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Analysis of a drift-diffusion model for perovskite solar cells

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Abstract

This paper deals with the analysis of an instationary drift-diffusion model for perovskite solar cells including Fermi–Dirac statistics for electrons and holes and Blakemore statistics for the mobile ionic vacancies in the perovskite layer. The free energy functional is related to this choice of the statistical relations.

Exemplary simulations varying the mobility of the ionic vacancy demonstrate the necessity to include the migration of ionic vacancies in the model frame. To prove the existence of weak solutions, first a problem with regularized state equations and reaction terms on any arbitrarily chosen finite time interval is considered. Its solvability follows from a time discretization argument and passage to the time-continuous limit. Applying Moser iteration techniques, a priori estimates for densities, chemical potentials and the electrostatic potential of its solutions are derived that are independent of the regularization level, which in turn ensure the existence of solutions to the original problem.

1 Introduction

Perovskite solar cells (PSCs) have emerged as a groundbreaking technology in photovoltaics, promising a significant impact on the renewable energy landscape. This progress is rooted in perovskite materials' outstanding optical and electronic properties [29]. Since perovskites do not describe one concrete material but belong to a class of crystalline semiconductors, they have several advantages such as adjustable band gaps, high absorption coefficients, and low exciton binding energies. With remarkable power conversion efficiency rates exceeding 30% [26], perovskite-silicon tandem solar cells surpass the efficiency of widely used silicon solar cells under laboratory conditions. Despite specific architectures demonstrating lower production costs than conventional solar cells, substantial challenges exist, including concerns regarding stability, limited lifespan, and toxicity issues [29]. Furthermore, the diffusion engineering of ionic migration is an important task to overcome the previously mentioned challenges. Several experimental observations and simulations indicate the occurrence of ionic vacancy accumulation near the perovskite interfaces [8, 23, 29].

The presence of additional ionic vacancy migration within perovskite materials is a significant difference from classical drift-diffusion charge transport models used for (in)organic semiconductors. Equally important is the need to constrain the accumulation of vacancies properly. Accumulating an excessive number of vacancies is physically unrealistic, potentially damaging the crystal structure and resulting in unrealistically high vacancy concentrations. Initial drift-diffusion models for PSCs incorporating ionic movement, such as [10, 28, 30, 32], did not impose limits on the vacancy density by choosing Boltzmann statistics. Subsequent models were introduced to address this limitation [2, 7, 9], reflected by the choice of statistics equal to a Blakemore approximation. Concerning the simulation, one-dimensional (partially) open-access software tools for simulating vacancy-assisted charge

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transport in PSCs are available [7, 9, 22]. However, multi-dimensional models and software are indispensable, especially when analyzing charge transport in structures like nanotextured PSCs [33], where one-dimensional simulations fall short. Therefore, as an alternative approach, we rely on the open-source software `ChargeTransport.jl` [3] for simulating charge transport in semiconductors using the Voronoi finite volume method in multi-dimensions. The discretization scheme was formulated and analyzed in [1]. In particular, the existence of discrete solutions was proven.

The mathematical analysis of semiconductor drift-diffusion systems is commonly restricted to Boltzmann statistical relations for electrons and holes [6, 14, 34]. In more sophisticated models where elevated carrier densities play a crucial role, one must consider Fermi–Dirac statistical relations, as detailed in [16], for a rigorous mathematical analysis. Both statistical relations share the characteristic that as the chemical potentials of the species approach infinity, the charge carrier densities also tend towards infinity.

In contrast, in organic semiconductor materials the so-called Gauss–Fermi statistics hold that feature bounded carrier densities. The mathematical analysis in the setting of organic semiconductor devices, incorporating this behavior along with adapted mobility laws, was conducted in [17]. In our current model framework, we have to deal with both, non-bounded relations for electron and holes and bounded statistical relations for the additional ionic vacancies. Furthermore, the continuity equations for the latter are confined to the subdomain corresponding to the perovskite material. The electric contacts of the device are realized in form of Dirichlet boundary conditions for electrons and holes as well as the electrostatic potential. Conversely, the total number of ionic vacancies constitutes a conserved quantity; hence, no-flux boundary conditions and no reactions are assumed. In a related study [19], a drift-diffusion system modeling memristive devices with an additional ionic species is explored. However, Boltzmann statistics for all species and one common domain is considered. Finally, in photovoltaic applications, as addressed in our text, the continuity equations for electrons and holes incorporate an additional photogeneration rate. This rate accounts for the absorption of light and the subsequent generation of an electron-hole pair.

The paper is organized as follows: In Section 2, there is a concise overview of the fundamental model for perovskite materials, incorporating extra mobile ionic vacancies as outlined in [2]. The significance of including these additional species is highlighted in Section 3, where simulation results are presented. The model analysis is detailed in Sections 4 and 5. Section 4 introduces key assumptions, the weak formulation of the problem, and initial energy estimates. The proof of the existence result is then provided in Section 5. Lastly, Section 6 offers a concluding summary.

2 Drift-diffusion modeling of perovskite solar cells

In this section, we formulate a rescaled drift-diffusion model for describing the charge transport in PSCs. This model, derived in [2], includes the fundamental reaction rates and initial and boundary conditions. In Section 4.1, suitable assumptions on the data will be formulated to continue with the model analysis.

2.1 Drift-diffusion system

Let $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, denote the spatial domain of the solar cell and I be the index set of moving carriers. Additionally to the movement of electrons and holes in Ω, we consider the migration of ionic vacancy carriers with the index set $I_0 \subset I$ in $\Omega_0 \subset \Omega$. We define the densities of electrons, holes, and vacancies as $u_i, i \in I := \{n, p\} \cup I_0$, where $i = n$ and $i = p$ refer to electrons and holes, respectively. The considered drift-diffusion model is given by a Poisson equation for the electrostatic potential ψ

$$-\nabla \cdot (\varepsilon \nabla \psi) = \begin{cases} C + z_n u_n + z_p u_p & \text{in } (0, \infty) \times (\Omega \setminus \overline{\Omega_0}), \\ C + z_n u_n + z_p u_p + \sum_{i \in I_0} z_i u_i & \text{in } (0, \infty) \times \Omega_0, \end{cases} \tag{2.1a}$$

where ε corresponds to a rescaled dielectric permittivity, z_i to the charge number of a species $i \in I$ and C corresponds to the fixed doping density. The Poisson equation is self-consistently coupled to the continuity equations

$$\frac{\partial u_i}{\partial t} - \nabla \cdot (z_i \mu_i u_i \nabla \varphi_i) = G - R, \; i = n, p, \qquad \text{in } (0, \infty) \times \Omega, \tag{2.1b}$$

$$\frac{\partial u_i}{\partial t} - \nabla \cdot (z_i \mu_i u_i \nabla \varphi_i) = 0, \quad i \in I_0, \qquad \text{in } (0, \infty) \times \Omega_0, \tag{2.1c}$$

where μ_i are the rescaled carrier mobilities. The generation/recombination terms G and R entering the continuity equations of electrons and holes (2.1b) are discussed in Section 2.3. For the ionic vacancy species $i \in I_0$ we do not take into account any reactions.

The crucial statistical relation that connects the potentials φ_i and ψ to the charge carrier densities u_i is given by

$$u_i = N_i \mathcal{F}_i(z_i(\varphi_i - \psi) + \zeta_i) = N_i \mathcal{F}_i(v_i + \zeta_i), \quad \text{where} \quad \varphi_i = \frac{1}{z_i} v_i + \psi, \quad i \in I, \tag{2.2}$$

with the effective densities of state N_i, the chemical potentials v_i and $\zeta_i := z_i \mathrm{E}_i$, $i \in I$, where E_i is the band-edge energy. The function $\mathcal{F}_i$, called statistics function, will be discussed in Section 2.2.

In comparison to the model in [2], we rescaled the electrostatic potential ψ and the quasi Fermi potentials φ_i by the thermal voltage $U_T = k_B T/q$. Here, k_B refers to the Boltzmann constant, T to the (constant) temperature and q to the elementary charge. Furthermore, we rescaled the chemical potentials v_i and the band-edge energies E_i by $k_B T$. Lastly, we multiply the dielectric permittivity ε by U_T/q and the mobilities μ_i by U_T.

We highlight that the introduced setting with a unified domain $\Omega_i = \Omega_0$, $i \in I_0$, for the vacancies, is only for notational simplicity. Our analysis would also allow (with simple adaptions) to handle different Ω_i for the different ions. Also the situation that on the whole domain Ω we have all the considered ions, $\Omega_i = \Omega$, $i \in I$, is included in our setting.

2.2 Statistical functions

For classical (inorganic) semiconductors the statistics functions for electrons and holes is given by the Fermi–Dirac integral of order $1/2$ (see e.g., [31])

$$F_{1/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2}}{\exp(\xi - z) + 1} \, \mathrm{d}\xi, \quad \text{for } z \in \mathbb{R} \tag{2.3}$$

i.e., $\mathcal{F}_n = \mathcal{F}_p = F_{1/2}$. In the case of small to moderate carrier densities [31], the Fermi–Dirac integral of order $1/2$ can be approximated by an exponential, called 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

$$\begin{cases} \text{(i)}\;\; \mathcal{F}_i \in C^1(\mathbb{R}), \quad \lim_{z\to-\infty} \mathcal{F}_i(z) = 0, \quad \lim_{z\to+\infty} \mathcal{F}_i(z) = +\infty, \\ \text{(ii)}\;\; z \leq c(1+\mathcal{F}_i(z)) \quad \text{for } z \in \mathbb{R}_+, \\ \text{(iii)}\;\; 0 < \mathcal{F}_i'(z) \leq \mathcal{F}_i(z) \leq \mathrm{e}^z \quad \text{for } z \in \mathbb{R}. \end{cases} \qquad i = n, p. \tag{2.4}$$

Concerning the ionic vacancy carriers, accumulating too many vacancies is physically unrealistic as it can destroy the crystal structure and lead to unrealistically high vacancy concentrations. This means, we need to adequately limit the vacancy concentration which can be done via a proper choice of statistics function. Following [2], we choose as statistics function the Fermi–Dirac integral of order -1 (which corresponds to the Blakemore statistics $F_{B,\gamma}$ function with $\gamma = 1$)

$$F_{-1}(z) = F_{B,1}(z), \quad \text{where} \quad F_{B,\gamma}(z) = \frac{1}{\mathrm{e}^{-z} + \gamma} \quad \text{for } z \in \mathbb{R}, \tag{2.5}$$

i.e., $\mathcal{F}_i = F_{-1}$ for all $i \in I_0$. As for the statistics functions of electrons and holes, we assume that the statistics function of the vacancy carriers satisfies the following properties

$$\begin{cases} \text{(i)}\;\; \mathcal{F}_i \in C^2(\mathbb{R}), \quad \lim_{z\to-\infty} \mathcal{F}_i(z) = 0, \quad \lim_{z\to+\infty} \mathcal{F}_i(z) = 1, \\ \text{(ii)}\;\; \mathcal{F}_i'(z) < \mathcal{F}_i(z) < \mathrm{e}^z \quad \text{for } z \in \mathbb{R}., \\ \text{(iii)}\;\; \mathcal{F}_i''(z) < 0, \quad \dfrac{|\mathcal{F}_i''(z)|}{\mathcal{F}_i'(z)} < 1 \quad \text{for } z \in \mathbb{R}_+, \\ \text{(iv)}\;\; 1 < (\mathrm{e}^z \mathcal{F}_i'(z))^{-1} < c, \quad \text{for } z \in \mathbb{R}_+. \end{cases} \qquad i \in I_0. \tag{2.6}$$

The Fermi–Dirac integral of order $1/2$ and the Boltzmann statistics indeed satisfy these properties (2.4) while the Fermi–Dirac integral of order -1 satisfies (2.6), see also Appendix A.

2.3 Generation-recombination and photogeneration term

Following the depiction in [13], we assume for the generation-recombination term R in (2.1b) an expression of the form

$$R = r(u_n, u_p)\big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big), \quad \text{with} \quad r(u_n, u_p) = r_0(u_n, u_p)\, u_n u_p, \tag{2.7}$$

where the non-negative function r_0 is given by the sum of all recombination processes relevant in photovoltaics. For instance, for PSCs the function r_0 is given as the sum of the Shockley-Read-Hall (SRH) and the radiative recombination rate [2], namely

$$r_0(u_n, u_p) = \frac{1}{\tau_p(u_n + u_{n,\tau}) + \tau_n(u_p + u_{p,\tau})} + r_{0,\text{rad}}, \tag{2.8}$$

where τ_n, τ_p are the carrier lifetimes and $u_{n,\tau}, u_{p,\tau}$ some reference carrier densities. Moreover, $r_{0,\text{rad}}$ is the constant rate coefficient.

For Boltzmann statistics, (2.7) is equivalent to the widely used form $R = r_0(u_n, u_p)(u_n u_p - n_i^2)$, where n_i is the intrinsic carrier density. The expression for the rate in (2.7) is compatible with thermodynamic equilibrium. In particular, it reflects the fact that in equilibrium the quasi Fermi levels of electrons and holes have to coincide.

The photogeneration rate $G \in L^\infty_+(\Omega)$ is assumed to be constant in time. In the simplest case, one assumes a Lambert–Beer generation profile in the vertical direction x_{vert}, i.e.,

$$G(x) = F_{\mathrm{ph}} \alpha_G \, \mathrm{e}^{-\alpha_G x_{\mathrm{vert}}} \quad \text{for } x = (\overline{x}, x_{\mathrm{vert}}) \tag{2.9}$$

with the incident photon flux F_{ph} and an material absorption coefficient α_G.

2.4 Initial and boundary conditions

For the densities u_i, $i \in I$, we prescribe initial values

$$u_i(0) = u_i^0 \quad \text{in } \Omega, \quad i = n, p, \quad u_i(0) = u_i^0 \quad \text{in } \Omega_0, \quad i \in I_0. \tag{2.10}$$

We decompose the boundary of the domain $\partial\Omega$ into an ohmic contact Γ_D and the semiconductor-insulator interface Γ_N. The ohmic contact Γ_D corresponds to the semiconductor-metal interfaces and are model via Dirichlet boundary conditions

$$\psi = \psi_0 + U(t), \quad \varphi_n = \varphi_p = U(t), \quad \text{on } \mathbb{R}_+ \times \Gamma_D, \tag{2.11}$$

where U denotes an externaly applied time-dependent voltage and ψ_0 some given potential [13]. In contrast to (2.11), we assume in the framework of our work time-independent boundary conditions. More precisely, let the Dirichlet values $\psi^D, \varphi^D \in W^{1,\infty}(\Omega)$ be given. Then, we take the following boundary conditions into account

$$\psi = \psi^D, \quad \varphi_n = \varphi_p = \varphi^D, \quad \text{on } \mathbb{R}_+ \times \Gamma_D. \tag{2.12a}$$

The semiconductor-insulator interface is realized by no-flux boundary conditions

$$\varepsilon \nabla \psi \cdot \nu = \mu_i u_i \nabla \varphi_i \cdot \nu = 0, \quad i = n, p, \quad \text{on } \mathbb{R}_+ \times \Gamma_N, \tag{2.12b}$$

where ν denotes the outer normal vector. At the boundary of the perovskite domain $\partial\Omega_0$ with outer normal vector ν_0 we assume no normal flux of ion vacancies

$$\mu_i u_i \nabla \varphi_i \cdot \nu_0 = 0 \quad \text{on } \mathbb{R}_+ \times \partial\Omega_0, \; i \in I_0. \tag{2.12c}$$

Due to the regularity assumptions in the weak formulation stated in Section 4.2 we are not in need of additional conditions for electrons and holes on the internal boundaries.

3 Physically meaningful simulations

Before we proceed with the analysis of the charge transport model, we highlight the practical significance of additional ionic vacancy carriers from an application perspective. Mobile vacancies profoundly impact the model's potentials, densities, and consequently, the current-voltage curves and the efficiency of the solar cells.

To this end, we examine a three-layer perovskite solar cell (PSC), illustrated in Figure 3.1, with methylammonium lead iodide (MAPI) as an extensively studied perovskite material. Given that the hopping of iodide has the lowest energy barrier within MAPI [11], we assume the movement of only one ionic vacancy for the simulations, precisely corresponding to the iodide vacancies of MAPI. We denote this carrier by a, i.e., $I_0 = \{a\}$, with the charge number $z_a = 1$. In total, the set of unknowns is given by the quasi Fermi potentials of electrons, holes, and ionic vacancy and the electrostatic potential $(\varphi_n, \varphi_p, \varphi_a, \psi)$. Subsequently, the charge carrier densities can be calculated via (2.2). Moreover, we use PCBM as electron transport layer (ETL) material and PEDOT:PSS as hole transport layer (HTL) material [29]. For electrons and holes, we have a present photogeneration (2.9) and a recombination rate, given by (2.7) and (2.8), entering the model via the right-hand side of the continuity equations (2.1b). We set $\mathcal{F}_n = \mathcal{F}_p = F_{1/2}$ and $\mathcal{F}_a = F_{-1}$. All relevant physical parameters needed for the simulations are stated in Table 3.1.

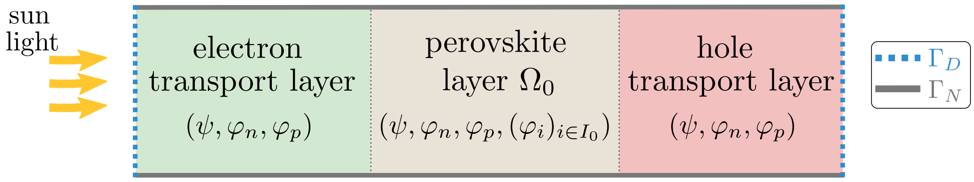

Figure 3.1: A possible three-layer PSC geometry Ω, divided into three subdomains: two transport layers and the perovskite material layer Ω_0. Furthermore, the relevant potentials are stated for each subdomain, indicating that we only allow ionic vacancies in Ω_0.

In practice, time-dependent scan protocols involving varying applied voltages are applied to analyze the behavior of PSCs. Mathematically, this procedure is achieved using the boundary conditions (2.11). For our simulations, we impose a linear voltage at the right contact with a scan rate of 40 mV/s. We utilize an implicit Euler scheme for the temporal and a two-point flux finite volume approximation scheme for the spatial discretization [1], where also the existence of discrete solutions for the used scheme was established.

In the following, we investigate the impact of the vacancy mobility parameter μ_a, entering the current density in (2.1c), on the charge transport dynamics within PSCs. We use the same initial configuration for all simulations, depicted in Figure 3.2.

Physical quantity	Symbol	Value			Unit
		ETL	MAPI	HTL	
Layer thickness		60	300	50	nm
Dielectric permittivity	ε	3	23.0	4	ε_0
Conduction band-edge energy	E_n	-3.8	-3.8	-3.0	eV
Valence band-edge energy	E_p	-6.2	-5.4	-5.1	eV
Eff. conduction band DoS	N_n	1×10^{25}	1.0×10^{25}	1×10^{26}	m^{-3}
Eff. valence band DoS	N_p	1×10^{25}	1×10^{25}	1×10^{26}	m^{-3}
Doping density	C	2.09×10^{24}	-1.0×10^{24}	-2.09×10^{24}	m^{-3}
Electron mobility	μ_n	1.0×10^{-7}	2.0×10^{-3}	1.0×10^{-5}	$\mathrm{m}^2/(\mathrm{Vs})$
Hole mobility	μ_p	1.0×10^{-7}	2.0×10^{-3}	1.0×10^{-5}	$\mathrm{m}^2/(\mathrm{Vs})$
Radiative recombination coeff.	$r_{0,\mathrm{rad}}$	6.8×10^{-17}	3.6×10^{-18}	6.3×10^{-17}	m^3/s
SRH lifetime, electrons	τ_n	1.0×10^{-6}	1.0×10^{-7}	1.0×10^{-6}	s
SRH lifetime, holes	τ_p	1.0×10^{-6}	1.0×10^{-7}	1.0×10^{-6}	s
SRH density, electrons	$u_{\tau,n}$	7×10^4	3.6×10^{11}	2.3×10^8	m^{-3}
SRH density, holes	$u_{\tau,p}$	7×10^4	3.6×10^{11}	2.3×10^8	m^{-3}
Inc. photon flux	F_{ph}	1.4×10^{21}	1.4×10^{21}	1.4×10^{21}	$1/(\mathrm{m}^2\mathrm{s})$
Absorption coefficient	α_G	0.0	4.2×10^6	0.0	m^{-1}

Table 3.1: Parameter values from [7] for the simulation of a three-layer PSC at a temperature $T = 300$ K with PCBM as electron transport layer material and PEDOT:PSS as hole transport layer material. Here, ε_0 denotes the vacuum permittivity.

As can be seen in Figure 3.2 (right) the initial vacancy density u_a depletes near the ETL/perovskite interface and accumulates near the perovskite/HTL interface. Note that due to a present photogeneration rate the initial electron and hole quasi Fermi potentials do not coincide and are not zero Figure 3.2 (left).

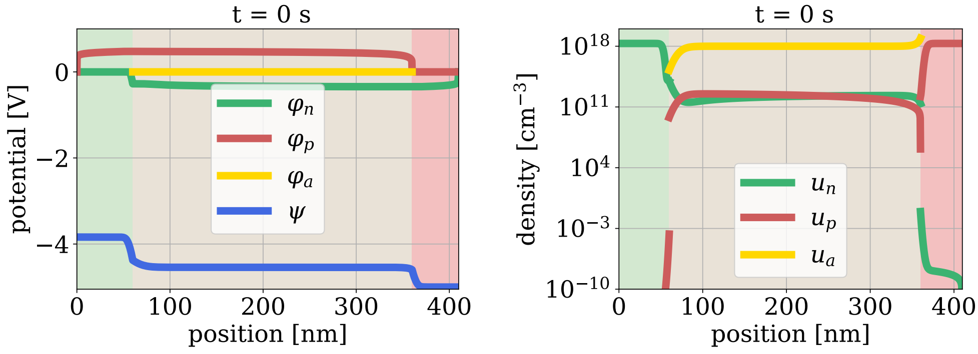

Figure 3.2: Initial potentials (left) and charge carrier densities (right) used for all simulations, which are independent of the choice of vacancy mobility μ_a. The transport layers and the perovskite layer are shaded in the respective colors, introduced in Figure 3.1.

The power conversion efficiency (PCE) and the open circuit voltage (OCV) are crucial performance indicators for solar cells, offering insights into how effectively these cells convert sunlight into usable electrical energy [27]. These metrics can be derived from information deduced from the current-voltage (I-V) curve.

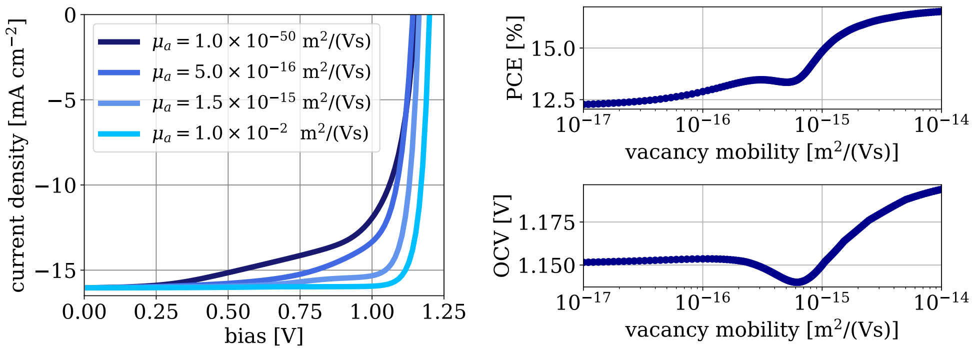

Figure 3.3: Left: The current-voltage characteristics for selected vacancy mobilities (left). Brighter color indicates a larger vacancy mobility. Right: The power conversion efficiency (PCE) and the open circuit voltage (OCV) in dependence on the vacancy mobility.

As Figure 3.3 illustrates, the mobility of vacancies μ_a substantially impacts the current-voltage characteristics, the PCE, and the OCV. As the vacancy mobility tends to either zero or infinity, no significant changes can be observed in the I-V curve (Figure 3.3, left) and, consequently, the PCE and the OCV saturate (Figure 3.3, right). Within the range of $\mu_a \in [10^{-17}, 10^{-14}]$ m$^2/(\mathrm{Vs})$, we observe a notable change in the I-V curve. Higher vacancy mobilities shift the total current to the right (Figure 3.3, left), thereby increasing the PCE and OCV (Figure 3.3, right).

The variations in the I-V curves correspond to changes in the carrier densities in dependence on the vacancy mobility, as shown in Figure 3.4. Larger vacancy mobilities decrease the depletion at the ETL/perovskite interface while increasing the depletion on the perovskite/HTL interface (Figure 3.4, first column). This behavior influences the electron and hole densities u_n, u_p near these boundaries

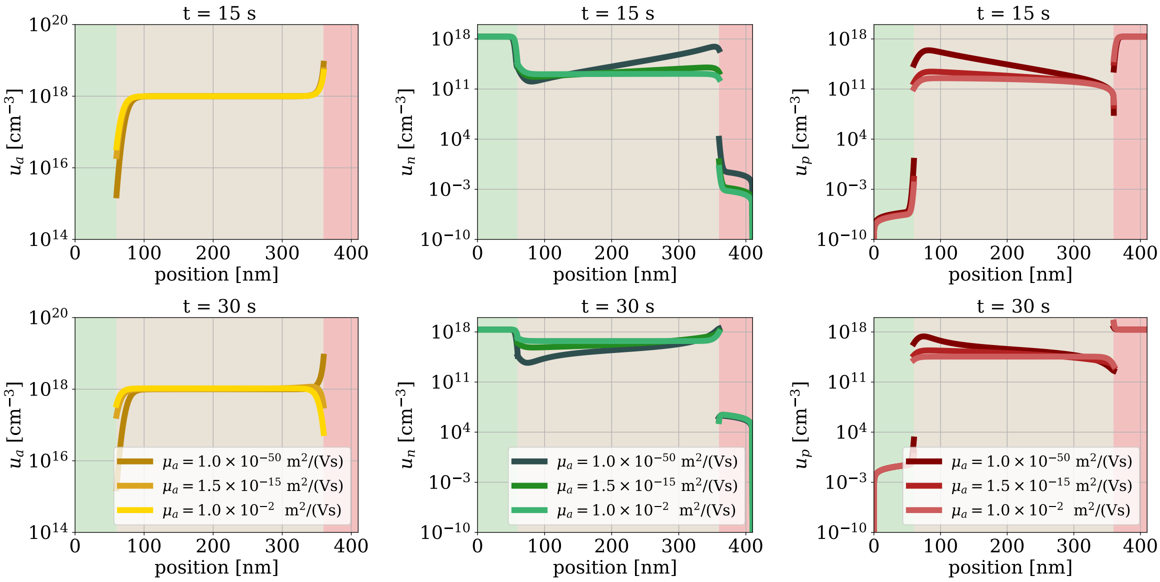

Figure 3.4: Densities of vacancies, electrons and holes at time $t = 15$ s (first row) and at the end time $t = 30$ s (second row). Brighter color indicates a larger vacancy mobility.

by several orders of magnitudes (Figure 3.4, second and third column). For higher mobilities, u_n, u_p become more uniform within the perovskite layer. Consequently, this more uniform distribution contributes to a delayed increase in the total current, as observed in Figure 3.3 (left) for higher mobilities.

4 Analysis of the instationary drift-diffusion model

4.1 Assumptions on the data

We work with 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 define $W_D^{1,p}(\Omega)$ as the closure of the set

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

in the Sobolev space $W^{1,p}(\Omega)$, and we set $W_D^{-1,p}(\Omega) := W_D^{1,p'}(\Omega)^*$, 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, we allow them to change from line to line.

We investigate the instationary drift-diffusion model under the following assumptions:

(A1) $\Omega_0 \subseteq \Omega \subset \mathbb{R}^2$ are bounded Lipschitz domains, $\Omega \cup \Gamma_N$ is regular in the sense of Gröger [18], $\Gamma_D, \Gamma_N \subset \Gamma =: \partial\Omega$ disjoint subsets such that $\overline{\Gamma_D \cup \Gamma_N} = \Gamma$ and $\mathrm{mes}(\Gamma_D) > 0$, $\Omega_n = \Omega_p := \Omega$, $\Omega_i := \Omega_0$, $i \in I_0$.

(A2) $\mathcal{F}_i$, $i = n, p$, fulfill (2.4), $\mathcal{F}_i$, $i \in I_0$, fulfill (2.6), $N_i,\ \mu_i \in L^\infty(\Omega_i)$, $\zeta_i =$ const, $0 < \underline{N} \le N_i \le \overline{N}$, $0 < \underline{\mu} \le \mu_i \le \overline{\mu}$ a.e. in Ω_i, $i \in I$, and $C,\ \varepsilon \in L^\infty(\Omega)$, $0 < \underline{\varepsilon} \le \varepsilon$ a.e. in Ω, $z_n = -1$, $z_p = 1$, $z_i \in \mathbb{Z}$, $i \in I_0$, $v_0^D := \psi^D,\ \varphi^D \in W^{1,\infty}(\Omega)$.

(A3) $R = r(x, u_n, u_p)\big(1 - \mathrm{e}^{\varphi_n - \varphi_p}\big)$, 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 Caratheodory function with $0 \leq r_0(x, u_n, u_p) \leq \overline{r}$ for a.a. $x \in \Omega$ and for all $(u_n, u_p) \in [0, +\infty)^2$, $G \in L^\infty(\mathbb{R}_+; L^\infty_+(\Omega))$.

(A4) $u_i^0 \in L^\infty(\Omega)$, $0 < \underline{u} \leq u_i^0 \leq \overline{u}$, $i = n, p$,
$u_i^0 \in L^\infty(\Omega_0)$, $0 < \underline{u} \leq u_i^0 \leq \overline{u_i} < N_i$ a.e. in Ω_0, $i \in I_0$.

In the following, we suppress in the writing the spatial position x in the reaction coefficients r and r_0, respectively.

4.2 Weak formulation

We define the functions $e_i : \mathbb{R} \to (0, \infty)$, $i = n, p$, $e_i : \mathbb{R} \to (0, 1)$, $i \in I_0$, by

$$e_i(z) = \mathcal{F}_i(z + \zeta_i), \quad i = n, p, \quad e_i(z) = \mathcal{F}_i(z + \zeta_i), \quad i \in I_0. \tag{4.1}$$

Then, Assumption (A2) guarantees

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

Note that the inverses e_i^{-1} are well-defined on $(0, \infty)$ for $i = n, p$, and on $(0, 1)$ for $i \in I_0$.

We introduce the following function spaces

$$V_D := \{y \in H^1(\Omega) : y|_{\Gamma_D} = 0\}, \quad V_0 := H^1(\Omega_0), \quad V := V_D^3 \times V_0^{\# I_0},$$
$$H := V_D \times L^2(\Omega)^2 \times L^\infty(\Omega_0)^{\# I_0}, \quad Z := H^1(\Omega) \times L^\infty(\Omega)^2 \times L^\infty(\Omega_0)^{\# I_0},$$
$$U := \big\{u \in V_D^* \times L^\infty(\Omega)^2 \times L^2(\Omega_0)^{\# I_0} : \ln u_i \in L^\infty(\Omega),\ i = n, p,$$
$$0 < \operatorname*{ess\,inf}_{x \in \Omega_0} u_i/N_i \leq \operatorname*{ess\,sup}_{x \in \Omega_0} u_i/N_i < 1,\ i \in I_0\big\}.$$

As in [15–17], we will use a weak formulation of (2.1) in the form

$$u' + A(v, v) = 0,\ u = E(v),\ u(0) = u^0$$

with the variables $v = (v_0, v_n, v_p, (v_i)_{i \in I_0}) = (\psi, \psi - \varphi_n, \varphi_p - \psi, (z_i(\varphi_i - \psi))_{i \in I_0})$ (potentials), $u := (u_0, u_n, u_p, (u_i)_{i \in I_0})$ and $u^0 := (u_0^0, u_n^0, u_p^0, (u_i^0)_{i \in I_0})$ (densities), where u_0 denotes the total charge density. The initial total charge density u_0^0 is given via $\langle u_0^0, w \rangle_{V_D} = \sum_{i \in I} \int_{\Omega_i} z_i u_i^0 w \,\mathrm{d}x + \int_\Omega C w \,\mathrm{d}x$ for all $w \in V_D$. Here, $z_n = -1$, $z_p = 1$, and z_i, $i \in I_0$, stand for the charge number of the ion vacancies. Thus, we have the relations

$$v_i = z_i(\varphi_i - v_0), \quad \text{and} \quad \varphi_i = \frac{1}{z_i} v_i + v_0, \quad i \in I. \tag{4.2}$$

In these variables, our problem reads

$$\begin{aligned}
&- \nabla \cdot (\varepsilon \nabla v_0) = \begin{cases} C + z_n u_n + z_p u_p, & \text{in } (0, \infty) \times (\Omega \setminus \overline{\Omega_0}) \\ C + z_n u_n + z_p u_p + \sum_{i \in I_0} z_i u_i, & \text{in } (0, \infty) \times \Omega_0 \end{cases}, \\
&\frac{\partial u_i}{\partial t} - \nabla \cdot (\mu_i u_i (\nabla v_i + z_i \nabla v_0)) = G - R, \quad i = n, p, \\
&\frac{\partial u_i}{\partial t} - \nabla \cdot (\mu_i u_i (\nabla v_i + z_i \nabla v_0)) = 0, \quad i \in I_0,
\end{aligned} \tag{4.3}$$

with $R = r(u_n, u_p)\big(1 - \mathrm{e}^{-v_n - v_p}\big)$ and $u_i = N_i e_i(v_i)$, $i \in I$.

Moreover, we introduce the Dirichlet values $v_n^D := v_0^D - \varphi^D$, $v_p^D := \varphi^D - v_0^D$. For the ionic vacancies we do not have to prescribe a Dirichlet value. But, for a unified notion we set $v^D := (v_0^D, v_n^D, v_p^D, (0)_{i\in I_0})$.

We consider operators $E_0 : v_0^D + V_D \to V_D^*$, $E : (v^D + V) \cap Z \to V^*$, $A : Z \times (v^D + V) \to V^*$,

$$
\begin{aligned}
\langle E_0(v_0), \overline{v}_0\rangle_{V_D} &:= \int_\Omega \varepsilon \nabla v_0 \cdot \nabla \overline{v}_0 \,\mathrm{d}x, \\
E(v) &:= (E_0(v_0), (N_i e_i(v_i))_{i\in I}), \\
\langle A(w, v), \overline{v}\rangle_V &:= \sum_{i\in I} \int_{\Omega_i} N_i e_i(w_i)\mu_i \nabla(v_i + z_i v_0) \cdot \nabla(\overline{v}_i + z_i \overline{v}_0)\,\mathrm{d}x \\
&\quad + \int_\Omega \big[r(N_n e_n(w_n), N_p e_p(w_p))\big(1 - \mathrm{e}^{-w_n - w_p}\big) - G\big](\overline{v}_n + \overline{v}_p)\,\mathrm{d}x \\
&= \sum_{i\in I} \int_{\Omega_i} z_i^2 N_i e_i(w_i)\mu_i \nabla\varphi_i \cdot \nabla\overline{\varphi}_i \,\mathrm{d}x \\
&\quad + \int_\Omega \big[r(N_n e_n(w_n), N_p e_p(w_p))\big(1 - \mathrm{e}^{\xi_n - \xi_p}\big) - G\big](\overline{\varphi}_p - \overline{\varphi}_n)\,\mathrm{d}x,
\end{aligned}
$$

for all $\overline{v}_0,\ \overline{v}_n,\ \overline{v}_p \in V_D$, $\overline{v}_i \in V_0,\ i \in I_0$, where $\xi_i = w_0 + \frac{1}{z_i} w_i$, $\varphi_i = v_0 + \frac{1}{z_i} v_i$, $\overline{\varphi}_i = \overline{v}_0 + \frac{1}{z_i}\overline{v}_i$, $i \in I$. Note that the element $u_0 := E_0(v_0)$ represents the total charge density of the device under consideration, we treat u_0 as one of the unknowns of the problem.

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 $v_i^0 := e_i^{-1}(u_i^0/N_i)$, $i \in I$, and $v^0 := (v_0^0, (v_i^0)_{i\in I})$.

The weak formulation of the drift-diffusion system (2.1), (2.10), and (2.12) is Problem

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

The set

$$
U_0 := \Big\{ u \in U : \langle u_0 - C + u_n - u_p, y\rangle_{V_D} - \sum_{i\in I_0} z_i \langle u_i, y|_{\Omega_0}\rangle_{V_0} = 0 \quad \forall y \in V_D \Big\}
$$

can be interpreted as the set of all possible states of the PSC device. Note that by definition $u_0^0 \in U_0$, and $u(t) \in U_0$ for all $t \ge 0$ has to be verified for solutions (u, v) to (P).

Remark 4.1 *Let (u, v) be a solution to (P). Then,*

$$
\int_{\Omega_0} u_i(t)\,\mathrm{d}x = \int_{\Omega_0} u_i^0 \,\mathrm{d}x, \quad i \in I_0, \quad \text{for all } t \in \mathbb{R}_+.
$$

For $i \in I_0$ this is obtained for any $t \in \mathbb{R}_+$ by testing $u' + A(v, v) = 0$ by the test function being 1 in the i-th component and 0 in all other components that belongs to $L^2(0, t; V)$.

4.3 Energy estimates for weak solutions

In the analytical treatment of drift-diffusion problems, entropy methods [15, 16, 20] play an important part. We will work with a free energy functional (4.6) containing an electrostatic part and a chemical part that is related to the statistical relations of the different types of species. The operator E is a strictly monotone operator with the potential $\Phi : v^D + V \to \mathbb{R} \cup \{+\infty\}$,

$$\Phi(v) := \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2\Big\}\mathrm{d}x + \sum_{i\in I}\int_{\Omega_i} N_i \int_{v_i^D}^{v_i} e_i(y)\,\mathrm{d}y\,\mathrm{d}x, \tag{4.4}$$

note that $v_i^D = 0$ for $i \in I_0$. The conjugate functional of Φ (see [12]) is

$$\Psi : V^* \to \overline{\mathbb{R}}, \quad \Psi(u) := \Phi^*(u) = \sup_{w\in V}\{\langle u, w\rangle_V - \Phi(w + v^D)\}. \tag{4.5}$$

Both functionals are convex. Note that the values of $\Phi(v)$ and $\Psi(u)$ may be $+\infty$. Because of $\Phi(v^D) = 0$, we obtain $\Psi(u) \geq 0$ for all $u \in V^*$. Since the functional Φ is continuous, strictly convex, and Gâteaux differentiable, it is also subdifferentiable and satisfies $\partial\Phi(v) = \{Ev\}$ if $v \in (v^D + V) \cap Z$.

For states $u = Ev \in V^*$, $u \in U$ we calculate

$$\begin{aligned}\Psi(u) &= \langle E(v), v - v^D\rangle_V - \Phi(v)\\ &= \int_\Omega \frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2\,\mathrm{d}x + \sum_{i\in I}\int_{\Omega_i}\int_{v_i^D}^{v_i}[u_i - N_i e_i(y)]\mathrm{d}y\,\mathrm{d}x,\end{aligned} \tag{4.6}$$

where we took advantage from $E_0 v_0 = u_0$. Let $\omega := \int_{v_i^D}^{v_i}(u_i - N_i e_i(y))\,\mathrm{d}y$. By separately considering different cases and exploiting that e_i is monotonically increasing we derive:

A) If $v_i^D < v_i$ and $|v_i^D - v_i| \leq 1$ then

$$\omega \geq [u_i - N_i e_i(v_i^D + 1)](v_i - v_i^D) \geq [u_i - N_i e_i(v_i^D + 1)]\cdot 1.$$

B) If $v_i^D < v_i$ and $|v_i^D - v_i| > 1$ then

$$\omega \geq \int_{v_i^D}^{v_i^D+1}(u_i - N_i e_i(y))\,\mathrm{d}y \geq [u_i - N_i e_i(v_i^D + 1)]\cdot 1.$$

C) If $v_i^D > v_i$ then

$$\omega = \int_{v_i}^{v_i^D+1}(N_i e_i(y) - u_i)\,\mathrm{d}y + \int_{v_i^D}^{v_i^D+1}(u_i - N_i e_i(y))\,\mathrm{d}y \geq [u_i - N_i e_i(v_i^D + 1)]\cdot 1.$$

Therefore, we obtain from (4.6) for these arguments $u = E(v)$ that

$$\|u_n\|_{L^1(\Omega)} + \|u_p\|_{L^1(\Omega)} + \sum_{i\in I_0}\|u_i\|_{L^1(\Omega_0)} + \|v_0 - v_0^D\|_{H^1}^2 \leq c(1 + \Psi(u)). \tag{4.7}$$

For a state $u \in V^*$ the quantity $\Psi(u)$ can be interpreted as the free energy of the state u.

Note that in case of $\mathcal{F}_i = F_{-1}$ the part of the chemical energy for the ionic vacancies $i \in I_0$ in (4.6) can be written as

$$\int_{\Omega_0}\int_0^{v_i}[u_i - N_i e_i(y)]\mathrm{d}y\,\mathrm{d}x = \int_{\Omega_0}\Big(u_i \ln\frac{u_i}{N_i} + (N_i - u_i)\ln\Big(1 - \frac{u_i}{N_i}\Big) + N_i \ln 2\Big)\,\mathrm{d}x$$

which forces the ionic vacancy density u_i to stay in $(0, N_i)$.

Theorem 4.1 *Let* (A1) – (A4) *be fulfilled. There exists a constant* $c > 0$ *such that for any weak solution* (u, v) *to the instationary Problem* (P) *the free energy fulfills*

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

Additionally, if the Dirichlet values are compatible with thermodynamic equilibrium (meaning $v_0^D,\ \varphi^D =$ *const) and if the photogeneration rate* G *is identically zero, then the free energy* $\Psi(u(t))$ *is monotonically decreasing.*

Proof. Let $t \in \mathbb{R}_+$ be arbitrarily given. We test $u' + A(v, v) = 0$ by $v - v^D \in L^2(0, t; V)$. Since $u(s) = E(v(s))$ f.a.a. $s \in [0, t]$ we obtain $v(s) - v^D \in \partial\Psi(u(s))$ f.a.a. $s \in [0, t]$ and the Brézis formula (cf. [5, Lemma 3.3]) ensures the chain rule

$$\begin{aligned}
\Psi(u(t))-\Psi(u(0)) &= \int_0^t \langle u'(s), v(s)-v^D\rangle_V \,\mathrm{d}s = -\int_0^t \langle A(v(s), v(s)), v(s)-v^D\rangle_V \,\mathrm{d}s \\
&= -\int_0^t \Big[\int_\Omega \sum_{i=n,p} \mu_i u_i \nabla\varphi_i \cdot \nabla(\varphi_i-\varphi^D)\,\mathrm{d}x \ + \int_{\Omega_0} \sum_{i\in I_0} z_i^2 \mu_i u_i \nabla\varphi_i \cdot \nabla(\varphi_i-v_0^D)\,\mathrm{d}x\Big]\mathrm{d}s \\
&\quad - \int_0^t \int_\Omega [r(\mathrm{e}^{\varphi_n-\varphi_p} - 1) + G](\varphi_n - \varphi_p)\,\mathrm{d}x\,\mathrm{d}s \\
&\leq \int_0^t \int_\Omega \sum_{i=n,p} \frac{u_i}{2}(-\mu_i|\nabla(\varphi_i - \varphi^D)|^2 + c|\nabla\varphi^D|^2)\,\mathrm{d}x\,\mathrm{d}s \\
&\quad + \int_0^t \int_{\Omega_0} \sum_{i\in I_0} z_i^2 \frac{u_i}{2}(-\mu_i|\nabla\varphi_i|^2 + c|\nabla v_0^D|^2)\,\mathrm{d}x\,\mathrm{d}s + \int_0^t \int_\Omega G(v_n + v_p)\,\mathrm{d}x\,\mathrm{d}s \\
&\leq c\int_0^t \int_\Omega \Big((u_n + u_p)|\nabla\varphi^D|^2 + v_n^+ + v_p^+\Big)\,\mathrm{d}x\,\mathrm{d}s + c\int_0^t \int_{\Omega_0} |\nabla v_0^D|^2\,\mathrm{d}x\,\mathrm{d}s \\
&\leq c\int_0^t \sum_{i=n,p} (\|u_i\|_{L^1} + \|v_i^+\|_{L^1} + 1)\,\mathrm{d}x\,\mathrm{d}s \leq c\int_0^t \sum_{i=n,p} (\|u_i\|_{L^1} + 1)\,\mathrm{d}x\,\mathrm{d}s.
\end{aligned} \tag{4.8}$$

In (4.8), we applied Young's inequality and toke into account the monotonicity of the exponential function and that $u_i \leq N_i$, $i \in I_0$, on solutions (since $u(t) = E(v(t))$ f.a.a. t). By assumption we have $v_0^D,\ \varphi^D \in W^{1,\infty}(\Omega)$, and $G \in L^\infty(\mathbb{R}_+; L^\infty_+(\Omega))$. According to the assumption (ii) in (2.4) we have $\|v_i^+\|_{L^1} \leq c(1 + \|u_i\|_{L^1})$, $i = n, p$. Moreover, (4.7) ensures an estimate of $\|u_i(s)\|_{L^1(\Omega)}$, $i = n, p$, in terms of $\Psi(u(s)) + c$.

Then, we apply Gronwall's lemma to get $\Psi(u(t)) \leq (\Psi(u(0))+c)\mathrm{e}^{ct}$ for all $t > 0$. The last assertion, for data compatible with thermodynamic equilibrium, directly results from (4.8). □

5 Existence result

In this section, $T > 0$ denotes an arbitrary finite time horizon. We consider the time interval $S := [0, T]$ and introduce the problem

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

In the treatment of the instationary drift-diffusion model for PSCs, we have to overcome the following essential problems compared to the classical van Roosbroeck system [14, 16]: (i) the statistical relation for the ion vacancies does not satisfy the standard assumption in Gajewski/Gröger [16, (2.3)] (see also [15, (3.5)] also for the treatment of non-Boltzmann statistics). In particular, we have finite charge carrier densities in the case $e_i(y) = F_{-1}(y + \zeta_i)$ such that we do not have the property that $\lim_{y\to+\infty} e_i(y) = +\infty$. However, the estimate $e_i'(y) \le ce_i(y)$ for all $y \in \mathbb{R}$ remains true in that case which is of importance for the proof of lower bounds for the ionic vacancy densities. (ii) The continuity equations for electron and holes feature the additional photogeneration rate G, which models the absorption of light and subsequent generation of an electron-hole pair. This additional term has to be included in the a priori estimates.

The guideline for the existence proof is as follows: To show the existence of a weak solution for any arbitrarily chosen finite time interval $S = [0, T]$, we first discuss a regularized problem ($\mathrm{P_M}$) on the finite time interval S, where the state equations as well as the reaction term are regularized (with parameter M). We ensure the solvability of ($\mathrm{P_M}$) by time discretization, derivation of suitable a priori estimates, and passage to the limit (see Lemma 5.2). Up to here, estimates are allowed to depend on the regularization level M.

Then, we provide a priori estimates for solutions to ($\mathrm{P_M}$) that are independent of M (see Lemma 5.6, here we use Moser techniques to get positive lower bounds for the carrier densities and Lemma 5.7, where we derive upper bounds for the densities not depending on M). Thus a solution to ($\mathrm{P_M}$) is a solution to (P) on S, if M is chosen sufficiently large.

5.1 A regularized problem ($\mathrm{P_M}$)

For

$$M > M^* := \max\Big\{ \max_{i\in I} \|e_i^{-1}(u_i^0/N_i)\|_{L^\infty(\Omega_i)}, \|v_n^D\|_{L^\infty}, \|v_p^D\|_{L^\infty} \Big\}, \tag{5.1}$$

we define the cut off function $d_M : \mathbb{R} \to [-M, M]$, $d_M(z) := \min\{\max\{z, -M\}, M\}$ (and use it also for vectors componentwise), and the regularized statistical relations

$$u_i = N_i e_i(d_M(v_i)) =: N_i e_{Mi}(v_i), \quad i \in I.$$

For our problem, we regularize the statistical relations and the reaction term, and consider regularized operators $E_M : v^D + V \to V^*$, $A_M : (v^D + V)^2 \to V^*$,

$$\begin{aligned} E_M(v) &:= (E_0 v_0, (N_i e_{Mi}(v_i))_{i\in I}), \\ \langle A_M(w, v), \overline{v}\rangle_V &:= \sum_{i\in I} \int_{\Omega_i} z_i^2 N_i e_{Mi}(w_i)\mu_i \nabla\varphi_i \cdot \nabla\overline{\varphi}_i \,\mathrm{d}x \\ &\quad + \int_{\Omega_0} \sum_{i\in I_0} z_i\big(z_i\varphi_i - d_M(z_i w_0) - d_M(w_i)\big)\overline{\varphi}_i \,\mathrm{d}x \\ &\quad + \int_\Omega \rho_M(w)[r(N_n e_n(w_n), N_p e_p(w_p))\big(1 - \mathrm{e}^{-w_n - w_p}\big) - G](\overline{v}_n + \overline{v}_p) \,\mathrm{d}x, \end{aligned} \tag{5.2}$$

for all $\overline{v}_0$, $\overline{v}_n$, $\overline{v}_p \in V_D$, and $\overline{v}_i \in V_0$, $i \in I_0$, where $\varphi_i = v_0 + \frac{1}{z_i} v_i$, $\overline{\varphi}_i = \overline{v}_0 + \frac{1}{z_i}\overline{v}_i$, $i \in I$, and $\rho_M : \mathbb{R}^{\#I+1} \to [0, 1]$ is a continuous function such that

$$\rho_M(v) = \begin{cases} 0, & \text{if } \max\{|v_n|, |v_p|\} \ge M, \\ 1, & \text{if } \max\{|v_n|, |v_p|\} < M/2. \end{cases}$$

Note that $\rho_M(v) = \rho_M(d_M(v))$. Then we consider the problem

$$u' + A_M(v,v) = 0,\ u = E_M(v),\ u(0) = u^0,\ u \in H^1(S,V^*),\ v - v^D \in L^2(S,V). \qquad (\mathrm{P_M})$$

Remark 5.1 *Let (u,v) be a solution to the problem* ($\mathrm{P_M}$) *and let us assume that*

$$(1+\max_{i\in I_0}|z_i|)\|v_0\|_{L^\infty(S,L^\infty(\Omega))} \le M, \quad \|v_i\|_{L^\infty(S,L^\infty(\Omega))} \le \tfrac{M}{2},\ i=n,p,$$

and $\|v_i\|_{L^\infty(S,L^\infty(\Omega_0))} \le M$, $i\in I_0$, then (u,v) solves ($\mathrm{P_S}$).

We solve the Problem ($\mathrm{P_M}$) by time discretization. For any Banach space X and $k \in \mathbb{N}$ we define $h_k := \frac{T}{k}$ and $C_k(S,X)$ as the space of all functions $u : S \to X$ being constant on each of the intervals $((l-1)h_k, lh_k]$, $l = 1,\dots,k$. Let u^l denote the value of $u \in C_k(S,X)$ on $((l-1)h_k, lh_k]$ and introduce the maps τ_k and Δ_k from $C_k(S,X)$ into itself via

$$(\tau_k u)^l := u^{l-1}, \quad (\Delta_k u)^l := \frac{1}{h_k}(u^l - u^{l-1}), \quad l = 1,\dots,k,$$

with the given initial value u^0. Additionally, we work with the continuous, piecewise linear function

$$(K_k u_k)(t) := u^0 + \int_0^t (\Delta_k u_k)(s)\,\mathrm{d}s.$$

The time-discrete analogon of ($\mathrm{P_M}$) now reads

$$\Delta_k u_k + A_M(v_k,v_k) = 0,\ u_k = E_M(v_k),\ v_k - v^D \in C_k(S,V) \qquad (5.3)$$

or written in more detail

$$E_M(v_k^l) + h_k A_M(v_k^l, v_k^l) = E_M(v_k^{l-1}) \text{ for } l = 1,\dots,k \text{ and } u_k^0 = E_M(v_k^0) = u^0. \qquad (5.4)$$

Lemma 5.1 *We assume* (A1) – (A4). *Then for all $k \in \mathbb{N}$ there exists a unique solution (u_k, v_k) to problem* (5.3). *Additionally,*

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

Proof. 1. The operator $v \mapsto \frac{1}{h_k}E_M(v) + A_M(v,v)$ with the given argument splitting in the definition of the operator A_M is an operator of variational type (see [25, p. 182]). Note that the main part (in the argument v in (5.2)) is monotone, continuous and bounded and the regularized reaction term (in the argument w) is bounded and Lipschitz continuous. Together with the coercivity of $v \mapsto \frac{1}{h_k}E_M(v) + A_M(v,v)$ this ensures for any given v_k^{l-1} a solution v_k^l to (5.4). Thus, we can successively compose from the solution for each time step a solution to (5.3).

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

$$\begin{aligned} \Phi_M(v) &:= \int_\Omega \Big\{\frac{\varepsilon}{2}|\nabla v_0|^2 - \frac{\varepsilon}{2}|\nabla v_0^D|^2\Big\}\,\mathrm{d}x + \sum_{i\in I}\int_{\Omega_i} N_i \int_{v_i^D}^{v_i} e_{Mi}(y)\,\mathrm{d}y\,\mathrm{d}x, \\ \Psi_M(u) &:= \sup_{w\in V}\{\langle u,w\rangle_V - \Phi_M(w+v^D)\}, \quad u \in V^*. \end{aligned} \qquad (5.5)$$

Note that by definition $v_i^D = 0$ for $i \in I_0$. The functional Φ_M has the Fréchet derivative $\Phi'_M = E_M$, and the conjugate functional Ψ_M for arguments $u = E_M(v)$ is obtained by

$$\Psi_M(u) = \langle u, v - v^D\rangle_V - \Phi_M(v) = \big\langle \big(E_0 v_0, (N_i e_{Mi}(v_i))_{i\in I}\big), v - v^D\big\rangle_V - \Phi_M(v). \tag{5.6}$$

Moreover, we have $v - v^D \in \partial\Psi_M(u)$ provided that $u = E_M(v)$ for $v \in v^D + V$. Exploiting (5.5) and (5.6), we estimate the regularized free energy $\Psi_M(u)$ for $u = E_M(v)$ where $v \in v^D + V$ from below by

$$\begin{aligned}
\Psi_M(u) &= \int_\Omega \frac{\varepsilon}{2}|\nabla(v_0 - v_0^D)|^2\,\mathrm{d}x + \sum_{i\in I}\int_{\Omega_i}\int_{v_i^D}^{v_i}(u_i - N_i e_{Mi}(y))\,\mathrm{d}y\,\mathrm{d}x \\
&\geq c\|v_0 - v_0^D\|_{H^1}^2 + \sum_{i\in I}\int_{\Omega_i}\int_{v_i^D}^{d_M(v_i)}(u_i - N_i e_i(y))\,\mathrm{d}y\,\mathrm{d}x \\
&\geq c\|v_0 - v_0^D\|_{H^1}^2 + \sum_{i\in I}\int_{\Omega_i}\big(u_i - N_i e_i(v_i^D + 1)\big)\,\mathrm{d}x.
\end{aligned}$$

The estimate in the last line results similar to the derivation of (4.7) by considering the different cases for $\omega_M := \int_{v_i^D}^{d_M(v_i)}(u_i - N_i e_i(y))\,\mathrm{d}y$. In summary, we obtain for arguments $u = E_M(v)$ that

$$\|u_n\|_{L^1(\Omega)} + \|u_p\|_{L^1(\Omega)} + \sum_{i\in I_0}\|u_i\|_{L^1(\Omega_0)} + \|v_0 - v_0^D\|_{H^1}^2 \leq c(1 + \Psi_M(u)). \tag{5.7}$$

Using (5.4), the subdifferential property, and the strong monotonicity of A_M in the second argument, we find for $l = 1, \ldots, k$,

$$\begin{aligned}
&\Psi_M(u_k^l) - \Psi_M(u^0) = \sum_{j=1}^{l}\big(\Psi_M(u_k^j) - \Psi_M(u_k^{j-1})\big) \leq \sum_{j=1}^{l}\big\langle u_k^j - u_k^{j-1}, v_k^j - v^D\big\rangle_V \\
&= -h_k\sum_{j=1}^{l}\big\langle A_M(v_k^j, v_k^j), v_k^j - v^D\big\rangle_V \\
&= -h_k\sum_{j=1}^{l}\Big\{\big\langle A_M(v_k^j, v_k^j) - A_M(v_k^j, v^D), v_k^j - v^D\big\rangle_V + \big\langle A_M(v_k^j, v^D), v_k^j - v^D\big\rangle_V\Big\} \\
&\leq -h_k\sum_{j=1}^{l}\Big\{\sum_{i=n,p}\underline{\mu}\underline{N}e_i(-M)\|\nabla(\varphi_{ki}^j - \varphi_i^D)\|_{L^2(\Omega)}^2 \\
&\qquad + \sum_{i\in I_0} z_i^2\big(\underline{\mu}\underline{N}e_i(-M)\|\nabla(\varphi_{ki}^j - v_0^D)\|_{L^2(\Omega_0)}^2 + \|\varphi_{ki}^j - v_0^D\|_{L^2(\Omega_0)}^2\big) \\
&\qquad + \big\langle A_M(v_k^j, v^D), v_k^j - v^D\big\rangle_V\Big\} \\
&\leq -\underline{c}\int_0^{lh_k}\Big\{\sum_{i=n,p}\|\nabla(\varphi_{ki} - \varphi_i^D)\|_{L^2(\Omega)}^2 + \sum_{i\in I_0}\|\varphi_{ki} - v_0^D\|_{V_0}^2 + \Big\}\mathrm{d}t + c_M,
\end{aligned} \tag{5.8}$$

where $c_M > 0$ does not depend on k. Here we used that for any test function $w \in L^2(S, V_D)$, we can estimate the generation and recombination term by

$$\begin{aligned}
&\int_S\int_\Omega \rho_M(v_k)[r(N_n e_{Mn}(v_{kn}), N_p e_{Mp}(v_{kp}))\big(1 - \mathrm{e}^{-v_{kn} - v_{kp}}\big) - G]w\,\mathrm{d}x\,\mathrm{d}t \\
&\qquad \leq c(M)\|\mathrm{e}^{2M} + 1 + \gamma\|_{L^2(S,L^2(\Omega))}\|w\|_{L^2(S,L^2(\Omega))}.
\end{aligned} \tag{5.9}$$

Because of $\Psi_M(u^0) < \infty$, the estimates (5.7), (5.8) guarantee that

$$\sup_{k\in\mathbb{N}} \big\{ \|v_{k0} - v_0^D\|_{L^\infty(S,V_D)} + \|v_k - v^D\|_{L^2(S,V)} \big\} < \infty. \tag{5.10}$$

Due to the regularizations in A_M, we find from (5.10) that $\sup_{k\in\mathbb{N}} \|A_M(v_k, v_k)\|_{L^2(S,V^*)} < \infty$ and $\sup_{k\in\mathbb{N}} \|\Delta_k u_k\|_{L^2(S,V^*)} < \infty$. Moreover, from $u_{k0} = E_0 v_{k0}$ and (5.10) we conclude that $\sup_{k\in\mathbb{N}} \|u_{k0}\|_{L^\infty(S,V_D^*)} < \infty$. Taking into account that $N_i e_i(-M) \le u_{ki} < N_i e_i(M)$, $i \in I$, 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 $t \in ((l-1)h_k, l h_k]$ we have $K_k u_k \in C(S, H^*)$ and $\sup_{k\in\mathbb{N}} \|K_k u_k\|_{C(S,H^*)} < \infty$. $\square$

Lemma 5.2 *We assume* (A1) – (A4)*. Then there exists a solution* (u, v) *to Problem* ($\mathrm{P_M}$)*.*

Proof. 1. Let $\{(u_k, v_k)\}_{k\in\mathbb{N}}$ be a sequence of solutions to the time discretized problems according to Lemma 5.1. Then, we find functions v and u and a non-relabelled subsequence such that

$$v_k - v^D \rightharpoonup v - v^D \text{ in } L^2(S,V), \quad K_k u_k \rightharpoonup u \text{ in } L^2(S,H) \text{ and } H^1(S,V^*). \tag{5.11}$$

We denote $\varphi_i := v_0 + \frac{1}{z_i} v_i$, $i \in I$.

2. Since for $w \in V$ and $t \in S$ the map $z \mapsto \langle z(t), w\rangle$, $z \in H^1(S,V^*)$, defines a continuous linear functional on $H^1(S,V^*)$ we get from (5.11) that $(K_k u_k)(t) \rightharpoonup u(t)$ in V^* for all $t \in S$. Moreover, the boundedness of $(K_k u_k)(t)$ in H then guarantees $(K_k u_k)(t) \rightharpoonup u(t)$ in H for $t \in S$. From $(K_k u_k)(0) = u^0$, $k \in \mathbb{N}$, we obtain $u(0) = u^0$.

3. Since $\|K_k u_k - u_k\|_{L^2(S,V^*)} \le h_k \|\Delta_k u_k\|_{L^2(S,V^*)} \to 0$ we find another non-relabelled subsequence such that $(K_k u_k - u_k)(t) \to 0$ in V^*, and $u_k(t) \rightharpoonup u(t)$ in H f.a.a. $t \in S$. Using that $u_{ki}/N_i = e_{Mi}(v_{ki}) < e_i(M)$, e_{Mi} are Lipschitzian, and $\{v_{ki}\}$ are bounded in $L^2(S, H^1(\Omega_i))$ we establish the boundedness of $\{u_{ki}/N_i\}$ in $L^2(S, H^1(\Omega_i))$, too. And Lebesgue's theorem ensures

$$u_{ki} \rightharpoonup u_i \text{ in } L^2(S, L^2(\Omega_i)), \quad i \in I. \tag{5.12}$$

Next, we take advantage of the inequality (6.40) in [24, p. 529]:

For all $\delta > 0$ there is a $L_\delta \in \mathbb{N}$ such that

$$\|y\|_{L^2}^2 \le \sum_{j=1}^{L_\delta} (y, \psi_j)_{L^2}^2 + \delta \|y\|_{H^1}^2 \quad \forall y \in H^1(\Omega_i) \quad (\{\psi_j\}_{j\in\mathbb{N}} \text{ ON-base in } L^2(\Omega_i)).$$

Setting $y = (u_{ki} - u_{li})/N_i$, we integrate this inequality over S. By the weak convergence in $L^2(\Omega_i)$ a.e. in S, the boundedness of $\{u_{ki}(t)\}$ in $L^2(\Omega_i)$ for $t \in S$, Lebesgue's theorem and the boundedness of $\{u_{ki}/N_i\}$ in $L^2(S, H^1(\Omega_i))$ we verify that $\{u_{ki}\}$ is a Cauchy sequence in $L^2(S, L^2(\Omega_i))$. And (5.12) ensures the strong convergence

$$u_{ki} \to u_i,\ u_{ki}/N_i \to u_i/N_i \ \text{ in } L^2(S, L^2(\Omega_i)), \quad i \in I. \tag{5.13}$$

In connection with $K_k u_k - u_k \to 0$ in $L^2(S,V^*)$ we conclude that $(K_k u_k - u)_i \to 0$ in $L^2(S, V_D^*)$ for $i = n, p$ and $(K_k u_k - u)_i \to 0$ in $L^2(S, V_0^*)$ for $i \in I_0$.

4. Sine $\big\langle A_M(v_k, v_k), (y, (-z_i y|_{\Omega_i})_{i\in I})\big\rangle_V = 0$ for any $y \in V_D$, we derive from (5.3) and partial integration that for any fixed indices k_1 and k_2 of our subsequence and every $y \in V_D$ and all $t \in S$

$$\begin{aligned} 0 &= \int_0^t \big\langle \Delta_{k_1} u_{k_1} - \Delta_{k_2} u_{k_2}, (y, (-z_i y|_{\Omega_i})_{i\in I})\big\rangle_V \,\mathrm{d}s \\ &= \big\langle (K_{k_1} u_{k_1} - K_{k_2} u_{k_2})(t), (y, (-z_i y|_{\Omega_i})_{i\in I})\big\rangle_V. \end{aligned}$$

Let J_D be the duality map of V_D. We set $y = y(t) = J_D^{-1}[(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0(t)]$ and obtain

$$\|(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0(t)\|_{V_D^*}^2 = \big\langle (K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0(t), J_D^{-1}[(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0(t)]\big\rangle$$

$$= \sum_{i=n,p} \big\langle (K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_i(t), J_D^{-1}[(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0(t)]\big\rangle_{V_D}$$

$$+ \sum_{i\in I_0} \big\langle (K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_i(t), J_D^{-1}[(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0(t)]|_{\Omega_0}\big\rangle_{V_0}.$$

After integration over S we arrive at

$$\|(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_0\|_{L^2(S,V_0^*)}$$
$$\le c\sum_{i=n,p} \|(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_i\|_{L^2(S,V_D^*)} + c\sum_{i\in I_0} \|(K_{k_1}u_{k_1} - K_{k_2}u_{k_2})_i\|_{L^2(S,V_0^*)}.$$

Thus, the last convergence results of Step 3 and the weak convergence in (5.11) ensure the strong convergences $(K_k u_k)_0 \to u_0$ in $L^2(S, V_D^*)$ and $K_k u_k \to u$ in $L^2(S, V^*)$. Again by Step 3, we also get $u_k \to u$ in $L^2(S, H)$, and for a non-relabelled subsequence, $u_k(t) \to u(t)$ in V^* f.a.a. $t \in S$.

5. We consider any subinterval $\widetilde{S}$ of S and $\widetilde{u} \in V^*$ with finite regularized free energy, $\Psi_M(\widetilde{u}) < \infty$. Since Ψ_M is lower semicontinuous and $v_k - v^D \in \partial\Psi_M(u_k)$ a.e. in S we estimate

$$\int_{\widetilde{S}} \langle \widetilde{u} - u(t), v(t) - v^D\rangle_V \,\mathrm{d}t = \lim_{k\to\infty} \int_{\widetilde{S}} \langle \widetilde{u} - u_k(t), v_k(t) - v^D\rangle \,\mathrm{d}t$$
$$\le \limsup_{k\to\infty} \int_{\widetilde{S}} (\Psi_M(\widetilde{u}) - \Psi_M(u_k(t)))\,\mathrm{d}t \le \int_{\widetilde{S}} (\Psi_M(\widetilde{u}) - \Psi_M(u(t)))\,\mathrm{d}t.$$

This guarantees for a.a. $t \in S$ that $\langle \widetilde{u} - u(t), v(t) - v^D\rangle_V \le \Psi_M(\widetilde{u}) - \Psi_M(u(t))$ meaning that for the limit functions $v(t) - v^D \in \partial\Psi_M(u(t))$ and $u(t) \in \partial\Phi_M(v(t)) = E_M(v(t))$ for a.a. $t \in S$. Applying the chain rule [5, Lemma 3.3] yields

$$\Psi_M(u(t)) - \Psi_M(u^0) = \int_0^t \langle u'(s), v(s) - v^D\rangle_V \,\mathrm{d}s \quad \forall\, t \in S. \tag{5.14}$$

6. Using the strong monotonicity of E_0 and $u_0(t) = E_0 v_0(t)$, $u_{k0}(t) = E_0 v_{k0}(t)$ a.e. in S we find for the subsequence by the test with $v_{k0} - v_0 \in V_D$ and integration over S

$$c\|v_{k0} - v_0\|_{L^2(S,V_D)}^2 \le \int_S \langle E_0 v_{k0} - E_0 v_0, v_{k0} - v_0\rangle_{V_D} \mathrm{d}t \le \|u_{k0} - u_0\|_{L^2(S,V_D^*)} \|v_{k0} - v_0\|_{L^2(S,V_D)}.$$

Thus, $c\|v_{k0} - v_0\|_{L^2(S,V_D)} \le \|u_{k0} - u_0\|_{L^2(S,V_D^*)} \to 0$ by Step 4. Additionally, from (5.13) and the Lipschitz continuity of e_i^{-1} on the interval $[e_i(-M), e_i(M)]$ we get

$$d_M(v_{ki}) = e_i^{-1}(u_{ki}/N_i) \to e_i^{-1}(u_i/N_i) \quad \text{in } L^2(S, L^2(\Omega_i)), \quad i \in I. \tag{5.15}$$

Let $\widehat{v} := (v_0, (e_i^{-1}(u_i/N_i))_{i\in I})$ and let $\widehat{A}(v) \in L^2(S, V^*)$ for $u = E_M v$ be defined by

$$\langle \widehat{A}(v), \overline{v}\rangle_V := \int_\Omega \big\{u_n\mu_n\nabla\varphi_n \cdot \nabla\overline{\varphi}_n + u_p\mu_p\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\big\}\,\mathrm{d}x$$
$$+ \int_{\Omega_0} \sum_{i\in I_0} \big\{z_i^2 u_i\mu_i\nabla\varphi_i \cdot \nabla\overline{\varphi}_i + z_i\big(z_i\varphi_i - d_M(z_i v_0) - \widehat{v}_i\big)\overline{\varphi}_i\big\}\,\mathrm{d}x$$
$$+ \int_\Omega \rho_M(\widehat{v})[r(u_n, u_p)\big(1 - \mathrm{e}^{-\widehat{v}_n - \widehat{v}_p}\big) - G](\overline{v}_n + \overline{v}_p)\,\mathrm{d}x.$$

Taking into account that $\rho_M(v_k) = \rho_M(d_M(v_k))$ we find

$$\begin{aligned}
&\rho_M(v_k) r(N_n e_n(v_{kn}), N_p e_p(v_{kp}))(1 - \mathrm{e}^{-v_{kn}-v_{kp}}) \\
&\qquad = \rho_M(d_M(v_k)) r(N_n e_n(d_M(v_{kn})), N_p e_p(d_M(v_{kp})))(1 - \mathrm{e}^{-d_M(v_{kn})-d_M(v_{kp})}).
\end{aligned}$$

Using additionally (5.13) and (5.15) and Lebesgue's dominated convergence theorem we derive for a non-relabelled subsequence the convergence

$$A_M(v_k, v) \to \widehat{A}(v) \quad \text{in } L^2(S, V^*). \tag{5.16}$$

7. Because (u_k, v_k) are solutions to (5.3), our convergence results for a subsequence obtained so far (see also Step 2 in the proof of Lemma 5.1) lead to

$$\begin{aligned}
0 &= \lim_{k\to\infty} \int_S \langle \Delta_k u_k + A_M(v_k, v_k), v_k - v\rangle_V \,\mathrm{d}t \\
&= \lim_{k\to\infty} \int_S \Big\{ \langle \Delta_k u_k, v_k - v^D\rangle_V - \langle u', v - v^D\rangle_V \\
&\quad + \big\langle A_M(v_k, v_k) - A_M(v_k, v), v_k - v\big\rangle_V + \big\langle A_M(v_k, v), v_k - v\big\rangle_V \Big\} \,\mathrm{d}t \\
&\geq \limsup_{k\to\infty} \Big\{ \Psi_M(u_k^k) - \Psi_M(u^0) \\
&\qquad + \int_S \Big[\langle u', v^D - v\rangle_V + \underline{c}\Big(\sum_{i=n,p} \|\nabla(\varphi_{ki} - \varphi_i)\|^2_{L^2(\Omega)} + \sum_{i\in I_0} \|\varphi_{ki} - \varphi_i\|^2_{V_0} \Big) \Big] \,\mathrm{d}t \Big\}.
\end{aligned}$$

Note that the limit of the last term in the third line is zero because of (5.16) and $v_k - v^D \rightharpoonup v - v^D$ in $L^2(S, V)$. The last two terms in the last line results from the strong monotonicity of A_M in the last argument. The weak lower continuity of Ψ_M on V^* yields

$$\limsup_{k\to\infty} \Psi_M(u_k^k) = \limsup_{k\to\infty} \Psi_M(u_k(T)) \geq \Psi_M(u(T)).$$

Therefore, using (5.14), the estimates of Step 7 ensure

$$\varphi_{ki} - \varphi_i \to 0 \text{ in } L^2(S, V_D), \quad i = n, p, \quad \varphi_{ki} \to \varphi_i \text{ in } L^2(S, V_0), \quad i \in I_0. \tag{5.17}$$

In Step 6 it was already proven that $\|v_{k0} - v_0\|_{L^2(S,V_0)} \to 0$. Thus, we also verify the convergence $\|v_{ki} - v_i\|_{L^2(S,V_D)} \to 0, i = n, p$, $\|v_{ki} - v_i\|_{L^2(S,V_0)} \to 0, i \in I_0$, and finally $\|v_k - v\|_{L^2(S,V)} \to 0$.

8. From $v_{ki} \to v_i$ in $L^2(S, L^2(\Omega_i))$ we obtain $d_M(v_{ki}) \to d_M(v_i)$ in $L^2(S, L^2(\Omega_i))$. By (5.15) we have $d_M(v_{ki}) \to e_i^{-1}(u_i/N_i)$ in $L^2(S, L^2(\Omega_i))$. The uniqueness of the limit gives $d_M(v_i) = e_i^{-1}(u_i/N_i) = \widehat{v}_i$, $i \in I$. Using again $\rho_M(v) = \rho_M(d_M(v))$ we establish that $\widehat{A}(v) = A_M(v, v)$ in $L^2(S, V^*)$. Therefore, for arbitrary $w \in L^2(S, V)$ we estimate

$$\begin{aligned}
\langle A_M(v_k, v_k) - A_M(v, v), w\rangle_V &= \langle A_M(v_k, v_k) - \widehat{A}(v), w\rangle_V \\
&= \langle A_M(v_k, v_k) - A_M(v_k, v), w\rangle_V + \langle A_M(v_k, v) - \widehat{A}(v), w\rangle_V \\
&\leq c\Big(\sum_{i=n,p} \|\varphi_{ki} - \varphi_i\|_{L^2(S,V_D)} + \sum_{i\in I_0} \|\varphi_{ki} - \varphi_i\|_{L^2(S,V_0)} \Big) \|w\|_{L^2(S,V)} \\
&\quad + \|A_M(v_k, v) - \widehat{A}(v)\|_{L^2(S,V^*)} \|w\|_{L^2(S,V)}.
\end{aligned}$$

Thus,

$$\|A_M(v_k,v_k)-A_M(v,v)\|_{L^2(S,V^*)} = \sup_{w\in L^2(S,V)} \frac{\langle A_M(v_k,v_k)-A_M(v,v),w\rangle_{L^2(S,V)}}{\|w\|_{L^2(S,V)}}$$
$$\leq c\sum_{i=n,p}\|\varphi_{ki}-\varphi_i\|_{L^2(S,V_D)} + c\sum_{i\in I_0}\|\varphi_{ki}-\varphi_i\|_{L^2(S,V_0)} + \|A_M(v_k,v)-\widehat{A}(v)\|_{L^2(S,V^*)}.$$

Due to (5.16) and (5.17), we obtain for that subsequence $A_M(v_k,v_k)\to A_M(v,v)$ in $L^2(S,V^*)$. Since Step 1 yields $A_M(v_k,v_k)=-\Delta_k u_k \rightharpoonup -u'$ in $L^2(S,V^*)$, we end up with the identity $u'+A_M(v,v)=0$. The relation $u=E_M v$ was already shown in Step 5 such that the limit (u,v) is indeed a solution to ($\mathrm{P_M}$), which completes the proof. □

5.2 A priori estimates for problem ($\mathbf{P_M}$)

By the choice of M in (5.1) and the definition of Ψ_M, the value of $\Psi_M(u^0)$ does not depend on M,

$$\Psi_M(u^0) = \int_\Omega \frac{\varepsilon}{2}|\nabla(v_0^0-v_0^D)|^2\,\mathrm{d}x + \sum_{i\in I}\int_{\Omega_i}\int_{v_i^D}^{v_i^0}(u_i^0 - N_i e_i(y))\,\mathrm{d}y\,\mathrm{d}x = \Psi(u^0).$$

Lemma 5.3 *We assume* (A1) – (A4)*. Let M fulfill* (5.1)*. Then, there exist $c,\ c^*>0$ not depending on M and u^0 such that*

$$\|v_0(t)-v_0^D\|^2_{H^1(\Omega)} + \sum_{i\in I}\|u_i(t)\|_{L^1(\Omega_i)} \leq c\mathrm{e}^{cT}(1+\Psi(u^0)) =: c_T \quad \forall t\in S,$$

$$\|v_0(t)\|_{H^1(\Omega)} + \|v_0(t)\|_{L^\infty(\Omega)} \leq c^*(1+\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}) \quad \forall t\in S,$$

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

Proof. 1. By means of the test function $v-v^D$ for $u'+A_M(v,v)=0$ we find for all $t\in S$

$$\begin{aligned}
0 &= \Psi_M(u(t)) - \Psi(u^0)\\
&\quad + \int_0^t \Big\{ \sum_{i\in I}\int_{\Omega_i} N_i e_{Mi}(v_i)\mu_i \nabla(v_i+z_i v_0)\cdot\nabla(v_i - v_i^D + z_i(v_0-v_0^D))\,\mathrm{d}x\\
&\qquad + \sum_{i\in I_0}\int_{\Omega_0}\big(v_i+z_iv_0 - d_M(v_i)-d_M(z_iv_0)\big)(v_i+z_i(v_0-v_0^D))\,\mathrm{d}x\\
&\qquad + \int_\Omega \rho_M(v)[r(N_ne_n(v_n),N_pe_p(v_p))\big(1-\mathrm{e}^{-v_n-v_p}\big)-G](v_n+v_p)\,\mathrm{d}x\Big\}\,\mathrm{d}s\\
&\geq \Psi_M(u(t)) - \Psi(u^0) + \int_0^t\Big\{\sum_{i\in I}\int_{\Omega_i}\frac{N_ie_{Mi}(v_i)\mu_i}{2}|\nabla(v_i-v_i^D+z_i(v_0-v_0^D))|^2\\
&\qquad + \sum_{i\in I_0}\int_{\Omega_0}\frac{1}{2}\big(v_i+z_iv_0-d_M(v_i)-d_M(z_iv_0)\big)^2\,\mathrm{d}x\\
&\qquad - c\int_\Omega\Big(\sum_{i\in I}|\nabla(v_i^D+z_iv_0^D)|^2 + |v_0^D|^2\Big)\,\mathrm{d}x\\
&\qquad + \int_\Omega \rho_M(v)[r(N_ne_n(v_n),N_pe_p(v_p))\big(1-\mathrm{e}^{-v_n-v_p}\big)-G](v_n+v_p)\,\mathrm{d}x\Big\}\,\mathrm{d}s.
\end{aligned}$$

Here we used the inequality $(f+g-d_M(f)-d_M(g))(f+g) \geq (f+g-d_M(f)-d_M(g))^2 \geq 0$. Moreover, note that φ^D, $v_0^D \in W^{1,\infty}(\Omega)$, the monotonicity of the exponential function, and that $\rho_M(v)(v_n+v_p) = \rho_M(v)(d_M(v_n)+d_M(v_p)) \leq \rho_M(v)(d_M(v_n)^+ + d_M(v_p)^+) \leq u_n+u_p+c$, see (2.4). We arrive at

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

Next, we use (5.7) and apply Gronwall's lemma to gain the first estimate of the lemma.

2. Since for arbitrarily given $y \in V_0$, $\langle A_M(v(s),v(s)),(y,(-z_i y|_{\Omega_i})_{i\in I})\rangle_V = 0$ we find

$$\begin{aligned} 0 &= \int_0^t \langle u'(s),(y,(-z_i y|_{\Omega_i})_{i\in I})\rangle_V\,\mathrm{d}s \\ &= \langle (u_0+u_n-u_p)(t) - u_0^0 - u_n^0 + u_p^0, y\rangle_{V_D} - \sum_{i\in I_0}\langle z_i(u_i(t)-u_i^0), y|_{\Omega_0}\rangle_{V_0} \quad \forall\, t\in S \end{aligned}$$

and thus $u(t) \in U_0$. Therefore, the test of $E_0 v_0(t) = u_0(t)$ by $v_0(t) - v_0^D$ yields

$$\|v_0(t)\|_{V_D} \leq c\Big(\sum_{i\in I}\|u_i(t)\|_{L^2(\Omega_i)}+1\Big) \leq c\Big(\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}+1\Big).$$

Here we toke into account that $v_0^D \in W^{1,\infty}(\Omega)$, $C\in L^\infty(\Omega)$, and $u_i \leq N_{i0}$ for $i\in I_0$.

3. Let $l \geq l_0 := \|v_0^D\|_{L^\infty}$ and $y := (v_0(t)-l)^+ - (v_0(t)+l)^- \in V_D$. Then the test of $E_0 v_0(t) = u_0(t)$ leads to

$$\begin{aligned} c_1\|y\|^2_{H^1(\Omega)} &\leq \int_\Omega \varepsilon\nabla v_0\cdot\nabla y\,\mathrm{d}x = \int_\Omega \Big(C+\sum_{i\in I}\chi_{\Omega_i} z_i u_i\Big) y\,\mathrm{d}x \\ &\leq c\big(\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}+1\big)\|y\|_{L^2(\Omega)} \leq c\big(\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}+1\big)\|y\|_{L^6(\Omega)} m_l^{1/3} \\ &\leq c\big(\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}+1\big)\|y\|_{H^1(\Omega)} m_l^{1/3}. \end{aligned}$$

Here, we used that $C\in L^\infty(\Omega)$, $u_i < N_i$ a.e. in Ω_0 for $i \in I_0$ and m_l is the Lebesgue measure of the set $\{x\in\Omega:\ |y(x)|>l\}$. The last inequality ensures

$$(k-l)m_k^{1/6} \leq \|y\|_{L^6(\Omega)} \leq c\big(\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}+1\big).$$

By [21, Lemma B.1] we conclude that $m_l = 0$ for $l \geq l_0 + c\big(\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)}+1\big)$. In other words, $\|v_0(t)\|_{L^\infty(\Omega)} \leq c(1+\sum_{i=n,p}\|u_i(t)\|_{L^2(\Omega)})$ for all $t\in S$. □

Exploiting the regularity result of Gröger [18, Theorem 1] for elliptic equations with non-smooth data and mixed boundary conditions in two spatial dimensions for the Poisson equation and using the boundedness of C and $u_i < N_i$, $i\in I_0$, we obtain

Lemma 5.4 *We assume* (A1) – (A4)*. Then, there exists a constant* $c>0$ *and an exponent* $\pi>2$ *(independent of* M *and* T*) such that for any solution* (u,v) *to* ($\mathrm{P_M}$)

$$\|v_0(t)\|_{W^{1,\pi}(\Omega)} \leq c\Big(1+\sum_{i=n,p}\|u_i(t)\|_{L^{\sigma'}(\Omega)}\Big) \quad \forall t\in S, \quad \textit{where } \sigma := \frac{2\pi}{\pi-2},\ \sigma' := \frac{2\pi}{\pi+2}.$$

The following three results are proven in such a way that their estimates can be used for Problem (P_M) as well as for Problem (P_S).

Lemma 5.5 *We assume* (A1) – (A4). *Let* $M \geq M^*$ *with* M^* *as in* (5.1). *Then, there exists a* $c_0 > 0$ *depending only on the data* (*but not on* M) *such that for any solution* (u, v) *to* (P_M)

$$u_i(t) \leq c_0(T) \quad \text{a.e. in}\, \Omega \quad \forall t \in S,\ i = n, p.$$

Proof. 1. Let (u, v) be a solution to (P_M) and $q \geq 2$ (not the elementary charge as in Section 2!). Let

$$K := \max\Big\{ \max_{i=n,p} \|e_i(z_i(\varphi^D - v_0^D))\|_{L^\infty(\Omega)}, \max_{i\in I} \|u_i^0/N_i\|_{L^\infty(\Omega_i)} \Big\}.$$

We define $w_i := (\frac{u_i}{N_i} - K)^+$, $i = n, p$, and use for the equation $u' + A_M(v, v) = 0$ the test function

$$q(0, w_n^{q-1}, w_p^{q-1}, 0, \dots, 0) \in L^2(S, V)$$

to obtain for all $t \in S$

$$\begin{aligned} \sum_{i=n,p} \|w_i(t)\|^q_{L^q(\Omega)} + \int_0^t \int_\Omega \sum_{i=n,p} \Big\{ & q\mu_i u_i \nabla(v_i + z_i v_0) \cdot \nabla w_i^{q-1} \\ & + q\rho_M(v)[r(1 - \exp\{-v_n - v_p\}) - G] w_i^{q-1} \Big\} \mathrm{d}x\, \mathrm{d}s = 0. \end{aligned} \tag{5.18}$$

2. Since in this proof all spatial integrations concern Ω, we leave out here the domain Ω in the notation for the norms. Using $e_i'(x) < e_i(x)$, $i = n, p$, and the characteristic function χ_{w_i} of the support of w_i, we estimate the diffusion term

$$\begin{aligned} \frac{u_i}{N_i} \nabla v_i \cdot \nabla w_i^{q-1} &= (q-1) w_i^{q-2} e_{iM}(v_i) \nabla v_i \cdot \nabla (e_{iM}(v_i) - K)^+ \\ &= (q-1) w_i^{q-2} e_{iM}(v_i) e_{iM}'(v_i) |\nabla v_i|^2 \chi_{w_i} \geq (q-1) w_i^{q-2} \chi_{w_i} e_{iM}'(v_i)^2 |\nabla v_i|^2 \\ &= (q-1) w_i^{q-2} |\nabla w_i|^2 = \tfrac{4(q-1)}{q^2} |\nabla w_i^{q/2}|^2 \geq \tfrac{2}{q} |\nabla w_i^{q/2}|^2. \end{aligned}$$

Using π and σ from Lemma 5.4, the essential drift part is estimated by

$$\int_\Omega \frac{u_i}{N_i} \nabla v_0 \cdot \nabla w_i^{q-1} \,\mathrm{d}x \leq c(\|w_i^{q/2}\|_{L^\sigma} + 1)(\|\nabla v_0\|_{L^\pi} + 1) \|\nabla w_i^{q/2}\|_{L^2}.$$

For the treatment of the reaction terms, note that due to $\mathcal{F}_n(x),\ \mathcal{F}_p(x) \leq \mathrm{e}^x$ we have $r\mathrm{e}^{-v_n - v_p} = r_0 N_n e_n(v_n) N_p e_p(v_p) \mathrm{e}^{-v_n - v_p} \leq c$. Moreover, $\rho_M(v) r \geq 0$ such that

$$q\rho_M(v)[G - r(1 - \exp\{-v_n - v_p\})] w_i^{q-1} \leq c q w_i^{q-1}.$$

In summary, the previous arguments ensure to conclude from (5.18) the inequality

$$\begin{aligned} \sum_{i=n,p} \|w_i(t)\|^q_{L^q} \leq \int_0^t \sum_{i=n,p} \Big\{ & - 2\underline{\mu}\underline{N} \|\nabla w_i^{q/2}\|^2_{L^2} + cq(\|w_i^{q/2}\|^2_{L^2} + 1) \\ & + cq(\|w_i^{q/2}\|_{L^\sigma} + 1)(\|\nabla v_0\|_{L^\pi} + 1) \|\nabla w_i^{q/2}\|_{L^2} \Big\} \,\mathrm{d}s. \end{aligned} \tag{5.19}$$

3. For $q = 2$ we obtain from (5.19) due to Lemma 5.4

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

Note that $u_i \leq N_i(w_i + K)$. For all $y \in H_D^1(\Omega)$ we estimate by Gagliardo-Nirenberg's inequality

$$\|y\|_{L^2}^2 \leq c\|y\|_{L^1}\|\nabla y\|_{L^2}, \quad \|y\|_{L^\sigma} \leq c\|y\|_{L^1}^{1/\sigma}\|\nabla y\|_{L^2}^{1/\sigma'}, \quad \|y\|_{L^{\sigma'}} \leq c\|y\|_{L^1}^{1/\sigma'}\|\nabla y\|_{L^2}^{1/\sigma},$$

such that after applying Young's inequality and the first estimate from Lemma 5.3 we find

$$\sum_{i=n,p} \|w_i(t)\|_{L^2}^2 \leq c(K)\int_0^t (\sum_{i=n,p} \|w_i\|_{L^1}^2 + 1) \,\mathrm{d}s \leq c(K)\int_0^T (c_T^2 + 1) \,\mathrm{d}s = \widehat{c}(T). \tag{5.20}$$

Because of $\sigma' < 2$ and $u_i \leq N_i(w_i + K)$, Lemma 5.4 ensures a T dependent bound

$$\kappa_T := (\|v_0\|_{C(S,W_D^{1,\pi}(\Omega))} + 1)^{2\sigma}. \tag{5.21}$$

4. For $q \geq 2$ we obtain from (5.19) under the use of Gagliardo-Nirenberg's and Young's inequality and (5.21) that

$$\sum_{i=n,p} \|w_i(t)\|_{L^q}^q \leq \overline{c} q^{2\sigma}\kappa_T T \sum_{i=n,p} (\sup_{t\in S} \|w_i\|_{L^{q/2}}^q + 1) \quad \forall t \in S. \tag{5.22}$$

Setting $q = 2^m$, $m \geq 0$, and $\omega_m := \sum_{i=n,p}(\sup_{t\in S} \|w_i(t)\|_{L^{2^m}}^{2^m} + 1)$ we find $\omega_m \leq \widetilde{c}^m\, 2\overline{c}\kappa_T T\omega_{m-1}^2$, $\widetilde{c} := 2^{2\sigma}$, and repeated application gives $\omega_m \leq (\widetilde{c}\, 2\overline{c}\kappa_T T\omega_0)^{2^m}$ which means

$$\sum_{i=n,p} \sup_{t\in S} \|w_i(t)\|_{L^{2^m}} \leq \widetilde{c}\, 2\overline{c}\kappa_T T \sum_{i=n,p} (\sup_{t\in S} \|w_i(t)\|_{L^1} + 1),$$

and leads in the limit $m \to \infty$ to

$$\sum_{i=n,p} \sup_{s\in S} \|w_i(t)\|_{L^\infty} \leq \widetilde{c}\, 2\overline{c}\kappa_T T \sum_{i=n,p} (\sup_{t\in S} \|w_i(t)\|_{L^1} + 1) \quad \forall t \in S. \tag{5.23}$$

Together with the inequality $w_i \leq u_i/N_i$ and the first estimate in Lemma 5.3, we obtain the bound $\sum_{i=n,p} \|w_i(t)\|_{L^\infty} \leq c(T)$ for all $t \in S$. This ensures that $u_i(t) \leq N_i(w_i(t) + K) \leq \overline{N}(w_i(t) + K) \leq \overline{N}(c(T) + K)$ for all $t \in S$. $\square$

Lemma 5.6 *We assume* (A1) – (A4)*. Let* $M \geq \max\{M^*, \max_{i\in I_0} |z_i|c^*(1 + 2c_0(T)|\Omega|^{1/2}\}$ *with* M^* *as in* (5.1)*,* c^* *from Lemma 5.3 and* $c_0(T)$ *from Lemma 5.5. Then, there exists* $c_1 > 0$ *depending only on the data* (*but not on* M) *so that for any solution* (u, v) *to* ($\mathsf{P_M}$)

$$u_i(t) \geq c_1(T) \quad \textit{a.e. in } \Omega_i \quad \forall t \in S,\ i \in I.$$

Proof. 1. Let (u, v) be a solution to ($\mathrm{P_M}$). We set

$$K := \max\Big\{ \max_{i=n,p} \|\ln e_i(v_i^D)\|_{L^\infty},\ \max_{i\in I} \|\big(\ln(u_i^0/N_i)\big)^-\|_{L^\infty},\ \max_{i\in I} \ln e_i(0)\Big\}.$$

Our choice of K ensures that $\big(\ln(u_i/N_i) + K\big)^-(0) = 0$, $i \in I$, and $\big(\ln(u_i/N_i) + K\big)^- \in L^2(S, V_D)$, $i = n, p$. First, we show the assertion for $i = n$ and use the test function

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

Analogously this can be done for $i = p$. Note that due to the definition of the reaction rate, the boundedness of r_0 and the charge carrier density (see Lemma 5.5) and the sign of the test function

$$\begin{aligned} &R\frac{w^{q-1}}{u_n/N_n} = r_0(u_n, u_p)N_n u_p\Big(1 - \exp\big\{-e_n^{-1}(u_n) - e_p^{-1}(u_p)\big\}\Big)w^{q-1} \leq c(T)w^{q-1},\\ &-G\frac{w^{q-1}}{u_n/N_n} \leq 0. \end{aligned} \tag{5.24}$$

We arrive at

$$\begin{aligned} \|w(t)\|_{L^q}^q &\leq \int_0^t \int_\Omega q\Big\{\mu_n u_n \nabla(v_n - v_0)\cdot\nabla\Big(\frac{w^{q-1}}{u_n/N_n}\Big) + c w^{q-1}\Big\}\,\mathrm{d}x\,\mathrm{d}s\\ &\leq \int_0^t \int_\Omega q\Big\{\mu_n N_n(\nabla v_n - \nabla v_0)\cdot\nabla w\Big((q-1)w^{q-2} + w^{q-1}\Big) + c(w^q + 1)\Big\}\,\mathrm{d}x\,\mathrm{d}s. \end{aligned} \tag{5.25}$$

Since $e_n'(y) \leq e_n(y)$ for all $y \in \mathbb{R}$ (see (iii) of (2.4)) we find

$$\nabla v_n \cdot \nabla w = -|\nabla v_n|^2 \frac{e_{Mn}'(v_n)\chi_{\mathsf{supp}\,w}}{e_{Mn}(v_n)} \leq -\Big(|\nabla v_n|\frac{e_{Mn}'(v_n)\chi_{\mathsf{supp}\,w}}{e_{Mn}(v_n)}\Big)^2 = -|\nabla w|^2. \tag{5.26}$$

Moreover, we rewrite

$$q(q-1)w^{q-2}|\nabla w|^2 = \frac{4(q-1)}{q}|\nabla w^{q/2}|^2, \quad q w^{q-1}|\nabla w|^2 = \frac{4q}{(q+1)^2}|\nabla w^{(q+1)/2}|^2.$$

We continue the estimate (5.25) with suitable $\delta > 0$ and $\widetilde{c}(T) > 1$ by

$$\begin{aligned} \|w(t)\|_{L^q}^q &\leq \int_0^t \Big\{ -\delta\|w^{q/2}\|_{H^1}^2 - \frac{\delta}{q}\|w^{(q+1)/2}\|_{H^1}^2 + c(T)q(\|w^{q/2}\|_{L^2}^2 + 1)\\ &\qquad + cq(\|w^{q/2}\|_{L^\sigma} + 1)(\|v_0\|_{L^\pi} + 1)\|\nabla w^{q/2}\|_{L^2}\Big\}\,\mathrm{d}s\\ &\leq \int_0^t -\frac{\delta}{q}\|w^{(q+1)/2}\|_{H^1}^2 + \widetilde{c}(T)q^{2\sigma}\kappa_T(\|w^{q/2}\|_{L^1}^2 + 1)\Big\}\,\mathrm{d}s. \end{aligned} \tag{5.27}$$

Here we used the definition (5.21) and again Gagliardo-Nirenberg's and Young's inequality.

2. With the estimate for values $\theta \in \mathbb{R}_+$ and the function $w \in V_0$

$$\theta\,\|w\|_{L^1}^2 \leq \theta\,c\,\|w\|_{L^{3/2}}^2 = \theta\,c\,\|w^{3/2}\|_{L^1}^{4/3} \leq \theta\,c\,\|w^{3/2}\|_{H^1}^{4/3} \leq \frac{\delta}{2}\|w^{3/2}\|_{H^1}^2 + c\,\theta^3,$$

we now consider the inequality (5.27) for $q = 2$ and get $\|w(t)\|_{L^2}^2 \leq c(T)$ for all $t \in S$. Therefore $\|w(t)\|_{L^1} \leq c\|w(t)\|_{L^2} \leq \overline{c}(T)$ for all $t \in S$.

For arbitrary $q \geq 2$, we exploit (5.27) and omit the first term on the right-hand side to obtain

$$\|w(t)\|^q_{L^q} \leq \widehat{c}(T) q^{2\sigma} \kappa_T (\sup_{s\in S} \|w^{q/2}(s)\|^2_{L^1} + 1). \tag{5.28}$$

3. Setting $q = 2^m$, $m \geq 0$, and $\omega_m := \sup_{t\in S} \|w(t)\|^{2^m}_{L^{2^m}} + 1$ we find $\omega_m \leq \widetilde{c}^m\, 2\widehat{c}(T)\kappa_T \omega^2_{m-1}$, $\widetilde{c} := 2^{2\sigma}$, and repeated application gives $\omega_m \leq (\widetilde{c}\, 2\widehat{c}(T)\kappa_T \omega_0)^{2^m}$ which means

$$\sup_{t\in S} \|w(t)\|_{L^{2^m}} \leq \widetilde{c}\, 2\widehat{c}(T)\kappa_T (\sup_{t\in S} \|w(t)\|_{L^1} + 1).$$

For the limit $m \to \infty$, we derive

$$\sup_{s\in S} \|w(t)\|_{L^\infty} \leq \widetilde{c}\, 2\widehat{c}(T)\kappa_T (\sup_{t\in S} \|w(t)\|_{L^1} + 1) \quad \forall t \in S.$$

Together with $\sup_{t\in S} \|w(t)\|_{L^1} \leq \overline{c}(T)$ we obtain $\|w(t)\|_{L^\infty} \leq 2\widetilde{c}\,\widehat{c}(T)\kappa_T(\overline{c}(T)+1)$ for all $t \in S$. Finally, this ensures for all $t \in S$

$$-\ln \frac{u_n(t)}{N_n} \leq K + 2\widetilde{c}\,\widehat{c}(T)\kappa_T(\overline{c}(T)+1), \quad c_1(T) := \underline{N} \mathrm{e}^{-K-2\widetilde{c}\,\widehat{c}(T)\kappa_T(\overline{c}(T)+1)} \leq u_n(t) \quad \text{a.e. in } \Omega.$$

4. The lower estimate for u_p follows exactly the same technique as presented for u_n. For u_i, $i \in I_0$ we use the test function with the i-th component $-q\frac{w^{q-1}}{u_i/N_i} \in L^2(S, V_0)$, $q \geq 2$, $w := \big(\ln u_i/N_i + K\big)^-$. All other components are zero. In contrast to the situation for u_n and u_p, here no parts coming from the generation-recombination of electrons and holes appear, but

$$\int_{\Omega_0} q(z_i\varphi_i - d_M(z_i v_0) - d_M(v_i)) \frac{w^{q-1}}{u_i/N_i}\, \mathrm{d}x = \int_{\Omega_0} q(z_i v_0 + v_i - d_M(z_i v_0) - d_M(v_i)) \frac{w^{q-1}}{u_i/N_i}\, \mathrm{d}x$$

has to be estimated on the right hand side. Our choice of M guarantees that $d_M(z_i v_0) = z_i v_0$ a.e. in Ω_0 for all $t \in S$. Therefore the last integral reduces to $\int_{\Omega_0} q(v_i - d_M(v_i))\frac{w^{q-1}}{u_i/N_i}\, \mathrm{d}x$ which is non-positive and can be neglected in the estimate. Note that our choice of K ensures that $v_i \leq 0$ in case that $w \neq 0$. The drift term is estimated as for electrons and holes using the expression κ_T such that we can proceed as in estimate (5.27) and follow the Steps 2 and 3 of the present proof. □

After obtaining the positive lower bound for u_i we are able to verify a suited upper bound for u_i less than N_i, $i \in I_0$, by choosing powers of the function $(\mathrm{e}^{v_i} - K)^+$, $i \in I_0$, for a Moser iteration technique (see Lemma 5.7).

Lemma 5.7 *We assume* (A1) – (A4)*. Let* $M \geq \max\{M^*, \max_{i\in I_0} |z_i| c^*(1 + 2c_0(T)|\Omega|^{1/2}\}$ *with* M^* *as in* (5.1)*,* c^* *from Lemma 5.3 and* $c_0(T)$ *from Lemma 5.5. Then, there exists a constant* c_2*,* $0 < c_2(T) < 1$*, depending only on the data (but not on* M*) such that for any solution* (u, v) *to* ($\mathrm{P_M}$)

$$u_i(t) \leq c_2(T) N_i \quad \textit{a.e. in } \Omega_0, \quad \forall t \in S, \quad i \in I_0.$$

Proof. 1. For the derivation of upper bounds for the density u_i strictly lower than N_i, $i \in I_0$, we verify a finite upper bound for the potential v_i, more precisely, for e^{v_i}. This is recommendable, since for test functions of the form

$$\frac{q\left[(\mathrm{e}^{v_i} - K)^+\right]^{q-1} \mathrm{e}^{v_i}}{e_i'(v_i)} \tag{5.29}$$

in a corresponding Moser iteration, all terms arising from the test of the continuity equation for u_i can be handled. Here the estimates in (2.6) play an important role. They ensure for $v_i > -\zeta_i$ the inequalities

$$\mathrm{e}^{\zeta_i} \leq \frac{1}{\mathrm{e}^{v_i} e_i'(v_i)} \leq c\mathrm{e}^{\zeta_i}, \quad \frac{|e_i''(v_i)|}{e_i'(v_i)} < 1, \quad e_i''(v_i) < 0. \tag{5.30}$$

However, we cannot use the function in (5.29) directly since it is not a priori clear that it belongs to $L^2(S, V_0)$. We have to approximate it by substituting v_i in (5.29) by $v_L := \min(v_i, L)$ for L large enough and considering the limit $L \to \infty$ in the resulting estimates.

2. Let (u, v) be a solution to ($\mathrm{P_M}$). We set $K := \max_{i\in I_0} \max\{\mathrm{e}^{\|e_i^{-1}(u_i^0/N_i)\|_{L^\infty(\Omega_0)}}, \mathrm{e}^{-\zeta_i}, 1\}$. Let $i \in I_0$ be arbitrarily fixed and $L > \ln K > 0$, $v_L := \min(v_i, L)$, $\widetilde{L} := N_i e_i(L)$, and $u_{\widetilde{L}} := \min(u_i, \widetilde{L})$. We use the test function with the i-th component

$$qW_L(v_i) := q\frac{w_L^{q-1}\mathrm{e}^{v_L}}{e_i'(v_L)}, \quad q \geq 2, \quad w_L := \big(\mathrm{e}^{v_L} - K\big)^+. \tag{5.31}$$

All other components are set to zero. Since $e_i'(y) > 0$ for all y and $\mathcal{F}_i''(\eta) < 0$ for all $\eta \geq 0$, we obtain $e_i'(v_L) \geq c(L) > 0$ for $v_i \geq \ln K$. Moreover, $\mathrm{e}^{v_L} < \widetilde{c}(L)$. (5.30) ensures an upper bound for $|e_i''(v_L)|$. Thus we find an estimate for

$$\nabla W_L(v_i) = \Big\{\frac{(q-1)[(\mathrm{e}^{v_L} - K)^+]^{q-2}\mathrm{e}^{2v_L}}{e_i'(v_L)} + \frac{[(\mathrm{e}^{v_L} - K)^+]^{q-1}\mathrm{e}^{v_L}}{e_i'(v_L)} - \frac{[(\mathrm{e}^{v_L} - K)^+]^{q-1}\mathrm{e}^{v_L}e_i''(v_L)}{(e_i'(v_L))^2}\Big\}\nabla v_i \; \chi_{\{x:\ln K \leq v_i \leq L\}}$$

such that $W_L(v_i) \in L^2(S, V_0)$ and (5.31) is an admissible test function. Moreover, our choice of K guarantees that $w_L(0) = 0$. Next, we rewrite

$$W_L(v_i) = \frac{[(\mathrm{e}^{e_i^{-1}(u_{\widetilde{L}})} - K)^+]^{q-1}\mathrm{e}^{e_i^{-1}(u_{\widetilde{L}})}}{e_i'(e_i^{-1}(u_{\widetilde{L}}))} =: \widetilde{u}_{\widetilde{L}}$$

and obtain

$$\int_0^t q\langle u_i', \widetilde{u}_{\widetilde{L}}\rangle_{V_0}\,\mathrm{d}s = \int_\Omega \big(g(u_i(t)) - g(u_i^0)\big)\,\mathrm{d}x, \tag{5.32}$$

where

$$g(y) := \int_0^y \frac{[(\mathrm{e}^{e_i^{-1}(\min(\tau,\widetilde{L}))} - K)^+]^{q-1}\mathrm{e}^{e_i^{-1}(\min(\tau,\widetilde{L}))}}{e_i'(e_i^{-1}(\min(\tau,\widetilde{L})))}\,\mathrm{d}\tau.$$

The validity of (5.32) is clear for smooth $u_i \in H^1(S, L^2)$. For general u_i the validity of this relation is obtained via approximation by smooth functions and passing to the limit. Note that due to the choice of K we have $g(u_i^0) = 0$. Additionally, we have the lower estimate

$$\begin{aligned} g(u_i) \geq g(\min(u_i, \widetilde{L})) = g(u_{\widetilde{L}}) &= \int_0^{\min(u_i,\widetilde{L})} \frac{[(\mathrm{e}^{e_i^{-1}(\min(\tau,\widetilde{L}))} - K)^+]^{q-1}\mathrm{e}^{e_i^{-1}(\min(\tau,\widetilde{L}))}}{e_i'(e_i^{-1}(\min(\tau,\widetilde{L})))}\,\mathrm{d}\tau \\ &= [(\mathrm{e}^{e_i^{-1}(\min(u_i,\widetilde{L}))} - K)^+]^q = [(\mathrm{e}^{\min(v_i,L)} - K)^+]^q = [(\mathrm{e}^{v_L} - K)^+]^q = w_L^q. \end{aligned}$$

3. The term resulting from the regularization

$$\begin{aligned} &\int_{\Omega_0} (d_M(z_i v_0) + d_M(v_i) - z_i\varphi_i)\frac{qw_L^{q-1}\mathrm{e}^{v_L}}{e_i'(v_L)}\,\mathrm{d}x \\ &\qquad = \int_{\Omega_0} (d_M(z_i v_0) + d_M(v_i) - z_i v_0 - v_i)\frac{qw_L^{q-1}\mathrm{e}^{v_L}}{e_i'(v_L)}\,\mathrm{d}x \end{aligned}$$

has to be estimated on the right hand side. Our choice of M guarantees that $d_M(z_i v_0) = z_i v_0$ a.e. in Ω_0 for all $t \in S$. Therefore the last term reduces to $\int_{\Omega_0} q(d_M(v_i) - v_i)\frac{w_L^{q-1} \mathrm{e}^{v_L}}{e_i'(v_L)}\,\mathrm{d}x$ which is non-positive (note that $w_L = 0$ for $v_i < 0$), and will be neglected.

4. Using the test function (5.31) and the relation (5.32), the estimate for the function g, and Step 3, it follows that

$$\begin{aligned}
\|w_L(t)\|^q_{L^q(\Omega_0)} &\leq -\int_0^t q \int_{\Omega_0} \mu_i u_i \nabla(v_i - z_i v_0) \cdot \nabla\Big(\frac{w_L^{q-1}\mathrm{e}^{v_L}}{e_i'(v_L)}\Big)\,\mathrm{d}x\,\mathrm{d}s \\
&= -\int_0^t q \int_{\Omega_0} \mu_i \big\{u_i\big(\Theta_1 + \Theta_2 + \Theta_3 + \Theta_4 + \Theta_5 + \Theta_6\big)\big\}\,\mathrm{d}x\,\mathrm{d}s,
\end{aligned} \tag{5.33}$$

where the terms Θ_i, $i = 1, \dots, 6$, are defined and estimated separately. Since here all spatial integrals are with respect to Ω_0, we will leave this out in the notation of the estimated norms in the rest of the poof. We use the properties $\nabla v_i \cdot \nabla w_L = |\nabla w_L|^2\,\mathrm{e}^{-v_L}$, $w_L < \mathrm{e}^{v_L}$, $\nabla v_i \cdot \nabla v_L = |\nabla v_L|^2$ and the estimates in (5.30) such that

$$\begin{aligned}
\Theta_1 &:= q(q-1)\nabla v_i \cdot \nabla w_L\, w_L^{q-2}\frac{\mathrm{e}^{v_L}}{e_i'(v_L)} \geq q(q-1)|\nabla w_L|^2\, w_L^{q-2}\frac{w_L}{\mathrm{e}^{v_L} e_i'(v_L)} \\
&= q(q-1)|\nabla w_L|^2\, w_L^{q-1}\frac{1}{\mathrm{e}^{v_L} e_i'(v_L)} = \frac{4q(q-1)}{(q+1)^2}\frac{|\nabla w_L^{(q+1)/2}|^2}{\mathrm{e}^{v_L} e_i'(v_L)} \geq c\mathrm{e}^{\zeta_i}|\nabla w_L^{(q+1)/2}|^2, \\
\Theta_2 &:= q|\nabla v_L|^2\, w_L^{q-1}\frac{\mathrm{e}^{v_L}}{e_i'(v_L)} \geq 0, \qquad \Theta_3 := -q\nabla v_i \cdot \nabla v_L\, w_L^{q-1}\frac{\mathrm{e}^{v_L} e_i''(v_L)}{(e_i'(v_L))^2} \geq 0.
\end{aligned}$$

The terms resulting from the drift are estimated as follows

$$\begin{aligned}
\Theta_4 &:= q(q-1)\nabla v_0 \cdot \nabla w_L\, w_L^{q-2}\frac{\mathrm{e}^{v_L}}{e_i'(v_L)} = q(q-1)\nabla v_0 \cdot \nabla w_L\, w_L^{\frac{q-1}{2}}\, w_L^{\frac{q-3}{2}}\,\frac{\mathrm{e}^{v_L}}{e_i'(v_L)} \\
&= \frac{2q(q-1)}{q+1}\nabla v_0 \cdot \nabla(w_L^{\frac{q+1}{2}})w_L^{\frac{q-3}{2}}\,\frac{\mathrm{e}^{v_L}\mathrm{e}^{v_L}}{\mathrm{e}^{v_L} e_i'(v_L)}, \\
|\Theta_4| &\leq cq|\nabla v_0||\nabla w_L^{\frac{q+1}{2}}|\big(|w_L^{\frac{q+1}{2}}| + 1\big)\frac{1}{\mathrm{e}^{v_L} e_i'(v_L)} \leq cq|\nabla v_0||\nabla w_L^{\frac{q+1}{2}}|\big(|w_L^{\frac{q+1}{2}}| + 1\big).
\end{aligned}$$

For the remaining terms Θ_5 and Θ_6, we argue

$$\begin{aligned}
\Theta_5 &:= q\nabla v_0 \cdot \nabla v_L\, w_L^{q-1}\frac{\mathrm{e}^{v_L}}{e_i'(v_L)} = q\nabla v_0 \cdot \nabla w_L w_L^{\frac{q-1}{2}}\, w_L^{\frac{q-1}{2}}\,\frac{\mathrm{e}^{v_L}}{\mathrm{e}^{v_L} e_i'(v_L)}, \\
|\Theta_5| &\leq c|\nabla v_0||\nabla w_L^{(q+1)/2}|\big(|w_L^{\frac{q+1}{2}}| + 1\big)\frac{1}{\mathrm{e}^{v_L} e_i'(v_L)} \leq c|\nabla v_0||\nabla w_L^{(q+1)/2}|\big(|w_L^{\frac{q+1}{2}}| + 1\big), \\
\Theta_6 &:= -q\nabla v_0 \cdot \nabla v_L\, w_L^{q-1}\frac{\mathrm{e}^{v_L} e_i''(v_L)}{(e_i'(v_L))^2} = -q\nabla v_0 \cdot \nabla w_L w_L^{\frac{q-1}{2}}\, w_L^{\frac{q-1}{2}}\,\frac{\mathrm{e}^{v_L}}{\mathrm{e}^{v_L} e_i'(v_L)}\,\frac{e_i''(v_L)}{e_i'(v_L)}, \\
|\Theta_6| &\leq c|\nabla v_0||\nabla w_L^{(q+1)/2}|\big(|w_L^{\frac{q+1}{2}}| + 1\big)\frac{1}{\mathrm{e}^{v_L} e_i'(v_L)}\,\frac{|e_i''(v_L)|}{e_i'(v_L)} \leq c|\nabla v_0||\nabla w_L^{(q+1)/2}|\big(|w_L^{\frac{q+1}{2}}| + 1\big).
\end{aligned}$$

By the estimates for Θ_i, $i = 1, \dots, 6$, $c_1(T) \leq u_i < N_i$ a.e. in Ω_0 (see Lemma 5.6), and (A2), we continue estimate (5.33) and ensure for a suitable $\delta = \delta(T) > 0$ (and π, σ and κ_T from (5.21)) that

$$\begin{aligned} \|w_L(t)\|_{L^q}^q &\le \int_0^t \Big\{ -\delta\|w_L^{\frac{q+1}{2}}\|_{H^1}^2 + cq(\|w_L^{\frac{q+1}{2}}\|_{L^2}^2+1) \\ &\qquad + cq\|\nabla v_0\|_{L^\pi}(\|w_L^{\frac{q+1}{2}}\|_{L^\sigma}+1)\|w_L^{\frac{q+1}{2}}\|_{H^1}\Big\}\,\mathrm{d}s \\ &\le \int_0^t \Big\{ -\frac{\delta}{2}\|w_L^{\frac{q+1}{2}}\|_{H^1}^2 + \widehat{c}q^{2\sigma}\kappa_T(\|w_L^{\frac{q+1}{2}}\|_{L^1}^2+1)\Big\}\,\mathrm{d}s. \end{aligned} \tag{5.34}$$

As in the estimate (5.28) in the proof of Lemma 5.6, we applied Hölder's, Gagliardo-Nirenberg's and Young's inequality, but now for the function $w_L^{\frac{q+1}{2}}$ instead of $w^{\frac{q}{2}}$.

5. Next, we calculate

$$\begin{aligned} \|w_L^{\frac{q+1}{2}}\|_{L^1}^2 &\le \Big(\|w_L^{\frac{q}{4}}\|_{L^2}\|w_L^{\frac{q+2}{4}}\|_{L^2}\Big)^{\frac{4}{q+1}} = \|w_L^{\frac{q}{2}}\|_{L^1}^{\frac{2}{q+1}}\|w_L^{\frac{q+1}{2}}\|_{L^{\frac{q+2}{q+1}}}^{\frac{2(q+2)}{(q+1)^2}} \le \widetilde{c}\|w_L^{\frac{q}{2}}\|_{L^1}^{\frac{2}{q+1}}\|w_L^{\frac{q+1}{2}}\|_{H^1}^{\frac{2(q+2)}{(q+1)^2}} \\ &\le \widetilde{c}\Big(\frac{4\delta\widehat{c}q^{2\sigma}\kappa_T}{4\delta\widehat{c}q^{2\sigma}\kappa_T}\Big)^{\frac{q+2}{(q+1)^2}}\|w_L^{\frac{q}{2}}\|_{L^1}^{\frac{2}{q+1}}\times\|w_L^{\frac{q+1}{2}}\|_{H^1}^{\frac{2(q+2)}{(q+1)^2}} \\ &\le \frac{\delta}{4}\frac{1}{\widehat{c}q^{2\sigma}\kappa_T}\|w_L^{\frac{q+1}{2}}\|_{H^1}^2 + \widetilde{c}^{\frac{(q+1)^2}{q^2+q-1}}\Big(\frac{4\widehat{c}q^{2\sigma}\kappa_T}{\delta}\Big)^{\frac{q+2}{q^2+q-1}}\|w_L^{\frac{w}{2}}\|_{L^1}^{\frac{2(q+1)}{q^2+q-1}} \\ &\le \frac{\delta}{4}\frac{1}{\widehat{c}q^{2\sigma}\kappa_T}\|w_L^{\frac{q+1}{2}}\|_{H^1}^2 + \widetilde{c}^{\frac{(q+1)^2}{q^2+q-1}}\Big(\frac{4\widehat{c}q^{2\sigma}\kappa_T}{\delta}\Big)^{\frac{q+2}{q^2+q-1}}(\|w_L^{\frac{q}{2}}\|_{L^1}^2+1). \end{aligned}$$

Inserting this estimate in (5.34) we find for a suitable $c_\delta > 1$ that

$$\begin{aligned} \|w_L(t)\|_{L^q}^q &\le \int_0^t \Big\{-\tfrac{\delta}{4}\|w_L^{\frac{q+1}{2}}\|_{H^1}^2 + \widetilde{c}^{\frac{(q+1)^2}{q^2+q-1}}\Big(\frac{4}{\delta}\Big)^{\frac{q+2}{q^2+q-1}}\Big(\widehat{c}q^{2\sigma}\kappa_T\Big)^{1+\frac{(q+1)^2}{q^2+q-1}}(\|w_L^{\frac{q}{2}}\|_{L^1}^2+1)\Big\}\,\mathrm{d}s \\ &\le \int_0^t\Big\{-\tfrac{\delta}{4}\|w_L^{\frac{q+1}{2}}\|_{H^1}^2 + c_\delta q^{6\sigma}(\|w_L^{\frac{q}{2}}\|_{L^1}^2+1)\Big\}\,\mathrm{d}s \qquad \forall t\in S. \end{aligned} \tag{5.35}$$

6. As in Step 2 of the proof of Lemma 5.6, we have for arbitrary $\theta \in \mathbb{R}_+$ that $\theta\,\|w_L\|_{L^1}^2 \le \frac{\delta}{2}\|w_L^{3/2}\|_{H^1}^2 + c\,\theta^3$. Inserting this in estimate (5.35) for $q=2$ we establish that $\|w_L(t)\|_{L^2} \le c(T)$ for all $t \in S$ and therefore also $\sup_{t\in S}\|w_L(t)\|_{L^1} \le c(T)$. Moreover, for arbitrary $q \ge 2$, it follows from (5.35) that

$$\|w_L(t)\|_{L^q}^q \le c_\delta q^{6\sigma-1}T\big(\sup_{s\in S}\|w_L^{\frac{q}{2}}(s)\|_{L^1}^2+1\big). \tag{5.36}$$

7. Defining

$$\omega_m = \sup_{s\in S}\|w_L(s)\|_{L^{2^m}}^{2^m}+1, \quad m = 0,1,2,\ldots$$

we find from (5.36) for $q = 2^m$, $m \ge 1$, and $\overline{c} := c_\delta T\,2^{6\sigma}$ that $\omega_m \le \overline{c}^m\omega_{m-1}^2$ and repeated application gives $\omega_m \le (\overline{c}\,\omega_0)^{2^m}$ which means $\|w_L(t)\|_{L^{2^m}} \le \overline{c}\,(\sup_{s\in S}\|w_L(s)\|_{L^1}+1)$, and leads in the limit $m\to\infty$ to

$$\|w_L(t)\|_{L^\infty} \le \overline{c}\,(\sup_{s\in S}\|w_L(s)\|_{L^1}+1) \quad \forall t\in S. \tag{5.37}$$

With $\sup_{t\in S}\|w_L(t)\|_{L^1} \le c(T)$ (see Step 6), (5.37) ensures that $\|w_L(t)\|_{L^\infty} \le c_\infty(T)$ for all $t\in S$.

8. Since the constant $c_\infty(T)$ does not depend on the choice of L, we can pass to the limit $L\to\infty$ in this estimate and derive $\|\big(\mathrm{e}^{v_i}-K\big)^+(t)\|_{L^\infty} \le c_\infty(T)$ and $\mathrm{e}^{v_i(t)} \le K + c_\infty(T)$,

$$v_i(t) \le \ln\big(K+c_\infty(T)\big), \quad \frac{u_i(t)}{N_i} \le e_i\big(\ln(K+c_\infty(T))\big) =: c_2(T) < 1 \quad \forall t\in S. \quad \square$$

5.3 Solvability of Problem (P)

Theorem 5.1 *We assume* (A1) – (A4)*. Then, for all* $T > 0$*,* $S = [0, T]$*, there exists a solution to Problem* ($\mathrm{P_S}$)*.*

Proof. For arbitrarily chosen $T > 0$, $S = [0, T]$ Problem ($\mathrm{P_M}$) has a solution, see Lemma 5.2. The a priori estimates for solutions to ($\mathrm{P_M}$) in Lemma 5.3, Lemma 5.5, Lemma 5.6 and Lemma 5.7 ensure that for $M \geq \max\{M^*, \max_{i\in I_0} |z_i|c^*(1 + 2c_0(T)|\Omega|^{1/2}\}$ (with M^* as in (5.1), c^* from Lemma 5.3 and $c_0(T)$ from Lemma 5.5) being sufficiently large (compare Remark 5.1, depending on T) namely

$$M \geq \max\Big\{ \max_{i\in I} |z_i|c^*(1 + 2c_0(T)|\Omega|^{1/2}), 2\max_{i=n,p} \big|e_i^{-1}\big(\tfrac{c_1(T)}{\overline{N}}\big)\big|, 2\max_{i=n,p} \big|e_i^{-1}\big(\tfrac{c_0(T)}{\underline{N}}\big)\big|,$$
$$\max_{i\in I_0} \big|e_i^{-1}\big(\tfrac{c_1(T)}{\overline{N}}\big)\big|, \max_{i\in I_0} \big|e_i^{-1}\big(c_2(T)\big)\big|\Big\}$$

every solution (u, v) to ($\mathrm{P_M}$) satisfies the equalities $d_M(v_i) = v_i$ for $i \in I$, $d_M(z_iv_0) = z_iv_0$ for $i \in I_0$. Since $\rho_M(v) = 1$, the reaction terms in $A_M(v, v)$ and $A(v, v)$ coincide. Moreover, the regularization terms $z_i\varphi_i - d_M(z_iv_0) - d_M(v_i)$ in the equations for the ionic vacancies disappear, and we have $E_M(v) = E(v)$, $A_M(v, v) = A(v, v)$ and the pair (u, v) is a solution to Problem ($\mathrm{P_S}$), too. □

5.4 Bounds for solutions to ($\mathrm{P_S}$)

Theorem 5.2 *We assume* (A1) – (A4)*. Then, for all* $T > 0$*,* $S = [0, T]$ *there exist* $c_0(T)$*,* $c_1(T)$*,* $c_2(T) > 0$ *with* $c_2(T) < 1$ *such that for any solution* (u, v) *to Problem* ($\mathrm{P_S}$) *and for all* $t \in S$

$$c_1(T) \leq u_i(t) \leq c_0(T) \quad \textit{a.e. in } \Omega,\ i = n, p, \quad c_1(T) \leq u_i(t) \leq c_2(T)N_i \quad \textit{a.e. in } \Omega_0,\ i \in I_0.$$

Proof. Let (u, v) be a solution to ($\mathrm{P_S}$). Theorem 4.1 and (4.7) ensure $\|v_0(t) - v_0^D\|^2_{H^1(\Omega)}$, $\|u_i(t)\|_{L^1(\Omega_i)}$ $\leq c(T)$ for all $t \in S$, $i \in I$. The estimates in the second line of Lemma 5.3 and the result of Lemma 5.4 remain also true for solutions (u, v) to ($\mathrm{P_S}$). For the upper bounds of u_n and u_p we argue exactly as in the proof of Lemma 5.5. Note that the estimate of the reaction term in Step 2 there works also in the non-regularized setting for ($\mathrm{P_S}$) without the factor ρ_M. Especially we again work with κ_T defined in (5.21) and do the Moser iteration technique.

To establish the positive lower bounds of u_i we proceed as in Lemma 5.6 and use also in the non-regularized setting for ($\mathrm{P_S}$) the inequality (5.24). Since in Step 4 of the proof of Lemma 5.6 the part stemming from the regularization term $z_i\varphi_i - d_M(z_iv_0) - d_M(v_i)$, $i \in I_0$, is only neglected and not explicitly used in the estimates, we can for ($\mathrm{P_S}$) exactly argue as in the proof of Lemma 5.6 to get the lower bound of u_i.

Finally, the upper bound for u_i, $i \in I_0$, is obtained following the lines of the proof of Lemma 5.7. Note that again, the part with the regularization term for ($\mathrm{P_M}$) is only neglected and not explicitly used in the estimates. □

Remark 5.2 *Using the global positive lower bounds for the charge carrier densities of solutions to* ($\mathrm{P_S}$) *established in Theorem 5.2 and the energy estimates performed in* (4.8) *in the proof of Theorem 4.1 we obtain the estimates* $\|\varphi_i\|_{L^2(S,H^1(\Omega_i))} \leq c(T)$*,* $i \in I$*, and* $\|v_0\|_{L^2(S,H^1(\Omega))} \leq c(T)$*. The relations of* φ_i *and* v_i *ensure the estimates* $\|v_i\|_{L^2(S,H^1(\Omega_i))} \leq c(T)$*,* $i \in I$*. Furthermore, the bounds of* u_i *from Theorem 5.2 and* $u_i = N_ie_i(v_i)$ *guarantee* L^∞ *bounds for* v_i*,* $i \in I$*, which lead to the estimates for the whole vectors*

$$\|A(v, v)\|_{L^2(S,V^*)},\ \|u'\|_{L^2(S,V^*)} \leq c(T).$$

6 Concluding remarks

We examined the drift-diffusion model introduced in [2] for the charge transport in perovskite solar cells, which includes the dynamics of multiple mobile ionic vacancies. We started by conducting simulations to underline the importance of including additional migrating vacancies from an application perspective. Furthermore, we demonstrated the existence of weak solutions to the problem and established positive lower and upper bounds for the densities depending on the length of the time interval $S = [0, T]$. The question of uniqueness of the solution to Problem (P) is still under consideration and rests upon higher regularity properties of the possible solutions.

In case of organic transport layer materials such as fullerene C_{60} (see [28]), Gauss-Fermi integrals have to be used for the statistical relation. According to [17, Subsec. 2.1], the Gauss-Fermi integrals satisfy similar essential properties as Blakemore statistics $F_{B,\gamma}$ for $\gamma = 1$ (cf. (2.5)) used in the presentation here. The methodologies for establishing positive lower and upper bounds on the number of transport states for charge carrier densities in organic semiconductor materials are elucidated in [17, proofs of Lemma 4.3, Thm. 5.2]. Note that Gauss-Fermi integrals can also be approximated by Blakemore statistics $F_{B,\gamma}$ for $\gamma = 0.27$.

In our model, we considered not only the movement of electrons and holes throughout the entire domain Ω but also accounted for the migration of ionic vacancies within a specific subdomain Ω_0, representing the perovskite material. It is noteworthy that the methods employed in our existence proof are versatile enough to accommodate scenarios involving distinct mobile ionic vacancies residing in various subdomains $\Omega_i \subset \Omega$, where $i \in I_0$. Furthermore, the scenario with $\Omega_i = \Omega$ for $i \in I_0$ is a valid configuration and encompasses the conditions observed in the study of memristive devices detailed in [19]. Therein, only one type of ionic species is considered, which is crucial for the analytical treatment of the model. The assumption includes applying Boltzmann statistics uniformly to all species, without the inclusion of generation/recombination terms and a photo-generation rate. The drift-diffusion system is analyzed in three spatial dimensions. Moreover, the model considers the distinct time scales associated with the motion of electrons/holes and ions, and it incorporates the fast-relaxation limit in two spatial dimensions.

A Properties of the statistics functions

Fermi–Dirac statistic $F_{1/2}$: The last two estimates in (2.4) follow from the inequalities

$$\frac{F_{1/2}(z)}{\mathrm{e}^z} = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2}}{\mathrm{e}^\xi + \mathrm{e}^z}\, \mathrm{d}\xi < \int_0^\infty \xi^{1/2} \mathrm{e}^{-\xi}\, \mathrm{d}\xi = 1,$$

$$(F_{1/2})'(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2} \exp(\xi - z)}{(\exp(\xi - z) + 1)^2}\, \mathrm{d}\xi \leq \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\xi^{1/2}}{\exp(\xi - z) + 1}\, \mathrm{d}\xi = F_{1/2}(z).$$

For the limit $z \to -\infty$, the value $F_{1/2}(z)$ decreases as e^z. In turn, for the limit $z \to +\infty$, the value $F_{1/2}(z)$ then increases as $\frac{4}{3\sqrt{\pi}} z^{3/2}$, see [4].

Fermi–Dirac statistic F_{-1}: To verify (ii) of (2.6), we estimate

$$\begin{aligned} F'_{-1}(z) &= \left[\frac{1}{\mathrm{e}^{-z} + 1}\right]' = \frac{\mathrm{e}^{-z}}{(\mathrm{e}^{-z} + 1)^2} = \frac{\mathrm{e}^{-z}}{\mathrm{e}^{-2z} + 2\mathrm{e}^{-z} + 1} \\ &< \frac{\mathrm{e}^{-z}}{\mathrm{e}^{-2z} + 2\mathrm{e}^{-z}} = \frac{1}{\mathrm{e}^{-z} + 2} < \frac{1}{\mathrm{e}^{-z} + 1} = F_{-1}(z) = \frac{\mathrm{e}^z}{1 + \mathrm{e}^z} < \mathrm{e}^z. \end{aligned}$$

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