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A coarse-grained electrothermal model for organic semiconductor devices

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Abstract

We derive a coarse-grained model for the electrothermal interaction of organic semiconductors. The model combines stationary drift-diffusion based electrothermal models with thermistor type models on subregions of the device and suitable transmission conditions. Moreover, we prove existence of a solution using a regularization argument and Schauder's fixed point theorem. In doing so, we extend recent work by taking into account the statistical relation given by the Gauss–Fermi integral and mobility functions depending on the temperature, charge-carrier density, and field strength, which is required for a proper description of organic devices.

1 Introduction

Charge transport in organic semiconductors can be modeled at very different scales, ranging from density functional theory for molecules, master equation approaches for carrier dynamics to drift-diffusion equations (see e.g. [19]). Transport properties in these materials are heavily influenced by temperature leading to self-heating effects which in turn have a strong impact on the performance of the device e.g., organic solar cells and transistors [26, 17]. Moreover, self-heating effects can lead to nonlinear phenomena like S-shaped current-voltage relations with regions of negative differential resistance. Furthermore, the interplay of self-heating and temperature activated hopping transport in combination with heat flow results in spatially inhomogeneous current flow and temperature distribution in large-area organic light emitting diodes [6, 5]. Therefore, we require models and simulations of the electrothermal interplay in multidimensional organic devices that are as accurate as necessary but computationally efficient. The idea is to derive a coarse-grained model that combines models for substructures with different model complexity. Such modeling approaches have already been used for inorganic semiconductor devices without taking into account the coupling to the heat flow, e.g., in [18, 25, 7].

Starting from a stationary drift-diffusion based electrothermal model (see (2.1)–(2.4)) for organic semiconductors introduced in [13], we construct a coarse-grained model that retains the strong coupling of the electrothermal effects but takes into account different depth in the characterization of the current flow. The model results from combining a drift-diffusion system in critical device subregions with coarser thermistor-like models that are limiting cases of the former for vanishing electron or hole densities for device substructures with highly n-doped or highly p-doped regions. Thus, we arrive at an effective model with different complexity and coupling interface conditions among the subregions.

The present paper deals with two tasks: First, we construct a coarse-grained model for the electrothermal behavior of organic semiconductors by applying coarser models in subregions which reduces the number of coupled equations. Hence, the full drift-diffusion model is applied only in the electronically relevant subregions of the device. In particular, the coarser, thermistor type models used for subregions of the device contain an equation for the net current flow coupled to the heat equation, namely

$$\begin{aligned} -\nabla\cdot(\widetilde{\sigma}(T,\nabla T,\nabla\varphi)\nabla\varphi) &= 0, \\ -\nabla\cdot(\lambda\nabla T) &= \widetilde{\sigma}(T,\nabla T,\nabla\varphi)|\nabla\varphi|^2, \end{aligned} \tag{1.1}$$

with an effective electrical conductivity function $\widetilde{\sigma}$ depending on the temperature and the gradients of temperature and potential.

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Second, we study analytical properties of this model concerning existence, boundedness and regularity of solutions. The key idea of this modeling approach is to use for device regions with doping of only one charge carrier type (e.g. near to contacts) a coarser description by a thermistor model combining heat flow and a simpler model for the current flow. The more detailed electrothermal drift-diffusion model is restricted to electronically relevant subregions where one balances electron and hole currents and generation/recombination processes. The decomposition of the semiconductor device into different subregions where different models are applied, requires transfer conditions at the interfaces among these different subregions to guarantee the continuity of the total current in the normal direction to the interface. Additionally, we have to ensure that at the interface between the n-doped (p-doped) subregions and the subregions where a full drift-diffusion type model is applied, the normal component of the electron (hole) current density as well as the electrochemical potentials of electrons (holes) are continuous. Moreover, we have to prescribe Dirichlet values for the Poisson equation at the interface to the drift-diffusion subregion. To ensure the required regularity of the Dirichlet function (see (2.18)), we restrict ourselves to two spatial dimensions.

A similar derivation was carried out in [12] for classical semiconductors under the assumption of Boltzmann statistics. In the organic setting, considered in the present paper, the mobility functions are temperature, density, and electric field strength dependent functions. Moreover, we have to take into consideration the special statistical relation given by Gauss–Fermi integrals, where its inverse cannot be given explicitly. Thus, in all derivations only qualitative properties of functions related to $\mathcal{G}$ can be used.

In Section 2, we introduce the considered coarse-grained model for the electrothermal behavior of organic semiconductor devices, formulate our assumptions and give our concept of solutions. Section 3 contains our main analytical results concerning a priori estimates (Theorem 3.1) and existence of weak solutions (Theorem 3.2). The proof of Theorem 3.2 is realized by regularization and Schauder's fixed point theorem in Section 4. Finally, we give an overview on properties related to Gauss–Fermi integrals in the Appendix.

2 Derivation of the coarse-grained model

If Ω denotes the domain of the device, the drift-diffusion model introduced in [13] (see also [3, 8]) that describes the interplay between electronic and heat transport in organic semiconductors is the following,

$$\begin{aligned} -\nabla\cdot(\varepsilon\nabla\psi) &= C-n+p,\\ -\nabla\cdot j_n &= -R,\ \ j_n=-n\mu_n\nabla\varphi_n,\\ \nabla\cdot j_p &= -R,\ \ j_p=-p\mu_p\nabla\varphi_p,\\ -\nabla\cdot(\lambda\nabla T) &= n\mu_n|\nabla\varphi_n|^2+p\mu_p|\nabla\varphi_p|^2+R(\varphi_p-\varphi_n). \end{aligned} \tag{2.1}$$

Here ψ denotes the electrostatic potential, φ_n, φ_p are the electrochemical potentials, T is the temperature, ε is the dielectric permittivity, $C := N_D^+ - N_A^-$ represents the charged donor and acceptor densities, respectively, and λ is the thermal conductivity. For organic materials, the mobilities of electrons $\mu_n = \mu_n(T, n, |\nabla\psi|)$ and holes $\mu_p = \mu_p(T, p, |\nabla\psi|)$ are considered to be temperature, density and electric field strength dependent functions, see e.g. [24, 19]. The chemical potentials are defined by $v_n := \psi - \varphi_n$ and $v_p := -(\psi - \varphi_p)$, the generation/recombination term R and the charge carrier densities n and p are given by,

$$\begin{aligned} R &= r_0(\cdot,n,p,T)\,n\,p\,\Big(1-\exp\frac{\varphi_n-\varphi_p}{T}\Big) = r_0(\cdot,n,p,T)\,n\,p\,\Big(1-\exp\frac{v_n+v_p}{T}\Big),\\ n &= N_{n0}\mathcal{G}\Big(\frac{\psi-\varphi_n+E_n}{T};\frac{\sigma_n}{T}\Big) = N_{n0}\mathcal{G}\Big(\frac{v_n+E_n}{T};\frac{\sigma_n}{T}\Big),\\ p &= N_{p0}\mathcal{G}\Big(\frac{E_p-(\psi-\varphi_p)}{T};\frac{\sigma_p}{T}\Big) = N_{p0}\mathcal{G}\Big(\frac{v_p+E_p}{T};\frac{\sigma_p}{T}\Big), \end{aligned} \tag{2.2}$$

with energy levels $E_n = -E_{\mathrm{LUMO}}$, $E_p = E_{\mathrm{HOMO}}$ related to the so called LUMO and HOMO energies (see e.g. [4]), the total densities of transport states N_{n0}, N_{p0} and the disorder parameters σ_n, σ_p. These parameters are only weakly temperature dependent, and we neglect for simplicity this temperature dependence. The function $\mathcal{G}$ results from the Gauss–Fermi integral

$$\mathcal{G}(\eta, z) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big(-\frac{\xi^2}{2}\Big) \frac{1}{\exp(z\xi - \eta) + 1} \,\mathrm{d}\xi, \tag{2.3}$$

see [23]. Properties of the function $\mathcal{G}$ needed for the analysis in this paper are collected or proven in Appendix A. The system (2.1), (2.2) is completed by mixed boundary conditions on $\Gamma := \partial\Omega$ for the drift-diffusion system and by Robin boundary conditions for the heat flow equation,

$$\begin{aligned} \psi = \psi^D, \quad \varphi_n = \varphi_n^D, \quad \varphi_p = \varphi_p^D \quad &\text{on } \Gamma_D, \\ \varepsilon\nabla\psi\cdot\nu = j_n\cdot\nu = j_p\cdot\nu = 0 \quad &\text{on } \Gamma_N, \\ \lambda\nabla T\cdot\nu + \kappa(T - T_a) = 0 \quad &\text{on } \partial\Omega, \end{aligned} \tag{2.4}$$

where Γ_D and Γ_N denote the Dirichlet and Neumann boundary parts, respectively, ν is the outer unit normal, and T_a is the ambient temperature.

Equations (2.1), (2.2), and (2.4) are already written in scaled form. A similar scaled model frame was used in [14] for classical inorganic semiconductors. In this model, thermoelectric effects (Peltier, Thomson, and Seebeck) are not included. Note that in [20, Sect. II.D] it is argued that in the case of organic semiconductors such effects are negligible as the thermal voltages are small compared to the applied voltage. For fully thermodynamically designed energy models for inorganic semiconductors including all these effects we refer e.g. to [1, 2, 16, 21], where [2, 16] discuss also numerical aspects.

The models (1.1) as well as (2.1) have heat source terms in the heat flow equation that are always nonnegative. This fact together with the Robin boundary conditions enforces that the temperature for solutions to the model equations (1.1), resp. (2.1), (2.4) has to fulfill $T \geq T_a$. A corresponding property the coarse-grained model retains.

2.1 Model reduction for strongly n–doped regions

In order to derive the coarser model, we assume that the energy levels E_i, the densities of transport states N_{i0} as well as the charged doping densities $\delta_n := N_D^+$, $\delta_p := N_A^-$ are spatially constant and that $\delta_i < N_{i0}$ for $i = n, p$. For illustrative purposes, we derive the coarser model for a strongly n-doped region, where the hole density is negligible with the opposite case running analogously.

We consider the limit $p \to 0$ for the model equations (2.1), (2.4) with the quantities $\nabla\varphi_p$, $\nabla\varphi_n$, ψ, $\nabla\psi$, v_n, n, T, and ∇T remaining bounded. We find $\frac{v_p}{T} \to -\infty$ using that $p = N_{p0}\mathcal{G}((v_p + E_p)/T; \sigma_p/T)$, $T \geq T_a$, and E_p is constant. Moreover, we have as a consequence,

$$\begin{aligned} &v_p \to -\infty, \quad p\mu_p\nabla\varphi_p \to 0, \quad p\mu_p|\nabla\varphi_p|^2 \to 0, \\ &R = npr_0(1 - \mathrm{e}^{\frac{v_n+v_p}{T}}) \to 0, \quad R(v_n + v_p) = npr_0(1 - \mathrm{e}^{\frac{v_n+v_p}{T}})(v_n + v_p) \to 0. \end{aligned} \tag{2.5}$$

For the last convergence, we have additionally to verify that $pv_p = \mathcal{G}((v_p + E_p)/T; \sigma_p/T)v_p \to 0$ which is obtained by the following steps: The boundedness of T ensures for $z > 0$ that

$$\lim_{\frac{v_p}{T}\to-\infty} \mathcal{G}\Big(\frac{v_p + E_p}{T}; z\Big)\frac{E_p}{T} = 0.$$

Next, we show that $\lim_{y\to-\infty} \mathcal{G}(y; z)y = 0$ for arguments $y < 0$ and $z > 0$. Since

$$\begin{aligned} 0 \geq \sqrt{2\pi}\mathcal{G}(y; z)y &= \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{\xi^2}{2}} \frac{y}{\mathrm{e}^{z\xi - y} + 1} \,\mathrm{d}\xi = \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{\xi^2}{2}} \frac{y\mathrm{e}^y}{\mathrm{e}^{z\xi} + \mathrm{e}^y} \,\mathrm{d}\xi > y\mathrm{e}^y \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{\xi^2}{2}}\mathrm{e}^{-z\xi} \,\mathrm{d}\xi \\ &= y\mathrm{e}^y \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}(\xi+z)^2 + \frac{z^2}{2}} \,\mathrm{d}\xi = y\mathrm{e}^y\mathrm{e}^{\frac{z^2}{2}} \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}(\xi+z)^2} \,\mathrm{d}\xi = y\mathrm{e}^y \,\text{const}, \end{aligned}$$

we find that, $0 \geq \lim_{y \to -\infty} \mathcal{G}(y;z)y \geq \lim_{y\to-\infty} y\mathrm{e}^y$ const $= 0$. In the case of Gauss–Fermi statistics we have, for $v_p + E_p < 0$ and $T \geq T_a$ the estimate $\mathcal{G}((v_p+E_p)/T;\sigma_p/T) \leq \mathcal{G}((v_p+E_p)/T;\sigma_p/T_a)$ (see [13, Lemma 2.1]). Therefore, we obtain,

$$\begin{aligned} 0 &\geq \lim_{\frac{v_p}{T}\to-\infty} \mathcal{G}\Big(\frac{v_p+E_p}{T};\frac{\sigma_p}{T}\Big)\frac{v_p}{T} \geq \lim_{\frac{v_p}{T}\to-\infty} \mathcal{G}\Big(\frac{v_p+E_p}{T};\frac{\sigma_p}{T_a}\Big)\frac{v_p}{T} \\ &= \lim_{\frac{v_p}{T}\to-\infty} \mathcal{G}\Big(\frac{v_p+E_p}{T};\frac{\sigma_p}{T_a}\Big)\frac{v_p+E_p}{T} - \lim_{\frac{v_p}{T}\to-\infty} \mathcal{G}\Big(\frac{v_p+E_p}{T};\frac{\sigma_p}{T_a}\Big)\frac{E_p}{T} = 0-0=0, \end{aligned}$$

establishing the last convergence in (2.5).

For the considered case of strong n-doping and negligible p-density ($\delta_n >> \delta_p \approx 0$), we additionally assume local charge neutrality. This means that the right-hand side of the Poisson equation in (2.1) fulfills $C - n + p = \delta_n - \delta_p - n + p = 0$, and that we obtain $n = \delta_n$ in the limit $p \to 0$. We recalculate a corresponding temperature dependent "chemical potentialöf electrons v_n as follows:

For parameters $0 < \delta < N_0$, $E \in \mathbb{R}$, $\sigma > 0$, and temperatures $T > 0$ we look for $v = V(T)$ such that

$$\mathcal{H}(T, V(T)) = 0, \text{ where } \mathcal{H}(T,v) := N_0\mathcal{G}\Big(\frac{v+E}{T};\frac{\sigma}{T}\Big) - \delta.. \tag{2.6}$$

Since for all fixed $T > 0$, $\sigma > 0$ the map $v \mapsto \mathcal{H}(T,v)$ is a strictly monotonously increasing function $\mathbb{R} \to (-\delta, N_0 - \delta)$ (see Appendix A), we find that for all $T > 0$, $\sigma > 0$, $N_0 > \delta > 0$ there is exactly one solution $v = V(T) = T\mathcal{G}^{-1}\Big(\frac{\delta}{N_0};\frac{\sigma}{T}\Big) - E$ such that $\mathcal{H}(T, V(T)) = 0$. Here $\mathcal{G}^{-1}(y;z)$ denotes the inverse of $\mathcal{G}$ with respect to y while z is held fixed.

In the case of strong n-doping, we introduce a notion of "chemical potential" of electrons $v_n := V_n(T)$, where the function $V_n(T)$ results from uniquely solving the equation (2.6), $\mathcal{H}(T, V_n(T)) = 0$ for the parameters $N_0 = N_{n0}$, $E = E_n$, $\sigma = \sigma_n$, $\delta = \delta_n$. Furthermore, we reconstruct an "electrostatic potential" via

$$\psi_n = \psi_n(\varphi_n, T) := \varphi_n + V_n(T).$$

Hence, in summary we describe the electrothermal interaction in a very coarse way by the interplay of the electrochemical potential of the electrons φ_n and the temperature T via the following reduced coupled system resulting from the continuity equation for φ_n and the heat flow equation by using the results of the described limit procedure,

$$\begin{aligned} -\nabla\cdot(\delta_n\mu_n(T,\delta_n,|\nabla\psi_n|)\nabla\varphi_n) &= 0 \quad \text{in } \Omega, \\ -\nabla\cdot(\lambda\nabla T) &= \delta_n\mu_n(T,\delta_n,|\nabla\psi_n|)|\nabla\varphi_n|^2 \quad \text{in } \Omega, \\ (\delta_n\mu_n(T,\delta_n,|\nabla\psi_n|)\nabla\varphi_n)\cdot\nu = 0 \quad \text{on } \Gamma_N, \quad \varphi_n &= \varphi_n^D \quad \text{on } \Gamma_D, \\ \lambda\nabla T\cdot\nu + \kappa(T - T_a) &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{2.7}$$

Setting the conductivity function $\widetilde{\sigma} = \delta_n\mu_n(T,\delta_n,|\nabla(\varphi_n + V_n(T))|)$, the potential $\varphi = \varphi_n$, the resulting problem is of the form (1.1).

In a completely analogous manner, for a strongly p-doped semiconductor region Ω with $\delta_p >> \delta_n \approx 0$ we obtain, under the assumption $n \to 0$ whereas the quantities $\nabla\varphi_n$, $\nabla\varphi_p$, ψ, $\nabla\psi$, v_p, p, T and ∇T remain bounded, the following reduced coupled system for the interaction of the electrochemical potential of the holes φ_p and the temperature T,

$$\begin{aligned} -\nabla\cdot(\delta_p\mu_p(T,\delta_p,|\nabla\psi_p|)\nabla\varphi_p) &= 0 \quad \text{in } \Omega, \\ -\nabla\cdot(\lambda\nabla T) &= \delta_p\mu_p(T,\delta_p,|\nabla\psi_p|)|\nabla\varphi_p|^2 \quad \text{in } \Omega, \\ (\delta_p\mu_p(T,\delta_p,|\nabla\psi_p|)\nabla\varphi_p)\cdot\nu = 0 \quad \text{on } \Gamma_N, \quad \varphi_p &= \varphi_p^D \quad \text{on } \Gamma_D, \\ \lambda\nabla T\cdot\nu + \kappa(T - T_a) &= 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{2.8}$$

with the reconstructed value $\psi_p = \psi_p(\varphi_p, T) := \varphi_p - V_p(T)$ for the "electrostatic potential", where the function $V_p(T)$ results from uniquely solving the equation (2.6), $\mathcal{H}(T, V_p(T)) = 0$ for the parameters $N_0 = N_{p0}$, $E = E_p$, $\sigma = \sigma_p$, and $\delta = \delta_p$. Note that, according to (2.2), and using $\mathcal{G}^{-1}(y; z)$ for the inverse of $\mathcal{G}$ with respect to y while z is held fixed,

$$V_i(T) = T\mathcal{G}^{-1}\Big(\frac{\delta_i}{N_{i0}}; \frac{\sigma_i}{T}\Big) - E_i, \quad i = n, p. \tag{2.9}$$

2.2 Notation and assumptions

In two spatial dimensions, we consider geometric situations as indicated schematically in Fig. 1 and use the following notation: Ω_{D} is the subregion of the device, where we consider the full electrothermal drift-diffusion model (2.1), Ω_{n} is the n-doped subregion, and Ω_{p} is the p-doped subregion of the device. The device region is defined as $\Omega :=$ int$(\overline{\Omega_{\mathrm{n}}} \cup \overline{\Omega_{\mathrm{D}}} \cup \overline{\Omega_{\mathrm{p}}})$. Moreover, we introduce $\Omega_{\mathrm{Dj}} :=$ int$(\overline{\Omega_{\mathrm{D}}} \cup \overline{\Omega_{\mathrm{j}}})$, $\Gamma_{\mathrm{Dj}} := \Gamma_D \cap \overline{\Omega_{\mathrm{j}}}$, $I_{\mathrm{j}} :=$ int$(\overline{\Omega_{\mathrm{D}}} \cap \overline{\Omega_{\mathrm{j}}})$ for $\mathrm{j} = \mathrm{n}, \mathrm{p}$, and $I := I_{\mathrm{n}} \cup I_{\mathrm{p}}$. By ν and ν_{D}, we denote the outer unit normals at $\partial\Omega$ and $\partial\Omega_{\mathrm{D}}$, respectively.

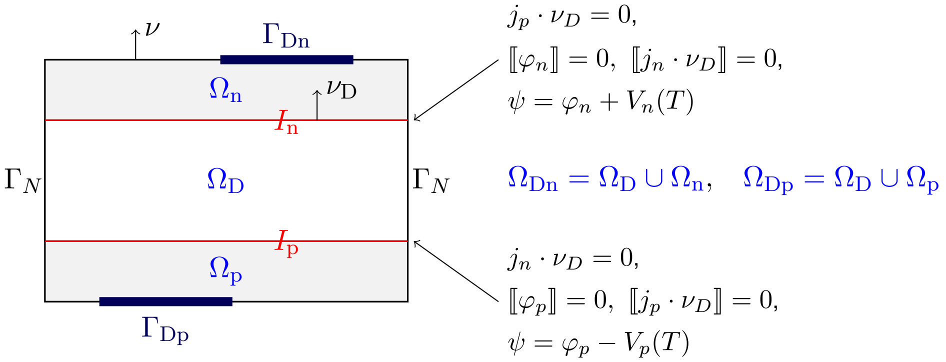

Figure 1: Schematic geometry of an organic semiconductor device partitioned into the different subregions and transfer conditions at interfaces, where $[\![\cdot]\!]$ denotes the jump of the argument over the respective interface.

To distinguish the energy levels E_i, the disorder parameters σ_i, and the number of transport states N_{i0} in the domains Ω_{i} (where they are assumed to be constants) from the corresponding parameters in Ω_{D}, we denote them now by $\widehat{E}_i$, $\widehat{\sigma}_i$, and $\widehat{N}_{i0}$, $i = n, p$. Moreover, δ_i denotes the corresponding doping density in Ω_{i}. Additionally, from now on, $V_i(T)$ means the functions resulting from uniquely solving the equation (2.6), $\mathcal{H}(T, V_i(T)) = 0$ for the parameters $N_0 = \widehat{N}_{i0}$, $E = \widehat{E}_i$, $\sigma = \widehat{\sigma}_i$, $\delta = \delta_i$, $i = n, p$.

We work with the Lebesgue spaces $L^p(\Omega)$ and the Sobolev spaces $W^{1,q}(\Omega)$. Moreover, we make use the following closed subspaces of H^1 functions: $H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}})$ indicates the closure of C^∞ functions with compact support in $\Omega_{\mathrm{Di}} \cup (\partial\Omega_{\mathrm{Di}} \setminus \Gamma_{\mathrm{Di}})$ with respect to the $H^1(\Omega_{\mathrm{Di}})$ norm, $H^1_I(\Omega_{\mathrm{D}})$ is the closure of C^∞ functions with compact support in $\Omega_{\mathrm{D}} \cup (\partial\Omega_{\mathrm{D}} \setminus I)$ with respect to the $H^1(\Omega_{\mathrm{D}})$ norm. In our estimates, positive constants, which 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 stationary electrothermal model, which we will introduce in Subsection 2.3 under the following general **Assumption (A).** In what follows, let $j = n, p$,

- $\Omega, \Omega_{\mathrm{D}}, \Omega_{\mathrm{Dj}} \subset \mathbb{R}^2$ are bounded Lipschitz domains with $\overline{\Omega_{\mathrm{n}}} \cap \overline{\Omega_{\mathrm{p}}} = \emptyset$, mes$(I_{\mathrm{j}}) > 0$, mes$(\Gamma_{\mathrm{Dj}}) > 0$ with $\mathrm{dist}(x, \overline{\Omega_{\mathrm{Dj}}}) \geq$ const > 0 for all $x \in \Gamma_{\mathrm{Di}}$, $\mathrm{i} \neq \mathrm{j}$, and $\widetilde{\Gamma}_{\mathrm{Nj}} := \partial\Omega_{\mathrm{Dj}} \setminus \Gamma_{\mathrm{Dj}}$, $\Omega_{\mathrm{Dj}} \cup \widetilde{\Gamma}_{\mathrm{Nj}}$ are regular in the sense of Gröger [15].
- $\varphi_j^D \in W^{1,\infty}(\Omega_{\mathrm{Dj}})$, $\left\|\varphi_j^D\right\|_{L^\infty(\Omega_{\mathrm{Dj}})} \leq K$, $\lambda \in L^\infty(\Omega)$, $0 < \lambda_0 \leq \lambda$ a.e. in Ω, $\lambda =$ const in Ω_{D}, $\kappa \in L^\infty_+(\Gamma)$, $\|\kappa\|_{L^1(\Gamma)} > 0$, $T_a =$ const > 0, $\varepsilon =$ const > 0.

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- The quantities $\widehat{N}_{j0}$, δ_j, $\widehat{\sigma}_j$ defined for Ω_{j} are positive constants, $\widehat{E}_j$ is constant. Moreover, $0 < \underline{N} \leq \widehat{N}_{j0} \leq \overline{N}$, $0 < \sigma_j \leq \overline{\sigma}$, $|\widehat{E}_j|, \leq \overline{E}$, $2\delta_j \leq \widehat{N}_{j0}$.
- $N_{j0}, \sigma_j \in L^\infty_+(\Omega_{\mathrm{D}})$, $C, E_j \in L^\infty(\Omega_{\mathrm{D}})$ such that $0 < \underline{N} \leq N_{j0} \leq \overline{N}$, $0 < \underline{\sigma} \leq \sigma_j \leq \overline{\sigma}$, $|E_j| \leq \overline{E}$, $|C| \leq \overline{C}$ a.e. in Ω_{D}.
- $r(\cdot, n, p, T) = npr_0(\cdot, n, p, T)$, where $r_0(\cdot, n, p, T) : \Omega_{\mathrm{D}} \times (0, \overline{N})^2 \times (0, \infty) \mapsto \mathbb{R}_+$ is a Caratheodory function and $r_0(\cdot, n, p, T) \leq \overline{r}$ a.e. in Ω_{D} for all $(n, p, T) \in (0, \overline{N})^2 \times (0, \infty)$.
- $\mu_j : \Omega_{\mathrm{Dj}} \times (0, \infty) \times (0, \overline{N}) \times [0, \infty) \mapsto \mathbb{R}_+$ are Caratheodory functions such that for all $\xi > 0$ there exists $\underline{\mu}_\xi$, $\overline{\mu}_\xi$ with $0 < \underline{\mu}_\xi \leq \mu_j(\cdot, T, y, z) \leq \overline{\mu}_\xi$ for all $(T, y, z) \in [\xi, \infty) \times (0, \overline{N}) \times [0, \infty)$ a.e. in Ω_{Dj}.

Henceforth, we set $\underline{\mu} := \underline{\mu}_{T_a}$, $\overline{\mu} := \overline{\mu}_{T_a}$.

From now on, we work with the approximations that (i) the built-in potential is nearly constant in homogeneously doped regions and (ii) that the voltage drop over strongly doped regions is very small in comparison to the voltage drop over the rest of the device. Under these approximations we substitute in Ω_{i} the mobility $\mu_i(T, \delta_i, |\nabla\psi_i|)$ by $\mu_i(T, \delta_i, 0)$, $i = n, p$, and consider the then resulting model equations.

2.3 Formulation of the coarse-grained model

In Ω_{D}, we use the quantities R, n, p as they were defined in (2.2). To simplify the presentation, we introduce the following quantities in the entire domain Ω,

$$\chi_n(x) = \begin{cases} 1 \text{ if } x \in \Omega_{\mathrm{Dn}} \\ 0 \text{ otherwise }, \end{cases} \qquad \chi_p(x) = \begin{cases} 1 \text{ if } x \in \Omega_{\mathrm{Dp}} \\ 0 \text{ otherwise }, \end{cases}$$

$$d_n(n, T, |\nabla\psi|) = \chi_n(1 - \chi_p)\delta_n\mu_n(T, \delta_n, 0) + \chi_n\chi_p n\mu_n(T, n, |\nabla\psi|), \tag{2.10}$$

$$d_p(p, T, |\nabla\psi|) = \chi_p(1 - \chi_n)\delta_p\mu_p(T, \delta_p, 0) + \chi_n\chi_p p\mu_p(T, p, |\nabla\psi|), \tag{2.11}$$

$$R_\Omega(n, p, T, \varphi_n, \varphi_p) = \chi_n\chi_p R(n, p, T, \varphi_n, \varphi_p), \tag{2.12}$$

$$\begin{aligned} &h_\Omega(n, p, T, z, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p) = \\ &\quad d_n(n, T, z)|\nabla\varphi_n|^2 + d_p(p, T, z)|\nabla\varphi_p|^2 + R_\Omega(n, p, T, \varphi_n, \varphi_p)(\varphi_p - \varphi_n). \end{aligned} \tag{2.13}$$

Using the above notation, the electrothermal behavior of the organic device occupying Ω is now described by the following stationary system of partial differential equations and transfer conditions:

Heat flow equation for T in Ω

$$\begin{aligned} -\nabla \cdot (\lambda\nabla T) &= h_\Omega(n, p, T, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p) && \text{in } \Omega, \\ \lambda\nabla T \cdot \nu + \kappa(T - T_a) &= 0 && \text{on } \Gamma. \end{aligned} \tag{2.14}$$

Continuity equation for electrons in Ω_{Dn}

$$\begin{aligned} \nabla \cdot (d_n(n, T, |\nabla\psi|)\nabla\varphi_n) &= -R_\Omega(n, p, T, \varphi_n, \varphi_p) && \text{in } \Omega_{\mathrm{Dn}}, \\ [\![\varphi_n]\!] = 0, \quad [\![d_n(n, T, |\nabla\psi|)\nabla\varphi_n \cdot \nu_{\mathrm{D}}]\!] &= 0 && \text{on } I_{\mathrm{n}}, \\ \varphi_n = \varphi_n^{\mathrm{D}} \text{ on } \Gamma_{\mathrm{Dn}}, \quad \nabla\varphi_n \cdot \nu &= 0 && \text{on } \partial\Omega_{\mathrm{Dn}} \backslash \Gamma_{\mathrm{Dn}}. \end{aligned} \tag{2.15}$$

Continuity equation for holes in Ω_{Dp}

$$\begin{aligned}-\nabla\cdot(d_p(p,T,|\nabla\psi|)\nabla\varphi_p) = -R_\Omega(n,p,T,\varphi_n,\varphi_p) \quad &\text{in } \Omega_{\mathrm{Dp}},\\ [\![\varphi_p]\!]=0,\quad [\![d_p(p,T,|\nabla\psi|)\nabla\varphi_p\cdot\nu_{\mathrm{D}}]\!]=0 \quad &\text{on } I_{\mathrm{p}},\\ \varphi_p=\varphi_p^{\mathrm{D}} \text{ on } \Gamma_{\mathrm{Dp}},\quad \nabla\varphi_p\cdot\nu=0 \quad &\text{on } \partial\Omega_{\mathrm{Dp}}\setminus\Gamma_{\mathrm{Dp}}.\end{aligned} \tag{2.16}$$

Poisson equation for the electrostatic potential ψ in Ω_{D}

$$\begin{aligned}-\nabla\cdot(\varepsilon\nabla\psi) = C-n+p \quad &\text{in } \Omega_{\mathrm{D}},\\ \psi=\psi^D \quad &\text{on } I,\\ \varepsilon\nabla\psi\cdot\nu=0 \quad &\text{on } \partial\Omega_{\mathrm{D}}\setminus I.\end{aligned} \tag{2.17}$$

The function $\psi^D(x)$ is defined as,

$$\psi^D(x) := (1-\tau(x))\big(\varphi_n+V_n(T(x))\big)+\tau(x)\big(\varphi_p-V_p(T(x))\big). \tag{2.18}$$

where V_n and V_p are defined in (2.9), and $\tau:\Omega_{\mathrm{D}}\to[0,1]$ is a $C^1(\overline{\Omega}_{\mathrm{D}})$ function such that,

$$\tau|_{I_{\mathrm{n}}}=0,\quad \tau|_{I_{\mathrm{p}}}=1,\quad |\nabla\tau|\le\widehat{c}. \tag{2.19}$$

For a more detailed description regarding the Dirichlet function ψ^D, we refer the interested reader to [12], where the Boltzmann case is considered.

Lemma 2.1 *Let $V_i(T)$ be the functions resulting from uniquely solving the equation* (2.6)*, $\mathcal{H}(T,V_i(T))=0$ for the constant parameters $N_0=\widehat{N}_{i0}$, $E=\widehat{E}_i$, $\sigma=\widehat{\sigma}_i$, $\delta=\delta_i$, $i=n,p$.*

1. If $T\in H^1(\Omega_{\mathrm{D}})$ and $\ln T\in L^\infty(\Omega_{\mathrm{D}})$, then $V_i(T)\in H^1(\Omega_{\mathrm{D}})\cap L^\infty(\Omega_{\mathrm{D}})$, $i=n,p$.

2. If $\varphi_n,\ \varphi_p,\ T\in H^1(\Omega_{\mathrm{D}})$ and $\varphi_n,\ \varphi_p,\ \ln T\in L^\infty(\Omega_{\mathrm{D}})$ then the function ψ^D defined in (2.18) *belongs to $H^1(\Omega_{\mathrm{D}})\cap L^\infty(\Omega_{\mathrm{D}})$.*

Proof. 1. The L^∞ property results directly from Lemma A.1. Thus it only remains to show that $\nabla V_i(T)\in L^2(\Omega)^2$. According to (A.6) we evaluate

$$\nabla V_i(T)=\frac{\mathrm{d}}{\mathrm{d}T}V_i(T)\nabla T=\Big\{\Big[\frac{\partial\mathcal{G}}{\partial\eta}(\eta_i,z_i)\Big]^{-1}\frac{\partial\mathcal{G}}{\partial z}(\eta_i,z_i)z_i+\mathcal{G}^{-1}\Big(\frac{\delta_i}{\widehat{N}_{i0}};\frac{\widehat{\sigma}_i}{T}\Big)\Big\}\nabla T, \tag{2.20}$$

where $\eta_i=\frac{V_i(T)+\widehat{E}_i}{T}$, $z_i=\frac{\widehat{\sigma}_i}{T}$. Because of $\ln T\in L^\infty(\Omega_{\mathrm{D}})$ and the lower bound of η_i from Lemma A.1, the estimates in [13, Subsec. 2.1] ensure that $\frac{\partial\mathcal{G}}{\partial\eta}(\eta_i,z_i)$ is positively bounded away from zero, and $\frac{\partial\mathcal{G}}{\partial z}(\eta_i,z_i)$ and $\mathcal{G}^{-1}\Big(\frac{\delta_i}{\widehat{N}_{i0}};\frac{\widehat{\sigma}_i}{T}\Big)$ are bounded from above which together with $T\in H^1(\Omega_{\mathrm{D}})$ in summary guarantees that $V_i(T)\in H^1(\Omega_{\mathrm{D}})$, $i=n,p$.

2. Due to the properties of $\tau,\ \varphi_n,\ \varphi_p$, the assertion follows directly from assertion 1. $\square$

3 Weak formulation, a priori estimates, and main result

3.1 Concept of solution for Problem (P)

We look for solutions to (2.14) – (2.17) in the following setting. Let $s>2$ denote an exponent which will finally be fixed in Theorem 3.1. A weak formulation of our model is as follows. Find $(\psi,\varphi_n,\varphi_p,T)\in\big[(\psi^D+H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}))\cap$

$L^\infty(\Omega_{\rm D})\big] \times \big[(\varphi_n^D + H^1_{\rm Dn}(\Omega_{\rm Dn})) \cap W^{1,s}(\Omega_{\rm Dn})\big] \times \big[(\varphi_p^D + H^1_{\rm Dp}(\Omega_{\rm Dp})) \cap W^{1,s}(\Omega_{\rm Dp})\big] \times \{T \in H^1(\Omega) : \ln T \in L^\infty(\Omega)\}$, such that

$$\begin{aligned}
&\int_{\Omega_{\rm D}} \varepsilon \nabla\psi \cdot \nabla\overline{\psi}\,\mathrm{d}x = \int_{\Omega_{\rm D}} (C-n+p)\overline{\psi}\,\mathrm{d}x \qquad \forall \overline{\psi} \in H^1_{\rm I}(\Omega_{\rm D}),\\
&\int_{\Omega_{\rm Dn}} d_n(n,T,|\nabla\psi|)\nabla\varphi_n \cdot \nabla\overline{\varphi}_n\,\mathrm{d}x + \int_{\Omega_{\rm Dp}} d_p(p,T,|\nabla\psi|)\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\,\mathrm{d}x\\
&= \int_{\Omega_{\rm D}} r(n,p,T)\Big(1-\exp\frac{\varphi_n-\varphi_p}{T}\Big)(\overline{\varphi}_n - \overline{\varphi}_p)\,\mathrm{d}x \quad \forall \overline{\varphi}_i \in H^1_{\rm Di}(\Omega_{\rm Di}),\ i=n,p,\\
&\int_\Omega \lambda\nabla T\cdot\nabla\overline{T}\,\mathrm{d}x + \int_\Gamma \kappa(T-T_a)\overline{T}\,\mathrm{d}\Gamma\\
&= \int_\Omega h_\Omega(n,p,T,|\nabla\psi|,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)\overline{T}\,\mathrm{d}x \quad \forall \overline{T}\in H^1(\Omega),
\end{aligned} \tag{P}$$

where d_n, d_p, and h_Ω are defined in (2.10), (2.11), and (2.13) respectively. We remark that the choice of the definition sets for $(\psi,\varphi_n,\varphi_p,T)$ and Assumption (A) ensure, $n,p \in L^\infty(\Omega_{\rm D})$, $\mu_n(T,n,|\nabla\psi|)$, $\mu_p(T,p,|\nabla\psi|)$, $r(n,p,T) \in L^\infty(\Omega_{\rm D})$, $\mu_i(T,\delta_i,0) \in L^\infty(\Omega_{\rm i})$, $d_i \in L^\infty(\Omega_{\rm Di})$, $i=n,p$, $h_\Omega \in L^{s/2}(\Omega)$, and $\psi^D \in H^1(\Omega)\cap L^\infty(\Omega)$ by Lemma 2.1.

If there is no problem of misunderstanding we leave out the arguments in $d_n,\ d_p,\ r,\ h_\Omega$.

3.2 A priori estimates

The proof of a priori estimates uses similar techniques applied for the inorganic coarse-grained model in [12], however, some essential modifications related to the statistical relation and the mobility functions have to be taken into account that are pointed out here.

Theorem 3.1 *Under Assumption* (A) *all solutions $(\psi,\varphi_n,\varphi_p,T)$ to* (P) *satisfy $T \ge T_a$ and $\|\varphi_n\|_{L^\infty(\Omega_{\rm Dn})}$, $\|\varphi_p\|_{L^\infty(\Omega_{\rm Dp})} \le K$ with T_a and K from Assumption* (A). *Moreover, there are exponents $s,\ t > 2$ and constants $c_{\varphi,s},\ c_{T,t},\ c_{T,\infty},\ c_{\psi,\infty} > 0$ depending only on the data and the underlying geometry such that*

$$\|\varphi_i\|_{W^{1,s}(\Omega_{\rm Di})} \le c_{\varphi,s},\ i=n,p,\ \ \|T\|_{W^{1,t}(\Omega)} \le c_{T,t},\ \ \|T\|_{L^\infty(\Omega)} \le c_{T,\infty},\ \ \|\psi\|_{L^\infty(\Omega_{\rm D})} \le c_{\psi,\infty},$$

for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P).

Proof. 1. As in [12, Lemma 3.1] it is verified that $T \ge T_a$ a.e. in Ω for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P).

2. Since the densities and the mobility functions μ_i are bounded, the techniques in [12, Lemma 3.2] ensure also in the organic case a constant $c_h > 0$, depending only on the data, such that

$$\begin{aligned}
\|h_\Omega(n,p,T,|\nabla\psi|,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)\|_{L^1(\Omega)} &\le c_h,\\
\|\varphi_n\|_{L^\infty(\Omega_{\rm Dn})},\ \|\varphi_p\|_{L^\infty(\Omega_{\rm Dp})} &\le K.
\end{aligned} \tag{3.1}$$

3. As in [12, Lemma 3.3], we derive constants $c_q > 0$, and $c_T > 0$, depending only on the data, such that $\|T\|_{W^{1,q}(\Omega)} \le c_q$, $q \in [1,2)$, $\|T\|_{L^2(\Gamma)} \le c_T$ for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P).

4. Next we aim to find a constant $c_{\psi/T} > 0$, depending only on the data, such that,

$$\|\psi/T\|_{L^\infty(\Omega_{\rm D})} \le c_{\psi/T} \tag{3.2}$$

for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (P). For this purpose we define in the organic case

$$K_1 := \max_{i=n,p}\Big\{\Big|\mathcal{G}^{-1}\Big(\frac{\delta_i}{\widehat{N}_{i0}};\frac{\widehat{\sigma}_i}{T_a}\Big)\Big|\Big\}.$$

Have in mind the definition of ψ^D in (2.18) and Lemma 2.1. For $L > 0$ and $\xi^+ := \max\{0,\xi\}$, $\xi^- := \max\{0,-\xi\}$ we use $mz_L^{m-1} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$, resp. $-m\overline{z}_L^{m-1} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ with

$$z_L := \min\{L, (\psi - K - \overline{E} - K_1 T)^+\}, \quad \overline{z}_L := \min\{L, (\psi + K + \overline{E} + K_1 T)^-\}, \quad m = 2^k,\ k \in \mathbb{N},$$

simultaneously as test functions for the Poisson and heat flow equation (on Ω_{D}). By a Moser iteration technique, we thus derive upper and lower bounds for ψ/T. Taking into account that in the organic setting $|C - n + p| \le \overline{C} + 2\overline{N}$ a.e. in Ω_{D} and adapting the Steps 1 and 2 in the proof of [12, Lemma 3.4] we establish the desired estimate.

5. The obtained estimates for T, φ_n, φ_p, and ψ/T as well as the properties of the Gauss–Fermi integral (see especially Lemma 2.1 and [13, Lemma 2.1]) ensure a.e. in Ω_{D}

$$\underline{c}_d \le n = N_{n0}\mathcal{G}\Big(\frac{\psi - \varphi_n + E_n}{T}; \frac{\sigma_n}{T}\Big),\ p = N_{p0}\mathcal{G}\Big(\frac{E_p - (\psi - \varphi_p)}{T}; \frac{\sigma_p}{T}\Big) < \overline{N}, \tag{3.3}$$

where

$$\underline{c}_d := \underline{N}\mathcal{G}\Big(-\frac{K+\overline{E}}{T_a} - c_{\psi/T}; 0\Big) \le \underline{N}\mathcal{G}\Big(-\frac{K+\overline{E}}{T_a} - c_{\psi/T}; \frac{\sigma_n}{T}\Big) \le \underline{N}\mathcal{G}\Big(\frac{\psi - \varphi_n + E_n}{T}; \frac{\sigma_n}{T}\Big)$$

depends only on the data and the underlying geometry. Using additionally the upper and lower bounds of the mobilities μ_i and δ_i, $i = n,p$, the estimates (3.3), and the upper bound for r_0 and Step 2, we find that the L^∞ norms of the right-hand sides of the continuity equations is bounded by a constant $c_R > 0$. The supposed regularity of φ_n^D, φ_p^D and the regularity result of Gröger [15, Theorem 1] for elliptic problems guarantee an exponent $s > 2$ and a $c_{\varphi,s} > 0$ depending only on the data and the underlying geometry such that

$$\varphi_i \in W^{1,s}(\Omega_{\mathrm{Di}}) \text{ and } \|\varphi_i\|_{W^{1,s}(\Omega_{\mathrm{Di}})} \le c_{\varphi,s}, \quad i = n,p.$$

6. Consequently, the right-hand side of the heat flow equation (2.14) belongs to $L^{s/2}(\Omega)$ and the $L^{s/2}(\Omega)$ norm is bounded by some constant $c > 0$. Here, we used for the reaction heat that $T \ge T_a$ a.e. in Ω and $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K$, $i = n,p$. We apply regularity results for second order elliptic equations with non-smooth data in the 2D case. According to [15, Theorem 1], there is a $t^* > 2$ such that the strongly monotone, Lipschitz continuous operator $\Lambda :\ H^1(\Omega) \mapsto H^1(\Omega)^*$,

$$\langle \Lambda T, w\rangle := \int_\Omega (\lambda \nabla T \cdot \nabla w + Tw)\,\mathrm{d}x, \quad w \in H^1(\Omega),$$

maps $W^{1,\tilde{t}}(\Omega)$ into and onto $W^{-1,\tilde{t}}(\Omega)$ for all $\tilde{t} \in [2,t^*]$. Here, $W^{-1,\tilde{t}}(\Omega)$ means $W^{1,\tilde{t}'}(\Omega)^*$ with $\frac{1}{\tilde{t}} + \frac{1}{\tilde{t}'} = 1$. Next we define $t \in (2,t^*]$ by

$$t := \begin{cases} t^* & \text{if } \dfrac{s}{s-2} \in \Big[1, \dfrac{2t^*}{t^*-2}\Big] \\ \dfrac{2s}{4-s} & \text{if } \dfrac{s}{s-2} > \dfrac{2t^*}{t^*-2} \end{cases}, \qquad \frac{1}{t} + \frac{1}{t'} = 1.$$

This definition guarantees that $L^{s/2}(\Omega) \hookrightarrow W^{-1,t}(\Omega) := W^{1,t'}(\Omega)^*$. Remark 13 in [15] then ensures $W^{1,t}$-estimates for solutions to problems of the form $\Lambda T = \mathcal{F}(T)$, where $\mathcal{F}$ is any mapping from $W^{1,2}(\Omega)$ into $W^{-1,t}(\Omega)$. In our case, we use

$$\begin{aligned}\langle \mathcal{F}(T), w\rangle := \int_\Omega \Big(h_\Omega(n,p,T,|\nabla\psi|,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p) + T\Big)\, w\,\mathrm{d}x \\ + \int_\Gamma \kappa(T_a - T)\, w\,\mathrm{d}\Gamma \quad \forall w \in W^{1,t'}(\Omega).\end{aligned}$$

Thus, we find a $c_{T,t} > 0$ such that the weak solution T to the heat flow equation belongs to $W^{1,t}(\Omega)$ and $\|T\|_{W^{1,t}(\Omega)} \le c_{T,t}$. The continuous embedding of $W^{1,t}(\Omega)$ in $L^\infty(\Omega)$ ensures $\|T\|_{L^\infty(\Omega)} \le c_{T,\infty}$. Moreover, together with (3.2) we therefore obtain $\|\psi\|_{L^\infty(\Omega_{\mathrm{D}})} \le c_{\psi,\infty}$, which finishes the proof. $\square$

3.3 Main result

Theorem 3.2 *Under Assumption* (A) *there exists a solution* $(\psi, \varphi_n, \varphi_p, T)$ *to Problem* (P).

We give the detailed existence proof in Section 4. It consists of the following steps: First, we consider a regularized Problem (P$_M$) with regularization parameter M. Second, for solutions to (P$_M$) we ensure a priori estimates and higher integrability properties for the electrostatic potential, quasi Fermi potentials, and the temperature that are independent of M (Theorem 4.1). Finally, we prove the solvability of (P$_M$) via Schauder's fixed point theorem. The regularization of Problem (P) consists of a manipulation of the statistical relation (see (4.1)) giving regularized densities which in the right-hand side of the Poisson equation, the flux terms, reaction coefficient, and the source term of the heat equation. Thus, if we choose $M > c_{\psi/T}$ with $c_{\psi/T}$ from (3.2), the manipulation of the statistical relation in the regularized problem does not become active. Therefore, by solving the regularized Problem (P$_M$), the proof of Theorem 3.2 is completed. Moreover, let us note that the regularization argument is necessary since we can not apply the Moser technique for the fixed point iterations to obtain a priori estimates, computed in (3.2), also for the expression $\psi/\widetilde{T}$ with the frozen argument $\widetilde{T}$, since $\widetilde{T}$ does not have to fulfill the heat equation.

As for the electrothermal drift-diffusion model and the thermistor model, uniqueness of the solution to (P) is not to be expected since organic semiconductor devices have the potential for S-shaped current-voltage relations with regions of negative differential resistance, see e.g. [3, 5].

As a consequence of Theorem 3.2 we obtain the following result concerning the thermodynamic equilibrium.

Corollary 3.1 *We suppose in addition to Assumption* (A) *that* $\varphi_i^D = const$ *in* Ω_{Di}, $i = n, p$, *and* $\varphi_n^D = \varphi_p^D$ *in* Ω_{D}. *Then there exists a unique solution to Problem* (P). *Moreover, it is the thermodynamic equilibrium and has the form* $(\psi^*, \varphi_n^*, \varphi_p^*, T^*) = (\psi^*, \varphi_n^D, \varphi_p^D, T_a)$, *where* $\psi^* \in H^1(\Omega_{\mathrm{D}})$ *is the unique solution to the nonlinear Poisson equation in* Ω_{D},

$$-\nabla \cdot (\varepsilon \nabla \psi^*) = C - N_{n0}\mathcal{G}\Big(\frac{\psi^* - \varphi_n^D + E_n}{T_a}; \frac{\sigma_n}{T_a}\Big) + N_{p0}\mathcal{G}\Big(\frac{E_p - (\psi^* - \varphi_p^D)}{T_a}; \frac{\sigma_p}{T_a}\Big),$$

with the boundary conditions $\psi^* = \psi^{D*}$ *on* I, $\varepsilon \nabla \psi^* \cdot \nu = 0$ *on* $\partial\Omega_{\mathrm{D}} \setminus I$, *where*

$$\psi^{D*} := (1-\tau)\big(\varphi_n^D + V_n(T_a)\big) + \tau\big(\varphi_p^D - V_p(T_a)\big). \tag{3.4}$$

Proof. Let $(\psi, \varphi_n, \varphi_p, T)$ be an arbitrary solution to (P) guaranteed by Theorem 3.2. The test function $(\varphi_n - \varphi_n^D, \varphi_p - \varphi_p^D) \in H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}) \times H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})$ for the continuity equations yields under the additional assumption of the corollary that

$$0 = \sum_{i=n,p} \int_{\Omega_{\mathrm{Di}}} d_i |\nabla \varphi_i|^2 \,\mathrm{d}x + \int_{\Omega_{\mathrm{D}}} r(n,p,T) \left(\exp\frac{\varphi_n - \varphi_p}{T} - 1\right)(\varphi_n - \varphi_p)\,\mathrm{d}x.$$

The integrands in all occurring integrals are nonnegative and the positivity of d_i in Ω_{Di} for $i = n, p$ guarantees that $\nabla \varphi_i = 0$ a.e. in Ω_{Di}. From the prescribed boundary values we obtain $\varphi_n = \varphi_n^D = \varphi_p^D = \varphi_p$. Therefore, all source terms in the heat equation (2.14) vanish. This ensures together with the Robin boundary condition that $T \equiv T_a$. Thus it remains to solve the Poisson equation where n and p on the right-hand side are substituted according to Gauss–Fermi statistics

$$n = N_{n0}\mathcal{G}\Big(\frac{\psi^* - \varphi_n^D + E_n}{T_a}; \frac{\sigma_n}{T_a}\Big), \quad p = N_{p0}\mathcal{G}\Big(\frac{E_p - (\psi^* - \varphi_p^D)}{T_a}; \frac{\sigma_p}{T_a}\Big).$$

As Dirichlet function the function ψ^{D*} defined in (3.4) has to be prescribed. $\square$

4 Proof of main result

4.1 The regularized Problem (P_M)

Let $M > 0$ and $k_M(y) := \min\{\max\{y, -M\}, M\}$. Our problem reads as follows: Find $(\psi, \varphi_n, \varphi_p, T) \in \big[(\psi^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})) \cap L^\infty(\Omega_{\mathrm{D}})\big] \times \big[(\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \cap W^{1,s}(\Omega_{\mathrm{Dn}})\big] \times \big[(\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})) \cap W^{1,s}(\Omega_{\mathrm{Dp}})\big] \times \{T \in H^1(\Omega) : \ln T \in L^\infty(\Omega)\}$ with

$$
\begin{aligned}
&\int_{\Omega_{\mathrm{D}}} \varepsilon \nabla\psi \cdot \nabla\overline{\psi}\,\mathrm{d}x = \int_{\Omega_{\mathrm{D}}} (C - n_M + p_M)\overline{\psi}\,\mathrm{d}x \qquad \forall\, \overline{\psi} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}),\\
&\int_{\Omega_{\mathrm{Dn}}} d_n(n_M, T, |\nabla\psi|)\nabla\varphi_n \cdot \nabla\overline{\varphi}_n\,\mathrm{d}x + \int_{\Omega_{\mathrm{Dp}}} d_p(p_M, T, |\nabla\psi|)\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\,\mathrm{d}x\\
&= \int_{\Omega_{\mathrm{D}}} r(n_M, p_M, T)\Big(1 - \exp\frac{\varphi_n - \varphi_p}{T}\Big)(\overline{\varphi}_n - \overline{\varphi}_p)\,\mathrm{d}x \quad \forall\, \overline{\varphi}_i \in H^1_{\mathrm{Di}}(\Omega_{\mathrm{Di}}),\ i = n, p,\\
&\int_{\Omega} \lambda \nabla T \cdot \nabla\overline{T}\,\mathrm{d}x + \int_{\Gamma} \kappa\,(T - T_a)\,\overline{T}\,\mathrm{d}\Gamma\\
&= \int_{\Omega} h_\Omega(n_M, p_M, T, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)\overline{T}\,\mathrm{d}x \quad \forall \overline{T} \in H^1(\Omega),
\end{aligned}
\tag{P_M}
$$

where the regularized densities n_M and p_M have to be determined pointwise by

$$
n_M = N_{n0}\mathcal{G}\Big(k_M\Big(\frac{\psi}{T}\Big) - \frac{\varphi_n - E_n}{T}; \frac{\sigma_n}{T}\Big), \quad p_M = N_{p0}\mathcal{G}\Big(\frac{E_p + \varphi_p}{T} - k_M\Big(\frac{\psi}{T}\Big); \frac{\sigma_p}{T}\Big). \tag{4.1}
$$

4.2 A priori estimates for solutions to Problem (P_M)

Theorem 4.1 *Under Assumption* (A)*, each weak solution $(\psi, \varphi_n, \varphi_p, T)$ to the regularized Problem* (P_M) *fulfills the estimates $T \geq T_a$ a.e. in Ω,*

$$
\begin{aligned}
&\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \leq K, \quad \|\varphi_i\|_{W^{1,s}(\Omega_{\mathrm{Di}})} \leq c_{\varphi,s},\ i = n, p, \quad \|\psi/T\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi/T},\\
&\|T\|_{L^2(\Gamma)} \leq c_T, \quad \|T\|_{W^{1,t}(\Omega)} \leq c_{T,t}, \quad \|T\|_{L^\infty(\Omega)} \leq c_{T,\infty}, \quad \|\psi\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi,\infty}
\end{aligned}
$$

with the exponents $s, t > 2$ from Theorem 3.1, the constants $T_a,\ K$ from Assumption (A) *and $c_T,\ c_{\psi/T}, c_{\varphi,s}, c_{T,t}, c_{T,\infty}$, and $c_{\psi,\infty}$ from Theorem 3.1.*

Proof. 1. We apply the techniques used in the proof of Theorem 3.1. The estimates of the first three steps remain valid with the same constants for solutions to Problem (P_M) if one substitutes $h_\Omega(n, p, T, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$ by $h_\Omega(n_M, p_M, T, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$, see especially (3.1) and $\|T\|_{L^2(\Gamma)} \leq c_T$. In Step 4 of the proof of Theorem 3.1, we have now to use that the (regularized) right-hand side of the heat equation is nonnegative and $|C - n_M + p_M| \leq \overline{C} + 2\overline{N}$ a.e. in Ω_{D}. Then exactly the same arguments ensure that $\|\psi/T\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi/T}$ with $c_{\psi/T}$ from (3.2).

2. The bounds $T \geq T_a$, $\|\psi/T\|_{L^\infty(\Omega_{\mathrm{D}})} \leq c_{\psi/T}$, $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \leq K$ guarantee the estimates $\underline{c}_d \leq n_M, p_M \leq \overline{N}$ for the regularized densities a.e. in Ω_{D} (with $\underline{c}_d$ defined in (3.3)) not depending on the regularization level M. Thus, we can repeat the Steps 5 and 6 of the proof of Theorem 3.1 with the same constants now for solutions to Problem (P_M). $\square$

4.3 Existence result for the regularized Problem (P_M)

Theorem 4.2 *Under Assumption* (A)*, there exists a weak solution $(\psi, \varphi_n, \varphi_p, T)$ to the regularized Problem* (P_M)*.*

The proof of Theorem 4.2 is based on Schauder's fixed point theorem. First, we introduce the iteration scheme, then we discuss subproblems with frozen arguments, then we verify the needed continuity properties of the fixed point map, and finally we prove the solvability of the regularized Problem (P_M). In the following, the constants are allowed to depend on the regularization level M.

4.3.1 Iteration scheme

We work with the non-empty, bounded, closed, convex set

$$\begin{aligned}\mathcal{N} := \Big\{(\varphi_n, \varphi_p, T) \in H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}}) \times W^{1,t_M}(\Omega) :\ \|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})} \le c_{M,H^1},\\ \|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K,\ i = n,p,\ \|T\|_{W^{1,t_M}(\Omega)} \le c_{T,t_M},\ T \ge T_a \quad \text{a.e. in } \Omega\Big\},\end{aligned} \tag{4.2}$$

where $c_{M,H^1} > 0$ will be defined in (4.8) and Lemma 4.2; $t_M > 2$ and $c_{T,t_M} > 0$ will be introduced in (4.10) and Lemma 4.3. In particular, we find a constant T_u such that $T_a \le T \le T_u$ for all $(\varphi_n, \varphi_p, T) \in \mathcal{N}$. For a simpler notation, we use the auxiliary function

$$\mathcal{U}(\psi, \varphi_n, \varphi_p, T) := N_{p0}\mathcal{G}\Big(\frac{E_p+\varphi_p}{T} - k_M\big(\frac{\psi}{T}\big); \frac{\sigma_p}{T}\Big) - N_{n0}\mathcal{G}\Big(k_M\big(\frac{\psi}{T}\big) - \frac{\varphi_n - E_n}{T}; \frac{\sigma_n}{T}\Big). \tag{4.3}$$

The fixed point map $\mathcal{Q} : \mathcal{N} \to \mathcal{N}$, $(\varphi_n, \varphi_p, T) = \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ is defined by the following three steps:

1. For given $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$, functions V_n, V_p defined in (2.9), and τ from Subsection 2.3 we construct the $H^1(\Omega_{\mathrm{D}})$ function

$$\widetilde{\psi}^D := (1-\tau)\big(\widetilde{\varphi}_n + V_n(\widetilde{T})\big) + \tau\big(\widetilde{\varphi}_p - V_p(\widetilde{T})\big) \tag{4.4}$$

(see Lemma 2.1). By Lemma 4.1 there is a unique weak solution $\psi \in \widetilde{\psi}^D + H^1_I(\Omega_{\mathrm{D}})$ to the nonlinear Poisson equation

$$\begin{aligned}-\nabla\cdot(\varepsilon\nabla\psi) &= C + \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \quad \text{in } \Omega_{\mathrm{D}},\\ \psi &= \widetilde{\psi}^D \quad \text{on } I, \quad \varepsilon\nabla\psi\cdot\nu = 0 \quad \text{on } \partial\Omega_{\mathrm{D}}\backslash I.\end{aligned} \tag{4.5}$$

2. We introduce the quantities

$$\widetilde{n}_M := N_{n0}\mathcal{G}\Big(k_M\big(\frac{\psi}{\widetilde{T}}\big) - \frac{\widetilde{\varphi}_n - E_n}{\widetilde{T}}; \frac{\sigma_n}{\widetilde{T}}\Big), \quad \widetilde{p}_M := N_{p0}\mathcal{G}\Big(\frac{E_p + \widetilde{\varphi}_p}{\widetilde{T}} - k_M\big(\frac{\psi}{\widetilde{T}}\big); \frac{\sigma_p}{\widetilde{T}}\Big). \tag{4.6}$$

With frozen coefficients $d_n(\widetilde{n}_M, \widetilde{T}, |\nabla\psi|)$, $d_p(\widetilde{p}_M, \widetilde{T}, |\nabla\psi|)$ and reaction rate coefficient $\widetilde{r} := r(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T})$, we solve (4.7) to obtain a weak solution (φ_n, φ_p):

$$\begin{aligned}&-\nabla\cdot(d_n(\widetilde{n}_M, \widetilde{T}, |\nabla\psi|)\nabla\varphi_n) = R_\Omega(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}, \varphi_n, \varphi_p) \text{ in } \Omega_{\mathrm{Dn}},\\ &[\![\varphi_n]\!] = 0 \text{ on } I_{\mathrm{n}}, \quad \Big[\!\!\Big[d_n(\widetilde{n}_M, \widetilde{T}, |\nabla\psi|)\nabla\varphi_n\cdot\nu_D\Big]\!\!\Big] = 0 \text{ on } I_{\mathrm{n}},\\ &\varphi_n = \varphi_n^D \text{ on } \Gamma_{\mathrm{Dn}}, \quad \nabla\varphi_n\cdot\nu = 0 \text{ elsewhere},\\ &-\nabla\cdot(d_p(\widetilde{p}_M, \widetilde{T}, |\nabla\psi|)\nabla\varphi_p) = -R_\Omega(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}, \varphi_n, \varphi_p) \text{ in } \Omega_{\mathrm{Dp}},\\ &[\![\varphi_p]\!] = 0 \text{ on } I_{\mathrm{p}}, \quad \Big[\!\!\Big[d_p(\widetilde{p}_M, \widetilde{T}, |\nabla\psi|)\nabla\varphi_p\cdot\nu_D\Big]\!\!\Big] = 0 \text{ on } I_{\mathrm{p}},\\ &\varphi_p = \varphi_p^D \text{ on } \Gamma_{\mathrm{Dp}}, \quad \nabla\varphi_p\cdot\nu = 0 \text{ elsewhere}.\end{aligned} \tag{4.7}$$

According to Lemma 4.2 we obtain a unique weak solution $(\varphi_n, \varphi_p) \in (\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \times (\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}))$ to (4.7). For some exponent $s_M > 2$, the solution fulfills the following estimates

$$\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{Di}})} \le K, \quad \|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})} \le c_{M,H^1}, \quad \|\varphi_i\|_{W^{1,s_M}(\Omega_{\mathrm{Di}})} \le c_{Ms},\ i = n,p, \tag{4.8}$$

which are uniform with respect to $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$.

3. These estimates together with $\widetilde{n}_M, \widetilde{p}_M < \overline{N}$ guarantee that the right-hand side of the heat equation,

$$\begin{aligned} -\nabla\cdot(\lambda\nabla T) &= h_\Omega(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p) \quad &&\text{in } \Omega,\\ \lambda\nabla T\cdot\nu + \kappa(T - T_a) &= 0 &&\text{on } \Gamma \end{aligned} \tag{4.9}$$

belongs to $L^{s_M/2}(\Omega)$ with uniform $L^{s_M/2}$ bound for all possible $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$. Lemma 4.3 ensures a unique weak solution $T \in H^1(\Omega)$ to (4.9). For some $t_M > 2$ it fulfills

$$\|T\|_{W^{1,t_M}(\Omega)} \le c_{T,t_M} \quad \text{and} \quad T \ge T_a, \tag{4.10}$$

which in summary demonstrates that $\mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) := (\varphi_n, \varphi_p, T) \in \mathcal{N}$.

4.3.2 Solvability of subproblems and estimates for their solutions

Lemma 4.1 (Poisson equation) *We assume* (A). *Let* $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ *be arbitrarily given and* $\widetilde{\psi}^D$ *be defined by* (4.4). *Then there exists a unique weak solution* $\psi \in \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ *to the nonlinear Poisson equation* (4.5). *There exists a constant* $c_{\psi,H^1} > 0$, *not depending on the choice of* $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$, *such that* $\|\psi\|_{H^1} \le c_{\psi,H^1}$.

Proof. 1. Using Assumption (A) and Lemma 2.1, we have $\left\|\widetilde{\psi}^D\right\|_{H^1(\Omega_{\mathrm{D}})} \le c$ for all $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ for $\widetilde{\psi}^D$ as in (4.4). Note that $\left\|\widetilde{T}\right\|_{W^{1,t_M}} \le c_{T,t_M}$ implies $\left\|\widetilde{T}\right\|_{L^\infty} \le T_u$ (comp. (4.2)). By the properties of the Gauss–Fermi integral, for given $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ the operator $B_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})} : \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}) \to (H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}))^*$,

$$\langle B_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})}\psi, \overline{\psi}\rangle := \int_{\Omega_{\mathrm{D}}} \varepsilon\nabla\psi\cdot\nabla\overline{\psi}\,\mathrm{d}x - \int_{\Omega_{\mathrm{D}}} \Big(\mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) + C\Big)\overline{\psi}\,\mathrm{d}x,\ \forall\,\overline{\psi} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$$

is strongly monotone and Lipschitz continuous (where we use that $\|\nabla\cdot\|_{L^2}$ is an equivalent norm on $H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ since $\mathrm{mes}(I) > 0$, that $\frac{\partial\mathcal{G}}{\partial\eta}(\eta; z) \in (0,1)$ for all $\eta \in \mathbb{R}$, $z > 0$, and that $\widetilde{T} \ge T_a$). Thus, the unique solution $\psi \in \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ to $B_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})}\psi = 0$ is the unique weak solution to (4.5).

2. Applying the test function $\psi - \widetilde{\psi}^D \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$, we derive

$$\left\|\psi - \widetilde{\psi}^D\right\|^2_{H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})} \le c\left\|\psi - \widetilde{\psi}^D\right\|_{H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})}\left\|\widetilde{\psi}^D\right\|_{H^1(\Omega_{\mathrm{D}})} + c(M)\left\|\psi - \widetilde{\psi}^D\right\|_{L^1(\Omega_{\mathrm{D}})}.$$

With Young's inequality and the fact that $\left\|\widetilde{\psi}^D\right\|_{H^1(\Omega_{\mathrm{D}})} \le c$, we estimate $\|\psi\|_{H^1} \le c_{\psi,H^1}$ independently of the choice of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$, which gives the desired constant. $\square$

Taking into account that $\widetilde{T} \ge T_a$, that $z \mapsto \mathcal{G}(\eta, z)$ is monotone increasing for negative arguments η, and that $\eta \mapsto \mathcal{G}(\eta, z)$ is monotone increasing for positive z (see Appendix A), we find

$$\begin{aligned} \underline{c_M} := \underline{N}\mathcal{G}\Big(-\frac{K+\overline{E}}{T_a} - M; 0\Big) &\le \underline{N}\mathcal{G}\Big(-\frac{K+\overline{E}}{T_a} - M; \frac{\sigma_n}{\widetilde{T}}\Big)\\ &\le N_{n0}\mathcal{G}\Big(k_M\Big(\frac{\psi}{\widetilde{T}}\Big) - \frac{\widetilde{\varphi}_n - E_n}{\widetilde{T}}; \frac{\sigma_n}{\widetilde{T}}\Big) = \widetilde{n}_M. \end{aligned}$$

Similarly, we obtain for $\widetilde{p}_M$ defined in (4.6) that

$$\underline{c_M} \le \widetilde{n}_M,\ \widetilde{p}_M < \overline{N} \text{ a.e. in } \Omega_{\mathrm{D}}. \tag{4.11}$$

Additionally, taking into account the boundedness of the mobility functions, upper and lower bounds for the ionized dopant densities δ_i in Ω_i, $i=n,p$, we find constants $c_{Ml},\ c_{Mu}>0$ such that

$$\begin{aligned} c_{Ml} &\le \widetilde{d}_{nM} := d_n(\widetilde{n}_M,\widetilde{T},|\nabla\psi|) \le c_{Mu} \quad \text{a.e. in } \Omega_\mathrm{Dn}, \\ c_{Ml} &\le \widetilde{d}_{pM} := d_p(\widetilde{p}_M,\widetilde{T},|\nabla\psi|) \le c_{Mu} \quad \text{a.e. in } \Omega_\mathrm{Dp}. \end{aligned} \tag{4.12}$$

Moreover, note that the reaction rate coefficient $\widetilde{r}:=r(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T})$ is non-negative and has a uniform upper bound on Ω_D. Having at hand the estimates (4.12) for $\widetilde{d}_{iM}$ and the upper bound for $\widetilde{r}$, we can apply the same arguments as in the proof of Lemma 4.2 in [13] to verify the following result.

Lemma 4.2 (Continuity equations) *We assume* (A). *Let* $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$. *Then* (4.7) *has a unique weak solution* $(\varphi_n,\varphi_p)\in(\varphi_n^D+H^1_\mathrm{Dn}(\Omega_\mathrm{Dn}))\times(\varphi_p^D+H^1_\mathrm{Dp}(\Omega_\mathrm{Dp}))$. *For some exponent* $s_M>2$, *it fulfills* $\|\varphi_i\|_{L^\infty(\Omega_\mathrm{Di})}\le K$, $\|\varphi_i\|_{H^1(\Omega_\mathrm{Di})}\le c_{M,H^1}$, $\|\varphi_i\|_{W^{1,s_M}(\Omega_\mathrm{Di})}\le c_{Ms}$, $i=n,p$. *These estimates and* s_M *are uniform with respect to* $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$.

Lemma 4.3 (Solution to the heat equation) *We assume* (A). *Let* $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$. *Then there exists a unique weak solution* $T\in H^1(\Omega)$ *to* (4.9). *It satisfies* $T\ge T_a$ *a.e. in* Ω. *Additionally, there is an exponent* $t_M>2$ *and a constant* $c_{T,t_M}>0$ *independent of the choice of* $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$ *such that* $\|T\|_{W^{1,t_M}(\Omega)}\le c_{T,t_M}$.

Proof. Lemma 4.2, (4.12) and the boundedness of $\widetilde{r}$ guarantee a $c_{HM}>0$ such that

$$\begin{aligned} &\Big\|\widetilde{d}_{iM}|\nabla\varphi_i|^2\Big\|_{L^{s_M/2}(\Omega_\mathrm{Di})}\le c_{HM},\ i=n,p, \\ &\Big\|\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-1\Big)(\varphi_n-\varphi_p)\Big\|_{L^{s_M/2}(\Omega_\mathrm{D})}\le c_{HM}. \end{aligned} \tag{4.13}$$

Thus, the right-hand side $h_\Omega(\widetilde{n}_M,\widetilde{p}_M,\widetilde{T},|\nabla\psi|,\nabla\varphi_n,\nabla\varphi_p,\varphi_n,\varphi_p)$ of equation (4.9) has a uniformly bounded $L^{s_M/2}(\Omega)$ norm ($s_M/2>1$) for all $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$. Therefore, there is exactly one solution $T\in H^1(\Omega)$ to the linear heat equation (4.9) with Robin boundary conditions. We introduce the exponent $\widehat{s}_M$ via

$$2<\widehat{s}_M:=\frac{4s_M}{2+s_M}<s_M \tag{4.14}$$

and find by Gröger's regularity result [15] (analogously to Step 6 of the proof of Theorem 3.1 with $\widehat{s}_M,\ t_M^*,\ t_M$ instead of $s,\ t^*,\ t$) an exponent $t_M>2$,

$$t_M:=\begin{cases} t_M^* & \text{if } \dfrac{\widehat{s}_M}{\widehat{s}_M-2}\in\Big[1,\dfrac{2t_M^*}{t_M^*-2}\Big] \\ \dfrac{2\widehat{s}_M}{4-\widehat{s}_M} & \text{if } \dfrac{\widehat{s}_M}{\widehat{s}_M-2}>\dfrac{2t_M^*}{t_M^*-2} \end{cases},\qquad \frac{1}{t_M}+\frac{1}{t_M'}=1,$$

(depending only on the data and the geometric setting) and a constant $c_{T,t_M}>0$ such that $\|T\|_{W^{1,t_M}(\Omega)}\le c_{T,t_M}$ uniformly for all $(\widetilde{\varphi}_n,\widetilde{\varphi}_p,\widetilde{T})\in\mathcal{N}$. (Here we applied (4.13) and the fact that the definition of t_M ensures the embeddings $L^{s_M/2}(\Omega)\hookrightarrow L^{\widehat{s}_M/2}(\Omega)\hookrightarrow W^{-1,t_M}(\Omega)=W^{1,t_M'}(\Omega)^*$.) Since the right-hand side of the heat equation (4.9) is nonnegative, the test of (4.9) by $-(T-T_a)^-$ leads to $T\ge T_a$ a.e. in Ω. ☐

4.3.3 Complete continuity of the fixed point map $\mathcal{Q}$

Here we prove the complete continuity of the fixed point map $\mathcal{Q}:\mathcal{N}\mapsto\mathcal{N}$, which directly implies the continuity of $\mathcal{Q}$. This proof is done in several steps: Let $\widetilde{\varphi}_i^l\rightharpoonup\widetilde{\varphi}_i$ in $H^1(\Omega_\mathrm{Di})$, $i=n,p$, and $\widetilde{T}^l\rightharpoonup\widetilde{T}$ in $W^{1,t_M}(\Omega)$. Then we verify

1. $\widetilde{\psi}^{Dl} \rightharpoonup \widetilde{\psi}^{D}$ in $H^1(\Omega_{\mathrm{D}})$ (Lemma 4.4),

2. $\psi^l \rightharpoonup \psi$ in $H^1(\Omega_{\mathrm{D}})$ for solutions to (4.5) (Lemma 4.5).

3. For each non-relabeled subsequence $\{l\}$, there is a sub-subsequence $\{l_j\}$ such that $\nabla\psi^{l_j}(x) \to \nabla\psi(x)$, $\psi^{l_j}(x) \to \psi(x)$ a.e. in Ω_{D} (Lemma 4.6).

4. Solutions $(\varphi_n^l, \varphi_p^l)$ to (4.7) converge strongly to (φ_n, φ_p) in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}})$ (Step 2 in the proof of Theorem 4.3).

5. Solutions T^l to (4.9) converge strongly to T in $W^{1,t_M}(\Omega)$ (Step 3 in the proof of Theorem 4.3).

Lemma 4.4 *We assume* (A). *Let* $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$, $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) \in \mathcal{N}$ *for all* l. *If* $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) \rightharpoonup (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ *in* $H^1(\Omega_{\mathrm{D}})^2 \times W^{1,t_M}(\Omega)$ *then* $\widetilde{\psi}^{Dl} \rightharpoonup \widetilde{\psi}^{D}$ *in* $H^1(\Omega_{\mathrm{D}})$ *for the Dirichlet functions constructed by* (4.4).

Proof. 1. Have in mind the definitions (2.18), (4.4) and the proof of Lemma 2.1. Let $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) \rightharpoonup (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in $H^1(\Omega_{\mathrm{D}})^2 \times W^{1,t_M}(\Omega)$. The convergence of the terms in (4.4) with $\widetilde{\varphi}_i$ follows directly from $\widetilde{\varphi}_i^l \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, and the definition of τ in (2.19). The difficult part are the convergences of $V_i(\widetilde{T}^l)$.

Since the triples belong to $\mathcal{N}$, we have uniform L^∞ bounds for $\widetilde{\varphi}_i^l$, $\widetilde{\varphi}_i$, $i = n, p$, $0 < T_a \le \widetilde{T}^l$, $\widetilde{T} \le T_u$. The results of Appendix A, especially Lemma A.2, ensure the needed continuity and differentiability properties of $T \mapsto V_i(T)$ for $T_a < T < T_u$. We use the notation of Appendix A and demonstrate the weak convergence of $\tau V_i(\widetilde{T}^l) \rightharpoonup \tau V_i(\widetilde{T})$ in $H^1(\Omega_{\mathrm{D}})$.

The compact embedding of $W^{1,t_M}(\Omega)$ into $L^\infty(\Omega)$ ensures $\widetilde{T}^l \to \widetilde{T}$ in $L^\infty(\Omega_{\mathrm{D}})$. Moreover, $\widetilde{T}^l \rightharpoonup \widetilde{T}$ in $W^{1,t_M}(\Omega)$ yields that $\nabla\widetilde{T}^l \rightharpoonup \nabla\widetilde{T}$ in $L^2(\Omega_{\mathrm{D}})^2$. Let $v \in H^1(\Omega_{\mathrm{D}})$ be arbitrary. Due to the continuous differentiability of the map $T \to V_i(T)$ and Lemma A.2 we have

$$\int_{\Omega_{\mathrm{D}}} \tau\Big(V_i(\widetilde{T}^l) - V_i(\widetilde{T})\Big) v \,\mathsf{d}x \le c\,\|v\|_{L^2} \left\|\widetilde{T}^l - \widetilde{T}\right\|_{L^2} \max_{\theta\in[T_a,T_u]} \left|\frac{\mathsf{d}V_i}{\mathsf{d}T}(\theta)\right| \to 0.$$

For the gradients of τV_i, we use the following decomposition

$$\int_{\Omega_{\mathrm{D}}} \nabla\Big[\tau\Big(V_i(\widetilde{T}^l) - V_i(\widetilde{T})\Big)\Big] \cdot \nabla v \,\mathsf{d}x = I_1 + I_2 + I_3,$$

where

$$\begin{aligned}
\Big|I_1\Big| &:= \Big|\int_{\Omega_{\mathrm{D}}} \Big(V_i(\widetilde{T}^l) - V_i(\widetilde{T})\Big)\nabla\tau \cdot \nabla v \,\mathsf{d}x\Big| \le c\,\|v\|_{H^1} \left\|\widetilde{T}^l - \widetilde{T}\right\|_{L^2} \max_{\theta\in[T_a,T_u]} \left|\frac{\mathsf{d}V_i}{\mathsf{d}T}(\theta)\right| \to 0,\\
\Big|I_2\Big| &:= \Big|\int_{\Omega_{\mathrm{D}}} \tau\Big[\frac{\mathsf{d}V_i}{\mathsf{d}T}(\widetilde{T}^l) - \frac{\mathsf{d}V_i}{\mathsf{d}T}(\widetilde{T})\Big]\nabla\widetilde{T}^l \cdot \nabla v \,\mathsf{d}x\Big|\\
&\le c\,\|v\|_{H^1} \left\|\widetilde{T}^l\right\|_{H^1} \left\|\widetilde{T}^l - \widetilde{T}\right\|_{L^\infty} \max_{\theta\in[T_a,T_u]} \left|\frac{\mathsf{d}^2V_i}{\mathsf{d}T^2}(\theta)\right| \to 0.
\end{aligned}$$

In the last estimate, we used $\left\|\widetilde{T}^l\right\|_{H^1(\Omega_{\mathrm{D}})} \le c$, $v \in H^1(\Omega_{\mathrm{D}})$, $\widetilde{T}^l \to \widetilde{T}$ in $L^\infty(\Omega_{\mathrm{D}})$, and the boundedness of $\frac{\mathsf{d}^2V_i}{\mathsf{d}T^2}(\theta)$. Moreover, we have

$$I_3 := \int_{\Omega_{\mathrm{D}}} \nabla(\widetilde{T}^l - \widetilde{T}) \cdot \nabla v\, \tau \frac{\mathsf{d}V_i}{\mathsf{d}T}(\widetilde{T}) \,\mathsf{d}x \to 0$$

since the product of τ, $\frac{\mathsf{d}V_i}{\mathsf{d}T}(\widetilde{T})$, and ∇v can be used as test function for the weak convergence of $\nabla\widetilde{T}^l \rightharpoonup \nabla\widetilde{T}$ in $L^2(\Omega_{\mathrm{D}})^2$. $\square$

Lemma 4.5 *We assume* (A) *and consider* $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ *with* $\widetilde{\varphi}_i^l \rightharpoonup \widetilde{\varphi}_i$ *in* $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, *and* $\widetilde{T}^l \rightharpoonup \widetilde{T}$ *in* $W^{1,t_M}(\Omega)$. *Let* ψ^l *and* ψ *denote the unique weak solutions to* (4.5) *corresponding to the Dirichlet functions* $\widetilde{\psi}^{Dl}$ *and* $\widetilde{\psi}^D$. *Then* $\psi^l \rightharpoonup \psi$ *in* $H^1(\Omega_{\mathrm{D}})$ *and* $\psi^l \to \psi$ *in* $L^r(\Omega_{\mathrm{D}})$ *for all* $r \in [1, \infty)$.

Proof. 1. Let ψ be the solution to (4.5) corresponding to the boundary function $\widetilde{\psi}^D$ and let $\widehat{\psi}^l \in \widetilde{\psi}^{Dl} + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ be the unique solution to the linear elliptic problem

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \widehat{\psi}^l) &= C + \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \quad \text{in } \Omega_{\mathrm{D}}, \\ \widehat{\psi}^l &= \widetilde{\psi}^{Dl} \quad \text{on } I, \quad \varepsilon \nabla \widehat{\psi}^l \cdot \nu = 0 \quad \text{on } \partial\Omega_{\mathrm{D}} \backslash I. \end{aligned} \tag{4.15}$$

Thus, $w^l := \psi - \widehat{\psi}^l$ is the solution of $-\nabla \cdot (\varepsilon \nabla w^l) = 0$ with mixed boundary conditions, where the Dirichlet function is given by $w^{Dl} = \widetilde{\psi}^D - \widetilde{\psi}^{Dl}$. The map that associates the solution $w^l \in w^{Dl} + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ to w^{Dl} is bounded and linear, and therefore continuous. According to [22, Prop. 4.2, p. 159] it is also continuous with respect to the weak topology meaning that $w^{Dl} \rightharpoonup 0$ in $H^1(\Omega_{\mathrm{D}})$ implies $w^l = \psi - \widehat{\psi}^l \rightharpoonup 0$ in $H^1(\Omega_{\mathrm{D}})$ and $\widehat{\psi}^l \to \psi$ in $L^r(\Omega_{\mathrm{D}})$, $r \in [1, \infty)$.

2. Using the test function $\psi^l - \widehat{\psi}^l \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ for problem (4.5) with solution ψ^l and for problem (4.15) with solution $\widehat{\psi}^l$ yields

$$\begin{aligned} &c \left\| \psi^l - \widehat{\psi}^l \right\|^2_{H^1(\Omega_{\mathrm{D}})} \\ &\leq \int_{\Omega_{\mathrm{D}}} \Big(\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \Big) (\psi^l - \widehat{\psi}^l) \,\mathrm{d}x \\ &= \int_{\Omega_{\mathrm{D}}} \Big(\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) + \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \Big) (\psi^l - \widehat{\psi}^l) \,\mathrm{d}x. \end{aligned}$$

The monotonicity of $\eta \to \mathcal{G}(\eta, z)$ gives $\big(\mathcal{U}(\psi^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)\big)(\psi^l - \widehat{\psi}^l) \leq 0.$

Since $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ (uniform bounds and especially the lower bound T_a for the temperatures are available) , we have continuous and bounded derivatives $\frac{\partial \mathcal{G}}{\partial \eta}$, $\frac{\partial \mathcal{G}}{\partial z}$ in the considered arguments that guarantees

$$|\mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})| \leq c_M \big(|\widehat{\psi}^l - \psi| + |\widetilde{\varphi}_n^l - \widetilde{\varphi}_n| + |\widetilde{\varphi}_p^l - \widetilde{\varphi}_p| + |\widetilde{T}^l - \widetilde{T}| \big).$$

In summary, we obtain

$$\begin{aligned} \left\| \psi^l - \widehat{\psi}^l \right\|^2_{H^1(\Omega_{\mathrm{D}})} \leq c_M \Big(&\left\| \widehat{\psi}^l - \psi \right\|_{L^2(\Omega_{\mathrm{D}})} + \left\| \widetilde{\varphi}_n^l - \widetilde{\varphi}_n \right\|_{L^2(\Omega_{\mathrm{D}})} \\ &+ \left\| \widetilde{\varphi}_p^l - \widetilde{\varphi}_p \right\|_{L^2(\Omega_{\mathrm{D}})} + \left\| \widetilde{T}^l - \widetilde{T} \right\|_{L^2(\Omega_{\mathrm{D}})} \Big) \left\| \psi^l - \widehat{\psi}^l \right\|_{L^2(\Omega_{\mathrm{D}})}, \end{aligned}$$

which ensures the convergence $\psi^l - \widehat{\psi}^l \to 0$ in $H^1(\Omega_{\mathrm{D}})$ because of Step 1 and $\widetilde{\varphi}_n^l \to \widetilde{\varphi}_n$, $\widetilde{\varphi}_p^l \to \widetilde{\varphi}_p$, $\widetilde{T}^l \to \widetilde{T}$ in $L^2(\Omega_{\mathrm{D}})$. Together with $\widehat{\psi}^l \rightharpoonup \psi$ in $H^1(\Omega_{\mathrm{D}})$ from Step 1, this yields $\psi^l \rightharpoonup \psi$ in $H^1(\Omega_{\mathrm{D}})$ and thus, $\psi^l \to \psi$ in $L^r(\Omega_{\mathrm{D}})$ for all $r \in [1, \infty)$ as $l \to \infty$. $\square$

Lemma 4.6 *We assume* (A). *Let* $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ *with* $\widetilde{\varphi}_i^l \rightharpoonup \widetilde{\varphi}_i$ *in* $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, *and* $\widetilde{T}^l \rightharpoonup \widetilde{T}$ *in* $W^{1,t_M}(\Omega)$, *let* ψ^l *and* ψ *denote the corresponding unique weak solutions to* (4.5). *Then for all non-relabeled subsequences* $\{l\}$ *there exists a sub-subsequence* $\{l_k\}$ *such that* $\psi^{l_k}(x) \to \psi(x)$ *and* $\nabla \psi^{l_k}(x) \to \nabla \psi(x)$ *a.e. in* Ω_{D}.

Proof. 1. We exhaust the Lipschitz domain $\Omega_{\mathrm{D}} \subset \mathbb{R}^2$ from inside by subdomains ω_k^1, $\omega_k^2 \subset\subset \Omega_{\mathrm{D}}$ as follows: We define

$$\Omega_{Dh} := \{x \in \Omega_{\mathrm{D}} : \mathrm{dist}(x, \partial\Omega_{\mathrm{D}} > h\}, \quad \Omega_{D2h} := \{x \in \Omega_{\mathrm{D}} : \mathrm{dist}(x, \partial\Omega_{\mathrm{D}} > 2h\}.$$

Since Ω_{D} is Lipschitz, we find some $0 < h_0 < 1/2$ such that for all $0 < h < h_0$ the set Ω_{D2h} is a nonempty simply connected subdomain of Ω_{D}. We set now $h = h_0^k$, $k \in \mathbb{N}$, and $\omega_k^1 := \Omega_{Dh_0^k}$, and $\omega_k^2 := \Omega_{D2h_0^k}$. Then by construction, $\omega_k^2 \subset \omega_{k+1}^2$, $k \in \mathbb{N}$, and $\lim_{k\to\infty} \text{mes}\,(\Omega_{\mathrm{D}} \setminus \omega_k^2) = 0$.

2. For arbitrary fixed $k \in \mathbb{N}$, let $\gamma_k \in C_0^\infty(\Omega_{\mathrm{D}})$ be such that $\gamma_k(x) = 1$ in ω_k^2 and $\gamma_k(x) = 0$ in $\Omega_{\mathrm{D}} \setminus \omega_k^1$. Then $u_k^l := \gamma_k \overline{\psi}^l$ where $\overline{\psi}^l := (\widehat{\psi}^l - \psi)$ with $\widehat{\psi}^l$ from the proof of Lemma 4.5 has zero boundary values on the entire boundary $\partial\Omega_{\mathrm{D}}$ and $\|u_k^l\|_{W^{1,2}(\Omega_{\mathrm{D}})} \le c$ for all l. Moreover, since $\nabla \cdot (\nabla \overline{\psi}^l) = 0$ ($\varepsilon = $ const), it results

$$\begin{aligned}\nabla \cdot (\nabla u_k^l) &= \nabla \cdot (\nabla(\gamma_k \overline{\psi}^l)) = \gamma_k \nabla \cdot (\nabla \overline{\psi}^l) + 2\nabla\gamma_k \cdot \nabla\overline{\psi}^l + \overline{\psi}^l \nabla \cdot (\nabla\gamma_k)\\ &= 2\nabla\gamma_k \cdot \nabla\overline{\psi}^l + \overline{\psi}^l \nabla \cdot (\nabla\gamma_k) =: f_k^l.\end{aligned}$$

Since $\left\|\overline{\psi}^l\right\|_{H^1(\Omega_{\mathrm{D}})}$ are uniformly bounded and $\gamma_k \in C^\infty(\Omega_{\mathrm{D}})$ we find that for fixed k the right hand sides f_k^l are uniformly bounded in $L^2(\Omega_{\mathrm{D}})$. Since $\omega_k^2 \subset\subset \Omega_{\mathrm{D}}$ and $u_k^l = \overline{\psi}^l$ on ω_k^2, we obtain according to Theorem 8.8 (p. 173) in [10] the uniform estimates on ω_k^2

$$\left\|\overline{\psi}^l\right\|_{W^{2,2}(\omega_k^2)} = \left\|u_k^l\right\|_{W^{2,2}(\omega_k^2)} \le c(\left\|u_k^l\right\|_{W^{1,2}(\Omega_{\mathrm{D}})} + \left\|f_k^l\right\|_{L^2(\Omega_{\mathrm{D}})}) \le c.$$

Thus, we find a subsequence $\{l_{k_j}\}$ and $\psi^* \in W^{2,2}(\omega_k^2)$ such that $\overline{\psi}^{l_{k_j}} \rightharpoonup \psi^*$ in $W^{2,2}(\omega_k^2)$ and therefore $\overline{\psi}^{l_{k_j}} \to \psi^*$ in $W^{1,2}(\omega_k^2)$. By Lemma 4.5 we know $\overline{\psi}^l \rightharpoonup 0$ in $H^1(\omega_k^2)$, the uniqueness of the weak limit ensures $\psi^* = 0$, meaning $\widehat{\psi}^{l_{k_j}} \to \psi$ in $H^1(\omega_k^2)$.

3. The construction of a subsequence $\{\widehat{\psi}^{l_k}\}$ of $\{\widehat{\psi}^l\}$ for the whole domain Ω_{D} is as follows: For all $k \in \mathbb{N}$, we choose some $\widehat{\psi}^{l_k} \in \{\widehat{\psi}^{l_{k_j}}\}$ with $\left\|\widehat{\psi}^{l_k} - \psi\right\|_{W^{1,1}(\omega_k^2)} \le \frac{1}{2^k}$ (which is possible due to Step 2), and we obtain

$$\begin{aligned}&\lim_{k\to\infty} \left\|\nabla(\widehat{\psi}^{l_k} - \psi)\right\|_{L^1(\Omega_{\mathrm{D}})} = \lim_{k\to\infty} \Big(\int_{\omega_k^2} |\nabla(\widehat{\psi}^{l_k} - \psi)|\,\mathrm{d}x + \int_{\Omega_{\mathrm{D}}\setminus\omega_k^2} |\nabla(\widehat{\psi}^{l_k} - \psi)|\,\mathrm{d}x \Big)\\ &\le \lim_{k\to\infty} \frac{1}{2^k} + \lim_{k\to\infty} c\big(\left\|\widehat{\psi}^{l_k}\right\|_{H^1(\Omega_{\mathrm{D}})} + \|\psi\|_{H^1(\Omega_{\mathrm{D}})} \big)\,\text{mes}(\Omega_{\mathrm{D}} \setminus \omega_k^2)^{1/2} = 0\end{aligned}$$

since $\left\|\widehat{\psi}^{l_k}\right\|_{H^1(\Omega_{\mathrm{D}})}$ and $\|\psi\|_{H^1(\Omega_{\mathrm{D}})}$ have a uniform bound and mes $(\Omega_{\mathrm{D}} \setminus \omega_k^2) \to 0$. This L^1 convergence ensures a non-relabeled subsequence such that $\nabla\widehat{\psi}^{l_k}(x) \to \nabla\psi(x)$ a.e. in Ω_{D}. Since $\widehat{\psi}^l - \psi^l \to 0$ in $H^1(\Omega_{\mathrm{D}})$ by Step 2 of the proof of Lemma 4.5, we find for a non-relabeled subsequence that also $\nabla\psi^{l_k}(x) \to \nabla\psi(x)$ a.e. in Ω_{D}.

4. The convergence $\psi^{l_k}(x) \to \psi(x)$ a.e. in Ω_{D} for a subsequence follows directly from Lemma 4.5. □

Theorem 4.3 *Under Assumption* (A)*, the map* $\mathcal{Q} : \mathcal{N} \to \mathcal{N}$ *is completely continuous.*

Proof. 1. Let $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l)$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ with $\widetilde{\varphi}_i^l \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$, and $\widetilde{T}^l \rightharpoonup \widetilde{T}$ in $W^{1,t_M}(\Omega)$. We have to show that $(\varphi_n^l, \varphi_p^l, T^l) := \mathcal{Q}(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) \to (\varphi_n, \varphi_p, T) := \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}}) \times W^{1,t_M}(\Omega)$.

The assumed weak convergences imply the strong convergences $\widetilde{\varphi}_i^l \to \widetilde{\varphi}_i$ in $L^r(\Omega_{\mathrm{Di}})$, $i = n, p$, and $\widetilde{T}^l \to \widetilde{T}$ in $L^r(\Omega)$ for all $r \in [1, \infty)$. Lemma 4.5 guarantees for the corresponding unique weak solutions to (4.5) that also $\psi^l \to \psi$ in $L^r(\Omega_{\mathrm{D}})$, $r \in [1, \infty)$ and Lemma 4.6 ensures that for any non-relabeled subsequence of solutions ψ^l we can find a sub-subsequence such that $\psi^{lj}(x) \to \psi(x)$ and $\nabla\psi^{lj}(x) \to \nabla\psi(x)$ a.e. in Ω_{D}.

2. In this step we verify the strong convergence $\varphi_i^l \to \varphi_i$ in $H^1(\Omega_{\mathrm{Di}})$, $i = n, p$. By Lemma 4.2 we have for the solutions φ_i^l to (4.7) that $\|\varphi_i^l\|_{H^1(\Omega_{\mathrm{Di}})} \le c_{M,H^1}$. We show that all weakly convergent subsequences of

$\{(\varphi_n^l, \varphi_p^l)\}$ in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}})$ converge weakly to the same limit (φ_n, φ_p). Then using [9, Lemma 5.4] we have $(\varphi_n^l, \varphi_p^l) \rightharpoonup (\varphi_n, \varphi_p)$ in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}})$ for the entire sequence and as a consequence $\varphi_i^l \to \varphi_i$ in $L^2(\Omega_{\mathrm{Di}})$.

Let $\{(\varphi_n^{l_k}, \varphi_p^{l_k})\}$ be a subsequence that converges weakly to some $(\varphi_n^*, \varphi_p^*)$ in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}})$. We verify that $\varphi_i^* = \varphi_i$. Since $\widetilde{\varphi}_i^{l_k} \to \widetilde{\varphi}_i$ in $L^2(\Omega_{\mathrm{Di}})$, $\widetilde{T}^{l_k} \to \widetilde{T}$ in $L^2(\Omega)$, and because of Lemma 4.6 we obtain, for a further, non-relabeled subsequence, that $\widetilde{\varphi}_i^{l_k} \to \widetilde{\varphi}_i$ a.e. in Ω_{Di}, $\widetilde{T}^{l_k} \to \widetilde{T}$ a.e. in Ω, $\psi^{l_k} \to \psi$ and $\nabla\psi^{l_k} \to \nabla\psi$ a.e. in Ω_{D}. Due to the continuity of the functions $(\psi, \varphi_n, T) \mapsto N_{n0}\mathcal{G}(\frac{\psi-\varphi_n+E_n}{T}; \frac{\sigma_n}{T})$, $(\psi, \varphi_p, T) \mapsto N_{p0}\mathcal{G}(\frac{E_p-(\psi-\varphi_p)}{T}; \frac{\sigma_p}{T})$, $(n,p,T) \mapsto r(n,p,T)$ for $T \geq T_a$ as well as the continuity of the functions d_i (with respect to T, n, p, and $|\nabla\psi|$) and because of the L^∞ bounds and the lower bound for the temperature for $(\widetilde{\varphi}_n^{l_k}, \widetilde{\varphi}_p^{l_k}, \widetilde{T}^{l_k})$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ we find for that subsequence

$$
\begin{aligned}
&\widetilde{n}_M^{l_k} := N_{n0}\mathcal{G}\Big(k_M\big(\tfrac{\psi^{l_k}}{\widetilde{T}^{l_k}}\big) - \tfrac{\widetilde{\varphi}_n^{l_k}-E_n}{\widetilde{T}^{l_k}}; \tfrac{\sigma_n}{\widetilde{T}^{l_k}}\Big) \to \widetilde{n}_M := N_{n0}\mathcal{G}\Big(k_M\big(\tfrac{\psi}{\widetilde{T}}\big) - \tfrac{\widetilde{\varphi}_n-E_n}{\widetilde{T}}; \tfrac{\sigma_n}{\widetilde{T}}\Big),\\
&\widetilde{p}_M^{l_k} := N_{p0}\mathcal{G}\Big(\tfrac{E_p+\widetilde{\varphi}_p^{l_k}}{\widetilde{T}^{l_k}} - k_M\big(\tfrac{\psi^{l_k}}{\widetilde{T}^{l_k}}\big); \tfrac{\sigma_p}{\widetilde{T}^{l_k}}\Big) \to \widetilde{p}_M := N_{p0}\mathcal{G}\Big(\tfrac{E_p+\widetilde{\varphi}_p}{\widetilde{T}} - k_M\big(\tfrac{\psi}{\widetilde{T}}\big); \tfrac{\sigma_p}{\widetilde{T}}\Big),\\
&\widetilde{r}^{l_k} := r(\widetilde{n}_M^{l_k}, \widetilde{p}_M^{l_k}, \widetilde{T}^{l_k}) \to \widetilde{r} := r(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}) \quad \text{a.e. in } \Omega_{\mathrm{D}},\\
&\widetilde{d}_{nM}^{l_k} := d_n(\widetilde{n}_M^{l_k}, \widetilde{T}^{l_k}, |\nabla\psi^{l_k}|) \to \widetilde{d}_{nM} := d_n(\widetilde{n}_M, \widetilde{T}, |\nabla\psi|) \text{ a.e. in } \Omega_{\mathrm{Dn}},\\
&\widetilde{d}_{pM}^{l_k} := d_p(\widetilde{p}_M^{l_k}, \widetilde{T}^{l_k}, |\nabla\psi^{l_k}|) \to \widetilde{d}_{pM} := d_p(\widetilde{p}_M, \widetilde{T}, |\nabla\psi|) \text{ a.e. in } \Omega_{\mathrm{Dp}}.
\end{aligned}
\tag{4.16}
$$

Using $(\varphi_n^{l_k} - \varphi_n, \varphi_p^{l_k} - \varphi_p)$ as test function in (4.7) gives

$$
\begin{aligned}
&\sum_{i=n,p} \int_{\Omega_{\mathrm{Di}}} \big\{\widetilde{d}_{iM}^{l_k}\nabla\varphi_i^{l_k} - \widetilde{d}_{iM}\nabla\varphi_i\big\} \cdot \nabla(\varphi_i^{l_k} - \varphi_i)\,\mathrm{d}x\\
&= \int_{\Omega_{\mathrm{D}}} \Big(\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}} - 1\Big) - \widetilde{r}^{l_k}\Big(\exp\frac{\varphi_n^{l_k}-\varphi_p^{l_k}}{\widetilde{T}^{l_k}} - 1\Big)\Big)\Big(\varphi_n^{l_k}-\varphi_n - \varphi_p^{l_k}+\varphi_p\Big)\,\mathrm{d}x.
\end{aligned}
\tag{4.17}
$$

We write

$$
\begin{aligned}
\widetilde{d}_{iM}^{l_k}\nabla\varphi_i^{l_k} &= \widetilde{d}_{iM}^{l_k}\nabla(\varphi_i^{l_k} - \varphi_i) + \widetilde{d}_{iM}^{l_k}\nabla\varphi_i\,,\\
\widetilde{r}^{l_k}\exp\frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\widetilde{T}^{l_k}} &= (\widetilde{r}^{l_k} - \widetilde{r})\exp\frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\widetilde{T}^{l_k}}\\
&\quad + \widetilde{r}\Big[\exp\frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\widetilde{T}^{l_k}} - \exp\frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\widetilde{T}}\Big] + \widetilde{r}\exp\frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\widetilde{T}}.
\end{aligned}
$$

Having in mind that $\widetilde{T}$, $\widetilde{T}^{l_k} \geq T_a$ a.e. in Ω, φ_i, $\varphi_i^{l_k} \in [-K, K]$ a.e. in Ω_{Di}, $\exp\frac{\varphi_n^{l_k}-\varphi_p^{l_k}}{\widetilde{T}^{l_k}} \leq c$, the Lipschitz continuity of the map $T \mapsto \exp\frac{\varphi_n-\varphi_p}{T}$ for $(\varphi_n, \varphi_p, T) \in [-K,K]^2 \times [T_a, \infty)$, the bounds from (4.12) and $\mathrm{mes}(\Gamma_{\mathrm{Di}}) > 0$ we derive from (4.17) the estimate

$$
\begin{aligned}
&c\sum_{i=n,p}\Big\|\varphi_i^{l_k} - \varphi_i\Big\|^2_{H^1(\Omega_{\mathrm{Di}})} + \int_{\Omega_{\mathrm{D}}} \widetilde{r}\Big(\exp\frac{\varphi_n^{l_k} - \varphi_p^{l_k}}{\widetilde{T}} - \exp\frac{\varphi_n - \varphi_p}{\widetilde{T}}\Big)\Big(\varphi_n^{l_k} - \varphi_n - \varphi_p^{l_k} + \varphi_p\Big)\,\mathrm{d}x\\
&\quad\leq c\sum_{i=n,p}\Big\|\nabla(\varphi_i^{l_k} - \varphi_i)\Big\|_{L^2(\Omega_{\mathrm{Di}})}\Big(\int_{\Omega_{\mathrm{Di}}} \big|\widetilde{d}_{iM}^{l_k} - \widetilde{d}_{iM}\big|^2|\nabla\varphi_i|^2\,\mathrm{d}x\Big)^{\frac12}\\
&\qquad + c\sum_{i=n,p}\Big\|\varphi_i^{l_k} - \varphi_i\Big\|_{L^2(\Omega_{\mathrm{Di}})}\Big(\Big(\int_{\Omega_{\mathrm{D}}} \big|\widetilde{r}^{l_k} - \widetilde{r}\big|^2\mathrm{d}x\Big)^{\frac12} + \Big\|\widetilde{T}^{l_k} - \widetilde{T}\Big\|_{L^2}\Big).
\end{aligned}
$$

Due to (4.12) and $\|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})} \leq c_{M,H^1}$ the first integral on the right-hand side has an integrable majorant. Since by assumption, the function r is bounded also the integrand of the integral in the last line has an integrable majorant. Using (4.16) we apply Lebesgue's dominated convergence theorem for both integrals to show that they tend to zero, and by assumption, $\widetilde{T}^{l_k} \to \widetilde{T}$ in $L^2(\Omega)$. Therefore, in summary it follows $\left\|\varphi_i^{l_k} - \varphi_i\right\|_{H^1(\Omega_{\mathrm{Di}})} \to 0$ for the subsequence related to the a.e. convergence of $\widetilde{\varphi}_n^{l_k}, \widetilde{\varphi}_p^{l_k}, \widetilde{T}^{l_k}, \psi^{l_k}, \nabla\psi^{l_k}$. Since by assumption $\varphi_n^{l_k}$ also weakly converges to φ_i^* for this subsequence, we find that $\varphi_i^* = \varphi_i$ and that the entire subsequence converges weakly to φ_i, $i = n, p$.

Since the subsequence was arbitrary, we verified that all weakly convergent subsequences of $\{(\varphi_n^l, \varphi_p^l)\}$ converge weakly to (φ_n, φ_p). Thus, by [9, Lemma 5.4] it follows $(\varphi_n^l, \varphi_p^l) \rightharpoonup (\varphi_n, \varphi_p)$ in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}})$ for the entire sequence.

In summary, we know that the subsequence $\{\varphi_i^{l_k}\}$ is strongly convergent, $\varphi_i^{l_k} \to \varphi_i$ in $H^1(\Omega_{\mathrm{Di}})$, and the entire sequence $\varphi_i^l \rightharpoonup \varphi_i$ in $H^1(\Omega_{\mathrm{Di}})$. The uniqueness of the weak limit guarantees that every strongly converging subsequence converges to φ_i. If there would be any subsequence $\{\varphi_i^{l_n}\}$ that does not contain any converging subsequence then there would be a $\alpha > 0$ such that $\left\|\varphi_i^{l_n} - \varphi_i\right\|_{H^1} \geq \alpha$ for all l_n. We lead this to a contradiction again by the method of this Step 2 using the convergences a.e. of $\widetilde{\varphi}_i^{l_n}, \widetilde{T}^{l_n}, \psi^{l_n}$, and $\nabla\psi^{l_n}$ for a corresponding non-relabeled subsequence. Therefore, we obtain $\varphi_i^l \to \varphi_i$ in $H^1(\Omega_{\mathrm{Di}})$ for the entire sequence, $i = n, p$.

3. It remains to verify that $T^l \to T$ in $W^{1,t_M}(\Omega)$ for the corresponding solutions to (4.9). According to Lemma 4.3 we have $\left\|T^l\right\|_{W^{1,t_M}} \leq c_{T,t_M}$ for all l. First, we show that all weakly convergent subsequences of $\{T^l\}$ in $W^{1,t_M}(\Omega)$ converge weakly to T. Then, we have $T^l \rightharpoonup T$ in $W^{1,t_M}(\Omega)$ for the entire sequence ([9, Lemma 5.4]). Let for some subsequence $\{T^{l_k}\}$ and some $T^* \in W^{1,t_M}(\Omega)$ hold true that $T^{l_k} \rightharpoonup T^*$ in $W^{1,t_M}(\Omega)$. We verify that $T^* = T$. We consider a further non-relabeled subsequence, where especially $\varphi_i^{l_k} \to \varphi_i$ in $H^1(\Omega_{\mathrm{Di}})$, $\varphi_i^{l_k} \to \varphi_i$ a.e. in Ω_{Di}, $\widetilde{T}^{l_k} \to \widetilde{T}$ a.e. in Ω, $\psi^{l_k} \to \psi$ and $\nabla\psi^{l_k} \to \nabla\psi$ a.e. in Ω_{D}, $i = n, p$. Our construction of $\widehat{s}_M$ and $t_M > 2$ in Lemma 4.3 ensures the embedding $L^{\widehat{s}_M/2}(\Omega) \hookrightarrow W^{-1,t_M}(\Omega) = W^{1,t'_M}(\Omega)^*$, where $\frac{1}{t_M} + \frac{1}{t'_M} = 1$. The result of Gröger [15] for the linear heat equation guarantees the estimate,

$$\left\|T^{l_k} - T\right\|_{W^{1,t_M}(\Omega)} \leq c\left\|\widetilde{h}_\Omega^{l_k} - \widetilde{h}_\Omega\right\|_{W^{1,t_M{}'}(\Omega)^*} \leq c\left\|\widetilde{h}_\Omega^{l_k} - \widetilde{h}_\Omega\right\|_{L^{\widehat{s}_M/2}(\Omega)}, \tag{4.18}$$

with the right-hand sides $\widetilde{h}_\Omega^{l_k} := h_\Omega(\widetilde{n}_M^{l_k}, \widetilde{p}_M^{l_k}, \widetilde{T}^{l_k}, |\nabla\psi^{l_k}|, \nabla\varphi_n^{l_k}, \nabla\varphi_p^{l_k}, \varphi_n^{l_k}, \varphi_p^{l_k})$ and $\widetilde{h}_\Omega := h_\Omega(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$. We have to show $\left\|\widetilde{h}_\Omega^{l_k} - \widetilde{h}_\Omega\right\|_{L^{\widehat{s}_M/2}(\Omega)} \to 0$. Since

$$\begin{aligned}
&\left|\widetilde{d}_{iM}^{l_k}|\nabla\varphi_i^{l_k}|^2 - \widetilde{d}_{iM}|\nabla\varphi_i|^2\right| \\
&\leq \widetilde{d}_{iM}^{l_k}|\nabla(\varphi_i^{l_k} - \varphi_i)||\nabla\varphi_i^{l_k}| + \widetilde{d}_{iM}^{l_k}|\nabla\varphi_i||\nabla(\varphi_i^{l_k} - \varphi_i)| + |\widetilde{d}_{iM}^{l_k} - \widetilde{d}_{iM}||\nabla\varphi_i|^2
\end{aligned}$$

we find with (4.14)

$$\begin{aligned}
&\left\|\widetilde{d}_{iM}^{l_k}|\nabla\varphi_i^{l_k}|^2 - \widetilde{d}_{iM}|\nabla\varphi_i|^2\right\|_{L^{\widehat{s}_M/2}}^{\widehat{s}_M/2} \\
&\leq c\int_{\Omega_{\mathrm{Di}}} \Big(|\nabla(\varphi_i^{l_k} - \varphi_i)|^{\widehat{s}_M/2}|\nabla\varphi_i^{l_k}|^{\widehat{s}_M/2} + |\nabla\varphi_i|^{\widehat{s}_M/2}|\nabla(\varphi_i^{l_k} - \varphi_i)|^{\widehat{s}_M/2} \\
&\qquad + |\widetilde{d}_{iM}^{l_k} - \widetilde{d}_{iM}|^{\widehat{s}_M/2}|\nabla\varphi_i|^{\widehat{s}_M}\Big)\,\mathrm{d}x \\
&\leq c\left\|\varphi_i^{l_k} - \varphi_i\right\|_{H^1}^{\widehat{s}_M/2}\left(\left\|\varphi_i^{l_k}\right\|_{W^{1,s_M}}^{\widehat{s}_M/2} + \|\varphi_i\|_{W^{1,s_M}}^{\widehat{s}_M/2}\right) + c\int_{\Omega_{\mathrm{Di}}} |\widetilde{d}_{iM}^{l_k} - \widetilde{d}_{iM}|^{\widehat{s}_M/2}|\nabla\varphi_i|^{\widehat{s}_M}\,\mathrm{d}x.
\end{aligned}$$

Using the a.e. convergence $\widetilde{d}_{iM}^{l_k} \to \widetilde{d}_{iM}$ and the integrable majorant $c|\nabla\varphi_i|^{\widehat{s}_M}$, Lebesgue's dominated convergence theorem gives the convergence to zero of the last integral. Since $\left\|\varphi_i^{l_k} - \varphi_i\right\|_{H^1} \to 0$ and $\left\|\varphi_i^{l_k}\right\|_{W^{1,s_M}}, \|\varphi_i\|_{W^{1,s_M}} \leq c_{M,s}$ the right-hand side tends to zero for the considered subsubsequence.

Moreover, exploiting

$$\widetilde{r}^{l_k} \to \widetilde{r} \text{ and } \exp\frac{\varphi_n^{l_k}-\varphi_p^{l_k}}{\widetilde{T}^{l_k}} \to \exp\frac{\varphi_n-\varphi_p}{\widetilde{T}} \text{ a.e. in } \Omega_{\rm D},$$

and the integrable majorant $(4K\overline{r}\overline{N}^2\exp\frac{2K}{T_a})^{\widehat{s}_M/2}$ Lebesgue's dominated convergence theorem gives for this subsequence

$$\int_{\Omega_{\rm D}}\Big|\widetilde{r}^{l_k}\Big(\exp\frac{\varphi_n^{l_k}-\varphi_p^{l_k}}{\widetilde{T}^{l_k}}-1\Big)(\varphi_n^{l_k}-\varphi_p^{l_k})-\widetilde{r}\Big(\exp\frac{\varphi_n-\varphi_p}{\widetilde{T}}-1\Big)(\varphi_n-\varphi_p)\Big|^{\widehat{s}_M/2}\,\mathrm{d}x \to 0.$$

Thus, in summary we have $\big\|\widetilde{h}_\Omega^{l_k}-\widetilde{h}_\Omega\big\|_{L^{\widehat{s}_M/2}(\Omega)} \to 0$. Due to (4.18) this ensures $T^{l_k} \to T$ in $W^{1,t_M}(\Omega)$. According to [15], the solution to (4.9) with right hand side $\widetilde{h}_\Omega$ is unique, and it follows that $T^{l_k} \rightharpoonup T^* = T$ in $W^{1,t_M}(\Omega)$, for this subsequence. Since we verified for arbitrary weakly convergent subsequences $T^{l_k} \rightharpoonup T^*$ in $W^{1,t_M}(\Omega)$ that $T^*=T$, we obtain the weak convergence of the entire sequence $T^l \rightharpoonup T$ in $W^{1,t_M}(\Omega)$.

To conclude: We know that at least for one subsequence $\{T^{l_k}\}$ is strongly convergent, $T^{l_k} \to T$ in $W^{1,t_M}(\Omega)$, and for the entire sequence $T^l \rightharpoonup T$ in $W^{1,t_M}(\Omega)$. The method of Step 3 and the uniqueness of the weak limit guarantees that every strongly converging subsequence converges to T. If there would be any subsequence $\{T^{l_n}\}$ that does not contain any converging subsequence then there would be a $\alpha > 0$ such that $\|T^{l_n}-T\|_{W^{1,t_M}(\Omega)} \geq \alpha$ for all l_n. As in Step 3, we lead this to a contradiction using the convergences a.e. for a corresponding non-relabeled subsequence. Finally, the entire sequence T^l must strongly converge to T in $W^{1,t_M}(\Omega)$ which finishes the proof. □

4.3.4 Solvability of (P_M)

Here we prove Theorem 4.2. The set $\mathcal{N}$ is nonempty, closed, and convex in $H^1(\Omega_{\rm Dn})\times H^1(\Omega_{\rm Dp})\times W^{1,t_M}(\Omega)$. Applying Theorem 4.3 and Schauder's fixed point theorem, we obtain at least one fixed point $(\varphi_n,\varphi_p,T)\in\mathcal{N}$ of $\mathcal{Q}$. For this fixed point, we define as in (2.18) the Dirichlet function

$$\psi^D := (1-\tau)\big(\varphi_n+V_n(T)\big)+\tau\big(\varphi_p-V_p(T)\big) \in H^1(\Omega_{\rm D})\cap L^\infty(\Omega_{\rm D}),$$

solve by Lemma 4.1 the problem $B_{(\varphi_n,\varphi_p,T)}\psi = 0$, and gain a unique weak solution $\psi \in \psi^D + H^1_{\rm I}(\Omega_{\rm D})$ to the nonlinear Poisson equation (4.5). It remains to show that the quadruple $(\psi,\varphi_n,\varphi_p,T)$ lies in the correct spaces in the sense of (P$_M$).

The definition of $\mathcal{N}$ ensures $T \in \{u\in H^1(\Omega): \ln u \in L^\infty(\Omega)\}$. Since (φ_n,φ_p,T) is a fixed point of $\mathcal{Q}$, the regularized continuity equations (middle equation in (P$_M$)) hold true and Step 2 of the proof of Theorem 3.1 for Problem (P) can be applied with the same constants for the regularized situation, see especially (3.1). Therefore, the estimates in Step 3 of that proof remain valid with the same constants, now for the heat equation with the regularized right-hand side, giving especially $\|T\|_{L^2(\Gamma)} \leq c_T$. Since (φ_n,φ_p,T) is a fixed point of $\mathcal{Q}$, Lemma 4.2 guarantees $\varphi_i \in W^{1,s_M}(\Omega_{\rm Di})$, $i=n,p$. Now the Poisson equation and the heat equation (first and last equation in (P$_M$)) are simultaneously fulfilled. Thus, we can repeat the arguments in Step 4 in the proof of Theorem 3.1 (see also Step 1 in the proof of Theorem 4.1) to obtain an L^∞ estimate for ψ/T with exactly the same bound $c_{\psi/T}$. Now we proceed as in Step 2 in the proof of Theorem 4.1 and repeat Step 5 in the proof of Theorem 3.1 to ensure that $\varphi_i \in W^{1,s}(\Omega_{\rm Di})$, $i=n,p$. Therefore, $(\psi,\varphi_n,\varphi_p,T)$ solves Problem (P$_M$) which proves Theorem 4.2.

Therefore, also the proof of Theorem 3.2 is finished.

5 Discussion

In this paper, we studied a coarse-grained model for the electrothermal behavior of organic semiconductor devices under some simplifying model assumptions. For example, we neglected the temperature dependence of E_n and E_p, the disorder parameters $\sigma_n,\ \sigma_p$, the total density of transport states N_{i0} and the charged doping densities N_D^+ and N_A^-. This was done so as not to overload the analytical estimates and to concentrate on the main coupling mechanisms and their analytical treatment in the case of organic semiconductor devices. In [12], we presented an existence proof for a coarse-grained model in the inorganic case with Boltzmann statistics where the temperature dependencies of band edges, effective density of state and charged doping densities are fully contained.

A Appendix: Properties of the Gauss–Fermi integral

Here we collect needed properties of the statistical relation for organic semiconductors from [4, Section 2.1], [11, Lemma 2.1], [13, Lemma 2.1] and derive some further needed properties. The Gauss–Fermi integral is given by

$$\mathcal{G}(\eta, z) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big(-\frac{\xi^2}{2}\Big) \frac{1}{\exp(z\xi-\eta)+1}\, \mathrm{d}\xi. \tag{A.1}$$

Note that $\mathcal{G}(0,z) = \frac{1}{2}$ for all $z > 0$. For $\eta \in \mathbb{R}$ and $z > 0$, the partial derivatives of first and second order exist and are given via

$$\begin{aligned}
\frac{\partial \mathcal{G}}{\partial \eta}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big\{-\frac{\xi^2}{2}\Big\} \frac{\exp(z\xi-\eta)}{[\exp(z\xi-\eta)+1]^2}\, \mathrm{d}\xi, \\
\frac{\partial}{\partial z}\mathcal{G}(\eta; z) &= -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big\{-\frac{\xi^2}{2}\Big\} \frac{\exp(z\xi-\eta)\xi}{[\exp(z\xi-\eta)+1]^2}\, \mathrm{d}\xi, \\
\frac{\partial^2 \mathcal{G}}{\partial \eta^2}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big\{-\frac{\xi^2}{2}\Big\} \frac{\exp(z\xi-\eta)[\exp(z\xi-\eta)-1]}{[\exp(z\xi-\eta)+1]^3}\, \mathrm{d}\xi, \\
\frac{\partial^2 \mathcal{G}}{\partial z \partial \eta}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big\{-\frac{\xi^2}{2}\Big\} \frac{\xi\exp(z\xi-\eta)[1-\exp(z\xi-\eta)]}{[\exp(z\xi-\eta)+1]^3}\, \mathrm{d}\xi, \\
\frac{\partial^2 \mathcal{G}}{\partial z^2}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\Big\{-\frac{\xi^2}{2}\Big\} \frac{\xi^2\exp(z\xi-\eta)[\exp(z\xi-\eta)-1]}{[\exp(z\xi-\eta)+1]^3}\, \mathrm{d}\xi.
\end{aligned} \tag{A.2}$$

They satisfy

$$\frac{\partial \mathcal{G}}{\partial \eta}(\eta; z) \in (0,1) \quad \text{and} \quad \lim_{\eta\to+\infty} \frac{\partial \mathcal{G}}{\partial \eta}(\eta; z) = \lim_{\eta\to-\infty} \frac{\partial \mathcal{G}}{\partial \eta}(\eta; z) = 0,$$

and

$$\frac{\partial}{\partial z}\mathcal{G}(\eta; z) \begin{cases} > 0 & \text{if } \eta < 0 \\ = 0 & \text{if } \eta = 0 \\ < 0 & \text{if } \eta > 0 \end{cases} \quad \text{and} \quad \Big|\frac{\partial}{\partial z}\mathcal{G}(\eta; z)\Big| \le \frac{1}{z}(1+\exp|\eta|) \quad \forall z > 0,\, \forall \eta \in \mathbb{R} \tag{A.3}$$

which ensures a constant $c_{k,\underline{z}} > 0$ such that $\Big|\frac{\partial}{\partial z}\mathcal{G}(\eta; z)\Big| \le c_{k,\underline{z}}$ for all $\eta \in \mathbb{R}$ with $|\eta| \le k$ and all z with $z \ge \underline{z} > 0$. Moreover, we find some $c_{k,\overline{z}} > 0$ such that

$$\frac{\partial \mathcal{G}}{\partial \eta}(\eta, z) \ge c_{k,\overline{z}} \quad \text{for all } \eta \in \mathbb{R} \text{ with } |\eta| \le k \text{ and all } z \text{ with } \overline{z} \ge z > 0. \tag{A.4}$$

This estimate follows directly from the inequalities

$$\begin{aligned}
\frac{\partial \mathcal{G}}{\partial \eta}(\eta, z) &> \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \exp\big(-\frac{\xi^2}{2}\big) \frac{\exp(z\xi-\eta)}{[\exp(z\xi-\eta)+1]^2}\, \mathrm{d}\xi \\
&\ge \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \exp\big(-\frac{\xi^2}{2}\big)\, \mathrm{d}\xi \ \frac{\exp(-\overline{z}-|\eta|)}{[\exp(\overline{z}+|\eta|)+1]^2} \\
&\ge \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} \exp\big(-\frac{\xi^2}{2}\big)\, \mathrm{d}\xi \ \frac{\exp(-\overline{z}-k)}{[\exp(\overline{z}+k)+1]^2} =: c_{k,\overline{z}}.
\end{aligned}$$

By $\mathcal{G}^{-1}(y;z)$, we denote the inverse of $\mathcal{G}$ with respect to the first variable and for fixed z. For parameters $0<\delta<N_0$, $E\in\mathbb{R}$, $\sigma>0$, and $T>0$, let the quantity $V(T)=T\mathcal{G}^{-1}(\frac{\delta}{N_0};\frac{\sigma}{T})-E$ be the unique solution to $\mathcal{H}(T,V(T))=0$ as in (2.6), where $\mathcal{H}(T,v):=N_0\mathcal{G}(\frac{v+E}{T};\frac{\sigma}{T})-\delta$.

Lemma A.1 *1. If $T\ge T_l$ for some $T_l>0$, $2\delta\le N_0$, and $V(T)$ solves $\mathcal{H}(T,V(T))=0$ then*

$$T\mathcal{G}^{-1}\Big(\frac{\delta}{N_0};\frac{\sigma}{T_l}\Big)-E\le V(T)\le -E. \tag{A.5}$$

Proof. By $\delta=N_0\mathcal{G}(\eta;z)$ and $2\delta\le N_0$ we get $\eta=\frac{V(T)+E}{T}<0$ which ensures the upper estimate $V(T)<-E$. According to [13, Lemma 2.1] we find

$$\frac{\delta}{N_0}=\mathcal{G}\Big(\eta;\frac{\sigma}{T}\Big)\le\mathcal{G}\Big(\eta;\frac{\sigma}{T_l}\Big).$$

Since $\mathcal{G}$ is monotone increasing in the first argument, it follows $\frac{V(T)+E}{T}\ge\mathcal{G}^{-1}\Big(\frac{\delta}{N_0};\frac{\sigma}{T_l}\Big)$, which gives the desired lower estimate. □

Lemma A.2 *We assume $2\delta\le N_0$, $0<T_l\le T\le T_u$ for some T_l, T_u, and $\sigma>\underline{\sigma}>0$. Let $V(T)$ solve $\mathcal{H}(T,V(T))=0$. Then the derivatives $\frac{\mathrm{d}V}{\mathrm{d}T}(T)$ and $\frac{\mathrm{d}^2V}{\mathrm{d}T^2}(T)$ are bounded by constants depending on T_l, T_u.*

Proof. 1. Since $\frac{\partial\mathcal{H}}{\partial v}(T,v)=\frac{N_0}{T}\frac{\partial\mathcal{G}}{\partial\eta}\Big(\frac{v+E}{T};\frac{\sigma}{T}\Big)>0$ for all $v\in\mathbb{R}$ the implicit function theorem can be used to obtain with the abbreviations $\eta(T)=\frac{V(T)+E}{T}$, $z=\frac{\sigma}{T}$ the relation

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}T}(T)&=-\Big[\frac{\partial\mathcal{H}}{\partial v}(T,V(T))\Big]^{-1}\frac{\partial\mathcal{H}}{\partial T}(T,V(T))\\&=\Big[\frac{\partial\mathcal{G}}{\partial\eta}\Big(\eta(T);z\Big)\Big]^{-1}\Big[\frac{\partial\mathcal{G}}{\partial\eta}\Big(\eta(T);z\Big)\eta(T)+\frac{\partial\mathcal{G}}{\partial z}\Big(\eta(T);z\Big)z\Big]\\&=\Big[\frac{\partial\mathcal{G}}{\partial\eta}\Big(\eta(T);z\Big)\Big]^{-1}\frac{\partial\mathcal{G}}{\partial z}\Big(\eta(T);z\Big)z+\mathcal{G}^{-1}\Big(\frac{\delta}{N_0};z\Big)\end{aligned}\tag{A.6}$$

for all $T>0$. Note that for temperatures with upper and lower bounds, we get bounds for $\frac{\mathrm{d}V(T)}{\mathrm{d}T}$, see (A.3), (A.4), and Lemma A.1. Therefore, using $|V(T)-V(T_1)|\le|\frac{\mathrm{d}V}{\mathrm{d}T}(T_\theta)||T-T_1|$ for some $T_\theta\in[T_l,T_u]$, we obtain the continuity of the map $T\mapsto V(T)$.

2. Moreover, implicit differentiation gives (here we leave out the arguments)

$$\frac{\partial^2\mathcal{H}}{\partial T^2}+2\frac{\partial^2\mathcal{H}}{\partial v\partial T}\frac{\mathrm{d}V}{\mathrm{d}T}(T)+\frac{\partial^2\mathcal{H}}{\partial v^2}\Big(\frac{\mathrm{d}V}{\mathrm{d}T}(T)\Big)^2+\frac{\partial\mathcal{H}}{\partial v}\frac{\mathrm{d}^2V}{\mathrm{d}T^2}(T)=0$$

and results in

$$\frac{\mathrm{d}^2V}{\mathrm{d}T^2}(T)=-\Big(\frac{\partial\mathcal{H}}{\partial v}\Big)^{-1}\Big[\frac{\partial^2\mathcal{H}}{\partial T^2}+2\frac{\partial^2\mathcal{H}}{\partial v\partial T}\frac{\mathrm{d}V}{\mathrm{d}T}(T)+\frac{\partial^2\mathcal{H}}{\partial v^2}\Big(\frac{\mathrm{d}V}{\mathrm{d}T}(T)\Big)^2\Big],$$

where it remains to show that the term in the bracket stays bounded for temperatures with upper and lower bounds to establish the boundedness of $\frac{\mathrm{d}^2V}{\mathrm{d}T^2}(T)$. Note that

$$\begin{aligned}\frac{\partial^2\mathcal{H}}{\partial v^2}&=\frac{N_0}{T^2}\frac{\partial^2\mathcal{G}}{\partial\eta^2},\\\frac{\partial^2\mathcal{H}}{\partial T\partial v}&=-\frac{N_0}{T^2}\Big[\frac{\partial\mathcal{G}}{\partial\eta}+\frac{\partial^2\mathcal{G}}{\partial\eta^2}\eta+\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}z\Big],\\\frac{\partial^2\mathcal{H}}{\partial T^2}&=\frac{N_0}{T^2}\Big[\frac{\partial\mathcal{G}}{\partial\eta}\eta+\frac{\partial\mathcal{G}}{\partial z}z+\frac{\partial^2\mathcal{G}}{\partial\eta^2}\eta^2+\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}z\eta+\frac{\partial\mathcal{G}}{\partial\eta}\eta+\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}z\eta+\frac{\partial^2\mathcal{G}}{\partial z^2}z^2+\frac{\partial\mathcal{G}}{\partial z}z\Big]\\&=\frac{N_0}{T^2}\Big[2\frac{\partial\mathcal{G}}{\partial\eta}\eta+2\frac{\partial\mathcal{G}}{\partial z}z+\frac{\partial^2\mathcal{G}}{\partial\eta^2}\eta^2+2\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}z\eta+\frac{\partial^2\mathcal{G}}{\partial z^2}z^2\Big].\end{aligned}$$

Next, we verify the boundedness of $\frac{\partial^2\mathcal{G}}{\partial\eta^2}$, $\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}$, $\frac{\partial^2\mathcal{G}}{\partial z^2}$ for $0 < T_l < T < T_u$, $\sigma > \underline{\sigma} > 0$, and $|v| \leq c$. Because of $\left|\frac{y(y-1)}{(y+1)^3}\right| < 1$ for all $y \geq 0$, we find from (A.2) that

$$\Big|\frac{\partial^2\mathcal{G}}{\partial\eta^2}(\eta, z)\Big| \leq \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\exp\Big\{-\frac{\xi^2}{2}\Big\}\,\mathrm{d}\xi = 1.$$

In the expressions for $\frac{\partial^2\mathcal{G}}{\partial z^2}$ and $\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}$, respectively, in (A.2) we write

$$\frac{\xi^2\exp(z\xi-\eta)[\exp(z\xi-\eta)-1]}{[\exp(z\xi-\eta)+1]^3} = \frac{\xi^2\exp(z\xi)}{(\exp(z\xi)+1)^2}\frac{(\exp(z\xi)+1)^2\exp(-\eta)[\exp(z\xi-\eta)-1]}{[\exp(z\xi-\eta)+1]^3}$$

and

$$\frac{\xi\exp(z\xi-\eta)[1-\exp(z\xi-\eta)]}{[\exp(z\xi-\eta)+1]^3} = \frac{\xi\exp(z\xi)}{(\exp(z\xi)+1)^2}\frac{(\exp(z\xi)+1)^2\exp(-\eta)[1-\exp(z\xi-\eta)]}{[\exp(z\xi-\eta)+1]^3}.$$

Since $\frac{|y^2\exp(y)|}{(\exp(y)+1)^2}, \frac{|y\exp(y)|}{(\exp(y)+1)^2} \leq 1$ for all $y \in \mathbb{R}$, we can estimate the absolute value of the first factor on the right-hand side of the first equation by $\frac{1}{z^2}$ and in the second equation by $\frac{1}{z}$. To handle the absolute value of the second factor in both equalities, we set $a := \exp(z\xi)$, $b := \exp(-\eta)$ and have to estimate

$$\frac{|(a+1)^2b(ab-1)|}{(ab+1)^3} = \frac{|a^3b^2+a^2(2b^2-b)+a(b^2-2b)-b|}{a^3b^3+3a^2b^2+3ab+1} \quad \text{for } a, b > 0.$$

In case of $b \geq 1$ (meaning $\eta \leq 0$) we estimate

$$\frac{|(a+1)^2b(ab-1)|}{(ab+1)^3} \leq \frac{a^3b^4+2a^2b^3+ab^2+b}{a^3b^3+3a^2b^2+3ab+1} = \frac{b(a^3b^3+2a^2b^2+ab+1)}{a^3b^3+3a^2b^2+3ab+1} \leq b.$$

For the case $b < 1$ (meaning $\eta > 0$) we find

$$\frac{|(a{+}1)^2b(ab{-}1)|}{(ab+1)^3} = \frac{|a^3b^3{+}a^2(2b^3{-}b^2){+}ab(b^2{-}2b){-}b^2|}{b(a^3b^3+3a^2b^2+3ab+1)} \leq \frac{a^3b^3+a^2b^2+2ab+1}{b(a^3b^3+3a^2b^2+3ab+1)} \leq \frac{1}{b}.$$

Therefore, in both integrands of $\frac{\partial^2\mathcal{G}}{\partial z^2}$ and $\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}$, the absolute value of the second factor in both equalities can be estimated by $\exp(|\eta|)$. In summary, we end up with

$$\Big|\frac{\partial^2\mathcal{G}}{\partial z^2}(\eta, z)\Big| \leq \frac{1}{z^2}\exp(|\eta|), \quad \Big|\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}(\eta, z)\Big| \leq \frac{1}{z}\exp(|\eta|).$$

This guarantees for arguments $\eta = \frac{v+E}{T}$ and $z = \frac{\sigma}{T}$ with $|v| \leq c$, $|E| \leq c_0$, and $0 < T_l < T < T_u$ uniform bounds for all the second derivatives of $\mathcal{G}$. $\square$

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