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Abstract

The paper deals with drift-diffusion models for semiconductor heterostructures with Schottky contacts at all metal-semiconductor interfaces. Our analytical investigations allow for Boltzmann as well as Fermi–Dirac statistics for the charge-carrier densities. We verify the existence and boundedness of weak solutions of the instationary van Roosbroeck system in this context. Moreover, under additional assumptions the uniqueness and the higher regularity of the solution are demonstrated. Here, higher regularity results for scalar quasilinear parabolic PDEs are used.

1 Introduction

In this paper, we study drift-diffusion problems for the charge transport in semiconductors, where the passage of the charge carriers through the metal-semiconductor interfaces is realized via Schottky contacts, see [23, 24, 26]. Such boundary conditions are of particular relevance because Schottky barriers strongly influence injection, extraction, and recombination processes at the interfaces. Accurate models for these contacts are therefore essential in applications such as memristive devices, where interface effects have a strong influence on charge separation and overall device efficiency, see [25]. Hence, understanding and correctly capturing the physics of Schottky contacts plays a central role in predicting device performance and optimizing semiconductor design.

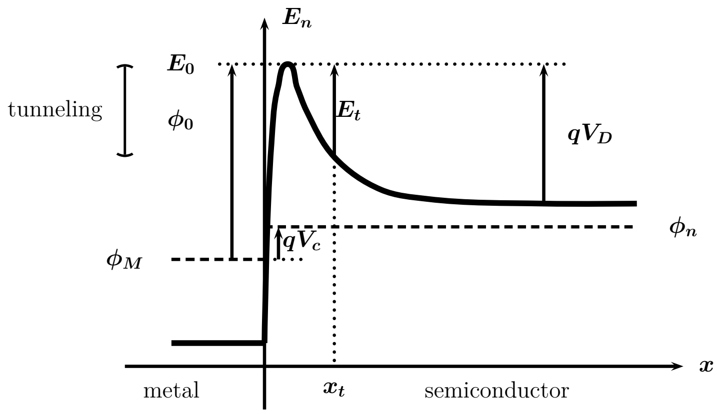

Figure 1: Energy band diagram of a metal-semiconductor contact for the conduction band where electrons are assumed to be the majority carriers, compare [24, p. 274].

Fig. 1 shows a schematic energy band diagram (conduction band edge E_n) of a metal-semiconductor contact. In equilibrium, depletion region arises in the semiconductor close to the interface. Thus, for the case of electron conduction there is an energy band bending upwards. This band bending introduces a barrier for the electron flow with barrier height ϕ_0 and E_0 corresponds to the top energy of the

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barrier. We indicate the Fermi level of the metal ϕ_M as well as the Fermi level of the semiconductor ϕ_n by dashed lines. At the interface the Fermi level makes a jump which is related to the voltage drop V_c at this contact. The two relevant current transport mechanisms at a metal-semiconductor contact are the thermionic emission over the top of the barrier and the tunneling of electrons through the barrier. The doping of the semiconductor determines which of the both processes is dominant near to the equilibrium situation. For high doping the space charge and the corresponding band curvature is high. Thus, the barrier becomes thin which forces a higher tunneling probability and induces a low contact resistance. In this case results an Ohmic contact. In the case of low doping the barrier becomes thick, tunneling very unlikely, and thermionic emission is the dominant transport mechanism. This characterizes a Schottky contact. For intermediate doping densities both current transport mechanisms have to be taken into account. In [24, Sec. 4], a model for such a non-ideal contact is established that assumes that tunneling through the barrier takes place for energies in the range of E_t below the top value E_0 and with a maximal tunnel length x_t from the junction, see Fig. 1. This model reduces to the model with Schottky contact in the limit of low doping density. A Schottky barrier refers to a metal-semiconductor contact having a large barrier height (i.e. $\phi_0 > k_B T)$ and low doping concentration that is less than the density of states in the conduction band or valence band.

For the charge transport in semiconductor devices, the underlying PDE system is the known van Roosbroeck system. It couples a Poisson equation for the electrostatic potential self-consistently to the continuity equations for the charge-carrier densities. But in the present paper, the usually considered Dirichlet boundary conditions at the electrical contacts at semiconductor-metal interfaces are substituted by so called Schottky boundary conditions. These prescribe Dirichlet values for the electrostatic potential and some kind of boundary conditions of third kind for the continuity equations, see Subsection 1.2 below for details. As usual, at semiconductor-isolator interfaces no-flux boundary conditions are formulated.

Whereas for the van Roosbroeck system with mixed Dirichlet/no flux boundary conditions comprehensive analytical investigations are available (see e.g. [6, 9, 18, 20] and references therein), the case of only Schottky contacts and isolating boundary conditions, relevant e.g. for memristor devices [23], is not treated from a mathematical analysis point of view. In the present paper, we discuss drift-diffusion problems for semiconductor heterostructures under assumptions allowing for Boltzmann as well as Fermi–Dirac statistics for the charge-carrier densities. We start with the underlying model equations and the formulation of the relevant mixed boundary conditions including Schottky contacts.

1.1 The underlying PDEs

The van Roosbroeck system describing the charge transport in semiconductor heterostructures consists of a *Poisson equation* for the electrostatic potential ψ that is self-consistently coupled to *continuity equations* for charge-carrier densities u_n and u_p of electrons and holes

$$-\nabla\cdot(\varepsilon_0\varepsilon_r\nabla\psi) = qC + \sum_{i=n,p} q_i u_i \quad \text{in } (0,\infty)\times\Omega, \tag{1.1}$$

$$q_i\partial_t u_i + \nabla\cdot j_i = -q_i R, \quad j_i = -q\overline{\mu}_i u_i\nabla\varphi_i, \quad \text{in } (0,\infty)\times\Omega, \quad i=n,p, \tag{1.2}$$

with the vacuum dielectric permittivity ε_0, the relative dielectric permittivity ε_r, the fixed doping density C, the elementary charge q, and $z_n=-1,\ z_p=1,\ q_i := z_i q$. The reaction rate

$$R = r(u_n,u_p)\big(1-\mathrm{e}^{\frac{q\varphi_n - q\varphi_p}{k_B T}}\big) \quad \text{with} \quad r(u_n,u_p) = r_0(u_n,u_p)u_n u_p$$

(see e.g. [8, Sect. 3]) incorporates the generation/recombination rates of electrons and holes. Moreover, j_i denotes the current densities, $\overline{\mu}_i$ are the carrier mobilities, and φ_i are the quasi-Fermi potentials. The latter are connected to the charge-carrier densities and the electrostatic potential via the statistical relations

$$u_i = u_i(\psi, \varphi_i, T) = N_i \mathcal{F}_i(\eta_i), \quad \eta_i = \frac{q_i(\varphi_i - \psi) + z_i E_i}{k_B T}, \quad i = n, p, \tag{1.3}$$

where T is the temperature, k_B is Boltzmann's constant, N_n and N_p are the effective densities of state of conduction and valence band, and E_i denote the (intrinsic) band edge energies.

For classical (inorganic) semiconductors the statistics functions for electrons and holes are usually given by the Fermi–Dirac integral of order $1/2$ (see e.g., [26])

$$F_{1/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2}}{\exp(\xi - z) + 1} \, \mathrm{d}\xi, \quad \text{for } z \in \mathbb{R}$$

i.e., $\mathcal{F}_n = \mathcal{F}_p = F_{1/2}$. In the case of small to moderate carrier densities [26], the Fermi–Dirac integral of order $1/2$ can be approximated by Boltzmann statistics, i.e., $F_{1/2}(z) \approx \mathrm{e}^z$. The proof of the existence of solutions is not restricted to these specific choices, but can be established under the following general properties of $\mathcal{F}_i$, $i = n, p$,

$$\begin{cases} \text{(i)} \;\; \mathcal{F}_i \in C^1(\mathbb{R}), \quad \lim\limits_{z \to -\infty} \mathcal{F}_i(z) = 0, \quad \lim\limits_{z \to +\infty} \mathcal{F}_i(z) = +\infty, \\ \text{(ii)} \;\; z \le c(1 + \mathcal{F}_i(z)) \quad \text{for } z \in \mathbb{R}_+, \\ \text{(iii)} \;\; 0 < \mathcal{F}_i'(z) \le \mathcal{F}_i(z) \le \mathrm{e}^z \quad \text{for } z \in \mathbb{R}. \end{cases} \tag{1.4}$$

These properties (1.4) are fulfilled for Boltzmann as well as Fermi–Dirac statistics.

1.2 Boundary conditions

We decompose the semiconductor boundary $\partial\Omega$ into the metal-semiconductor contacts $\Gamma_S \subset \partial\Omega$ and the semiconductor-insulator interface $\partial\Omega \backslash \Gamma_S$, and we fix the following mixed boundary conditions. At Γ_S we formulate so called Schottky boundary conditions. This is related to a metal-semiconductor contact having a large barrier height (i.e. $\phi_0 > k_B T$) and low doping concentration C that is less than the densities of states N_n or N_p in the conduction band or valence band, respectively. The potential barrier between the metal and the semiconductor can be identified on an energy band diagram. According to [5, 23, 25], [26, Chap. 3.3.3], we formulate *at the metal-semiconductor contacts* Γ_S thermionic emission conditions with the thermionic recombination velocities $\overline{a}_n$ and $\overline{a}_p$, i.e., for the normal fluxes of electrons and holes we impose

$$j_n \cdot \nu = q_n \overline{a}_n (u_n - u_{n,0}), \quad j_p \cdot \nu = q_p \overline{a}_p (u_p - u_{p,0}) \quad \text{on } (0, \infty) \times \Gamma_S. \tag{1.5}$$

In inorganic semiconductors, explicit formulas for $\overline{a}_n$ and $\overline{a}_p$ in terms of the effective masses m_n^* and m_p^* of electrons and holes hold

$$\overline{a}_n = \frac{4\pi m_n^* (k_B T)^2}{h^3 N_n}, \quad \overline{a}_p = \frac{4\pi m_p^* (k_B T)^2}{h^3 N_p}, \tag{1.6}$$

where h is Planck's constant. The quasi-equilibrium carrier densities are given via

$$u_{n,0} = N_n \mathcal{F}_n\Big(-\frac{\phi_0}{k_B T}\Big), \quad u_{p,0} = N_p \mathcal{F}_p\Big(-\frac{E_G - \phi_0}{k_B T}\Big).$$

Here, the intrinsic Schottky barrier $\phi_0 = \phi_0(x)$ is a fixed material and device dependent quantity and $E_G = E_n - E_p$ denotes the intrinsic band gap, such that also $u_{n,0}$ and $u_{p,0}$ can be considered as material and device dependent given quantity. Note that for n-type semiconductors ($C > 0$) the barrier height is obtained from $\phi_{0n} = \phi_m - \chi$, where ϕ_m is the work function of the metal and χ is the electron affinity. For p-type material ($C < 0$), the barrier height is given by the difference between the valence band edge and the Fermi energy in the metal, $\phi_{0p} = \frac{E_G}{q} + \chi - \phi_m$.

For the electrostatic potential ψ, at Γ_S, Dirichlet boundary conditions

$$\psi = \psi_0 + \psi_{appl}, \quad \psi_0 = (\phi_0 - E_n)/q_n \quad \text{on } (0,\infty) \times \Gamma_S$$

are formulated, where ψ_{appl} is the applied electrostatic potential at the contact.

At the isolated parts (isolator-semiconductor interface) of the boundary $\partial\Omega \setminus \Gamma_S$ zero-flux boundary conditions for the Poisson equation as well as the continuity equations are prescribed

$$\varepsilon_0 \varepsilon_r \nabla\psi \cdot \nu = 0, \quad j_n \cdot \nu = j_p \cdot \nu = 0 \quad \text{on } (0,\infty) \times (\partial\Omega \setminus \Gamma_S).$$

The analysis of the model equation differs significantly from the usual treatment of the van Roosbroeck system with mixed Dirichlet/Neumann boundary conditions if no Dirichlet contact is present and only Schottky contacts appear. Note that the simultaneous treatment of Dirichlet and Schottky contacts would be possible by adapting the technique e.g. in [9] and treating the additional boundary terms on Γ_S given by (1.5). For the present paper, we now assume that *all* metal-semiconductor contacts are of Schottky type. Especially concerning the regularizations and the treatment of the regularized problems novel ideas in the existence proof are necessary. We point out the new aspects in the proofs and combine them with known proof techniques for the Dirichlet case which can be applied in both situations. Moreover, for boundedness and uniqueness results, additional boundary terms have to be handled.

The paper is organized as follows: In Section 2, we formulate our assumptions and give a weak formulation of the scaled model equations. While Section 3 is devoted to energy estimates, the existence of weak solutions and their boundedness are demonstrated in Section 4. Under the additional assumption (A3), in Section 5 the uniqueness of the weak solution is demonstrated using a higher regularity result that is proven in Section 6. The paper ends with concluding remarks in Section 7.

2 Weak formulation

2.1 Scaling of the model equations for the analysis

For a simpler notation in the analysis, we work with the following scaled quantities: The potentials ψ, ψ_{app} and quasi-Fermi potentials φ_i, $i = n, p$, are scaled by the thermal voltage $U_T := k_{\mathrm{B}}T/q$. The chemical potentials, the Schottky barrier ϕ_0, and the (intrinsic) band edges E_i are divided by $k_{\mathrm{B}}T$, and we denote $\zeta_i := z_i \frac{E_i}{k_{\mathrm{B}}T}$. We define $\mu_i = \overline{\mu}_i U_T$ and $\varepsilon := \varepsilon_0 \varepsilon_r U_T/q$. After dividing the Poisson equation (1.1) by q, the continuity equations (1.2) by $q z_i$, and denoting the scaled potentials by the same symbol as the original ones, we obtain

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \psi) &= C + z_n u_n + z_p u_p, \quad \text{in } (0,\infty) \times \Omega, \\ \frac{\partial u_i}{\partial t} - \nabla \cdot (z_i \mu_i u_i \nabla \varphi_i) &= -R, \quad i = n, p, \quad \text{in } (0,\infty) \times \Omega \end{aligned} \tag{2.1}$$

with $u_i = N_i\mathcal{F}_i\big(z_i(\varphi_i - \psi) + \zeta_i\big)$, $v_i = z_i(\varphi_i - \psi)$, $i = n, p$, $R = r(u_n, u_p)\big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)$. The initial and boundary conditions remain of the form

$$u_n(0) = u_n^0, \quad u_p(0) = u_p^0 \quad \text{in } \Omega \tag{2.2}$$

$$\begin{aligned} \psi = \psi^D, \quad \mu_i u_i \nabla\varphi_i \cdot \nu = a_i\Big(\frac{u_i}{N_i} - \frac{u_{i,0}}{N_i}\Big), \quad i = n, p, \quad \text{on } (0,\infty) \times \Gamma_S, \\ \varepsilon\nabla\psi \cdot \nu = \mu_i u_i \nabla\varphi_i \cdot \nu = 0, \quad i = n, p, \quad \text{on } (0,\infty) \times \Gamma_N \end{aligned} \tag{2.3}$$

with $\psi^D := \phi_0 + \zeta_n + \psi_{app}$ and $a_i := qN_i\overline{a}_i$, $i = n, p$.

2.2 Notation and assumptions on the data

We use the Lebesgue spaces $L^p(\Omega)$ and the Sobolev spaces $W^{1,p}(\Omega)$, $p \in [1, \infty]$, and $H^1(\Omega) = W^{1,2}(\Omega)$. For $p \in [1, \infty]$, we introduce $W^{1,p}_S(\Omega)$ as the closure of the set

$$\{y|_\Omega : y \in C_0^\infty(\mathbb{R}^d),\ \operatorname{supp} y \cap \Gamma_S = \emptyset\}$$

in the Sobolev space $W^{1,p}(\Omega)$, and we set $W^{-1,p}_S(\Omega) := W^{1,p'}_S(\Omega)^*$, where $1/p + 1/p' = 1$. In our estimates, positive constants that may depend at most on the data of our problem are denoted by c. In particular, they can change from line to line.

We study the van Roosbroeck system with Schottky boundary conditions under the following assumptions:

(A1) $\Omega \subset \mathbb{R}^2$ is a bounded Lipschitz domain, $\Omega \cup \Gamma_N$ is regular in the sense of Gröger [15], $\Gamma_S,\ \Gamma_N \subset \Gamma := \partial\Omega$ are disjoint subsets such that $\overline{\Gamma_S \cup \Gamma_N} = \Gamma$ and $\operatorname{mes}(\Gamma_S) > 0$.

(A2) $\mathcal{F}_i$, $i = n, p$, fulfill (1.4), $N_i,\ \mu_i \in L^\infty(\Omega)$, $\zeta_i =$ const,
$0 < \underline{N} \le N_i \le \overline{N}$, $0 < \underline{\mu} \le \mu_i \le \overline{\mu}$ a.e. in Ω, $i = n, p$, and $C,\ \varepsilon \in L^\infty(\Omega)$,
$0 < \underline{\varepsilon} \le \varepsilon$ a.e. in Ω, $z_n = -1$, $z_p = 1$, $a_i \in L^\infty_+(\Gamma_S)$ with $\int_{\Gamma_S} a_i \,\mathrm{d}\Gamma > 0$, $i = n, p$,
$v_0^D := \psi^D$, $v_n^S := -(\phi_0 + \zeta_n)$, $v_p^S := -v_n^S = \phi_0 + \zeta_n \in W^{1,\infty}(\Omega)$,
$R = r(x, u_n, u_p)\big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)$, such that $r(x, u_n, u_p) = r_0(x, u_n, u_p)\, u_n\, u_p$, where
$r_0 : \Omega \times [0, +\infty)^2 \to \mathbb{R}$ is a Carathéodory function with
$0 \le r_0(x, u_n, u_p) \le \overline{r}$ for a.a. $x \in \Omega$ and for all $(u_n, u_p) \in [0, +\infty)^2$,
$u_i^0 \in L^\infty(\Omega)$, $0 < \underline{u} \le u_i^0 \le \overline{u}$, a.e. in Ω, $i = n, p$.

We will suppress the spatial position x in the writing of the reaction coefficients r and r_0.

2.3 Weak formulation

We introduce the statistical functions $e_i : \mathbb{R} \to (0, \infty)$ by $e_i(z) := \mathcal{F}_i(z + \zeta_i)$, $i = n, p$. Assumption (A2) and $u_i = N_i e_i(v_i) = N_i\mathcal{F}_i(v_i + \zeta_i)$ ensure

$$v_i = e_i^{-1}(\tfrac{u_i}{N_i}) = \mathcal{F}_i^{-1}(\tfrac{u_i}{N_i}) - \zeta_i, \quad \nabla\tfrac{u_i}{N_i} = \mathcal{F}_i'(v_i + \zeta_i)\nabla v_i = e_i'(v_i)\nabla v_i. \tag{2.4}$$

Have in mind that the inverses e_i^{-1}, $i = n, p$, are well-defined on $(0, \infty)$. Because of

$$\mathcal{F}_n(-\phi_0) = \mathcal{F}_n(-(\phi_0 + \zeta_n) + \zeta_n) = e_n(-(\phi_0 + \zeta_n)),$$
$$\mathcal{F}_p(-E_G + \phi_0) = \mathcal{F}_p(E_p - E_n + \phi_0 - \zeta_p + \zeta_p) = \mathcal{F}_p(\phi_0 + \zeta_n + \zeta_p) = e_p(\phi_0 + \zeta_n),$$

our definitions in (A2) ensure that $u_{i,0} = N_i e_i(v_i^S)$, $i = n, p$.

We work with a weak formulation of (2.1) in the form $u' + A(v, v) = 0,\ u = E(v),\ u(0) = u^0$ with the vectors $v = (v_0, v_n, v_p) = (\psi, \psi - \varphi_n, \varphi_p - \psi)$ (potentials), $u := (u_0, u_n, u_p)$ (densities, where u_0 represents the total charge density, i.e., the right-hand side of (1.1)). The vector of initial densities is denoted $u^0 := (u_0^0, u_n^0, u_p^0)$, where the initial total charge density u_0^0 is defined as $\langle u_0^0, w\rangle_{V_S} = \int_\Omega (\sum_{i=n,p} z_i u_i^0 w \,\mathrm{d}x + Cw)\,\mathrm{d}x$ for all $w \in V_S$, where we define the function spaces

$$V_S := \{y \in H^1(\Omega) : y|_{\Gamma_S} = 0\}, \quad V := V_S \times H^1(\Omega)^2, \quad Z := H^1(\Omega) \times L^\infty(\Omega)^2,$$
$$H := V_S \times L^2(\Omega)^2, \quad U := \big\{u \in V_S^* \times L^\infty(\Omega)^2 : \ln u_i \in L^\infty(\Omega),\ i = n, p\big\}.$$

For the boundary data, we set $v^S := (v_0^D, v_n^S, v_p^S)$ and use the operators $E_0 : v_0^D + V_S \to V_S^*$, $E : (v^S + V) \cap Z \to V^*$, $A : ((v^S + V) \cap Z)^2 \to V^*$,

$$\langle E_0(v_0), \overline{v}_0\rangle_{V_S} := \int_\Omega \varepsilon \nabla v_0 \cdot \nabla \overline{v}_0 \,\mathrm{d}x, \qquad E(v) := (E_0(v_0), N_n e_n(v_n), N_p e_p(v_p)),$$
$$\begin{aligned}\langle A(w, v), \overline{v}\rangle_V := &\sum_{i=n,p} \int_\Omega N_i e_i(w_i) \mu_i \nabla(v_i + z_i v_0) \cdot \nabla(\overline{v}_i + z_i \overline{v}_0) \,\mathrm{d}x \\ &+ \int_\Omega r(N_n e_n(w_n), N_p e_p(w_p))\big(1 - \mathrm{e}^{-w_n - w_p}\big)(\overline{v}_n + \overline{v}_p) \,\mathrm{d}x \\ &+ \sum_{i=n,p} \int_{\Gamma_S} a_i(e_i(w_i) - e_i(v_i^S)) \overline{v}_i \,\mathrm{d}\Gamma \qquad \forall \overline{v} \in V.\end{aligned}$$

Note that the test functions are such that $\overline{v}_0 = 0$ on Γ_S, thus, in the boundary contribution to A, we can write $\overline{v}_i$ instead of $\overline{v}_i + z_i \overline{v}_0$.

For the initial state u^0, we denote by v_0^0 the unique solution to $E_0(v_0) = u_0^0$ (note that E_0 is strongly monotone and Lipschitz continuous). Moreover, let $v_i^0 := e_i^{-1}(u_i^0/N_i)$, $i = n, p$, and $v^0 := (v_0^0, v_n^0, v_p^0)$ for the initial values. The weak formulation of the scaled drift-diffusion system with Schottky boundary conditions (2.1), (2.2), and (2.3) is problem

$$\begin{aligned}&u' + A(v, v) = 0, \quad u = E(v) \quad \text{a.e. on } \mathbb{R}_+, \quad u(0) = u^0, \\ &u \in H^1_{\text{loc}}(\mathbb{R}_+, V^*), \quad v - v^S \in L^2_{\text{loc}}(\mathbb{R}_+, V) \cap L^\infty_{\text{loc}}(\mathbb{R}_+, Z).\end{aligned} \tag{P}$$

3 Energy estimates for weak solutions

Entropy methods [9, 10, 17] are an efficient tool in the analytical treatment of drift-diffusion problems. Our free energy functional Ψ in (3.1) consists of an electrostatic part and a chemical part that is derived from the underlying statistical relations. The above defined operator E is strictly monotone and has the potential $\Phi : v^S + V \to \mathbb{R} \cup \{+\infty\}$,

$$\Phi(v) := \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2 + \sum_{i=n,p} N_i \int_{v_i^S}^{v_i} e_i(y)\,\mathrm{d}y\Big\}\mathrm{d}x.$$

The functional Φ and its conjugate functional (see [7]) $\Psi : V^* \to \overline{\mathbb{R}}$, defined via

$$\Psi(u) := \Phi^*(u) = \sup_{w\in V} \big\{\langle u, w\rangle_V - \Phi(w + v^S)\big\},$$

are convex. Since $\Phi(v^S) = 0$, we have $\Psi(u) \geq 0$ for all $u \in V^*$. Because Φ is continuous, strictly convex, and Gâteaux differentiable, it is also subdifferentiable on $v^S + V$ and it holds that $\partial\Phi(v) = \{Ev\}$ if $v \in (v^S + V) \cap Z$. For states $u = Ev \in V^*$, $u \in U$ we obtain

$$\begin{aligned}\Psi(u) &= \langle E(v), v - v^S\rangle_V - \Phi(v)\\ &= \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2 + \sum_{i=n,p}\int_{v_i^S}^{v_i} [u_i - N_i e_i(y)]\mathrm{d}y\Big\}\mathrm{d}x.\end{aligned} \tag{3.1}$$

By separately discussing the different cases $v_i^S < v_i$, $v_i^S > v_i$, as well as $|v_i^S - v_i| > 1$ and $|v_i^S - v_i| \leq 1$ and using that e_i is monotonically increasing, we find $\int_{v_i^S}^{v_i}(u_i - N_i e_i(y))\,\mathrm{d}y \geq [u_i - N_i e_i(v_i^S + 1)]$. Therefore, it results from (3.1) that

$$\|u_n\|_{L^1} + \|u_p\|_{L^1} + \|v_0 - v_0^D\|_{H^1}^2 \leq c(1 + \Psi(u)). \tag{3.2}$$

Theorem 3.1 *We assume* (A1) *and* (A2)*. There exists a constant $c > 0$ such that for any solution (u, v) to Problem* (P) *the free energy along the solution can be estimated by*

$$\Psi(u(t)) \leq \big(\Psi(u(0)) + c\big)\mathrm{e}^{ct} \quad \forall\ t > 0.$$

Moreover, if v_0^D and $v_n^S = -v_p^S$ are constants then $\Psi(u(t))$ is monotonically decreasing.

Proof. 1. For arbitrarily given $t \in \mathbb{R}_+$, we test $u' + A(v, v) = 0$ by $v - v^S \in L^2(0, t; V)$. Because of $u(s) = E(v(s))$ f.a.a. $s \in [0, t]$, we obtain $v(s) - v^S \in \partial\Psi(u(s))$ f.a.a. $s \in [0, t]$ and the Brézis formula (cf. [4, Lemma 3.3]) guarantees the chain rule

$$\begin{aligned}\Psi(u(t)) - \Psi(u(0)) &= \int_0^t \langle u'(s), v(s) - v^S\rangle_V\,\mathrm{d}s = -\int_0^t \langle A(v(s), v(s)), v(s) - v^S\rangle_V\,\mathrm{d}s\\ &= -\int_0^t\int_\Omega \Big[\sum_{i=n,p} \mu_i u_i \nabla\varphi_i \cdot \nabla(\varphi_i - v_0^D - z_i v_i^S) + r(\mathrm{e}^{\varphi_n - \varphi_p} - 1)(\varphi_n - \varphi_p)\Big]\,\mathrm{d}x\,\mathrm{d}s\\ &\quad - \int_0^t\int_{\Gamma_S}\sum_{i=n,p} a_i(e_i(v_i) - e_i(v_i^S))(v_i - v_i^S)\,\mathrm{d}\Gamma\,\mathrm{d}s\\ &\leq \int_0^t \sum_{i=n,p}\int_\Omega \frac{u_i}{2}(-\mu_i|\nabla\varphi_i|^2 + c|\nabla v_0^D|^2 + c|\nabla v_i^S|^2)\,\mathrm{d}x\,\mathrm{d}s.\end{aligned} \tag{3.3}$$

Here we used $\varphi_i = v_0 + \frac{1}{z_i}v_i$, the monotonicity of e_i and the exponential function. Moreover, we applied Young's inequality. In particular, the estimate (3.3) ensures for constant v_0^D and $v_n^S = -v_p^S$ that the free energy $\Psi(u(t))$ is monotonically decreasing.

2. Because of $v_0^D, v_i^S \in W^{1,\infty}(\Omega)$, we derive from (3.3) that

$$\Psi(u(t)) - \Psi(u(0)) \leq c\int_0^t\int_\Omega \sum_{i=n,p} u_i(|\nabla v_0^D|^2 + |\nabla v_i^S|^2)\,\mathrm{d}x\,\mathrm{d}s \leq c\int_0^t \sum_{i=n,p}\|u_i\|_{L^1}\,\mathrm{d}s.$$

Since (3.2) guarantees an estimate of $\|u_i(s)\|_{L^1(\Omega)}$, $i = n, p$, in terms of $\Psi(u(s)) + c$, Gronwall's lemma ensures $\Psi(u(t)) \leq (\Psi(u(0)) + c)\mathrm{e}^{ct}$ for all $t > 0$. $\square$

4 Existence result

For any arbitrary finite time horizon $T > 0$, let $I := [0, T]$. We consider the problem

$$u' + A(v, v) = 0, \quad u = E(v) \text{ a.e. on } I, \quad u(0) = u^0,$$
$$u \in H^1(I, V^*), \quad v - v^S \in L^2(I, V) \cap L^\infty(I, Z). \tag{$\mathsf{P_I}$}$$

To show the existence of a weak solution to ($\mathsf{P_I}$), we first consider a regularized problem ($\mathsf{P_M}$), where the state equations $u_i = N_i e_i(v_i)$, reaction and boundary terms are regularized, and gradient contributions are suitably completed to obtain coercivity in H^1 (with parameter M, see the definition of the operators E_M and A_M below). We verify the solvability of ($\mathsf{P_M}$) by time discretization, derivation of suitable a priori estimates, and passing to the limit in Lemma 4.3. Here, the estimates can depend on the regularization level M. Next, we derive a priori estimates for solutions to ($\mathsf{P_M}$) that are independent of M (see Lemma 4.5 below for upper bounds and Lemma 4.6 below for positive lower bounds for the carrier densities). Therefore any solution to ($\mathsf{P_M}$) is also a solution to ($\mathsf{P_I}$), if we take the parameter M sufficiently large.

4.1 The regularized problem ($\mathsf{P_M}$)

In this subsection, all estimates are allowed to depend on the regularization level M. For

$$M > M^* := \max\big\{\max_{i=n,p} \|e_i^{-1}(u_i^0/N_i)\|_{L^\infty}, \|v_n^S\|_{L^\infty}\big\}, \tag{4.1}$$

we introduce the cut-off function $d_M : \mathbb{R} \to [-M, M]$, $d_M(z) := \min\{\max\{z, -M\}, M\}$ and the regularized statistical relations $u_i = N_i e_i(d_M(v_i)) =: N_i e_{Mi}(v_i)$, $i = n, p$. We regularize the reaction and boundary terms by means of a continuous function

$$\rho_M : \mathbb{R}^3 \to [0, 1] \quad \text{with} \quad \rho_M(v) = \begin{cases} 0, & \text{if } \max\{|v_n|, |v_p|\} \geq M, \\ 1, & \text{if } \max\{|v_n|, |v_p|\} < M/2. \end{cases}$$

We write $\varphi_i = v_0 + z_i v_i$, $\overline{\varphi}_i = \overline{v}_0 + z_i \overline{v}_i$, $i = n, p$, and work with the regularized operators $E_M : v^S + V \to V^*$, $A_M : (v^S + V)^2 \to V^*$,

$$\begin{aligned} E_M(v) &:= (E_0 v_0, N_n e_{Mn}(v_n), N_p e_{Mp}(v_p)), \\ \langle A_M(w, v), \overline{v}\rangle_V &:= \int_\Omega \sum_{i=n,p} \Big\{ N_i e_{Mi}(w_i) \mu_i \nabla\varphi_i \cdot \nabla\overline{\varphi}_i + \big(\varphi_i - d_M(w_0) - z_i d_M(w_i)\big)\overline{\varphi}_i \Big\} \mathrm{d}x \\ &\quad + \int_{\Gamma_S} \sum_{i=n,p} \rho_M(w) a_i \big((e_i(w_i) - e_i(v_i^S)\big)\overline{v}_i \, \mathrm{d}\Gamma \\ &\quad + \int_\Omega \rho_M(w) r(N_n e_n(w_n), N_p e_p(w_p)) \big(1 - \mathrm{e}^{-w_n - w_p}\big)(\overline{v}_n + \overline{v}_p) \, \mathrm{d}x, \end{aligned} \tag{4.2}$$

for all $\overline{v} \in V$. Note that $\rho_M(v) = \rho_M(d_M(v))$ and $\rho_M(v) e_i(v_i) = \rho_M(v) e_{Mi}(v_i)$ and $\overline{\varphi}_i = \overline{v}_i$ on Γ_S as $\overline{v}_0 = 0$ thereon. We study the problem

$$u' + A_M(v, v) = 0, \; u = E_M(v), \; u(0) = u^0, \; u \in H^1(I, V^*), \; v - v^S \in L^2(I, V). \tag{$\mathsf{P_M}$}$$

Remark 4.1 *Any solution* (u, v) *to* ($\mathrm{P_M}$) *with* $\|v_0\|_{L^\infty(I,L^\infty)} \le M$ *and* $\|v_i\|_{L^\infty(I,L^\infty)} \le \frac{M}{2}$, $i = n, p$, *is also a solution to* ($\mathrm{P_I}$).

We consider a time-discrete version of ($\mathrm{P_M}$). For $k \in \mathbb{N}$, let $h_k := \frac{T}{k}$. For any Banach space X, we define $C_k(I, X)$ as the space of all functions $u : I \to X$ being constant on each interval $((l-1)h_k, lh_k]$, $l = 1, \dots, k$. Let u^l denote the value of $u \in C_k(I, X)$ on $((l-1)h_k, lh_k]$ and introduce the map Δ_k from $C_k(I, X)$ into itself by $(\Delta_k u)^l := \frac{1}{h_k}(u^l - u^{l-1})$, $l = 1, \dots, k$, with the initial value u^0. Moreover, we use for $u \in C_k(I, X)$ the continuous, piecewise linear function $(K_k u)(t) := u^0 + \int_0^t (\Delta_k u)(s)\,\mathrm{d}s$. The corresponding time-discrete version of ($\mathrm{P_M}$) is to look for (u_k, v_k) such that

$$\Delta_k u_k + A_M(v_k, v_k) = 0,\ u_k = E_M(v_k),\ v_k - v^S \in C_k(I, V). \tag{4.3}$$

Lemma 4.2 *We suppose* (A1) *and* (A2). *Then, for all* $k \in \mathbb{N}$, *the problem* (4.3) *has a unique solution* (u_k, v_k). *Moreover, it satisfies the estimates*

$$\sup_{k\in\mathbb{N}} \big\{ \|v_k - v^S\|_{L^2(I,V)} + \|\Delta_k u_k\|_{L^2(I,V^*)} + \|K_k u_k\|_{C(I,H^*)} \big\} < \infty.$$

Proof. 1. Using the argument splitting in the definition of the operator A_M, the (regularized) operator $v \mapsto \frac{1}{h_k} E_M(v) + A_M(v, v)$ is an operator of variational type (see [19, p. 182]). We recall that the main part (in the argument v in (4.2)) is monotone, continuous and bounded and the regularized reaction and boundary terms (in the argument w) are bounded and Lipschitz continuous. Since additionally $v \mapsto \frac{1}{h_k} E_M(v) + A_M(v, v)$ is coercive, we obtain for any given v_k^{l-1} with $u_k^{l-1} = E_M(v_k^{l-1})$ a solution v_k^l to single time steps in (4.3). Therefore, we successively compose from the solution for each time step a solution to (4.3).

2. We work with the regularized functionals $\Phi_M : v^S + V \to \mathbb{R}$, $\Psi_M : V^* \to (-\infty, \infty]$,

$$\begin{aligned}
\Phi_M(v) &:= \int_\Omega \frac{\varepsilon}{2} \big\{ |\nabla v_0|^2 - |\nabla v_0^D|^2 \big\}\,\mathrm{d}x + \sum_{i=n,p} \int_\Omega N_i \int_{v_i^S}^{v_i} e_{Mi}(y)\,\mathrm{d}y\,\mathrm{d}x, \\
\Psi_M(u) &:= \sup_{w\in V} \{ \langle u, w\rangle_V - \Phi_M(w + v^S) \}, \quad u \in V^*.
\end{aligned}$$

The functional Φ_M is Fréchet differentiable with $\Phi_M' = E_M$, and the conjugate functional Ψ_M for arguments $u = E_M(v)$ is given by

$$\Psi_M(u) = \langle u, v - v^S\rangle_V - \Phi_M(v) = \big\langle \big(E_0 v_0, N_n e_{Mn}(v_n), N_p e_{Mp}(v_p)\big), v - v^S \big\rangle_V - \Phi_M(v).$$

Additionally, we have $v - v^S \in \partial\Psi_M(u)$ provided that $u = E_M(v)$ for $v \in v^S + V$. Because of $\int_{v_i^S}^{v_i} (u_i - N_i e_{Mi}(y))\,\mathrm{d}y = \int_{v_i^S}^{d_M(v_i)} (u_i - N_i e_i(y))\,\mathrm{d}y \ge u_i - N_i e_i(v_i^S + 1)$ we obtain

$$\Psi_M(u) \ge c\|v_0 - v_0^D\|_{H^1}^2 + \sum_{i=n,p} \int_\Omega \big(u_i - N_i e_i(v_i^S + 1)\big)\,\mathrm{d}x.$$

Similar to (3.2), it follows that

$$\|u_n\|_{L^1} + \|u_p\|_{L^1} + \|v_0 - v_0^D\|_{H^1}^2 \le c(1 + \Psi_M(u)). \tag{4.4}$$

By (4.3), the subdifferential property, and the strong monotonicity of the operator A_M in the second argument, we derive for $l = 1, \ldots, k$,

$$\begin{aligned}
\Psi_M(u_k^l) - \Psi_M(u^0) &= \sum_{j=1}^{l} \big(\Psi_M(u_k^j) - \Psi_M(u_k^{j-1})\big) \le \sum_{j=1}^{l} \big\langle u_k^j - u_k^{j-1}, v_k^j - v^S \big\rangle_V \\
&= -h_k \sum_{j=1}^{l} \Big\{ \big\langle A_M(v_k^j, v_k^j) - A_M(v_k^j, v^S), v_k^j - v^S \big\rangle_V + \big\langle A_M(v_k^j, v^S), v_k^j - v^S \big\rangle_V \Big\} \\
&\le -h_k \sum_{j=1}^{l} \Big\{ \sum_{i=n,p} \big(\underline{\mu}\underline{N} e_i(-M) \|\nabla(\varphi_{ki}^j - v_0^D - z_i v_i^S)\|_{L^2}^2 + \|\varphi_{ki}^j - v_0^D - z_i v_i^S\|_{L^2}^2\big) \\
&\qquad + \big\langle A_M(v_k^j, v^S), v_k^j - v^S \big\rangle_V \Big\} \\
&\le -\int_0^{lh_k} \sum_{i=n,p} \underline{c}_M \|\varphi_{ki} - v_0^D - z_i v_i^S\|_{H^1}^2 \,\mathrm{d}t + c_M,
\end{aligned} \tag{4.5}$$

where $c_M > 0$ does not depend on k. Since $\Psi_M(u^0) < \infty$, the estimates (4.4), (4.5) ensure

$$\sup_{k\in\mathbb{N}} \big\{ \|v_{k0} - v_0^D\|_{L^\infty(I,V_S)} + \|v_k - v^S\|_{L^2(I,V)} \big\} < \infty. \tag{4.6}$$

Due to the regularizations in A_M, we derive from (4.6) that $\sup_{k\in\mathbb{N}} \|A_M(v_k, v_k)\|_{L^2(I,V^*)} < \infty$ and therefore also $\sup_{k\in\mathbb{N}} \|\Delta_k u_k\|_{L^2(I,V^*)} < \infty$ by comparison. Furthermore, from $u_{k0} = E_0 v_{k0}$ and (4.6) it results $\sup_{k\in\mathbb{N}} \|u_{k0}\|_{L^\infty(I,V_S^*)} < \infty$. Using that $N_i e_i(-M) \le u_{ki} < N_i e_i(M)$, $i = n, p$, and $(K_k u_k)(t) = \big(\frac{t}{h_k} - l + 1\big) u_k^l + \big(l - \frac{t}{h_k}\big) u_k^{l-1}$ for $t \in ((l-1)h_k, lh_k]$ we obtain $K_k u_k \in C(I, H^*)$ with $\sup_{k\in\mathbb{N}} \|K_k u_k\|_{C(I,H^*)} < \infty$. $\square$

Lemma 4.3 *Under the Assumptions* (A1) *and* (A2) *there exists a solution* (u, v) *to* ($\mathrm{P_M}$).

Proof. 1. Let us start with a sequence $\{(u_k, v_k)\}_{k\in\mathbb{N}}$ of solutions to (4.3). According to Lemma 4.2, there are functions v and u and a non-relabelled subsequence such that

$$v_k - v^S \rightharpoonup v - v^S \text{ in } L^2(I,V), \quad K_k u_k \rightharpoonup u \text{ in } L^2(I,H) \text{ and } H^1(I,V^*). \tag{4.7}$$

For the limits, we denote $\varphi_i := v_0 + z_i v_i$, $i = n, p$. Since for any $w \in V$ and $t \in I$ the map $y \mapsto \langle y(t), w\rangle$, $y \in H^1(I, V^*)$, defines a continuous linear functional on $H^1(I, V^*)$, we get from (4.7) that $(K_k u_k)(t) \rightharpoonup u(t)$ in V^* for all $t \in I$. Additionally, the boundedness of $(K_k u_k)(t)$ in H then ensures $(K_k u_k)(t) \rightharpoonup u(t)$ in H for $t \in I$. By $(K_k u_k)(0) = u^0$, $k \in \mathbb{N}$, we conclude $u(0) = u^0$.

2. Arguing as in Step 3 of the proof of [1, Lemma 5.2] (for $I_0 = \emptyset$) it results

$$K_k u_k - u_k \to 0 \ \text{ in } L^2(I,V^*), \quad u_{ki} \to u_i, \ \frac{u_{ki}}{N_i} \to \frac{u_i}{N_i} \ \text{ in } L^2(I, L^2(\Omega)), \quad i = n, p. \tag{4.8}$$

Moreover, by $\|w\|_{L^2(S,L^2(\Gamma_S))}^2 \le c\|w\|_{L^2(S,L^2(\Omega))} \|w\|_{L^2(S,H^1)}$, the boundedness of $\{u_{ki}/N_i\}$ in $L^2(I, H^1(\Omega))$, and since $\{u_{ki}\}$ is a Cauchy sequence in $L^2(I, L^2(\Omega))$, we find that $\{u_{ki}\}$ is a Cauchy sequence in $L^2(I, L^2(\Gamma_S))$, too, and by the uniqueness of the limit

$$u_{ki}/N_i \to u_i/N_i \ \text{ in } L^2(I, L^2(\Gamma_S)), \quad i = n, p. \tag{4.9}$$

With $K_k u_k - u_k \to 0$ in $L^2(I,V^*)$ we conclude that $(K_k u_k)_i \to u_i$ in $L^2(I,H^1(\Omega)^*)$, $i=n,p$.

3. Because of $\big\langle A_M(v_k,v_k),(y,y,-y)\big\rangle_V = 0$ for all $y\in V_S$, we obtain from (4.3) and partial integration that for any fixed indices k_1 and k_2 of our subsequence

$$\int_0^t \big\langle \Delta_{k_1}u_{k_1}-\Delta_{k_2}u_{k_2},(y,y,-y)\big\rangle_V \,\mathrm{d}s = \big\langle (K_{k_1}u_{k_1}-K_{k_2}u_{k_2})(t),(y,y,-y)\big\rangle_V = 0$$

for all $y\in V_S$ and all $t\in I$. Let $J_S: V_S\to V_S^*$ denote the duality map of V_S. We take $y=y(t)=J_S^{-1}[(K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_0(t)]$ and obtain

$$\begin{aligned}&\|(K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_0(t)\|^2_{V_S^*} = \big\langle (K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_0(t), J_S^{-1}[(K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_0(t)]\big\rangle\\ &= \sum_{i=n,p} \big\langle (K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_i(t), J_S^{-1}[(K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_0(t)]\big\rangle_{H^1}\end{aligned}$$

and therefore $\|(K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_0\|_{L^2(I,V_S^*)} \le c\sum_{i=n,p}\|(K_{k_1}u_{k_1}-K_{k_2}u_{k_2})_i\|_{L^2(I,(H^1)^*)}$. The convergences (4.8) and the weak convergence in (4.7) ensure the strong convergences $(K_k u_k)_0\to u_0$ in $L^2(I,V_S^*)$ and $K_k u_k\to u$ in $L^2(I,V^*)$. Also using (4.8) we obtain $u_k\to u$ in $L^2(I,H)$, and $u_k(t)\to u(t)$ in V^* f.a.a. $t\in I$ for a non-relabelled subsequence.

4. As in Step 5 in the proof of [1, Lemma 5.2] we obtain $u(t)\in\partial\Phi_M(v(t))=E_M(v(t))$ f.a.a. $t\in I$ and the Brézis formula [4, Lemma 3.3] guarantees

$$\Psi_M(u(t))-\Psi_M(u^0) = \int_0^t \langle u'(s), v(s)-v^S\rangle_V \,\mathrm{d}s \quad \forall\, t\in I. \tag{4.10}$$

5. Exploiting the strong monotonicity of E_0 and $u_0(t)=E_0v_0(t)$, $u_{k0}(t)=E_0v_{k0}(t)$ a.e. in I we find with the test function $v_{k0}-v_0\in V_S$ and integration over I

$$c\|v_{k0}-v_0\|^2_{L^2(I,V_S)} \le \int_I \langle E_0v_{k0}-E_0v_0, v_{k0}-v_0\rangle_{V_S}\mathrm{d}t \le \|u_{k0}-u_0\|_{L^2(I,V_S^*)}\|v_{k0}-v_0\|_{L^2(I,V_S)}.$$

Step 3 then ensures $c\|v_{k0}-v_0\|_{L^2(I,V_S)} \le \|u_{k0}-u_0\|_{L^2(I,V_S^*)}\to 0$. Moreover, from (4.8), (4.9), and the Lipschitz continuity of e_i^{-1} on the interval $[e_i(-M),e_i(M)]$ we derive

$$d_M(v_{ki}) = e_i^{-1}(u_{ki}/N_i) \to e_i^{-1}(u_i/N_i) \quad \text{in } L^2(I,L^2(\Omega)),\ L^2(I,L^2(\Gamma_S)), \quad i=n,p. \tag{4.11}$$

Let $\widehat{v} := (v_0, e_n^{-1}(u_n/N_n), e_p^{-1}(u_p/N_p))$ and define $\widehat{A}\in L^2(I,V^*)$ by

$$\begin{aligned}\langle \widehat{A},\overline{v}\rangle_V :=& \int_\Omega \sum_{i=n,p}\big\{u_i\mu_i\nabla\varphi_i\cdot\nabla\overline{\varphi}_i + (\varphi_i - d_M(v_0)-z_i\widehat{v}_i)\overline{\varphi}_i\big\}\,\mathrm{d}x\\ &+\int_\Omega \rho_M(\widehat{v})r(u_n,u_p)\big(1-\mathrm{e}^{-\widehat{v}_n-\widehat{v}_p}\big)(\overline{v}_n+\overline{v}_p)\,\mathrm{d}x + \int_{\Gamma_S}\rho_M(\widehat{v})\sum_{i=n,p}a_i\big(\frac{u_i}{N_i}-e_i(v_i^S)\big)\overline{v}_i\,\mathrm{d}\Gamma.\end{aligned}$$

From $\rho_M(v_k)=\rho_M(d_M(v_k))$ we obtain $\rho_M(v_k)e_i(v_{ki})=\rho_M(d_M(v_k))e_i(d_M(v_{ki}))$ and

$$\begin{aligned}&\rho_M(v_k)r(N_ne_n(v_{kn}),N_pe_p(v_{kp}))(1-\mathrm{e}^{-v_{kn}-v_{kp}})\\ &\quad = \rho_M(d_M(v_k))r(N_ne_n(d_M(v_{kn})),N_pe_p(d_M(v_{kp})))(1-\mathrm{e}^{-d_M(v_{kn})-d_M(v_{kp})}).\end{aligned}$$

Together with (4.8), (4.9), (4.11), and Lebesgue's dominated convergence theorem we gain for a non-relabelled subsequence the convergence

$$A_M(v_k,v)\to\widehat{A} \quad \text{in } L^2(I,V^*). \tag{4.12}$$

6. Since (u_k, v_k) are solutions to (4.3), our convergence results for the subsequence obtained so far (compare also Step 2 in the proof of Lemma 4.2) give

$$\begin{aligned}
0 &= \lim_{k\to\infty} \int_I \langle \Delta_k u_k + A_M(v_k, v_k), v_k - v\rangle_V \,\mathrm{d}t \\
&= \lim_{k\to\infty} \int_I \Big\{ \langle \Delta_k u_k, v_k - v^S\rangle_V - \langle u', v - v^S\rangle_V \\
&\qquad\qquad + \big\langle A_M(v_k, v_k) - A_M(v_k, v), v_k - v\big\rangle_V + \big\langle A_M(v_k, v), v_k - v\big\rangle_V \Big\} \,\mathrm{d}t \\
&\geq \limsup_{k\to\infty} \Big[\Psi_M(u_k^k) - \Psi_M(u^0) + \int_I \Big\{ \langle u', v^S - v\rangle_V + \underline{c} \sum_{i=n,p} \|\varphi_{ki} - \varphi_i\|_{H^1}^2 \Big\} \,\mathrm{d}t \Big].
\end{aligned}$$

The limit of the last term in the third line is zero because of (4.12) and $v_k - v^S \rightharpoonup v - v^S$ in $L^2(I, V)$. The last term in the last line results from the strong monotonicity of A_M in the last argument. From the weak lower semi-continuity of Ψ_M, we obtain $\limsup_{k\to\infty} \Psi_M(u_k^k) = \limsup_{k\to\infty} \Psi_M(u_k(T)) \geq \Psi_M(u(T))$. Thus, with (4.10) and the estimates of Step 6, we conclude

$$\varphi_{ki} \to \varphi_i \quad \text{in } L^2(I, H^1(\Omega)), \quad i = n, p. \tag{4.13}$$

In Step 5, it was demonstrated that $\|v_{k0} - v_0\|_{L^2(I, V_S)} \to 0$. Therefore, we also derive the convergence $\|v_{ki} - v_i\|_{L^2(I, H^1)} \to 0$, $i = n, p$, and finally $\|v_k - v\|_{L^2(I,V)} \to 0$.

7. By $v_{ki} \to v_i$ in $L^2(I, L^2(\Omega))$ we find $d_M(v_{ki}) \to d_M(v_i)$ in $L^2(I, L^2(\Omega))$. With (4.11) we have $d_M(v_{ki}) \to e_i^{-1}(u_i/N_i)$ in $L^2(I, L^2(\Omega))$, $L^2(I, L^2(\Gamma_S))$. The uniqueness of the limit ensures $d_M(v_i) = e_i^{-1}(u_i/N_i) = \widehat{v}_i$, $i = n, p$. Using again $\rho_M(v) = \rho_M(d_M(v))$ we obtain that $\widehat{A} = A_M(v, v)$ in $L^2(I, V^*)$. For arbitrary $w \in L^2(I, V)$ we estimate

$$\begin{aligned}
\langle A_M(v_k, v_k) - A_M(v, v), w\rangle_V &= \langle A_M(v_k, v_k) - \widehat{A}, w\rangle_V \\
&= \langle A_M(v_k, v_k) - A_M(v_k, v), w\rangle_V + \langle A_M(v_k, v) - \widehat{A}, w\rangle_V \\
&\leq c \sum_{i=n,p} \|\varphi_{ki} - \varphi_i\|_{L^2(I,H^1)} \|w\|_{L^2(I,V)} + \|A_M(v_k, v) - \widehat{A}\|_{L^2(I,V^*)} \|w\|_{L^2(I,V)}.
\end{aligned}$$

This leads to

$$\|A_M(v_k, v_k) - A_M(v, v)\|_{L^2(I,V^*)} \leq c \sum_{i=n,p} \|\varphi_{ki} - \varphi_i\|_{L^2(S,H^1)} + \|A_M(v_k, v) - \widehat{A}\|_{L^2(I,V^*)}.$$

By (4.12) and (4.13), it follows for this subsequence that $A_M(v_k, v_k) \to A_M(v, v)$ in $L^2(I, V^*)$. Because Step 1 ensured $A_M(v_k, v_k) = -\Delta_k u_k \rightharpoonup -u'$ in $L^2(I, V^*)$, we obtain the identity $u' + A_M(v, v) = 0$. The equation $u = E_M(v)$ was already verified in Step 4. Thus, the limit (u, v) is a solution to ($\mathrm{P_M}$). □

4.2 A priori estimates for Problem ($\mathbf{P_M}$)

Now we look for estimates that do not depend on the cut-off threshold M. First, the choice of M in (4.1) and the definition of Ψ_M, ensure that for the initial value $\Psi_M(u^0) = \Psi(u^0)$.

Lemma 4.4 *We assume* (A1)*,* (A2)*, and* (4.1)*. Then, there exist* $c,\ c^*>0$ *and an exponent* $\pi>2$ *not depending on* M *and* u^0 *such that for any solution* (u,v) *to* $(\mathrm{P_M})$

$$\begin{aligned}
&\|v_0(t)-v_0^D\|_{H^1}^2+\textstyle\sum_{i=n,p}\|u_i(t)\|_{L^1}\le c\mathrm{e}^{cT}(1+\Psi(u^0))=:c_T,\\
&\|v_0(t)\|_{H^1}+\|v_0(t)\|_{L^\infty}\le c^*(1+\textstyle\sum_{i=n,p}\|u_i(t)\|_{L^2}),\\
&\|v_0(t)\|_{W^{1,\pi}}\le c\Big(1+\textstyle\sum_{i=n,p}\|u_i(t)\|_{L^{\sigma'}}\Big),\quad \textit{where } \sigma:=\tfrac{2\pi}{\pi-2},\ \sigma':=\tfrac{2\pi}{\pi+2}\qquad \forall t\in I.
\end{aligned}$$

Proof. 1. The test function $v-v^S$ for $u'+A_M(v,v)=0$ yields for all $t\in I$

$$\begin{aligned}
0&=\Psi_M(u(t))-\Psi(u^0)\\
&\quad+\int_0^t\Big\{\sum_{i=n,p}\int_\Omega N_ie_{Mi}(v_i)\mu_i\nabla(v_i+z_iv_0)\cdot\nabla(v_i-v_i^S+z_i(v_0-v_0^D))\,\mathrm{d}x\\
&\qquad+\sum_{i=n,p}\int_\Omega\big(v_i+z_iv_0-d_M(v_i)-d_M(z_iv_0)\big)(v_i-v_i^S+z_i(v_0-v_0^D))\,\mathrm{d}x\\
&\qquad+\int_\Omega\rho_M(v)r(N_ne_n(v_n),N_pe_p(v_p))\big(1-\mathrm{e}^{-v_n-v_p}\big)(v_n+v_p)\,\mathrm{d}x\\
&\qquad+\int_{\Gamma_S}\sum_{i=n,p}\rho_M(v)a_i\big((e_i(v_i)-e_i(v_i^S)\big)(v_i-v_i^S)\,\mathrm{d}\Gamma\Big\}\,\mathrm{d}s\\
&\ge\Psi_M(u(t))-\Psi(u^0)+\int_0^t\Big\{\sum_{i=n,p}\int_\Omega\tfrac{N_ie_{Mi}(v_i)\mu_i}{2}|\nabla(v_i-v_i^S+z_i(v_0-v_0^D))|^2\,\mathrm{d}x\\
&\qquad-c\int_\Omega\sum_{i=n,p}\Big(u_i(|\nabla v_i^S|^2+|\nabla v_0^D|^2)+|v_i^S|^2+|v_0^D|^2\Big)\,\mathrm{d}x\Big\}\,\mathrm{d}s.
\end{aligned}$$

Here we applied the inequality $(f+g-d_M(f)-d_M(g))(f+g)\ge(f+g-d_M(f)-d_M(g))^2$ to estimate $(v_i+z_iv_0-d_M(v_i)-d_M(z_iv_0))(v_i-v_i^S+z_i(v_0-v_0^D))\ge-(|v_i^S|^2+|v_0^D|^2)$. Additionally, we took into account the monotonicity of e_i and the exponential function. Noting that $v_i^S,\ v_0^D\in W^{1,\infty}(\Omega)$, we arrive at

$$\Psi_M(u(t))\le\Psi(u^0)+c\int_0^t\big(1+\sum_{i=n,p}\|u_i(s)\|_{L^1}\big)\,\mathrm{d}s.$$

Using (4.4) and applying Gronwall's lemma implies the first estimate of the lemma.

2. Because of $\langle A_M(v(s),v(s)),(y,y,-y)\rangle_V=0$ for all $y\in V_S$, we obtain

$$0=\int_0^t\langle u'(s),(y,y,-y)\rangle_V\,\mathrm{d}s=\langle u_0(t)-u_0^0,y\rangle_{V_S}+\langle u_n(t)-u_p(t)-u_n^0+u_p^0,y\rangle\quad\forall t\in I,$$

and the test of $E_0v_0(t)=u_0(t)$ by $v_0(t)-v_0^D$ gives $\|v_0(t)\|_{V_S}\le c\big(\sum_{i=n,p}\|u_i(t)\|_{L^2}+1\big)$ for all $t\in I$. Exactly as in Step 3 of the proof of [1, Lemma 5.3] (setting there $I_0=\emptyset$) we obtain $\|v_0(t)\|_{L^\infty}\le c(1+\sum_{i=n,p}\|u_i(t)\|_{L^2})$ for all $t\in I$.

3. The regularity result of Gröger [15, Theorem 1] for elliptic equations with non-smooth data and mixed boundary conditions in two spatial dimensions for the Poisson equation together with the boundedness of C, justifies the last estimate of the lemma. □

The techniques in the proofs of the following two lemmas are in such a way that they can be applied for Problem ($\mathrm{P_M}$) as well as for Problem ($\mathrm{P_I}$).

Lemma 4.5 *We assume* (A1) *and* (A2). *Let* $M \geq M^*$ *with* M^* *as in* (4.1). *Then, there exists a* $c_2 > 0$ *depending only on the data (but not on* M*) such that* $u_i(t) \leq c_2(T)$ *a.e. in* Ω *for all* $t \in I$*,* $i = n, p$*, for any solution* (u, v) *to* ($\mathsf{P_M}$).

Proof. 1. Let $K := \max_{i=n,p}\big\{\max\big\{\|e_i(v_i^S)\|_{L^\infty}, \|u_i^0/N_i\|_{L^\infty}, e_i(0)\big\}\big\}$ and let (u, v) be a solution to ($\mathsf{P_M}$). We introduce $w_i := (\frac{u_i}{N_i} - K)^+$, $i = n, p$ and use for $u' + A_M(v, v) = 0$ the test functions $q(0, w_n^{q-1}, w_p^{q-1}) \in L^2(I, V)$ with $q \geq 2$ to obtain for all $t \in I$

$$\begin{aligned}\sum_{i=n,p}\|w_i(t)\|_{L^q}^q &+ q\sum_{i=n,p}\int_0^t\int_\Omega \mu_i u_i \nabla(v_i{+}z_i v_0)\cdot\nabla w_i^{q-1}\mathrm{d}x\,\mathrm{d}s\\
&+ q\sum_{i=n,p}\int_0^t\int_\Omega [v_i - d_M(v_i) + z_i(v_0 - d_M(v_0))]w_i^{q-1}\mathrm{d}x\,\mathrm{d}s\\
&+ q\sum_{i=n,p}\int_0^t\int_\Omega \rho_M(v) r(1-\mathrm{e}^{-v_n-v_p})w_i^{q-1}\mathrm{d}x\,\mathrm{d}s\\
&+ q\sum_{i=n,p}\int_0^t\int_{\Gamma_S}\rho_M(v)a_i(e_i(v_i)-e_i(v_i^S))w_i^{q-1}\,\mathrm{d}\Gamma\,\mathrm{d}s = 0.\end{aligned}\tag{4.14}$$

Note that our choice of K ensures that $w_i(0) = 0$, $[e_i(v_i^S) - e_i(v_i)]w_i \leq 0$, $(v_i - d_M(v_i))w_i \geq 0$, and $-[v_i - d_M(v_i) + z_i(v_0 - d_M(v_0))]w_i \leq 2|v_0|w_i$. With this knowledge and the methods in the proof of [1, Lemma 5.6], we find with π, σ and σ' from Lemma 4.4 that

$$\begin{aligned}\sum_{i=n,p}\|w_i(t)\|_{L^q}^q \leq \int_0^t\sum_{i=n,p}\Big\{ &- 2\underline{\mu}\underline{N}\|w_i^{q/2}\|_{H^1}^2\\
&+ cq(\|w_i^{q/2}\|_{L^\sigma}+1)(\|\nabla v_0\|_{L^\pi}+1)\|\nabla w_i^{q/2}\|_{L^2}\\
&+ cq\|v_0\|_{L^\infty}\|w_i^{q-1}\|_{L^1} + cq^2(\|w_i^{q/2}\|_{L^2}^2+1)\Big\}\,\mathrm{d}s.\end{aligned}\tag{4.15}$$

2. First, for $q = 2$ we obtain from (4.15) due to Lemma 4.4 and $\|v_0\|_{L^\infty}\|w_i\|_{L^1} \leq \|v_0\|_{L^\infty}\|w_i\|_{L^2} \leq c\sum_{j=n,p}\|w_i\|_{L^2}^2 + c$ that

$$\begin{aligned}\sum_{i=n,p}\|w_i(t)\|_{L^2}^2 &\leq \int_0^t\sum_{i=n,p}\Big\{-2\underline{\mu}\underline{N}\|w_i\|_{H^1}^2 + c(\|w_i\|_{L^2}^2+1)\\
&\qquad + c(\|w_i\|_{L^\sigma}+1)(\|\nabla v_0\|_{L^\pi}+1)\|w_i\|_{H^1}\Big\}\,\mathrm{d}s\\
&\leq \int_0^T\sum_{i=n,p}\Big\{-2\underline{\mu}\underline{N}\|w_i\|_{H^1}^2 + c(\|w_i\|_{L^2}^2+1)\\
&\qquad + c(\|w_i\|_{L^\sigma}+1)(\sum_{j=n,p}\|u_j\|_{L^{\sigma'}}+1)\|w_i\|_{H^1}\Big\}\,\mathrm{d}s.\end{aligned}$$

Recall that $u_i \leq N_i(w_i + K)$. The Gagliardo–Nirenberg inequality yields

$$\|y\|_{L^2}^2 \leq c\|y\|_{L^1}\|y\|_{H^1},\quad \|y\|_{L^\sigma} \leq c\|y\|_{L^1}^{1/\sigma}\|y\|_{H^1}^{1/\sigma'},\quad \|y\|_{L^{\sigma'}} \leq c\|y\|_{L^1}^{1/\sigma'}\|y\|_{H^1}^{1/\sigma}\quad \forall y \in H^1(\Omega),$$

such that after applying Young's inequality and the first estimate in Lemma 4.4 we find

$$\sum_{i=n,p}\|w_i(t)\|_{L^2}^2 \leq c(K)\int_0^t\big(\sum_{i=n,p}\|w_i\|_{L^1}^2+1\big)\,\mathrm{d}s \leq c(K)\int_0^T(c_T^2+1)\,\mathrm{d}s = \widehat{c}(T).$$

3. Because of $\sigma' < 2$ and $u_i \le N_i(w_i+K)$, the last two estimates in Lemma 4.4 ensure T dependent bounds κ_T and $c_{T\infty}$ such that

$$(\|v_0\|_{C(I,W_S^{1,\pi}(\Omega))} + 1)^{2\sigma} \le \kappa_T, \quad \|v_0\|_{C(I,L^\infty(\Omega))} \le c_{T\infty}. \tag{4.16}$$

For $q \ge 2$ it results from (4.15), an application of Gagliardo–Nirenberg's and Young's inequality, and (4.16) that

$$\sum_{i=n,p} \|w_i(t)\|_{L^q}^q \le \bar{c} q^{2\sigma} \kappa_T T \sum_{i=n,p} (\sup_{t\in I} \|w_i\|_{L^{q/2}}^q + 1) \quad \forall t \in I.$$

Now, we follow the Moser iteration type arguments in the proof of [1, Lemma 5.6] to finalize our proof. □

Lemma 4.6 *We assume* (A1), (A2)*, and* $M \ge \max\{M^*, c_{T\infty}\}$ *with* M^* *from* (4.1) *and* $c_{T\infty}$ *from* (4.16)*. Then, there exists* $c_1 > 0$ *depending only on the data* (*but not on* M) *such that* $c_1(T) \le u_i(t)$ *a.e. in* Ω *for all* $t \in I$*,* $i = n, p$*, for any solution* (u, v) *to* ($\mathrm{P_M}$)*.*

Proof. We define $K := \max_{i=n,p} \big\{ \max \big\{ \|\ln e_i(v_i^S)\|_{L^\infty},\ \|\big(\ln(u_i^0/N_i)\big)^-\|_{L^\infty},\ \ln e_i(0)\big\}\big\}$. We validate the assertion for $i = n$ (analogously this can be done for $i = p$). Let (u, v) be any solution to ($\mathrm{P_M}$). Then, it holds that $\big(\ln(u_n/N_n) + K\big)^-(0) = 0$. We use the test functions

$$-q\Big(0, \frac{w^{q-1}}{u_n/N_n}, 0\Big) \in L^2(I, V), \quad w := \big(\ln u_n/N_n + K\big)^-, \quad q \ge 2.$$

We have to estimate on the right-hand side the expression

$$\int_\Omega q(\varphi_n - d_M(v_0) - z_n d_M(v_n)) \frac{z_n w^{q-1}}{u_n/N_n}\,\mathrm{d}x = \int_\Omega q(v_0 + z_n v_n - d_M(v_0) - z_n d_M(v_n)) \frac{z_n w^{q-1}}{u_n/N_n}\,\mathrm{d}x.$$

Our choice of M guarantees that $d_M(v_0) = v_0$ a.e. in Ω for all $t \in I$. Therefore, the last integral reduces to $\int_\Omega q(v_n - d_M(v_n)) \frac{w^{q-1}}{u_n/N_n}\,\mathrm{d}x$, which is non-positive and can be neglected in the estimate. Note that our choice of K ensures that $v_n \le 0$ and $v_n \le v_n^S$ in case that $w \ne 0$. Together with the monotonuous increase of e_i this guarantees that $(e_n(v_n) - e_n(v_n^S)) \frac{w^{q-1}}{u_n/N_n} \le 0$ and the boundary term can be neglected on the right-hand side, too.

With these additional informations, we follow the arguments in the proof of [1, Lemma 5.7] to establish with suitable $\delta > 0$ and $\widetilde{c}(T) > 1$ the estimate

$$\|w(t)\|_{L^q}^q \le \widehat{c}(T) q^{2\sigma} \kappa_T (\sup_{s\in I} \|w^{q/2}(s)\|_{L^1}^2 + 1)$$

with σ from Lemma 4.4 and κ_T from (4.16). Now, as in the proof of [1, Lemma 5.7] the desired lower bound is obtained by Moser iteration. □

4.3 Solvability of Problem (P)

Theorem 4.7 *We suppose* (A1) *and* (A2)*. Then, for all* $T > 0$*,* $I = [0, T]$*, there exists a solution to Problem* ($\mathrm{P_I}$)*.*

Proof. For arbitrarily chosen $T > 0$, $I = [0,T]$ Problem ($\mathrm{P_M}$) can be solved, see Lemma 4.3. The a priori estimates for solutions to ($\mathrm{P_M}$) in Lemma 4.4, Lemma 4.5, and Lemma 4.6 ensure that for

$$M \geq \max\left\{M^*, c_{T\infty}, 2\max_{i=n,p}\left|e_i^{-1}\left(\tfrac{c_1(T)}{\overline{N}}\right)\right|, 2\max_{i=n,p}\left|e_i^{-1}\left(\tfrac{c_2(T)}{\underline{N}}\right)\right|\right\}$$

(with M^* as in (4.1), $c_{T\infty}$ from (4.16)) every solution (u,v) to ($\mathrm{P_M}$) satisfies $d_M(v_i) = v_i$ for $i = 0,n,p$. Because of $\rho_M(v) = 1$, the reaction and boundary terms in $A_M(v,v)$ and $A(v,v)$ coincide. Furthermore, the regularizing terms $\varphi_i - d_M(v_0) - z_i d_M(v_i)$ disappear, and we have $A_M(v,v) = A(v,v)$ and $E_M(v) = E(v)$. Thus, (u,v) solves ($\mathrm{P_I}$), too. □

4.4 Bounds for solutions to ($\mathrm{P_I}$)

Theorem 4.8 *We suppose* (A1) *and* (A2)*. Then, for all $T > 0$, $I = [0,T]$ there exist constants $c_1(T)$, $c_2(T) > 0$ such that for any solution (u,v) to Problem* ($\mathrm{P_I}$)

$$c_1(T) \leq u_i(t) \leq c_2(T) \quad \textit{a.e. in}\ \Omega \quad \textit{for all}\ t \in I, \quad i = n,p.$$

Proof. Let (u,v) be any solution to ($\mathrm{P_I}$). By Theorem 3.1 and (3.2) we have $\|u_i(t)\|_{L^1}$, $\|v_0(t)-v_0^D\|^2_{H^1}$ $\leq c(T)$ for all $t \in I$, $i = n,p$. The estimates in the second and last line of Lemma 4.4 hold true also for solutions (u,v) to ($\mathrm{P_I}$). To get the upper bounds of u_i we proceed as in the proof of Lemma 4.5. Recall that the estimate of the reaction term and the boundary integrals therein work also in the non-regularized setting for ($\mathrm{P_I}$) without the factor ρ_M. Moreover, the parts resulting from the regularization terms $z_i\varphi_i - d_M(z_i v_0) - d_M(v_i)$, $i = n,p$, are only neglected and not explicitly used in the estimates. We again use κ_T defined in (4.16) and apply the Moser iteration.

For the positive lower bounds of u_i we argue as in Lemma 4.6. In the proof of Lemma 4.6, the parts stemming from the regularization terms $z_i\varphi_i - d_M(z_i v_0) - d_M(v_i)$, $i = n,p$, are only neglected and not explicitly used in the estimates, thus, we can proceed for ($\mathrm{P_I}$) exactly as in the proof of Lemma 4.6 to obtain the lower bounds of u_i. □

Remark 4.9 *Note that the bounds above in connection to the third estimate in Lemma 4.4 imply that $\|v_0(t)\|_{W^{1,q}} \leq c$ for all $1 \leq q \leq \pi$ and $t \in I$.*

5 Uniqueness result and regularity properties

Under the additional (restrictive) Assumption (A3), we establish uniqueness (Theorem 5.1) and regularity results (Theorem 5.2) for weak solutions to ($\mathrm{P_I}$).

(A3) Ω is a domain with Lipschitz boundary (strong Lipschitz domain in the sense of Grisvard [14, Chap. 1.2]); $r_0(x,\cdot)$ is locally Lipschitz continuous for a.e. $x \in \Omega$; $N_i =$ const, $\mathcal{F}_i \in C^2(\mathbb{R})$, $u_i^0 \in W^{1,\lambda}(\Omega)$ for some $\lambda > 2$, $i = n,p$.

Theorem 5.1 *Under the Assumptions* (A1) – (A3)*, the solution to* ($\mathrm{P_I}$) *is unique.*

The proof of Theorem 5.1 uses ideas from [13, Sec. 4 and 5] and the following regularity result for solutions to ($\mathrm{P_I}$), whose proof is postponed to Section 6.

Theorem 5.2 *We assume* (A1) – (A3)*, then, there exists an exponent* $q > 2$ *such that*

$$v_0 \in L^s(I, W_S^{1,q}(\Omega)), \quad u_i \in L^s(I, W^{1,q}(\Omega)) \cap W^{1,s}(I, W^{1,q'}(\Omega)^*), \quad i = n, p,$$

for all $s \geq 1$ *and for any solution* (u, v) *to Problem* (P$_\mathrm{I}$).

Proof of Theorem 5.1. 1. Since N_i are constant by (A3), we obtain for solutions (u, v) to (P$_\mathrm{I}$) by (2.4) that $\nabla u_i = N_i e_i'(v_i)\nabla v_i$ and the diffusive part in the flux term of the continuity equations in (2.1) can be rewritten by

$$\mu_i u_i \nabla v_i = \mu_i \frac{u_i}{N_i}(e_i^{-1})'\big(\frac{u_i}{N_i}\big)\nabla u_i = b_i(u_i)\nabla u_i, \quad \text{where } b_i(u_i) := \mu_i \frac{u_i}{N_i}(e_i^{-1})'\big(\frac{u_i}{N_i}\big), \tag{5.1}$$

$i = n, p$. According to the uniform positive lower and upper bounds of the carrier densities u_i guaranteed by Theorem 4.8, we find constants $\underline{b}$ and $\overline{b}$ such that $0 < \underline{b} \leq b_i(u_i(t)) \leq \overline{b}$ a.e. in Ω for all $t \in I$, $i = n, p$ and $u_i \in L^2(I, H^1(\Omega))$ for all solutions (u, v) to (P$_\mathrm{I}$). Since $e_i \in C^2(\mathbb{R})$ and $e_i'(x) > 0$ we obtain the local Lipschitz continuity of $(e_i^{-1})'$ and thus the Lipschitz continuity for bounded intervals of densities. Similarly, by (A3) we get the Lipschitz continuity of R,

$$R(u_n, u_p) := r(u_n, u_p)\big(1 - \mathrm{e}^{-e_n^{-1}(u_n/N_n) - e_p^{-1}(u_p/N_p)}\big) \tag{5.2}$$

for bounded intervals of densities.

2. Let (u, v) and $(\widehat{u}, \widehat{v})$ be two solutions to (P$_\mathrm{I}$) and $\overline{u} := u - \widehat{u}$ and $\overline{v} := v - \widehat{v}$. Then

$$E_0(v_0(t)) - E_0(\widehat{v}_0(t)) = \overline{u}_0(t) \quad \text{and} \quad \|\overline{v}_0(t)\|_{V_S} \leq c \sum_{i=n,p} \|\overline{u}_i(t)\|_{L^2} \quad \text{f.a.a. } t \in I. \tag{5.3}$$

3. We test $u' + A(v, v) = 0$ and $\widehat{u}\,' + A(\widehat{v}, \widehat{v}) = 0$ by

$$(0, \overline{u}_n, \overline{u}_p) = (0, N_n(e_n(v_n) - e_n(\widehat{v}_n)), N_p(e_p(v_p) - e_p(\widehat{v}_p)) \in L^2(I, V)$$

and find for all $t \in I$

$$\begin{aligned}
\frac{1}{2}\sum_{i=n,p} \|\overline{u}_i(t)\|_{L^2}^2 = \sum_{i=n,p} \int_0^t \Big\{ \int_\Omega \big\{ &-b_i(u_i)|\nabla \overline{u}_i|^2 + \big(R(\widehat{u}_n, \widehat{u}_p) - R(u_n, u_p)\big)\overline{u}_i \\
&- \big(\big(b_i(u_i) - b_i(\widehat{u}_i)\big)\nabla \widehat{u}_i + \mu_i \overline{u}_i z_i \nabla v_0 + \mu_i \widehat{u}_i z_i \nabla \overline{v}_0\big) \cdot \nabla \overline{u}_i \big\}\,\mathrm{d}x \\
&- \int_{\Gamma_S} N_i a_i (e_i(v_i) - e_i(\widehat{v}_i))^2\,\mathrm{d}\Gamma \Big\}\,\mathrm{d}t' \\
\leq \sum_{i=n,p} \int_0^t \int_\Omega \big\{ &-\underline{b}|\nabla \overline{u}_i|^2 + c|\overline{u}_i||\nabla \overline{u}_i|(|\nabla \widehat{u}_i| + |\nabla v_0|) \\
&+ c\widehat{u}_i|\nabla \overline{v}_0||\nabla \overline{u}_i| + c|\overline{u}_i|^2 \big\}\,\mathrm{d}x\,\mathrm{d}t'.
\end{aligned}$$

We use $q > 2$ from Theorem 5.2 and define s by $1/s = 1/2 - 1/q$. Note in particular, that $q < \pi$, where π is given in Lemma 4.4, thus, we get that $\|v_0(t)\|_{W^{1,q}} \leq c$ for all $t \in I$ (see Remark 4.9). We apply (5.3) and the Gagliardo–Nirenberg inequality $\|y\|_{L^s} \leq c\|y\|_{L^2}^{2/s}\|y\|_{H^1}^{1-2/s}$ for $y \in H^1(\Omega)$, to estimate the term under the time integral by

$$\begin{aligned}
&-\underline{b}\|\overline{u}_i\|_{H^1}^2 + c\|\overline{u}_i\|_{L^s}\|\overline{u}_i\|_{H^1}(\|\nabla \widehat{u}_i\|_{L^q} + \|\nabla v_0\|_{L^q}) + c\|\nabla \overline{v}_0\|_{L^2}\|\overline{u}_i\|_{H^1} + c\|\overline{u}_i\|_{L^2}^2 \\
\leq &-\underline{b}\|\overline{u}_i\|_{H^1}^2 + c\|\overline{u}_i\|_{L^s}\|\overline{u}_i\|_{H^1}(\|\nabla \widehat{u}_i\|_{L^q} + 1) + c\sum_{j=n,p}\|\overline{u}_j\|_{L^2}\|\overline{u}_i\|_{H^1} + c\|\overline{u}_i\|_{L^2}^2 \\
\leq &-\underline{b}\|\overline{u}_i\|_{H^1}^2 + c\|\overline{u}_i\|_{L^2}^{2/s}\|\overline{u}_i\|_{H^1}^{2-2/s}(\|\nabla \widehat{u}_i\|_{L^q} + 1) + c\sum_{j=n,p}\|\overline{u}_j\|_{L^2}\|\overline{u}_i\|_{H^1} + c\|\overline{u}_i\|_{L^2}^2.
\end{aligned}$$

Finally, we apply Young's inequality and establish the inequality

$$\sum_{i=n,p} \|\overline{u}_i(t)\|_{L^2}^2 \leq \sum_{i=n,p} \int_0^t c\|\overline{u}_i(t')\|_{L^2}^2 (\|\nabla \widehat{u}_i\|_{L^q}^s + 1)\,\mathrm{d}t' \quad \forall t \in I.$$

Since by Theorem 5.2, $\widehat{u}_i \in L^s(I, W^{1,q}(\Omega))$, $i = n, p$, Gronwall's lemma yields $\overline{u}_i = 0$, $v_i = \widehat{v}_i$, $i = n, p$. Inequality (5.3) guarantees $v_0 = \widehat{v}_0$, therefore also $u_0 = \widehat{u}_0$, and $(u, v) = (\widehat{u}, \widehat{v})$ which proves Theorem 5.1. □

Corollary 5.3 *Under the Assumptions* (A1) – (A3)*, the solution to Problem* (P) *is unique.*

Proof. If we had two different solutions (u^1, v^1) and (u^2, v^2) to Problem (P) then there would be some $T_0 > 0$ and $I_0 = [0, T_0]$ such that $(u^1|_{I_0}, v^1|_{I_0})$ and $(u^2|_{I_0}, v^2|_{I_0})$ are two different solutions to $(\mathrm{P}_{\mathrm{I}_0})$. This, however, would contradict to Theorem 5.1. □

6 Proof of higher regularity

We shortly outline the proof of Theorem 5.2, which adapts ideas from [13, Sec. 5]. Using the form (5.1) of the diffusive flux density, we apply for each continuity equation separately the regularity theory for single quasilinear parabolic equations [16, 22]. We will show the existence of some $q > 2$ such that for all solutions (u, v) to (P_I) and all $s \geq 1$ it holds true that $u_n,\ u_p \in L^s(I, W^{1,q}(\Omega))$.

We base our proof on a variant of the higher regularity result for scalar quasilinear parabolic equations of [22, Theorem 5.3] shortly summarized in Subsection 6.1. We apply it in Subsection 6.2 to our suitably regularized continuity equations where the electrostatic potential in the drift term, the carrier densities in the generation-recombination term as well as the chemical potentials in terms resulting from the Schottky boundary condition are fixed by a solution (u, v) to (P_I). The cut-offs in the regularizations are realized in such a way that they do not effect solutions to (P_I) according to Theorem 4.8.

Theorem 6.2 below ensures a unique solution $y_i \in L^s(I, W^{1,q}(\Omega))$ to the regularized continuity equation (comp. Problem (P_{iq}) later on). On the one hand, this solution solves also the auxiliary problem (P_{i2}), see Subsection 6.2. On the other hand, for any solution (u, v) to (P_I), u_i is a solution to the auxiliary problem (P_{i2}), too. In Lemma 6.4 we verify that $u_i = y_i$. Thus, we gain the higher integrability of ∇u_i, $i = n, p$. The better regularity of v_0 results from the regularity result by Gröger [15].

6.1 A higher regularity result for scalar quasilinear parabolic equations

For a bounded, measurable function $\rho : \Omega \to \mathbb{R}$ with $0 < \underline{\rho} \leq \rho(x) \leq \overline{\rho}$ a.e. in Ω, we define the operator denoted by $-\nabla \cdot \rho \nabla + 1 :\ W_S^{1,2}(\Omega) \to W_S^{-1,2}(\Omega)$ by

$$\langle (-\nabla \cdot \rho \nabla + 1) w, \overline{w} \rangle_{W_S^{1,2}(\Omega)} := \int_\Omega (\rho \nabla w \cdot \nabla \overline{w} + w \overline{w})\,\mathrm{d}x, \quad w, \overline{w} \in W_S^{1,2}(\Omega),$$

and adhere to this notation of the operator when the range space is restricted to the spaces $W_S^{-1,q}(\Omega)$ ($q > 2$). A similar notation is also used for the spaces without boundary conditions, i.e., we denote $-\nabla \cdot \rho \nabla + 1 :\ W^{1,2}(\Omega) \to W^{1,2}(\Omega)^*$ for

$$\langle (-\nabla \cdot \rho \nabla + 1) w, \overline{w} \rangle_{W^{1,2}(\Omega)} := \int_\Omega (\rho \nabla w \cdot \nabla \overline{w} + w \overline{w})\,\mathrm{d}x, \quad w, \overline{w} \in W^{1,2}(\Omega).$$

We briefly report on a special case of the regularity result [22, Theorem 5.3] for scalar quasilinear parabolic equations that we will apply to improve the integrability properties of the gradient of the charge-carrier densities for solutions to (P_I). We formulate it only for the case that no Dirichlet boundary conditions in the equation are assumed - which is permitted in [22, Theorem 5.3]. According to [22, Remark 2.5 iv)] and our additional Assumption (A3), Ω admits bi-Lipschitzian boundary charts which are volume preserving, and the Assumptions 2.2, 2.4 for [22, Theorem 5.3] are fulfilled in our case. The assumptions for the right-hand side of the parabolic problem for [22, Theorem 5.3] are:

Assumption (B) (Assumption 5.1 in [22]) The function $\mathcal{R} : I \times C(\overline{\Omega}) \to W^{1,q'}(\Omega)^*$ is a Carathéodory function, i.e., $\mathcal{R}(\cdot, y) : I \to W^{1,q'}(\Omega)^*$ is measurable for each $y \in C(\overline{\Omega})$ and $\mathcal{R}(t, \cdot) : C(\overline{\Omega}) \to W^{1,q'}(\Omega)^*$ is continuous for all $t \in I$. Moreover, for $s \in (1, \infty)$, we assume that the superposition operator $y \mapsto [t \mapsto \mathcal{R}(t, y(t))]$ is continuous from every bounded set of $C(\overline{I \times \Omega})$ to $L^s(I, W^{1,q'}(\Omega)^*)$ such that for some constant $c_{\mathcal{R}} > 0$

$$\sup_{y \in C(\overline{\Omega})} \|\mathcal{R}(\cdot, y)\|_{L^s(I, W^{1,q'}(\Omega)^*)} \leq c_{\mathcal{R}}.$$

Remark 6.1 *([22, Remark 5.2]) Note that Assumption* (B) *is satisfied for a Carathéodory function* $\mathcal{R}$ *if the boundedness property is fulfilled and for every* $\eta > 0$ *there exists a function* $L_\eta \in L^s(I)$ *such that* $\|\mathcal{R}(t, y_1) - \mathcal{R}(t, y_2)\|_{W^{1,q'}(\Omega)^*} \leq L_\eta \|y_1 - y_2\|_{C(\overline{\Omega})}$ *f.a.a.* $t \in I$, *for all* $y_1,\ y_2 \in C(\overline{\Omega})$ *with* $\|y_1\|_{C(\overline{\Omega})},\ \|y_2\|_{C(\overline{\Omega})} \leq \eta$.

Theorem 6.2 *(Special case of Theorem 5.3 in [22]) Let* $\Omega \subset \mathbb{R}^d$ *be a strong Lipschitz domain in the sense of Grisvard [14] with* $d \leq 3$. *Let* μ *be a measurable coefficient function on* Ω *with* $\underline{\mu} \leq \mu \leq \overline{\mu}$ *a.e. in* Ω. *We suppose that* $\theta : \mathbb{R} \to [\underline{\theta}, \overline{\theta}]$, *where* $0 < \underline{\theta} < \overline{\theta}$, *is Lipschitz continuous on bounded sets. Assume further that for some* $q > d$ *the map* $-\nabla \cdot \mu \nabla + 1 : W^{1,q}(\Omega) \to W^{1,q'}(\Omega)^*$ *is a topological isomorphism. Let* $s > 2(1 - \frac{d}{q})^{-1}$ *and* y^0 *in the real interpolation space* $(W^{1,q}(\Omega), W^{1,q'}(\Omega)^*)_{1/s,s}$, *and let* $\mathcal{R} : I \times C(\overline{\Omega}) \to W^{1,q'}(\Omega)^*$ *satisfy the Assumption* (B) *for this* s. *Then there exists a global solution* $y \in W^{1,s}(I, W^{1,q'}(\Omega)^*) \cap L^s(I, W^{1,q}(\Omega))$ *of the quasilinear equation*

$$y'(t) - \nabla \cdot \big(\theta(y(t))\mu \nabla y(t)\big) + y(t) = \mathcal{R}(t, y(t)), \quad y(0) = y^0.$$

If $\mathcal{R}$ *additionally satisfies the assumptions in Remark 6.1, then this solution is unique.*

Remark 6.3 *i) Theorem 5.3 in [22] is originally formulated for* $d = 3$. *A consultation of the authors, J. Rehberg and H. Meinlschmidt, confirmed the validity of the result of Theorem 5.3 in [22] for* $d \leq 3$, *see also [1]. A statement for quasilinear equations clearer formulated for space dimension* $d = 2$ *and* $d = 3$ *can be found in [21, Theorem 2.2.12].*

ii) In [16, Theorem 3.1], the result of [22, Theorem 5.3] was extended, and the existence and uniqueness of global-in-time solutions in the $W_D^{-1,q}$ *-* $W_D^{1,q}$*-setting was demonstrated (for* $d = 2, 3$*) for abstract quasilinear parabolic PDEs with non-smooth data and mixed boundary conditions, including a nonlinear source term with at most linear growth.*

6.2 Application of the regularity result in Theorem 6.2 to regularized continuity equations

The Assumptions (A1), (A2) allow us to apply [15, Theorem 1], which in turn guarantees the existence of $\pi > 2$ such that $-\nabla \cdot \varepsilon \nabla + 1 : W_S^{1,q}(\Omega) \to W_S^{-1,q}(\Omega)$ is a topological isomorphism for all $q \in [2, \pi]$.

For any given solution (u,v) to ($\mathrm{P_I}$) it results from $v_i \in L^2(I,H^1(\Omega)) \cap L^\infty(I,L^\infty(\Omega))$ that $v_i \in L^\infty(I,L^\infty(\Gamma_S))$ with $\|v_i\|_{L^\infty(I,L^\infty(\Gamma))} \le \|v_i\|_{L^\infty(I,L^\infty(\Omega))}$. Moreover, for constant N_i, we obtain $u_i = N_i e_i(v_i) \in L^2(I,H^1(\Omega)) \cap L^\infty(I,L^\infty(\Omega))$. Note that under Assumption (A3), for solutions to ($\mathrm{P_I}$) we have $u_i \in C(I,L^2(\Omega))$, $i=n,p$. (This follows from the fact that $\{u_i \in L^2(I,H^1(\Omega)) : u_i' \in L^2(I,H^1(\Omega)^*)\}$ is continuously embedded in $C(I,L^2(\Omega))$, see [11, p. 147]). Using the Lipschitz continuous dependence of $(-\nabla\cdot\varepsilon\nabla+1)^{-1} : W_S^{-1,\pi}(\Omega) \to W_S^{1,\pi}(\Omega)$ on a given right-hand side (see [15, Theorem 1]) and the continuous embedding $L^2(\Omega) \hookrightarrow W_S^{-1,\pi}(\Omega)$, it follows that $v_0 \in C(I,W^{1,\pi}(\Omega))$.

We use the bounds from Theorem 4.8 to introduce the functions

$$d_i(y) := \max\{c_1(T),\min\{y,c_2(T)\}\}, \quad \theta_i(y) := \frac{d_i(y)}{N_i}(e_i^{-1})'\Big(\frac{d_i(y)}{N_i}\Big), \quad i=n,p.$$

Since the functions $(e_i^{-1})'$ are bounded from below and above for arguments in $[\frac{c_1(T)}{N_i},\frac{c_2(T)}{N_i}]$, there are constants $0<\underline{\theta}<\overline{\theta}<\infty$ such that $\underline{\theta}\le\theta_i(y)\le\overline{\theta}$ for all $y\in\mathbb{R}$. Additionally, by $e_i\in C^2(\mathbb{R})$, the truncating functions θ_i are Lipschitz continuous, $i=n,p$.

We fix an arbitrary solution (u,v) to ($\mathrm{P_I}$) and use the corresponding functions $v_0(t)$, $v_i(t)$, and $u_i(t)$, $i=n,p$, to define right-hand sides $\mathcal{R}_i : I\times C(\overline{\Omega}) \to H^1(\Omega)^*$ by

$$\begin{aligned}\langle\mathcal{R}_i(t,y),\overline{w}\rangle_{H^1} := &-\int_\Omega \Big\{(\mu_i z_i d_i(y)\nabla v_0(t))\cdot\nabla\overline{w} + R(u_n(t),u_p(t))\overline{w} - u_i(t)\overline{w}\Big\}\,\mathrm{d}x \\ &-\int_{\Gamma_S} a_i(e_i(v_i(t))-e_i(v_i^S))\,\overline{w}\,\mathrm{d}\Gamma \quad \forall\overline{w}\in H^1(\Omega), \quad i=n,p,\end{aligned}$$

with R from (5.2).

We apply the result for scalar quasilinear parabolic equations formulated in Theorem 6.2 separately for the continuity equations for electrons and holes. For this purpose, we fix the exponent $q>2$ as follows: By (A1), (A2), [15, Theorem 1] ensures some $q^*>2$ such that $-\nabla\cdot\mu_i\nabla+1 : W^{1,q}(\Omega)\to W^{1,q'}(\Omega)^*$, $i=n,p$, are topological isomorphisms for all $q\in[2,q^*]$. With λ from (A3) we now define

$$q := \min\{\lambda,\pi,q^*\} > 2. \tag{6.1}$$

Separately, for $i=n$ and $i=p$ we apply Theorem 6.2 for the quantities $\mathcal{R}:=\mathcal{R}_i$, $\theta:=\theta_i$, $\mu:=\mu_i$, $y^0:=u_i^0$. Note that $y_i^0=u_i^0$, $i=n,p$, are admissible initial values for Theorem 6.2. By the definition of the $\mathcal{R}_i$ and the estimates for the solution (u,v) to ($\mathrm{P_I}$) from Theorem 4.8 (the bounds of the carrier densities, the arguments at the beginning of this subsection like the fact that $v_0\in C(I,W^{1,\pi}(\Omega))$), we establish that $\mathcal{R}_i : I\times C(\overline{\Omega})\to W^{1,q'}(\Omega)^*$ is a Carathéodory function. The measurability in t for each $y\in C(\overline{\Omega})$ follows immediately, and the continuity in y is due to

$$\|\mathcal{R}_i(t,y_1)-\mathcal{R}_i(t,y_2)\|_{(W^{1,q'})^*} \le c\|\nabla v_0\|_{C(S,L^q)}\|y_1-y_2\|_{C(\overline{\Omega})} \tag{6.2}$$

for all $y_1,\ y_2\in C(\overline{\Omega})$ with a constant $c>0$ (not depending on t) for all $t\in I$, $i=n,p$. Furthermore, for $s\in(1,\infty)$, we can estimate for the superposition operator

$$\|\mathcal{R}_i(\cdot,y_1(\cdot))-\mathcal{R}_i(\cdot,y_2(\cdot))\|_{L^s(I,(W^{1,q'})^*)} \le \|\nabla v_0\|_{C(I,L^q)}\|y_1-y_2\|_{C(\overline{I\times\Omega})}$$

for all $y_1,\ y_2\in C(\overline{I\times\Omega})$. By the definition of $\mathcal{R}_i$ and the a priori estimates for the solution (u,v) to ($\mathrm{P_I}$), we verify the boundedness result

$$\begin{aligned}\sup_{y\in C(\overline{\Omega})}\|\mathcal{R}_i(\cdot,y)\|_{L^s(I,(W^{1,q'})^*)} \le c(s,T)\big(&\|v_0\|_{L^s(I,W^{1,q})} + \|e_i(v_i)-e_i(v_i^S)\|_{L^\infty(I,L^\infty(\Gamma_S))} \\ &+ \|u_i\|_{L^\infty(I,L^\infty)} + \|R(u_n,u_p)\|_{L^\infty(I,L^\infty)}\big) \le \widehat{c}(s,T).\end{aligned}$$

Thus, Assumption (B) is fulfilled for all s, especially for $s > \frac{2q}{q-2}$. Therefore, in summary, Theorem 6.2, Remark 6.1 and (6.2) guarantee unique solutions y_i of the Problems

$$\begin{aligned} &y_i \in W^{1,s}(I, W^{1,q'}(\Omega)^*) \cap L^s(I, W^{1,q}(\Omega)) \quad \text{such that} \\ &y_i'(t) - \nabla \cdot \theta_i(y_i(t))\mu_i \nabla y_i(t) + y_i(t) = \mathcal{R}_i(t, y_i(t)), \quad y_i(0) = y_i^0, \end{aligned} \tag{P$_{iq}$}$$

$i = n, p$. Since I is finite and the initial values satisfy $y_i^0 \in W^{1,q}(\Omega)$ (see (A3) and (6.1)), we obtain the integrability $y_i \in W^{1,s}(I, W^{1,q'}(\Omega)^*) \cap L^s(I, W^{1,q}(\Omega))$ for all $s \geq 1$. Additionally, we consider the Problem (P$_{i2}$) with the weak formulation: Find

$$\begin{aligned} &w_i \in H^1(I, W^{1,2}(\Omega)^*) \cap L^2(I, W^{1,2}(\Omega)) \text{ such that} \\ &w_i'(t) + B_i(t, w_i(t)) = 0 \text{ a.e. in } I, \quad w_i(0) = y_i^0, \end{aligned} \tag{P$_{i2}$}$$

where

$$\begin{aligned} \langle B_i(t, w_i), \overline{w}_i \rangle_{H^1} := &\int_\Omega \big\{ \mu_i \theta_i(w_i) \nabla w_i \cdot \nabla \overline{w}_i + (w_i - u_i(t)) \overline{w}_i \big\} \,\mathrm{d}x, \\ &+ \int_\Omega \big\{ R(u_n(t), u_p(t)) \overline{w}_i + \mu_i z_i d_i(w_i) \nabla v_0(t) \cdot \nabla \overline{w}_i \big\} \,\mathrm{d}x, \\ &+ \int_{\Gamma_S} a_i (e_i(v_i(t)) - e_i(v_i^S)) \overline{w}_i \,\mathrm{d}\Gamma \end{aligned}$$

with R from (5.2) for the fixed solution (u, v) to (P$_\text{I}$). Then the solution y_i to (P$_{iq}$) is also a solution to Problem (P$_{i2}$). Additionally, by Assumption (A3) and Theorem 4.8 the function u_i is a solution to Problem (P$_{i2}$), too.

Lemma 6.4 *We assume* (A1) – (A3)*. Let* y_i *be the unique solution to*

$$y_i'(t) - \nabla \cdot \big(\theta_i(y_i(t))\mu_i \nabla y_i(t)\big) + y_i(t) = \mathcal{R}_i(t, y_i(t)), \quad y_i(0) = y_i^0$$

and let u_i *solve the continuity equation in* (P$_\text{I}$)*. Then* $y_i = u_i$ *holds true,* $i = n, p$*.*

Proof. For $i = n, p$, we test (P$_{i2}$) for the solutions u_i and y_i by $u_i - y_i \in L^2(I, W^{1,2}(\Omega))$, respectively, substract them and obtain (note that the boundary and reaction terms disappear)

$$\begin{aligned} \frac{1}{2}\|u_i(t) - y_i(t)\|_{L^2}^2 = &\int_0^t \int_\Omega \big\{ - \mu_i \theta(u_i) |\nabla(u_i - y_i)|^2 - (u_i - y_i)^2 \\ &\qquad - \mu_i(\theta_i(u_i) - \theta_i(y_i)) \nabla y_i \cdot \nabla(u_i - y_i) \\ &\qquad - \mu_i z_i (d_i(u_i) - d_i(y_i)) \nabla v_0 \cdot \nabla(u_i - y_i) \big\} \,\mathrm{d}x \,\mathrm{d}t' \\ \leq &\int_0^t \big\{ - \min\{1, \underline{\mu\theta}\} \|u_i - y_i\|_{H^1}^2 \\ &\qquad + c\|u_i - y_i\|_{L^2}^{2/\beta} \|u_i - y_i\|_{H^1}^{2-2/\beta} \big(\|\nabla y_i\|_{L^q} + \|\nabla v_0\|_{L^q} \big) \big\} \,\mathrm{d}t' \\ \leq c &\int_0^t \big\{ \|u_i - y_i\|_{L^2}^2 \big(\|\nabla y_i\|_{L^q}^\beta + \|\nabla v_0\|_{L^q}^\beta \big) \big\} \,\mathrm{d}t' \quad \forall t \in I, \end{aligned}$$

where $1/\beta + 1/q = 1/2$. Here, we used Gagliardo–Nirenberg's inequality, namely, $\|w\|_{L^\beta} \leq c\|w\|_{L^2}^{2/\beta} \|w\|_{H^1}^{1-2/\beta}$, and applied Young's inequality. According to Theorem 6.2 and Assumption (A3), $y_i \in L^\beta(I, W^{1,q}(\Omega))$. Moreover, Theorem 4.8 and the definition of q in (6.1) ensure that $v_0 \in L^\beta(I, W^{1,q}(\Omega))$. Thus, an application of Gronwall's lemma leads to $u_i = y_i$. $\square$

This result yields the higher regularity $u_i \in L^s(I, W^{1,q}(\Omega))$ for all $s \geq 1$, $i = n, p$, for the solution (u, v) we started with. Note that due to our choice in (6.1), the exponent q is uniform for all possible solutions (u, v) to Problem ($\mathrm{P_I}$).

With respect to the electrostatic potential, remember that [15, Theorem 1] guarantees some $\pi > 2$ such that $-\nabla \cdot \varepsilon\nabla + 1 : W_S^{1,q}(\Omega) \to (W_S^{1,q}(\Omega))^*$ is a topological isomorphism for all $q \in [2, \pi]$. Our choice of q in (6.1) ensures that $v_0 \in L^s(I, W_S^{1,q}(\Omega))$ for all $s \geq 1$ for any solution (u, v) to ($\mathrm{P_I}$). This completes the proof of Theorem 5.2.

7 Concluding remarks

We examined the drift-diffusion model for charge transport with Schottky boundary conditions at the metal-semiconductor interfaces instead of assuming Ohmic contacts and imposing Dirichlet boundary conditions. We established the existence of weak solutions and derived positive lower and upper bounds for the densities. Under the additional assumption (A3) we verified higher regularity properties of the solutions (see Theorem 5.2) that are used to establish the uniqueness of the weak solution (see Theorem 5.1).

7.1 Vacancy-assisted charge transport

For the description of different novel applications it is of importance to consider vacancy-assisted charge transport models since also the (much slower) motion of ions respectively the migration of vacancies plays an important part (e.g. in perovskite solar cells [1, 3] or memristor devices [2, 25]). Here, besides continuity equations for electrons and holes also balance equations for the ionic vacancies from an index set I_0 have to be taken into account, and the source term in the Poisson equation additionally contains parts stemming from the charged vacancy densities. Schottky contacts for electrons and holes (as treated in the present paper) together with no-flux boundary conditions for the ionic vacancies are especially relevant for the modeling of memristor devices as in [25]. Combining the methods of the present paper with the treatment of the ionic vacancies in [1] such vacancy-assisted charge transport models with Schottky boundary conditions can be handled, too.

7.2 Mixed Dirichlet, Schottky and no-flux boundary conditions

In the case that both types of boundary conditions, Dirichlet and Schottky contacts, are simultaneously present, $\Gamma_D,\, \Gamma_S \subset \partial\Omega$ with mes $\Gamma_D > 0$, $\Gamma_N = \partial\Omega \setminus (\Gamma_D \cup \Gamma_S)$, we can apply the techniques in [1] by setting $I_0 = \emptyset$ therein. Namely, supposing dist$(\Gamma_D, \Gamma_S) > 0$, $\overline{v}_0^D \in W^{1,\infty}(\Omega)$ such that $\overline{v}_0^D|_{\Gamma_D \cup \Gamma_S} = v_0^D$, $\overline{v}_i^D \in W^{1,\infty}(\Omega)$ such that $\overline{v}_i^D|_{\Gamma_D} = v_i^D$, $\overline{v}_i^D|_{\Gamma_S} = v_i^S$, $i = n, p$, and looking for $v \in v^D + (V_{DS} \times V_D^2)$, where $v^D = (\overline{v}_0^D, \overline{v}_n^D, \overline{v}_p^D)$, and V_{DS}, resp. V_D denote the closure of $\{y|_\Omega : y \in C_0^\infty(\mathbb{R}^2),\ \operatorname{supp} y \cap (\Gamma_D \cup \Gamma_S) = \emptyset\}$ resp. $\{y|_\Omega : y \in C_0^\infty(\mathbb{R}^2),\ \operatorname{supp} y \cap \Gamma_D = \emptyset\}$ in $H^1(\Omega)$ the methods there are applicable. Note that in the analytical treatment in [1], the additionally occurring boundary terms on Γ_S resulting from the thermionic emission description of Schottky contacts can be handled analogously to the methods developed in the present paper. Therefore, a corresponding existence and boundedness result can be obtained.

7.3 Organic semiconductors

For organic semiconductor materials, so-called Gauss–Fermi integrals have to be used in the statistical relation for electrons and holes in (1.3). Here, assumption (1.4) is not fulfilled, but the methodologies for establishing positive lower and upper bounds for charge-carrier densities in organic semiconductor materials are elucidated in [12, proofs of Lemma 4.3, Thm. 5.2]. Thus, for organic semiconductor devices with Schottky contacts, existence and boundedness of weak solutions and a uniqueness result (supposing (A3)) are to be expected, too.

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