t}\,(v_1^{\beta-1}, v_2^{\beta-1}, 0, \dots, 0) \in L^2(S, X)$, $\beta = 2^m$, $m \geq 1$, we obtain

$$\begin{aligned}
&\mathrm{e}^{\beta t}\sum_{i=1}^{2}\int_\Omega \overline{u}_i v_i(t)^\beta\,\mathrm{d}x \\
&= \int_0^t \beta\mathrm{e}^{\beta s}\Big\{\int_\Omega\Big\{\sum_{i=1}^{2}\big(\overline{u}_i v_i^\beta - D_i\overline{u}_i(\nabla v_i + \lambda_i b_i\nabla z)\cdot\nabla v_i^{\beta-1}\big) + G_{phot}(v_1^{\beta-1} + v_2^{\beta-1}) \\
&\qquad + k_0(\cdot, b_1, b_2)(1 - b_1 b_2)(v_1^{\beta-1} + v_2^{\beta-1})\Big\}\,\mathrm{d}x \\
&\quad + \sum_{j=1}^{l}\int_G\Big\{k_j^n((1+e_j^n)b_{2j+1} - b_1 b_{2j+2})v_1^{\beta-1} + k_j^p((1+e_j^p)b_{2j+2} - b_2 b_{2j+1})v_2^{\beta-1}\Big\}\,\mathrm{d}\mu_{2j+1}\Big\}\mathrm{d}s.
\end{aligned}$$

2. Having in mind (A3), (A4), (A2) and Lemma 3.2, applying Hölder's, Gagliardo-Nirenberg's and Young's inequality we proceed as follows

$$\begin{aligned}\epsilon_0\,\mathrm{e}^{\beta t}\sum_{i=1}^{2}\|v_i(t)\|_{L^\beta}^{\beta} &\le \int_0^t \mathrm{e}^{\beta s}\int_\Omega\sum_{i=1}^{2}\Big\{c\beta\big(b_i|\nabla z||\nabla v_i^{\beta-1}|+|v_i|^\beta+(\sum_{k=1}^{2}b_k+1)v_i^{\beta-1}\big)\\ &\qquad\qquad -\epsilon|\nabla v_i^{\beta/2}|^2\Big\}\,\mathrm{d}x\,\mathrm{d}s\\ &\le \int_0^t \mathrm{e}^{\beta s}\sum_{i=1}^{2}\Big\{c\beta\big(\|\nabla z\|_{L^q}(\|v_i^{\beta/2}\|_{L^r}+1)\|v_i^{\beta/2}\|_{H^1}\\ &\qquad\qquad + c\beta\big(\|v_i^{\beta/2}\|_{L^2}^2+1\big)-\epsilon\|v_i^{\beta/2}\|_{H^1}^2\Big\}\,\mathrm{d}s\\ &\le \int_0^t \mathrm{e}^{\beta s}\Big\{\kappa\, c\,\beta^{2r}\sum_{i=1}^{2}(\|v_i^{\beta/2}\|_{L^1}^2+1)\,\mathrm{d}s\Big\}\end{aligned}$$

with κ from (3.10). This guarantees the estimate

$$\sum_{i=1}^{2}\|v_i(t)\|_{L^\beta}^{\beta}\le c\beta^{2r}\kappa\sum_{i=1}^{2}\sup_{s\in S}(\|v_i(s)\|_{L^{\beta/2}}^{\beta}+1)\qquad \forall t\in S. \tag{3.11}$$

3. With the definition

$$\alpha_m=\sum_{i=1}^{2}\Big\{\sup_{s\in S}\|v_i(s)\|_{L^{2^m}}^{2^m}+1\Big\},\quad m=0,1,\ldots$$

(3.11) leads to

$$\alpha_m\le c^m\,\kappa\,\alpha_{m-1}^2\le c^{m+2(m-1)}\,\kappa^{1+2}\,\alpha_{m-2}^4\le\cdots\le c^{2^{m+1}-2-m}\,\kappa^{2^m-1}\,\alpha_0^{2^m},$$

and we continue estimate (3.11) by

$$\sum_{i=1}^{2}\|v_i(t)\|_{L^{2^m}}\le c\kappa\sum_{i=1}^{2}\Big\{\sup_{s\in S}\|v_i(s)\|_{L^1}+1\Big\}.$$

Taking the limit $m\to\infty$, we find

$$\sum_{i=1}^{2}\|v_i(t)\|_{L^\infty}\le c\kappa\sum_{i=1}^{2}\Big\{\sup_{s\in S}\|v_i(s)\|_{L^1}+1\Big\}\qquad\forall t\in S.$$

Since $u_i\le\overline{u}_i(v_i+\widehat{K})$, $b_i\le v_i+\widehat{K}$ this supplies the desired estimate for u_i and b_i, $i=1,2$. The result for z is a direct consequence of Remark 3.3 and the Sobolev embedding $W^{1,q}(\Omega)\hookrightarrow L^\infty(\Omega)$ in two space dimensions for $q>2$. □

4 Existence result for (P)

4.1 The regularized problem (P$_M$)

To prove the solvability of (P) we consider a regularized problem which is defined on an arbitrarily fixed time interval $S=[0,T]$. For $M\ge M^*:=\max\{1,\|U/\overline{u}\|_V\}$ let

$\rho_M : \mathbb{R}^{2l+2} \to [0,1]$ be a Lipschitz continuous function with the properties

$$\rho_M(b) = \begin{cases} 0 & \text{if } |b|_\infty \geq M, \\ 1 & \text{if } |b|_\infty \leq M/2 \end{cases}, \quad |b|_\infty = \max\{|b_1|, \dots, |b_{2l+2}|\}.$$

Moreover, we use the projection

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

and define the operators $\mathcal{R}_M : [X + b^D] \cap V_+ \to X^*$, $\mathcal{A}_M : (X + b^D) \times (Z + z^D) \to X^*$ by

$$\begin{aligned} \langle \mathcal{R}_M(b), \bar{b} \rangle_X := & \sum_{j=1}^{l} \int_G \rho_M(b)\, k_j^n \big(b_1 b_{2j+2} - (1 + e_j^n) b_{2j+1}\big)(\bar{b}_1 + \bar{b}_{2j+2} - \bar{b}_{2j+1})\, \mathrm{d}\mu_{2j+1} \\ & + \sum_{j=1}^{l} \int_G \rho_M(b)\, k_j^p \big(b_2 b_{2j+1} - (1 + e_j^p) b_{2j+2}\big)(\bar{b}_2 + \bar{b}_{2j+1} - \bar{b}_{2j+2})\, \mathrm{d}\mu_{2j+1} \\ & + \int_\Omega \Big\{ \rho_M(b)\, k_0 (b_1 b_2 - 1)(\bar{b}_1 + \bar{b}_2) - G_{phot}(\bar{b}_1 + \bar{b}_2) \Big\}\, \mathrm{d}x, \\ \langle \mathcal{A}_M(b, z), \bar{b} \rangle_X := & \int_\Omega \sum_{i=1}^{2} D_i \overline{u}_i \big(\nabla b_i + \lambda_i [\sigma_M(b_i)]^+ \nabla z\big) \cdot \nabla \bar{b}_i\, \mathrm{d}x, \quad \bar{b} \in X. \end{aligned}$$

We consider the regularized problem

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

Note that solutions (u, b, z) to (P_M) possess the regularity properties u, $b \in C(S, Y)$ and $z - z^D \in C(S, Z)$.

4.2 Existence result for (P_M)

The existence proof for (P_M) is inspired by [11]. In this subsection the constants may depend on M and S. First we give an equivalent formulation of (P_M). We write b in the form $b = (v, w)$, where $v = (b_1, b_2)$, $w = (b_3, \dots, b_{2l+2})$ and introduce the spaces

$$Y^2 = L^2(\Omega)^2,\ Y^{2l} = \textstyle\prod_{i=3}^{2l+2} L^2(G; \mathrm{d}\mu_i),\ X^2 = H_0^1(\Omega \cup \Gamma_N)^2,\ X^{2*} := (X^2)^*,$$

and the operators $\mathcal{B}_v : L^2(S, Y^2) \to L^2(S, Y^2)$, $\mathcal{B}_w : L^2(S, Y^{2l}) \to L^2(S, Y^{2l})$,

$$\mathcal{B}_v v = (\overline{u}_i\, v_i)_{i=1,2}, \quad \mathcal{B}_w w = (\overline{u}_{i+2}\, w_i)_{i=1,\dots,2l}.$$

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

$$\langle \mathcal{A}_v^0(v-v^D), \overline{v}\rangle_{L^2(S,X^2)} := \int_S \int_\Omega \sum_{i=1}^2 D_i \overline{u}_i \, \nabla(v_i - v_i^D) \cdot \nabla \overline{v}_i \, \mathrm{d}x \, \mathrm{d}s,$$

$$\langle \mathcal{A}_v(v,z), \overline{v}\rangle_{L^2(S,X^2)} := \int_S \int_\Omega \sum_{i=1}^2 D_i \overline{u}_i (\nabla v_i^D + \lambda_i \, [\sigma_M(v_i)]^+ \nabla z) \cdot \nabla \overline{v}_i \, \mathrm{d}x \, \mathrm{d}s,$$

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

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

For all given $v \in L^2(S,Y^2)$, $w \in L^2(S,Y^{2l})$ the vector $(\mathcal{B}_v v, \mathcal{B}_w w)$ lies in $L^2(S,Y)$. Thus, by Lemma 3.1 there is a unique solution z with $z - z^D \in L^2(S,Z) \cap (L^\infty(S, L^\infty(\Omega)))$ of

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

Let $\mathcal{T}_z \colon L^2(S,Y^2) \times L^2(S,Y^{2l}) \to L^2(S,Z) + z^D$ denote the corresponding solution operator such that $z = \mathcal{T}_z(v,w)$. Since $(\mathcal{B}_v v^D)' = 0$ and $(\mathcal{B}_w w)' = \mathcal{B}_w w'$, problem ($\mathrm{P}_M$) can be formulated equivalently as follows:

$$\begin{aligned} &(\mathcal{B}_v(v-v^D))' + \mathcal{A}_v^0(v-v^D) = -\mathcal{R}_v(v,w) - \mathcal{A}_v(v, \mathcal{T}_z(v,w)), \\ &(\mathcal{B}_v(v-v^D))(0) = (U_1,U_2) - \mathcal{B}_v v^D, \quad v - v^D \in W^2, \end{aligned} \tag{4.1}$$

$$w' + \mathcal{B}_w^{-1}[\mathcal{R}_w(v,w)] = 0, \quad w(0) = \mathcal{B}_w^{-1}(U_3,\dots,U_{2l+2}), \quad w \in H^1(S,Y^{2l}), \tag{4.2}$$

where

$$W^2 := \big\{ v \in L^2(S,X^2) \colon (\mathcal{B}_v v)' \in L^2(S,X^{2*}) \big\} \subset C(S,Y^2).$$

The existence result for (P_M) is shown by proving that the system (4.1), (4.2) can be solved. We start with a short overview of this proof. At the beginning we fix some $\widehat{v} \in W^2 + v^D$ and solve the initial value problem

$$w' + \mathcal{B}_w^{-1}[\mathcal{R}_w(\widehat{v},w)] = 0, \quad w(0) = \mathcal{B}_w^{-1}(U_3,\dots,U_{2l+2}), \quad w \in H^1(S,Y^{2l}), \tag{4.3}$$

obtain $w = \mathcal{T}_w \widehat{v}$ with a solution operator $\mathcal{T}_w \colon W^2 + v^D \to H^1(S,Y^{2l})$ (see Lemma 4.1). Next we treat the problem

$$\begin{aligned} (\mathcal{B}_v(v-v^D))' + \mathcal{A}_v^0(v-v^D) &= -\mathcal{R}_v(\widehat{v}, \mathcal{T}_w \widehat{v}) - \mathcal{A}_v(\widehat{v}, \mathcal{T}_z(\widehat{v}, \mathcal{T}_w \widehat{v})), \\ (\mathcal{B}_v(v-v^D))(0) &= (U_1,U_2) - \mathcal{B}_v v^D, \quad v - v^D \in W^2. \end{aligned} \tag{4.4}$$

According to Lemma 5.3 there is a unique solution $v = \mathcal{Q}\widehat{v}$ to this problem. The operator $\mathcal{Q}$ is completely continuous (see Lemma 4.2). Using Schauder's fixed point theorem we obtain a fixed point v of $\mathcal{Q}$ (see Lemma 4.3). Then $(v, \mathcal{T}_w v)$ is a solution to (4.1), (4.2).

Lemma 4.1 *We assume* (A1) – (A6). *Then for all* $\widehat{v} \in W^2 + v^D$ *there is exactly one solution to* (4.3). *Moreover*

$$\|\mathcal{T}_w\widehat{v}^1-\mathcal{T}_w\widehat{v}^2\|_{C(S,Y^{2l})} \le c\|\widehat{v}^1-\widehat{v}^2\|_{L^2(S,Y^2)}, \quad \|\mathcal{T}_w\widehat{v}^1\|_{C(S,Y^{2l})} \le c \quad \forall \widehat{v}^1,\, \widehat{v}^2 \in W^2+v^D.$$

Proof. Since for $w \in L^2(S,Y^{2l})$ the map $w \mapsto \mathcal{B}_w^{-1}[\mathcal{R}_w(\widehat{v},w)]$ is Lipschitz continuous uniformly w.r.t. $\widehat{v}$, by [8, Chapt. V, Theorem 1.3] problem (4.3) has a unique solution $w = \mathcal{T}_w\widehat{v}$ with a solution operator $\mathcal{T}_w\colon W^2+v^D \to H^1(S,Y^{2l})$. Moreover, taking into account that $\|\mathcal{R}_w(\widehat{v}^1,w^1)(t)-\mathcal{R}_w(\widehat{v}^2,w^2)(t)\|_{Y^{2l}} \le c(\|\widehat{v}^1(t)-\widehat{v}^2(t)\|_{Y^2}+\|w^1(t)-w^2(t)\|_{Y^{2l}})$ f.a.a $t \in S$, for all $(\widehat{v}^1,w^1)$, $(\widehat{v}^2,w^2) \in L^2(S,Y)$, testing (4.3) (for $(\widehat{v}^1,w^1)$ and $(\widehat{v}^2,w^2)$) by w^1-w^2 and using Gronwall's lemma we derive the estimates of Lemma 4.1. □

Lemma 4.2 *Under the assumptions* (A1) – (A6) *the mapping* $\mathcal{Q}\colon W^2+v^D \to W^2+v^D$ *is completely continuous.*

Proof. Let $\{\widehat{v}_n\} \subset W^2+v^D$ be bounded. Because of Lemma 5.2 we may assume that there exists an element $\widehat{v} \in W^2+v^D$ such that $\widehat{v}_n \to \widehat{v}$ in $L^2(S,Y^2)$. Let

$$v_n = \mathcal{Q}\widehat{v}_n,\ v = \mathcal{Q}\widehat{v},\ w_n = \mathcal{T}_w\widehat{v}_n,\ w = \mathcal{T}_w\widehat{v},\ z_n = \mathcal{T}_z(\widehat{v}_n,w_n),\ z = \mathcal{T}_z(\widehat{v},w).$$

By Lemma 4.1, Lemma 3.1 it follows that $w_n \to w$ in $L^2(S,Y^{2l})$ and $z_n - z \to 0$ in $L^2(S,Z)$. Testing (4.4) for $\widehat{v}_n$ and $\widehat{v}$ by $v_n - v \in L^2(S,X^2)$ we obtain according to Lemma 5.2

$$\begin{aligned}
&\frac{\epsilon_0}{2}\|(v_n-v)(t)\|_{Y^2}^2 + \int_0^t \epsilon\|v_n-v\|_{X^2}^2\,\mathrm{d}s \\
&\le c\int_0^t \Big\{ \int_\Omega \sum_{i=1}^2 \Big\{|[\sigma_M(\widehat{v}_{ni})]^+ - [\sigma_M(\widehat{v}_i)]^+||\nabla z|\,|\nabla(v_{ni}-v_i)| + |\nabla(z_n-z)||\nabla(v_{ni}-v_i)|\Big\}\,\mathrm{d}x \\
&\qquad + (\|\widehat{v}_n-\widehat{v}\|_{Y^2} + \|w_n-w\|_{Y^{2l}})\,\|v_n-v\|_{Y^2}\Big\}\,\mathrm{d}s \quad \forall t \in S.
\end{aligned}$$

Applying Hölder's inequality and Lemma 4.1 we arrive at

$$\begin{aligned}
&\|v_n-v\|_{L^2(S,X^2)}^2 \\
&\le c\|v_n-v\|_{L^2(S,X^2)}\Big\{\|\widehat{v}_n-\widehat{v}\|_{L^2(S,Y^2)} + \|z_n-z\|_{L^2(S,Z)} \\
&\qquad + \sum_{i=1}^2 \Big[\int_0^T \int_\Omega |[\sigma_M(\widehat{v}_{ni})]^+ - [\sigma_M(\widehat{v}_i)]^+|^2\,|\nabla z|^2\,\mathrm{d}x\,\mathrm{d}s\Big]^{1/2}\Big\}.
\end{aligned}$$

Properties of superposition operators ensure that the last square bracket term tends to zero if $n \to \infty$. Thus in summary we find that $v_n - v \to 0$ in $L^2(S,X^2)$. Next we obtain

$$\begin{aligned}
&\|(\mathcal{B}_v(v_n-v))'\|_{L^2(S,X^{2*})} \\
&\le \|\mathcal{R}_v(\widehat{v}_n,w_n)-\mathcal{R}_v(\widehat{v},w)\|_{L^2(S,X^{2*})} + \|\mathcal{A}_v^0(v_n-v)\|_{L^2(S,X^{2*})} + \|\mathcal{A}_v(\widehat{v}_n,z_n)-\mathcal{A}_v(\widehat{v},z)\|_{L^2(S,X^{2*})} \\
&\le c\Big\{\|v_n-v\|_{L^2(S,X^2)} + \|\widehat{v}_n-\widehat{v}\|_{L^2(S,Y^2)} + \|w_n-w\|_{L^2(S,Y^{2l})} + \|z_n-z\|_{L^2(S,Z)} \\
&\qquad + \sum_{i=1}^2 \Big[\int_0^T \int_\Omega |[\sigma_M(\widehat{v}_{ni})]^+ - [\sigma_M(\widehat{v}_i)]^+|^2\,|\nabla z|^2\,\mathrm{d}x\,\mathrm{d}s\Big]^{1/2}\Big\} \to 0 \text{ for } n \to \infty,
\end{aligned}$$

and we arrive at $v_n - v \to 0$ in W^2. The continuity of the operator $\mathcal{Q}$ can be shown by similar arguments. $\square$

Lemma 4.3 *Under the assumptions* (A1) – (A6) *the mapping* $\mathcal{Q}$ *has a fixed point.*

Proof. Let $\widehat{v} \in W^2 + v^D$, $z = \mathcal{T}_z(\widehat{v}, \mathcal{T}_w\widehat{v})$ and $v = \mathcal{Q}\widehat{v}$. We use $v^0 := v - v^D$ as test function for (4.4), take into account that $(\mathcal{B}_v(v - v^D))' = (\mathcal{B}_v v)'$, (A4) and (A6) and the Lipschitz continuity of $\mathcal{R}_v$ and apply Lemma 3.1, Lemma 4.1 and Young's inequality. Then

$$\begin{aligned} &\epsilon_0\|v^0(t)\|_{Y^2}^2 + 2\epsilon\int_0^t \|v^0\|_{X^2}^2\,\mathrm{d}s \\ &\le c + c\int_0^t \big(1 + \|v^0\|_{Y^2}^2 + \|\widehat{v} - v^D\|_{Y^2}^2 + \|z\|_{H^1}\|v^0\|_{X^2}\big)\,\mathrm{d}s \\ &\le c + \int_0^t \big(\epsilon\|v^0\|_{X^2}^2 + c\big(1 + \|v^0\|_{Y^2}^2 + \|\widehat{v} - v^D\|_{Y^2}^2\big)\big)\,\mathrm{d}s \quad \forall t \in S. \end{aligned} \tag{4.5}$$

Therefore we find a constant $\overline{c} > 0$ such that for all $k > 0$

$$\begin{aligned} &\mathrm{e}^{-kt}\Big(\|v^0(t)\|_{Y^2}^2 + \int_0^t \|v^0\|_{X^2}^2\,\mathrm{d}s\Big) \\ &\le \overline{c} + \overline{c}\mathrm{e}^{-kt}\int_0^t \Big\{\Big\{\|v^0\|_{Y^2}^2 + \|\widehat{v} - v^D\|_{Y^2}^2 + \int_0^s \big(\|v^0\|_{X^2}^2 + \|\widehat{v} - v^D\|_{X^2}^2\big)\,\mathrm{d}\tau\Big\}\mathrm{e}^{-ks}\mathrm{e}^{ks}\Big\}\,\mathrm{d}s \\ &\le \overline{c} + \overline{c}\mathrm{e}^{-kt}\sup_{s\in S}\Big\{\Big\{\|v^0(s)\|_{Y^2}^2 + \|\widehat{v}(s) - v^D\|_{Y^2}^2 + \int_0^s \big(\|v^0\|_{X^2}^2 + \|\widehat{v} - v^D\|_{X^2}^2\big)\,\mathrm{d}\tau\Big\}\mathrm{e}^{-ks}\Big\}\frac{\mathrm{e}^{kt}-1}{k}. \end{aligned}$$

Choosing now $k \ge 3\overline{c}$ we obtain

$$\begin{aligned} &\sup_{t\in S}\mathrm{e}^{-kt}\Big(\|v^0(t)\|_{Y^2}^2 + \int_0^t \|v^0(s)\|_{X^2}^2\,\mathrm{d}s\Big) \\ &\qquad \le \frac{3}{2}\overline{c} + \frac{1}{2}\sup_{t\in S}\Big\{\mathrm{e}^{-kt}\Big(\|\widehat{v}(t) - v^D\|_{Y^2}^2 + \int_0^t \|\widehat{v}(s) - v^D\|_{X^2}^2\,\mathrm{d}s\Big)\Big\}. \end{aligned}$$

Again using Lemma 3.1 and Lemma 4.1 we estimate

$$\begin{aligned} &\|(\mathcal{B}_v v^0)'\|_{L^2(S,X^{2*})} = \sup_{\|\overline{v}\|_{L^2(S,X^2)}\le 1} \langle -\mathcal{R}_v(\widehat{v}, \mathcal{T}_w\widehat{v}) - \mathcal{A}_v^0(v^0) - \mathcal{A}_v(\widehat{v}, z), \overline{v}\rangle_{L^2(S,X^2)} \\ &\le c\,\big(\|v^0\|_{L^2(S,X^2)} + \|z\|_{L^2(S,H^1)} + \|\widehat{v} - v^D\|_{L^2(S,Y^2)} + 1\big) \\ &\le c\,\Big(\|v^0\|_{L^2(S,X^2)} + \|\widehat{v} - v^D\|_{L^2(S,Y^2)} + 1\Big) \\ &\le \widetilde{c}\Big(\|v^0\|_{L^2(S,X^2)} + \Big[\sup_{t\in S}\Big\{\mathrm{e}^{-kt}\Big(\|\widehat{v}(t) - v^D\|_{Y^2}^2 + \int_0^t \|\widehat{v}(s) - v^D\|_{X^2}^2\,\mathrm{d}s\Big)\Big\}\mathrm{e}^{kT}\Big]^{1/2} + 1\Big). \end{aligned}$$

Now we define the set

$$\begin{aligned} \mathcal{M} = \Big\{v \in W^2 + v^D\colon\ &\sup_{t\in S}\Big\{\mathrm{e}^{-kt}\Big(\|v^0(t)\|_{Y^2}^2 + \int_0^t \|v^0\|_{X^2}^2\,\mathrm{d}s\Big)\Big\} \le 3\overline{c}, \\ &\|(\mathcal{B}_v v^0)'\|_{L^2(S,X^{2*})} \le \widetilde{c}\,\Big(2\sqrt{3\overline{c}}\mathrm{e}^{kT} + 1\Big)\Big\}. \end{aligned}$$

This set is a non-empty, bounded, closed and convex subset of W^2+v^D with the property that $\mathcal{Q}(\mathcal{M})\subset\mathcal{M}$. Since the mapping $\mathcal{Q}$ is completely continuous the assertion follows from Schauder's fixed point theorem. $\square$

Theorem 4.1 *Under the assumptions* (A1) – (A6) *there exists a solution* (u,b,z) *to* (P_M).

Proof. Because of Lemma 4.3 there exists a solution v of the problem

$$\begin{aligned}(\mathcal{B}_v(v-v^D))'+\mathcal{A}_v^0(v-v^D)&=-\mathcal{R}_v(v,\mathcal{T}_w v)-\mathcal{A}_v(v,\mathcal{T}_z(v,\mathcal{T}_w v)),\\ (\mathcal{B}_v(v-v^D))(0)&=(U_1,U_2)-\mathcal{B}_v v^D,\quad v-v^D\in W^2.\end{aligned}$$

We set $w=\mathcal{T}_w v\in H^1(S,Y^{2l})$. Then the pair (v,w) fulfills the equations (4.1) and (4.2) which represent an equivalent formulation of problem (P_M). $\square$

4.3 Energy estimates for solutions to (P_M)

Lemma 4.4 *We assume* (A1) – (A6). *Then, for any solution* (u,b,z) *to* (P_M) *and for every* $t\in S$ *the inequalities* $b_i(t)$, $u_i(t)\geq 0$ *a.e. on* Ω, $i=1,2$, $u_i(t)\in[0,1]$ μ_i*-a.e. in* G, $i=3,\ldots,2l+2$, *are fulfilled.*

Proof. Let (u,b,z) be a solution to (P_M). We use the test function $-b^-$. Taking into account that

$$\begin{gathered}(\nabla b_i+\lambda_i[\sigma_M(b_i)]^+\nabla z)\cdot\nabla b_i^-\leq 0,\quad -G_{phot}b_i^-\leq 0\quad i=1,2,\quad (b_1^+b_2^+-1)(b_1^-+b_2^-)\leq 0,\\ (b_1^+b_{2j+2}^+-(1+e_j^n)b_{2j+1}^+)(b_1^-+b_{2j+2}^--b_{2j+1}^-)\leq 0,\\ (b_2^+b_{2j+1}^+-(1+e_j^p)b_{2j+2}^+)(b_2^-+b_{2j+1}^--b_{2j+2}^-)\leq 0,\quad j=1,\ldots,l,\end{gathered}$$

we find that $\|b^-(t)\|_Y^2\leq 0$ for all $t\in S$. Arguing now as in the proof of Lemma 3.2 we verify the remaining results of the lemma. $\square$

We introduce a regularized free energy functional F_M which is compatible with the regularizations done in problem (P_M). Using the function

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

we define the functional $\widetilde{F}_{M2}:Y\to\overline{\mathbb{R}}$ by

$$\widetilde{F}_{M2}(u)=\int_\Omega\sum_{i=1}^{2}\int_{u_i^D}^{u_i}\big(l_M(\tfrac{y}{\overline{u}_i})-\ln b_i^D\big)\,\mathrm{d}y\,\mathrm{d}x+\sum_{i=3}^{2l+2}\int_G\int_{\overline{u}_i}^{u_i}\ln(\tfrac{y}{\overline{u}_i})\,\mathrm{d}y\,\mathrm{d}\mu_i\quad\text{if } u\in Y_+,$$

and $\widetilde{F}_{M2}(u)=+\infty$ for $u\in Y\setminus Y_+$. Moreover, we set

$$F_{M2}=(\widetilde{F}^*_{M2}|_X)^*:X^*\to\overline{\mathbb{R}},\quad F_M=F_1+F_{M2}:X^*\to\overline{\mathbb{R}},$$

where F_1 was introduced in Subsection 3.4. Since the function l_M has the same essential properties as the ln-function which occurs in the definition of F_2 we obtain the following results. F_M is proper, convex and lower semicontinuous. For $u \in Y_+$ it can be evaluated as $\widetilde{F}_1(u) + \widetilde{F}_{M2}(u)$. Due to the choice of M we have $F_M(U) = F(U)$. The restriction $F_M|_{Y_+}$ is continuous. If $u \in Y_+$ then $\lambda(z - z^D) \in \partial F_1(u)$ where z is the solution of $\mathcal{P}(z, u) = 0$. If $u \in Y$, $u \geq \delta > 0$ then $\big(l_M(b_1) - \ln b_1^D, l_M(b_2) - \ln b_2^D, l_M(b_3), \ldots, l_M(b_{2l+2})\big) \in \partial F_{M2}(u)$. By the definition of F_1 and l_M especially it follows for $u \in Y_+$ and b, z with $b = \mathcal{B}^{-1}u$, $\mathcal{P}(z, u) = 0$ that

$$\|z - z^D\|_Z^2,\ \|b_i \ln b_i\|_{L^1},\ \|u_i\|_{L^1} \leq cF_M(u) + \widetilde{c}, \quad i = 1, 2. \tag{4.6}$$

Lemma 4.5 *Let* (A1) – (A6) *be satisfied. Then there exist constants* $c_1(T) > 0$, $c_2(T) > 0$ *not depending on* M *such that*

$$F_M(u(t)) \leq c_1(T), \quad \|b_i(t) \ln b_i(t)\|_{L^1} \leq c_2(T), \quad i = 1, 2, \quad \forall t \in S$$

for any solution (u, b, z) *to* (P_M).

Proof. 1. We take δ as in (3.6), define $b^\delta := \max\{b, \delta\}$ and introduce the functional $\widetilde{F}^\delta_{M2} \colon Y \to \mathbb{R}$,

$$\begin{aligned}\widetilde{F}^\delta_{M2}(u) = \int_\Omega \sum_{i=1}^{2} \int_{u_i^D}^{u_i} \big(l_M(\max\{\tfrac{y}{\overline{u}_i}, \delta\}) - \ln b_i^D\big)\, \mathrm{d}y\, \mathrm{d}x \\ + \sum_{i=3}^{2l+2} \int_G \int_{\overline{u}_i}^{u_i} \ln(\max\{\tfrac{y}{\overline{u}_i}, \delta\})\, \mathrm{d}y\, \mathrm{d}\mu_i, \quad u \in Y_+\end{aligned}$$

and $\widetilde{F}^\delta_{M2}(u) = +\infty$ if $u \in Y \setminus Y_+$, and the functional $F^\delta_{M2} = (\widetilde{F}^{\delta *}_{M2}|_X)^* \colon X^* \to \overline{\mathbb{R}}$. Note that for $u \in Y$ we have $F^\delta_{M2}(u) \to F_{M2}(u)$ as $\delta \downarrow 0$.

2. Let (u, b, z) be a solution to (P_M). Then $u \in H^1(S, X^*)$, u, $b \geq 0$, $z - z^D \in L^2(S, Z)$,

$$w^\delta_M := (l_M(b^\delta_1) - \ln b_1^D, l_M(b^\delta_2) - \ln b_2^D, \ln(b^\delta_3), \ldots, \ln(b^\delta_{2l+2})) \in L^2(S, X)$$

(note that $l_M(b^\delta_i) = \ln b_i^D$ a.e. on $S \times \Gamma_D$, $i = 1, 2$) and $\lambda(z(t) - z^D) \in \partial F_1(u(t))$, $w^\delta_M(t) \in \partial F^\delta_{M2}(u(t))$ f.a.a. $t \in S$. Thus, according to Lemma 5.1, we obtain that the functions $t \mapsto F_1(u(t))$, $t \mapsto F^\delta_{M2}(u(t))$ are absolutely continuous on S and

$$\frac{\mathrm{d}}{\mathrm{d}t} F_1(u(t)) = \langle u'(t), \lambda(z(t) - z^D)\rangle_X, \quad \frac{\mathrm{d}}{\mathrm{d}t} F^\delta_{M2}(u(t)) = \big\langle u'(t), w^\delta_M(t)\big\rangle_X \text{ f.a.a. } t \in S.$$

3. We set $\zeta^\delta_M = w^\delta_M + \lambda(z - z^D)$ and obtain

$$\begin{aligned}\Big[F_1(u(t)) + F^\delta_{M2}(u(t))\Big]\Big|_0^t &= \int_0^t \langle u'(s), \zeta^\delta_M(s)\rangle_X\, \mathrm{d}s \\ &= -\int_0^t \langle R_M(b(s)) + A_M(b(s), z(s)), \zeta^\delta_M(s)\rangle_X\, \mathrm{d}s \\ &= -\int_0^t \langle R_M(b^\delta(s)) + A_M(b^\delta(s), z(s)), \zeta^\delta_M(s)\rangle_X + \theta^\delta(s)\, \mathrm{d}s,\end{aligned}$$

where $\theta^\delta = \langle R_M(b^\delta) - R_M(b) + A_M(b^\delta, z) - A_M(b, z), \zeta^\delta_M\rangle_X \to 0$ for $\delta \downarrow 0$. Since all the reaction terms containing the factor ρ_M become zero if $|b|_\infty > M$, we have for these terms only to discuss the situation $b^\delta_i \le M$, and here is $l_M(b^\delta_i) = \ln b^\delta_i$ such that we can argue as in Step 2 of the proof of Theorem 3.2 to arrive at

$$\begin{aligned}
&-\langle \mathcal{R}_M(b^\delta), \zeta^\delta_M\rangle_X \\
&\quad\le c(1 + \sum_{i=1}^{2} \|b^\delta_i\|_{L^1})\|\ln b^D_1 b^D_2\|_{L^\infty} + \|G_{phot}\|_{L^\infty}\Big\{\sum_{i=1}^{2}\big(\|b^\delta_i\|_{L^1} + \|\ln b^D_i\|_{L^1}\big) + \|z - z^D\|_{L^1}\Big\} \\
&\quad + c\sum_{j=1}^{l}\Big\{(\|b^\delta_1\|_{L^1} + 1)\|\ln \tfrac{1+e^n_j}{b^D_1}\|_{L^\infty(G,\mathrm{d}\mu_{2j+1})} + (\|b^\delta_2\|_{L^1} + 1)(\|\ln \tfrac{1+e^p_j}{b^D_2}\|_{L^\infty(G,\mathrm{d}\mu_{2j+1})}\Big\}.
\end{aligned}$$

Having in mind that on solutions $[\sigma_M(b^\delta_i)]^+ = \sigma_M(b^\delta_i) \le b^\delta_i$, $\nabla l_M(b^\delta_i) = \nabla(b^\delta_i)/\sigma_M(b^\delta_i)$, $i = 1, 2$, using (A4), (A5) and Young's inequality, and leaving out nonpositive terms we find

$$\begin{aligned}
&-\langle \mathcal{A}_M(b^\delta, z), \zeta^\delta_M\rangle_X \\
&\quad = -\int_\Omega \sum_{i=1}^{2} D_i \overline{u}_i \sigma_M(b^\delta_i)\Big\{|\nabla(l_M(b^\delta_i) + \lambda_i z)|^2 - \nabla(l_M(b^\delta_i) + \lambda_i z)\cdot\nabla(\ln b^D_i - \lambda_i z^D)\Big\}\,\mathrm{d}x \\
&\quad \le c\sum_{i=1}^{2}\|b^\delta_i\|_{L^1}\|\nabla(\ln b^D_i + \lambda_i z^D)\|^2_{L^\infty} \quad \text{a.e. on } S.
\end{aligned}$$

Taking $\delta \downarrow 0$ in the estimates of Step 3 and using (A3), (A4) and (4.6) we end up with

$$F_M(u(t)) - F_M(U) \le c\int_0^t (1 + F_M(u(s)))\,\mathrm{d}s,$$

where c depends on the data, but not on M. The choice of M guarantees that $F_M(U) = F(U)$. So Gronwall's lemma supplies the first assertion of the lemma. The remaining assertion of the lemma is a consequence of (4.6). □

4.4 Further estimates for solutions to (P_M)

Theorem 4.2 *We assume* (A1) – (A6). *Then there is a constant $c^*(T) > 0$ not depending on M such that for any solution (u, b, z) to* (P_M)

$$\|b\|_{L^\infty(S,V)} \le c^*(T). \tag{4.7}$$

Proof. 1. Let (u, b, z) be a solution to (P_M). Let $q > 2, r$ and r' be chosen as in Lemma 3.1 and (3.2). Due to Lemma 4.4 and Lemma 3.1 we get

$$\|z(t)\|_{W^{1,q}} \le c\Big[1 + \sum_{i=1,2}\|u_i(t)\|_{L^{r'}}\Big] \le c\Big[1 + \sum_{i=1,2}\|b_i(t)\|_{L^{r'}}\Big] \quad \forall t \in S. \tag{4.8}$$

2. We test (P_M) by $2(v_1, v_2, 0, \ldots, 0)$, where $v_i = (b_i - \widehat{K})^+$, $i = 1, 2$, with $\widehat{K}$ given in (3.8). Estimating $[\sigma_M(b_i)]^+$ by $v_i + \widehat{K}$, using Lemma 4.4, (4.8), (5.1), Young's inequality, Lemma 4.5 and (4.6) we find that

$$\sum_{i=1,2} \epsilon_0 \|v_i(t)\|_{L^2}^2$$
$$\leq \int_0^t \sum_{i=1,2} \big\{-2\epsilon\|v_i\|_{H^1}^2 + c(\|v_i\|_{L^r}\|z\|_{W^{1,q}}\|v_i\|_{H^1} + \|z\|_{H^1}\|v_i\|_{H^1} + \|v_i\|_{L^2}^2 + 1)\big\}\,\mathrm{d}s$$
$$\leq \int_0^t \sum_{i=1,2} \Big\{ -\epsilon\|v_i\|_{H^1}^2 + \overline{c}\|v_i\|_{L^r}\|v_i\|_{H^1} \sum_{k=1,2} \|v_k\|_{L^{r'}} + c\Big\}\,\mathrm{d}s.$$

Using $\|v_k\|_{L^{r'}} \leq \|v_k\|_{L^1}^{(r-2)/r}\|v_k\|_{L^2}^{2/r}$, the inequality (5.2) for $p = 2$ and Lemma 4.5 we have

$$\overline{c}\sum_{i=1,2}\|v_i\|_{L^r}\|v_i\|_{H^1}\sum_{k=1,2}\|v_k\|_{L^{r'}} \leq \sum_{i=1,2}\Big\{\frac{\epsilon}{2}\|v_i\|_{H^1}^2 + c\|v_i\|_{L^2}^2\sum_{k=1,2}\|v_k\|_{L^2}^2\Big\}$$
$$\leq \sum_{i=1,2}\Big\{\frac{\epsilon}{2}\|v_i\|_{H^1}^2 + \Big[\frac{\sqrt{\epsilon}}{2c_2(T)}\|v_i \ln v_i\|_{L^1}\|v_i\|_{H^1} + c\|v_i\|_{L^1}\Big]^2\Big\} \leq \sum_{i=1,2}\epsilon\|v_i\|_{H^1}^2 + c.$$

The previous estimates and the inequality (4.8) ensure the existence of positive constants $c(T)$, $\widetilde{\kappa}$ independent of M such that

$$\|v_i(t)\|_{L^2} \leq c_3(T)\,,\ i = 1, 2, \quad \|z(t)\|_{W^{1,q}}^{2r} + 1 \leq \widetilde{\kappa}(T) \quad \forall t \in S. \tag{4.9}$$

3. Following the estimates in the proof of Theorem 3.3, but estimating $[\sigma_M(b_i)]^+$ by $v_i + \widehat{K}$ and using $\widetilde{\kappa}(T)$ from (4.9) instead of κ we find that $\|v_i(t)\|_{L^\infty} \leq c(T)$ for all $t \in S$ which gives the desired upper bounds for b_i, $i = 1, 2$, on S. Since by Lemma 4.4 it is $b_i \leq 1/\overline{u}_i$ μ_i-a.e. in G for all $t \in S$, $i = 3, \ldots, 2l + 2$, the proof is finished. □

4.5 Existence result for (P)

Theorem 4.3 *We assume* (A1) – (A6). *Then there exists at least one solution to* (P).

Proof. It suffices to prove the existence of a solution to (P) on any finite time interval $S = [0, T]$. Such problems are denoted by (P_S). We choose $\overline{M} = 2\,c^*(T)$ (cf. Theorem 4.2). Then according to Theorem 4.1 there is a solution (u, b, z) to ($\mathrm{P}_{\overline{M}}$). The choice of $\overline{M}$ guarantees that the operators $\mathcal{R}_{\overline{M}}$ and $\mathcal{R}$ as well as the operators $\mathcal{A}_{\overline{M}}$ and $\mathcal{A}$ coincide on this solution. Therefore (u, b, z) is a solution to (P_S), too. □

5 Appendix

We suppose that $\Omega \subset \mathbb{R}^2$ is a bounded Lipschitzian domain. We use Sobolev's imbedding results (see [16]) and we apply the Gagliardo-Nirenberg inequality

$$\|w\|_{L^p} \leq c_p\,\|w\|_{L^1}^{1/p}\|w\|_{H^1}^{1-1/p} \quad \forall w \in H^1(\Omega)\,,\ 1 < p < \infty \tag{5.1}$$

(see [5, 19]). 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

$$\|w\|_{L^p}^p \le \delta \, \|w \ln |w|\|_{L^1} \, \|w\|_{H^1}^{p-1} + c_{\delta,p} \, \|w\|_{L^1} \quad \forall w \in H^1(\Omega). \tag{5.2}$$

This inequality is verified in [1] for bounded smooth domains and $p = 3$. But (5.2) is true for bounded Lipschitzian domains and $p \in (1,\infty)$ since (5.1) is valid in this situation, too. Additionally, we make use of the following chain rule, which can be obtained from [3, Lemma 3.3].

Lemma 5.1 *Let X be a Hilbert space, X^* its dual, $S = [0,T]$. Let $F : X^* \to \overline{\mathbb{R}}$ be proper, convex and semicontinuous. 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 $F \circ u : S \to \mathbb{R}$ is absolutely continuous, and*

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

Let $\overline{u} \in L^\infty(\Omega)$, $\operatorname{ess\,inf}_{x\in\Omega} \overline{u}(x) \ge c > 0$. We define $B\colon L^2(\Omega) \longrightarrow L^2(\Omega)$ by $Bw := \overline{u}\, w$, $w \in L^2(\Omega)$. For $S = [0,T]$, $T < \infty$, the extended operator $B\colon L^2(S,L^2(\Omega)) \longrightarrow L^2(S,L^2(\Omega))$ is given by $(Bw)(t) := B(w(t))$ f.a.a. $t \in S$. For the set

$$W_B = \big\{ w \in L^2(S, H_0^1(\Omega \cup \Gamma_N)\colon (Bw)' \in L^2(S, H_0^1(\Omega\cup\Gamma_N)^*)\big\}$$

the following assertions can be verified as in [8, 17, 22].

Lemma 5.2 *Equipped with the scalar product*

$$(w,\overline{w})_{W_B} = (w,\overline{w})_{L^2(S,H_0^1(\Omega\cup\Gamma_N))} + \big((Bw)', (B\overline{w})'\big)_{L^2(S,H_0^1(\Omega\cup\Gamma_N)^*)}$$

the linear space W_B is a Hilbert space, which is continuously embedded in $C(S,L^2(\Omega))$. The operator $B\colon W_B \to C(S,L^2(\Omega))$ is continuous. For $w \in W_B$ and t_1, $t_2 \in S$ the formula

$$\int_{t_1}^{t_2} \big\langle (Bw)'(s), w(s)\big\rangle_{H^1} \, ds = \frac{1}{2}\, ((Bw)(t_2), w(t_2))_{L^2} - \frac{1}{2}\, ((Bw)(t_1), w(t_1))_{L^2}$$

holds. The imbedding of W_B in $L^2(S,L^2(\Omega))$ is compact.

The following existence result can be proved as in [8, Chap. IV].

Lemma 5.3 *Let $A\colon L^2(S,H_0^1(\Omega\cup\Gamma_N)) \to L^2(S,H_0^1(\Omega\cup\Gamma_N)^*)$ be the operator*

$$\langle Aw, \overline{w}\rangle_{L^2(S,H_0^1(\Omega\cup\Gamma_N))} := \int_0^T \int_\Omega a\nabla w \cdot \nabla \overline{w} \, dx\, ds, \quad w,\, \overline{w} \in L^2(S,H_0^1(\Omega\cup\Gamma_N)),$$

where $a \in L^\infty(S\times\Omega)$ with $a(t,x) \ge c > 0$ f.a.a. $(t,x) \in S\times\Omega$. Then for every $f \in L^2(S,H_0^1(\Omega\cup\Gamma_N)^*)$ and every $U \in L^2(\Omega)$ there exists a unique solution to

$$(Bw)' + Aw = f, \quad (Bw)(0) = U, \quad w \in W_B.$$

Acknowledgment

This work was partially supported by the DFG Research Center Matheon "Mathematics for key technologies" under project D22.

References

1. P. Biler, W. Hebisch, and T. Nadzieja, *The Debye system: Existence and large time behavior of solutions*, Nonlinear Anal. **23** (1994), 1189–1209.

2. V. L. Bonch-Bruevich and S. G. Kalashnikov, *Halbleiterphysik*, Dt. Verlag d. Wiss., Berlin, 1982.

3. H. Brézis, *Opérateurs maximaux monotones et semi–groups de contractions dans les espaces de Hilbert*, North-Holland Math. Studies, vol. 5, North–Holland, Amsterdam, 1973.

4. I. Ekeland and R. Temam, *Convex analysis and variational problems*, Studies in Mathematics and its Applications, vol. 1, North–Holland, Amsterdam, 1976.

5. E. Gagliardo, *Ulteriori proprietà di alcune classi di funzioni in più variabili*, Ricerche Mat. **8** (1959), 24–51.

6. H. Gajewski, *Analysis und Numerik von Ladungstransport in Halbleitern (Analysis and numerics of carrier transport in semiconductors)*, Mitt. Ges. Angew. Math. Mech. **16** (1993), 35–57.

7. H. Gajewski and K. Gröger, *Initial boundary value problems modelling heterogeneous semiconductor devices*, Surveys on Analysis, Geometry and Math. Phys. Teubner-Texte zur Mathematik, vol. 117 (B. W. Schulze and H. Triebel, eds.), Teubner Verlag, Leipzig, 1990, pp. 4–53.

8. H. Gajewski, K. Gröger, and K. Zacharias, *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen*, Akademie–Verlag, Berlin, 1974.

9. A. Glitzky, *Elektro-Reaktions-Diffusionssysteme mit nichtglatten Daten*, Habilitationsschrift, Humboldt-Universität zu Berlin, 2001, Logos-Verlag, Berlin, 2002.

10. A. Glitzky, *Analysis of a spin-polarized drift-diffusion model*, Adv. Sci. Appl. **18** (2008), 401–427.

11. A. Glitzky and R. Hünlich, *Global existence result for pair diffusion models*, SIAM J. Math. Anal. **36** (2005), 1200–1225.

12. A. Glitzky and R. Hünlich, *Stationary energy models for semiconductor devices with incompletely ionized impurities*, Z. Angew. Math. Mech. **85** (2005), 778–792.

13. K. Gröger, *Initial–boundary value problems describing mobile carrier transport in semiconductor devices*, Comment. Math. Univ. Carolin. **26** (1985), 75–89.

14. K. Gröger, *A $W^{1,p}$–estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann. **283** (1989), 679–687.

15. H.-Ch. Kaiser, H. Neidhardt, and J. Rehberg, *Classical solutions of drift-diffusion equations for semiconductor devices: The two-dimensional case*, Nonlinear Anal. **71** (2009), 1584–1605.

16. A. Kufner, O. John, and S. Fučik, *Function spaces*, Academia, Prague, 1977.

17. J. L. Lions, *Quelques méthodes de résolution des problèmes aux limites non linéaires*, Dunod Gauthier–Villars, Paris, 1969.

18. M. S. Mock, *An initial value problem from semiconductor device theory*, SIAM J. Math. Anal. **5** (1974), 597–612.

19. L. Nirenberg, *An extended interpolation inequality*, Ann. Scuola Norm. Sup. Pisa **20** (1966), 733–737.

20. R. Stangl, C. Leendertz, and J. Haschke, *Numerical simulation of solar cells and solar cell characterization methods: the open-source on demand program AFORS-HET*, Solar Energy (R. D. Rugescu, ed.), INTECH, Croatia, 2010, pp. 319–352.

21. S. M. Sze and K. K. Ng, *Physics of semiconductor devices*, John Wiley & Sons, Inc., Hoboken, New Jersey, 2007.

22. R. Temam, *Navier–Stokes equations. Theory and numerical analysis*, Studies in Mathematics and its Applications, vol. 2, North–Holland, Amsterdam - New York - Oxford, 1979.

23. W. V. van Roosbroeck, *Theory of flow of electrons and holes in germanium and other semiconductors*, Bell Syst. Techn. J. **29** (1950), 560–607.

24. H. Wu, P. A. Markowich, and S. Zheng, *Global existence and asymptotic behavior for a semiconductor drift-diffusion-poisson model*, Math. Models Methods Appl. Sci. **18** (2008), 443–487.