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A coarse-grained electrothermal model for organic semiconductor devices

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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.

KEYWORDS

charge & heat transport, coarse-grained model, drift-diffusion, electrothermal interaction, organic semiconductor, weak solutions

MSC CLASSIFICATION

35J57; 35K05; 78A35

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., Kordt et al.[1]). 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, for example, organic solar cells and transistors.[2,3] 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.[4,5] Therefore, models and simulations of the electrothermal interplay in multidimensional organic devices are required that are as accurate as necessary but computationally efficient. Such effective descriptions can be obtained by combining models in substructures with different complexity. In the isothermal case, this approach has already been used for inorganic semiconductor devices, for example, in other studies.[6–8]

In the present paper, we consider organic devices and take the coupling to heat flow into account. Starting from a stationary drift-diffusion-based electrothermal model for organic semiconductors (see 2.1), we construct a coarse-grained model that retains the strong coupling of the electrothermal effects while simultaneously accounting for the different depth in the characterization of the electric current flow. The model results from combining a drift-diffusion system in critical subregions of the device with reduced thermistor-like models for device substructures with n-doped or p-doped regions. Hence, the full drift-diffusion model is applied only in the electronic relevant subregions of the device where one balances both electron and hole current as well as generation/recombination processes. In contrast, the thermistor-type models, which are derived as limiting cases of the full drift-diffusion model, contain only one equation for the net current flow coupled to the heat equation as follows,

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

with electric conductivity $\widetilde{\sigma}$ depending on the temperature, the gradient of the temperature, and the electric field.

Naturally, this model fragmentation applied on semiconductor devices requires suitable transfer conditions at the interfaces among the neighboring subregions that guarantee the continuity of 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.

It is worth noting that the proposed approach entailing the derivation of coarse-grained models for substructures of different physical complexity is firmly rooted in applications. Depending on the device geometry and doping, the subregions where reduced models are suitable can be quite large. For instance, in large-area thin-film organic LEDs the n-doped and p-doped layers cover together more than half of the height of the film, see the middle picture in fig. 2 of Zheng et al.[4] Furthermore, the simplicity of reduced models could be utilized to model the doped layers adjacent to the oxide in pinMOS structures, see Figure 1 in Zheng et al.[9]

In the main part of the paper, we study the analytical properties of the coarse-grained model, that os, existence, boundedness, and regularity of solutions. One crucial point thereby is the analytical treatment of the transfer and boundary conditions between the different subregions, especially the prescribed Dirichlet function for the Poisson equation at the interface to the drift-diffusion subregion. To ensure the required regularity of the latter (see 2.18), we restrict ourselves to two spatial dimensions. Similar investigations were carried out in Glitzky et al[10] for classical, inorganic semiconductors with Boltzmann statistics. In the present paper, the organic setting is treated, which gives rise to novel challenges concerning the analysis: (i) mobility functions depend on temperature, density, and electric field strength; (ii) special statistical relations given by Gauss–Fermi integrals $\mathcal{G}$ (see 2.3) have to be considered, whose inverses 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 A.

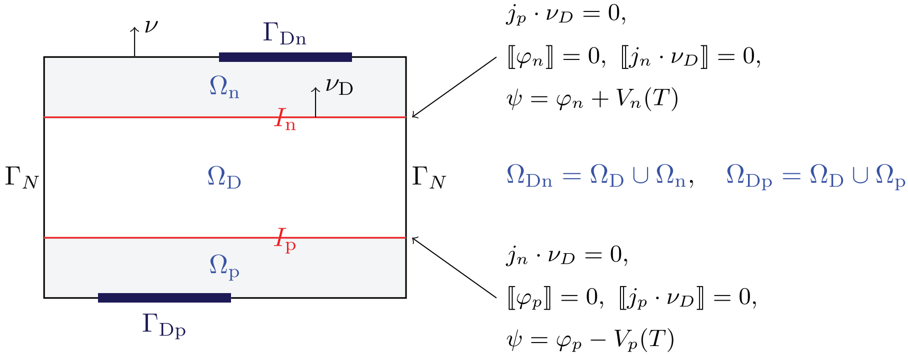

FIGURE 1 Schematic geometry of an organic semiconductor device partitioned into the different subregions and transfer conditions at interfaces, where $[\![\cdot]\!]$ denotes the jump of the argument over the respective interface [Colour figure can be viewed at wileyonlinelibrary.com]

2 | DERIVATION OF THE COARSE-GRAINED MODEL

If Ω denotes the domain of the device, the drift-diffusion model introduced in Glitzky et al.[11] (see also Doan et al[12] and Fuhrmann et al.[13]) 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, for example, Kordt et al[1] and Pasveer et al.[14] The chemical potentials are defined by $\nu_n := \psi - \varphi_n$ and $\nu_p := -(\psi - \varphi_p)$, the generation/recombination term R and the charge carrier densities n and p are given by

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

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., Doan et al.[27]), 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

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

see Paasch and Scheinert.[15] 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,

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

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 Griepentrog[16] for classical inorganic semiconductors. In this model, thermoelectric effects (Peltier, Thomson, and Seebeck) are not included. Note that in sect. II.D of Krikun and Zojer,[17] 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, for example, to other studies,[18–21] where the authors[19,20] discuss also numerical aspects.

The models (1.1) and (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,

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

For the last convergence, we also have 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

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

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

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

we find that, $0 \geq \lim_{y\to-\infty}\mathcal{G}(y; z)y \geq \lim_{y\to-\infty} y\mathrm{e}^y\,\mathrm{const} = 0$. 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 Lemma 2.1 in Glitzky et al.[11]). Therefore, we obtain

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

establishing the last convergence in (2.5).

For the considered case of strong n-doping and negligible p-density ($\delta_n \gg \delta_p \approx 0$), 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 potential" of 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

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

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 $v = V(T) = T\mathcal{G}^{-1}\left(\frac{\delta}{N_0}; \frac{\sigma}{T}\right) - E$ 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,

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

Setting the conductivity function $\tilde{\sigma} = \delta_n \mu_n(T, \delta_n, |\nabla(\varphi_n + V_n(T))|)$, 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 $\delta_p \gg \delta_n \approx 0$ we obtain, under the assumption $n \to 0$ whereas the quantities $\nabla\varphi_n, \nabla\varphi_p, \psi, \nabla\psi, \nu_p, p, T$ 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,

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

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,

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

2.2 | Notation and assumptions

In two spatial dimensions, we consider geometric situations as indicated schematically in Figure 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 $\Omega := \mathrm{int}(\overline{\Omega_\mathrm{n}} \cup \overline{\Omega_\mathrm{D}} \cup \overline{\Omega_\mathrm{p}})$. Moreover, we introduce $\Omega_\mathrm{Dj} := \mathrm{int}(\overline{\Omega_\mathrm{D}} \cup \overline{\Omega_\mathrm{j}})$, $\Gamma_\mathrm{Dj} := \Gamma_D \cap \overline{\Omega_\mathrm{j}}$, $I_\mathrm{j} := \mathrm{int}(\overline{\Omega_\mathrm{D}} \cap \overline{\Omega_\mathrm{j}})$ for j = n,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.

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 $\Omega_\mathrm{Di} \cup (\partial\Omega_\mathrm{Di} \backslash \Gamma_\mathrm{Di})$ 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 is introduced in Section 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 $\overline{\Omega_\mathrm{n}} \cap \overline{\Omega_\mathrm{p}} = \emptyset$, $\mathrm{mes}(I_\mathrm{j}) > 0$, $\mathrm{mes}(\Gamma_\mathrm{Dj}) > 0$ with $\mathrm{dist}(x, \overline{\Omega_\mathrm{Dj}}) \geq$ const > 0 for all $x \in \Gamma_\mathrm{Di}$, i≠j, and $\widetilde{\Gamma}_\mathrm{Nj} := \partial\Omega_\mathrm{Dj} \backslash \Gamma_\mathrm{Dj}$, $\Omega_\mathrm{Dj} \cup \widetilde{\Gamma}_\mathrm{Nj}$ are regular in the sense of Gröger.[22]

- $\varphi_j^D \in W^{1,\infty}(\Omega_{\mathrm{Dj}})$, $\|\varphi_j^D\|_{L^\infty(\Omega_{\mathrm{Dj}})} \le K$, $\lambda \in L^\infty(\Omega)$, $0 < \lambda_0 \le \lambda$ 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.
- The quantities $\widehat{N}_{j0}$, δ_j, $\widehat{\sigma}_j$ defined for Ω_{j} are positive constants, $\widehat{E}_j$ is constant. Moreover, $0 < \underline{N} \le \widehat{N}_{j0} \le \overline{N}$, $0 < \widehat{\sigma}_j \le \overline{\sigma}$, $|\widehat{E}_j| \le \bar{E}$, $2\delta_j \le \widehat{N}_{j0}$.
- $N_{j0}, \sigma_j \in L^\infty_+(\Omega_{\mathrm{D}})$, $C, E_j \in L^\infty(\Omega_{\mathrm{D}})$ such that $0 < \underline{N} \le N_{j0} \le \overline{N}$, $0 < \underline{\sigma} \le \sigma_j \le \overline{\sigma}$, $|E_j| \le \bar{E}$, $|C| \le \overline{C}$ 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 $r_0(\cdot, n, p, T) \le \bar{r}$ 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 $0 < \underline{\mu}_\xi \le \mu_j(\cdot, T, y, z) \le \overline{\mu}_\xi$ 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,

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

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

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

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

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

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}

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

Continuity equation for holes in Ω_{Dp}

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

Poisson equation for the electrostatic potential ψ in Ω_D

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

The function ψ^D is defined as

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

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

$$
\tau|_{I_n}=0,\ \ \tau|_{I_p}=1,\ \ |\nabla\tau|\le\hat{c}.
\tag{2.19}
$$

For a more detailed description regarding the Dirichlet function ψ^D, we refer the interested reader to Glitzky et al,[10] 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 $T\in H^1(\Omega_D)$ and $\ln T\in L^\infty(\Omega_D)$, then $V_i(T)\in H^1(\Omega_D)\cap L^\infty(\Omega_D)$, $i=n,p$.*
2. *If $\varphi_n,\varphi_p,T\in H^1(\Omega_D)$ and $\varphi_n,\varphi_p,\ln T\ \in\ L^\infty(\Omega_D)$ then the function ψ^D defined in (2.18) belongs to $H^1(\Omega_D)\cap L^\infty(\Omega_D)$.*

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 (A6), we evaluate

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

where $\eta_i = \frac{V_i(T)+\widehat{E}_i}{T}$, $z_i = \frac{\widehat{\sigma}_i}{T}$. Because of $\ln T\in L^\infty(\Omega_D)$ and the lower bound of η_i from Lemma A.1, the estimates in Subsection 2.1 of Glitzky et al[11] 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 $\mathcal{G}^{-1}\left(\frac{\delta_i}{\widehat{N}_{i0}};\frac{\widehat{\sigma}_i}{T}\right)$ are bounded from above which together with $T\in H^1(\Omega_D)$ in summary guarantees that $V_i(T)\in H^1(\Omega_D)$, $i=n,p$.
2. Due to the properties of τ,φ_n,φ_p, the assertion follows directly from Assertion 1. □

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

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

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, $n,p\in L^\infty(\Omega_\mathrm{D})$, $\mu_n(T,n,|\nabla\psi|),\mu_p(T,p,|\nabla\psi|), r(n,p,T)\in L^\infty(\Omega_\mathrm{D})$, $\mu_i(T,\delta_i,0)\in L^\infty(\Omega_\mathrm{i})$, $d_i\in L^\infty(\Omega_{\mathrm{D}i})$, $i=n,p$, $h_\Omega\in L^{s/2}(\Omega)$, 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_Ω.

3.2 | A priori estimates

The proof of a priori estimates uses similar techniques applied for the inorganic coarse-grained model in Glitzky et al.;[10] however, some essential modifications related to the statistical relation and the mobility functions (see 2.2–2.3 and the last assumption in **(A)**, respectively) have to be taken into account. The proof of the following theorem follows the arguments in,[10] all necessary modifications 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 $\|\varphi_n\|_{L^\infty(\Omega_{Dn})}, \|\varphi_p\|_{L^\infty(\Omega_{Dp})}\le K$ 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*

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

for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (3.1).

Proof.

1. As in Lemma 3.1 in[10] it is verified that $T\ge T_a$ a.e. in Ω for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (3.1).
2. Since the densities and the mobility functions μ_i are bounded, the techniques in Lemma 3.2[10] ensure also in the organic case a constant $c_h>0$, depending only on the data, such that

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

3. As in Lemma 3.3,[10] 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 (3.1).
4. Next we aim to find a constant $c_{\psi/T}>0$, depending only on the data, such that,

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

for any solution $(\psi,\varphi_n,\varphi_p,T)$ to (3.1). For this purpose, we define in the organic case

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

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. $-m\bar{z}_L^{m-1} \in H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ with

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

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 Lemma 3.4 in Glitzky et al[10] 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 Lemma 2.1 in Glitzky et al.[11]) ensure a.e. in Ω_{D}

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

where

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

depends only on the data and the underlying geometry. Using additionally the upper and lower bounds on 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 are bounded by a constant $c_R>0$. The supposed regularity of φ_n^D, φ_p^D and the regularity result Theorem 1 of Gröger[22] for elliptic problems guarantee an exponent $s>2$ and a constant $c_{\varphi,s}>0$ depending only on the data and the underlying geometry such that

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

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 $\|\varphi_i\|_{L^\infty(\Omega_{\mathrm{D}i})} \le K$, $i=n,p$. The test of (2.14) by T yields $\|T\|_{H^1} \le c$. We apply regularity results for second order elliptic equations with non-smooth data in the 2D case. According to Theorem 1 in Gröger,[22] there is $t^*>2$ such that the strongly monotone, Lipschitz continuous operator $\Lambda\colon H^1(\Omega) \mapsto H^1(\Omega)^*$,

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

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

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

This definition guarantees that $L^{s/2}(\Omega) \hookrightarrow W^{-1,t}(\Omega) := W^{1,t'}(\Omega)^*$. Remark 13 in[22] 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

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

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

3.3 | Main result

Theorem 3.2. *Under Assumption (A), there exists a solution $(\psi, \varphi_n, \varphi_p, T)$ to Problem (3.1).*

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 (3.1) consists of a manipulation of the statistical relation (see 4.1) giving regularized densities which occur 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 (3.1) 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, for example, Fischer et al[5] and Doan et al.[12]

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 (3.1). 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 $\psi^* \in H^1(\Omega_D)$ is the unique solution to the nonlinear Poisson equation in Ω_D,*

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

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

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

Proof. Let $(\psi, \varphi_n, \varphi_p, T)$ be an arbitrary solution to (3.1) guaranteed by Theorem 3.2. The test function $(\varphi_n - \varphi_n^D, \varphi_p - \varphi_p^D) \in H^1_{Dn}(\Omega_{Dn}) \times H^1_{Dp}(\Omega_{Dp})$ for the continuity equations yields under the additional assumption of the corollary that

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

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

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

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

4 | PROOF OF THEOREM 3.2

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 $(\psi, \varphi_n, \varphi_p, T) \in \left[(\psi^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})) \cap L^\infty(\Omega_{\mathrm{D}})\right] \times \left[(\varphi_n^D + H^1_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}})) \cap W^{1,s}(\Omega_{\mathrm{Dn}})\right] \times \left[(\varphi_p^D + H^1_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}})) \cap W^{1,s}(\Omega_{\mathrm{Dp}})\right] \times \{T \in H^1(\Omega) : \ln T \in L^\infty(\Omega)\}$ with

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

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

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

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,*

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

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 (4.1) 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).

□

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 (4.1).*

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, 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

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

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

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

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 Section 2.3, we construct the $H^1(\Omega_{\mathrm{D}})$ function
$$\widetilde{\psi}^D := (1-\tau)\left(\widetilde{\varphi}_n + V_n(\widetilde{T})\right) + \tau\left(\widetilde{\varphi}_p - V_p(\widetilde{T})\right) \tag{4.4}$$
(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
$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \psi) = C + \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \text{ in } \Omega_{\mathrm{D}}, \\ \psi = \widetilde{\psi}^D \text{ on } I,\ \varepsilon \nabla\psi \cdot \nu = 0 \text{ on } \partial\Omega_{\mathrm{D}} \backslash I. \end{aligned} \tag{4.5}$$

2. We introduce the quantities
$$\widetilde{n}_M := N_{n0}\mathcal{G}\left(k_M\left(\frac{\psi}{\widetilde{T}}\right) - \frac{\widetilde{\varphi}_n - E_n}{\widetilde{T}}; \frac{\sigma_n}{\widetilde{T}}\right),\ \widetilde{p}_M := N_{p0}\mathcal{G}\left(\frac{E_p + \widetilde{\varphi}_p}{\widetilde{T}} - k_M\left(\frac{\psi}{\widetilde{T}}\right); \frac{\sigma_p}{\widetilde{T}}\right). \tag{4.6}$$

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):

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

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

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

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,

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

belongs to $L^{s_M/2}(\Omega)$ with uniform $L^{s_M/2}$ bound for all $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$. 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 $\|\widetilde{\psi}^D\|_{H^1(\Omega_{\mathrm{D}})} \le c$ for all $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ for $\widetilde{\psi}^D$ as in (4.4). Note that $\|\widetilde{T}\|_{W^{1,t_M}} \le c_{T,t_M}$ implies $\|\widetilde{T}\|_{L^\infty} \le T_u$ (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 $B_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})} : \widetilde{\psi}^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}) \to (H^1_{\mathrm{I}}(\Omega_{\mathrm{D}}))^*$,

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

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

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

With Young's inequality and the fact that $\|\widetilde{\psi}^D\|_{H^1(\Omega_{\mathrm{D}})} \le c$, 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. □

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

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

Similarly, we obtain bounds for $\widetilde{p}_M$ defined in (4.6) such 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 μ_i (see last assumption in **(A)**), upper and lower bounds for the ionized dopant densities δ_i in Ω_i, $i=n,p$, we find $c_{Ml}, c_{Mu} > 0$ such that

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

Moreover, note that the reaction rate coefficient $\widetilde{r} := r(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T})$ is nonnegative 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 6.2 in Glitzky et al[10] 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 $(\varphi_n, \varphi_p) \in (\varphi_n^D + H^1_{Dn}(\Omega_{Dn})) \times (\varphi_p^D + H^1_{Dp}(\Omega_{Dp}))$. For some exponent $s_M > 2$, it fulfills $\|\varphi_i\|_{L^\infty(\Omega_{Di})} \le K$, $\|\varphi_i\|_{H^1(\Omega_{Di})} \le c_{M,H^1}$, $\|\varphi_i\|_{W^{1,s_M}(\Omega_{Di})} \le c_{Ms}$, $i = n, p$. 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 the existence of $c_{HM} > 0$ such that

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

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 satisfying $\|T\|_{H^1} \le C_{T,M,H^1}$. 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[22] (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 $t_M > 2$,

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

(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 Q

Here we prove the complete continuity of the fixed point map $Q : \mathcal{N} \mapsto \mathcal{N}$, which directly implies its continuity. 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 $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}), (\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l) \in \mathcal{N}$ for all l. If $(\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l) \rightharpoonup (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in $H^1(\Omega_D)^2 \times W^{1,t_M}(\Omega)$ then $\widetilde{\psi}^{Dl} \rightharpoonup \widetilde{\psi}^D$ in $H^1(\Omega_D)$ 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 $(\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l) \rightharpoonup (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in $H^1(\Omega_D)^2 \times W^{1,t_M}(\Omega)$. The convergence of the terms in (4.4) with $\widetilde{\varphi}_i$ follows directly from $\widetilde{\varphi}^l_i \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{Di})$, $i = n, p$, 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 $\widetilde{\varphi}^l_i$, $\widetilde{\varphi}_i$, $i = n, p$, $0 < T_a \leq \widetilde{T}^l, \widetilde{T} \leq T_u$. 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 $H^1(\Omega_D)$.

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

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

For the gradients of τV_i, we use the following decomposition:

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

where

$$|I_1| := \left| \int_{\Omega_D} \left(V_i(\widetilde{T}^l) - V_i(\widetilde{T}) \right) \nabla\tau \cdot \nabla v \,\mathrm{d}x \right| \leq c\|v\|_{H^1} \|\widetilde{T}^l - \widetilde{T}\|_{L^2} \max_{\theta \in [T_a, T_u]} \left| \frac{\mathrm{d}V_i}{\mathrm{d}T}(\theta) \right| \to 0,$$

$$|I_2| := \left| \int_{\Omega_D} \tau \left[\frac{\mathrm{d}V_i}{\mathrm{d}T}(\widetilde{T}^l) - \frac{\mathrm{d}V_i}{\mathrm{d}T}(\widetilde{T}) \right] \nabla\widetilde{T}^l \cdot \nabla v \,\mathrm{d}x \right| \leq c\|v\|_{H^1} \|\widetilde{T}^l\|_{H^1} \|\widetilde{T}^l - \widetilde{T}\|_{L^\infty} \max_{\theta \in [T_a, T_u]} \left| \frac{\mathrm{d}^2 V_i}{\mathrm{d}T^2}(\theta) \right| \to 0.$$

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

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

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

Lemma 4.5. *We assume (A) and consider $(\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l), (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ with $\widetilde{\varphi}^l_i \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{Di})$, $i = n, p$, 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 $H^1(\Omega_D)$ and $\psi^l \to \psi$ in $L^r(\Omega_D)$ 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 $\widehat{\psi}^l \in \widetilde{\psi}^{Dl} + H^1_I(\Omega_D)$ be the unique solution to the linear elliptic problem

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

   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 $w^l \in w^{Dl} + H^1_I(\Omega_D)$ to w^{Dl} is bounded and linear, and therefore continuous. According to Prop. 4.2, p. 159 in Morrison[23] it is also continuous with respect to the weak topology meaning that $w^{Dl} \rightharpoonup 0$ in $H^1(\Omega_D)$ implies $w^l = \psi - \widehat{\psi}^l \rightharpoonup 0$ in $H^1(\Omega_D)$ and $\widehat{\psi}^l \to \psi$ in $L^r(\Omega_D)$, $r \in [1, \infty)$.

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

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

The monotonicity of $\eta \to \mathcal{G}(\eta, z)$ gives $\left(\mathcal{U}(\psi^l, \widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l) - \mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l) \right) (\psi^l - \widehat{\psi}^l) \le 0.$

Since $(\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l), (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ (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

$$
|\mathcal{U}(\widehat{\psi}^l, \widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l) - \mathcal{U}(\psi, \widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})| \le c_M \left(|\widehat{\psi}^l - \psi| + |\widetilde{\varphi}^l_n - \widetilde{\varphi}_n| + |\widetilde{\varphi}^l_p - \widetilde{\varphi}_p| + |\widetilde{T}^l - \widetilde{T}| \right).
$$

In summary, we obtain

$$
\begin{aligned}
\|\psi^l - \widehat{\psi}^l\|^2_{H^1(\Omega_D)} \le c_M \big(&\|\widehat{\psi}^l - \psi\|_{L^2(\Omega_D)} + \|\widetilde{\varphi}^l_n - \widetilde{\varphi}_n\|_{L^2(\Omega_D)} \\
&+ \|\widetilde{\varphi}^l_p - \widetilde{\varphi}_p\|_{L^2(\Omega_D)} + \|\widetilde{T}^l - \widetilde{T}\|_{L^2(\Omega_D)} \big) \|\psi^l - \widehat{\psi}^l\|_{L^2(\Omega_D)},
\end{aligned}
$$

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

Lemma 4.6. *We assume (A). Let $(\widetilde{\varphi}^l_n, \widetilde{\varphi}^l_p, \widetilde{T}^l), (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}$ with $\widetilde{\varphi}^l_i \rightharpoonup \widetilde{\varphi}_i$ in $H^1(\Omega_{Di})$, $i = n, p$, 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 $\{l_j\}$ 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 $\Omega_D \subset \mathbb{R}^2$ from inside by subdomains $\omega^1_k, \omega^2_k \subset\subset \Omega_D$ as follows: We define

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

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 $h = h^k_0$, $k \in \mathbb{N}$, and $\omega^1_k := \Omega_{Dh^k_0}$, and $\omega^2_k := \Omega_{D2h^k_0}$. Then by construction, $\omega^2_k \subset \omega^2_{k+1}$, $k \in \mathbb{N}$, and $\lim_{k\to\infty} \mathrm{mes}(\Omega_D \backslash \omega^2_k) = 0$.

2. For arbitrary fixed $k \in \mathbb{N}$, let $\gamma_k \in C^\infty_0(\Omega_D)$ be such that $\gamma_k(x) = 1$ in ω^2_k and $\gamma_k(x) = 0$ in $\Omega_D \backslash \omega^1_k$. Then $u^l_k := \gamma_k \overline{\psi}^l$ 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 $\partial\Omega_D$ and $\|u^l_k\|_{W^{1,2}(\Omega_D)} \le c$ for all l. Moreover, since $\nabla \cdot (\nabla \overline{\psi}^l) = 0$ ($\varepsilon =$ const), it results

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

Since $\|\overline{\psi}^l\|_{H^1(\Omega_D)}$ are uniformly bounded and $\gamma_k \in C^\infty(\Omega_D)$ we find that for fixed k the right-hand sides f_k^l are uniformly bounded in $L^2(\Omega_D)$. Since $\omega_k^2 \subset\subset \Omega_D$ and $u_k^l = \overline{\psi}^l$ on ω_k^2, we obtain according to Theorem 8.8 (p. 173) in Gilbarg and Trudinger[24] the uniform estimates on ω_k^2

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

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 $\|\widehat{\psi}^{l_k} - \psi\|_{W^{1,1}(\omega_k^2)} \le \frac{1}{2^k}$ (which is possible due to Step 2), and we obtain

$$\lim_{k\to\infty} \|\nabla(\widehat{\psi}^{l_k} - \psi)\|_{L^1(\Omega_D)} = \lim_{k\to\infty}\left(\int_{\omega_k^2} |\nabla(\widehat{\psi}^{l_k} - \psi)|\,dx + \int_{\Omega_D\setminus\omega_k^2} |\nabla(\widehat{\psi}^{l_k} - \psi)|\,dx\right)$$
$$\le \lim_{k\to\infty} \frac{1}{2^k} + \lim_{k\to\infty} c\left(\|\widehat{\psi}^{l_k}\|_{H^1(\Omega_D)} + \|\psi\|_{H^1(\Omega_D)}\right) \mathrm{mes}(\Omega_D\setminus\omega_k^2)^{1/2} = 0$$

since $\|\widehat{\psi}^{l_k}\|_{H^1(\Omega_D)}$ and $\|\psi\|_{H^1(\Omega_D)}$ have a uniform bound and $\mathrm{mes}(\Omega_D\setminus\omega_k^2) \to 0$. 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 $H^1(\Omega_D)$ 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 $\psi^l(x) \to \psi(x)$ a.e. in Ω_D for a subsequence follows directly from Lemma 4.5. □

Theorem 4.3. *Under Assumption (A), the map $Q : \mathcal{N} \to \mathcal{N}$ 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 $H^1(\Omega_{Di})$, $i = n, p$, and $\widetilde{T}^l \rightharpoonup \widetilde{T}$ in $W^{1,t_M}(\Omega)$. We have to show that $(\varphi_n^l, \varphi_p^l, T^l) := Q(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l, \widetilde{T}^l) \to (\varphi_n, \varphi_p, T) := Q(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in $H^1(\Omega_{Dn}) \times H^1(\Omega_{Dp}) \times W^{1,t_M}(\Omega)$.
The assumed weak convergences imply the strong convergences $\widetilde{\varphi}_i^l \to \widetilde{\varphi}_i$ in $L^r(\Omega_{Di})$, $i = n, p$, 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 $L^r(\Omega_D)$, $r \in [1, \infty)$ and Lemma 4.6 ensures that for any non-relabeled subsequence of solutions ψ^l we can find a sub-subsequence such that $\psi^{l_j}(x) \to \psi(x)$ and $\nabla\psi^{l_j}(x) \to \nabla\psi(x)$ a.e. in Ω_D.
2. In this step, we verify the strong convergence $\varphi_i^l \to \varphi_i$ in $H^1(\Omega_{Di})$, $i = n, p$. By Lemma 4.2 we have for the solutions φ_i^l to (4.7) that $\|\varphi_i^l\|_{H^1(\Omega_{Di})} \le c_{M,H^1}$. We show that all weakly convergent subsequences of $\{(\varphi_n^l, \varphi_p^l)\}$ in $H^1(\Omega_{Dn}) \times H^1(\Omega_{Dp})$ converge weakly to the same limit (φ_n, φ_p). Then using Lemma 5.4 in Gajewski et al[25] we have $(\varphi_n^l, \varphi_p^l) \rightharpoonup (\varphi_n, \varphi_p)$ in $H^1(\Omega_{Dn}) \times H^1(\Omega_{Dp})$ for the entire sequence and as a consequence $\varphi_i^l \to \varphi_i$ in $L^2(\Omega_{Di})$.
Let $\{(\varphi_n^{l_k}, \varphi_p^{l_k})\}$ be a subsequence that converges weakly to some $(\varphi_n^*, \varphi_p^*)$ in $H^1(\Omega_{Dn}) \times H^1(\Omega_{Dp})$. We verify that $\varphi_i^* = \varphi_i$. Since $\widetilde{\varphi}_i^{l_k} \to \widetilde{\varphi}_i$ in $L^2(\Omega_{Di})$, $\widetilde{T}^{l_k} \to \widetilde{T}$ 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 $T \ge T_a$ 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 T_a 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

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

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

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

We write

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

Having in mind that $\widetilde{T}$, $\widetilde{T}^{l_k}\ge T_a$ a.e. in Ω, φ_i, $\varphi_i^{l_k}\in[-K,K]$ a.e. in Ω_{Di}, $\exp\frac{\varphi_n^{l_k}-\varphi_p^{l_k}}{\widetilde{T}^{l_k}}\le c$, 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

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

Due to (4.12) and $\|\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})}\le c_{M,H^1}$ 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 $\|\varphi_i^{l_k}-\varphi_i\|_{H^1(\Omega_{\mathrm{Di}})}\to 0$ for the subsequence related to the a.e. convergence of $\tilde{\varphi}_n^{l_k},\tilde{\varphi}_p^{l_k},\tilde{T}^{l_k},\psi^{l_k},\nabla\psi^{l_k}$. 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 $\varphi_i,\ i=n,p$.

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 Lemma 5.4 in Gajewski et al,[25] 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 was any subsequence $\{\varphi_i^{l_n}\}$ that does not contain any converging subsequence then there would be $\alpha > 0$ such that $\|\varphi_i^{l_n} - \varphi_i\|_{H^1} \geq \alpha$ for all l_n. We lead this to a contradiction again by the method of Step 2 using the convergence a.e. of $\tilde{\varphi}_i^{l_n}, \tilde{T}^{l_n}, \psi^{l_n}$, 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 $\|T^l\|_{W^{1,t_M}} \leq c_{T,t_M}$ 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 (Lemma 5.4 in[25]). 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 $\hat{s}_M$ and $t_M > 2$ in Lemma 4.3 ensures the embedding $L^{\hat{s}_M/2}(\Omega) \hookrightarrow W^{-1,t_M}(\Omega) = W^{1,t_M'}(\Omega)^*$, where $\frac{1}{t_M} + \frac{1}{t_M'} = 1$. The result of Gröger[22] for the linear heat equation guarantees the estimate

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

with $\widetilde{h}_\Omega^{l_k} := h_\Omega(\widetilde{n}_M^{l_k}, \widetilde{p}_M^{l_k}, \widetilde{T}^{l_k}, |\nabla\psi^{l_k}|, \nabla\varphi_n^{l_k}, \nabla\varphi_p^{l_k}, \varphi_n^{l_k}, \varphi_p^{l_k})$ and $\widetilde{h}_\Omega := h_\Omega(\widetilde{n}_M, \widetilde{p}_M, \widetilde{T}, |\nabla\psi|, \nabla\varphi_n, \nabla\varphi_p, \varphi_n, \varphi_p)$ and $\theta_{l_k} \to 0$ for $T^{l_k} \to T$ in $H^1(\Omega)$. We have to show $\|\widetilde{h}_\Omega^{l_k} - \widetilde{h}_\Omega\|_{L^{\hat{s}_M/2}(\Omega)} \to 0$. Since

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

we find with (4.14)

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

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

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

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

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

Thus, in summary, we have $\|\widetilde{h}_\Omega^{l_k} - \widetilde{h}_\Omega\|_{L^{\hat{s}_M/2}(\Omega)} \to 0$ such that especially $\|T^{k_l} - T\|_{H^1} \to 0$. Moreover, due to (4.18) this ensures $T^{l_k} \to T$ in $W^{1,t_M}(\Omega)$. According to[22] 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 was any subsequence $\{T^{l_n}\}$ that does not contain any converging subsequence then there would be $\alpha > 0$ 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 ($\mathrm{P}_{\boldsymbol{M}}$)

Here we prove Theorem 4.2. The set $\mathcal{N}$ is nonempty, closed, and convex in $H^1(\Omega_{\mathrm{Dn}}) \times H^1(\Omega_{\mathrm{Dp}}) \times W^{1,t_M}(\Omega)$. 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 Q. For this fixed point, we define as in (2.18) the Dirichlet function

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

solve by Lemma 4.1 the problem $B_{(\varphi_n,\varphi_p,T)}\psi = 0$, and gain a unique weak solution $\psi \in \psi^D + H^1_{\mathrm{I}}(\Omega_{\mathrm{D}})$ 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 (4.1).

The definition of $\mathcal{N}$ ensures $T \in \{u \in H^1(\Omega) : \ln u \in L^\infty(\Omega)\}$. Since $(\varphi_n, \varphi_p, T)$ is a fixed point of Q, the regularized continuity equations (middle equation in (4.1)) 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 $(\varphi_n, \varphi_p, T)$ is a fixed point of Q, Lemma 4.2 guarantees $\varphi_i \in W^{1,s_M}(\Omega_{\mathrm{Di}})$, $i = n, p$. Now the Poisson equation and the heat equation (first and last equation in (4.1)) 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 $\varphi_i \in W^{1,s}(\Omega_{\mathrm{Di}})$, $i = n, p$. Therefore, $(\psi, \varphi_n, \varphi_p, T)$ solves problem (4.1) 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 the energy levels E_n and E_p, the disorder parameters σ_n, σ_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 Glitzky et al,[10] 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.

An existence result for the coarse-grained model in the 3D case is completely open. The following techniques of the present paper fail: We would need that the Dirichlet functions ψ^D and $\widetilde{\psi}^D$, defined in (2.18) and (4.4), respectively, are at least $H^1(\Omega_{\mathrm{D}})$ functions. This especially ensures that the nonlinear Poisson Equation (4.5) in the iteration process has a unique solution (comp. Lemma 4.1). To guarantee that the Dirichlet functions are in $H^1(\Omega_{\mathrm{D}})$, T, resp. $\widetilde{T}$ has to belong also at least to $H^1(\Omega_{\mathrm{D}})$. Due to the Joule heating terms in the right-hand side of the heat equation, this can, however, only be achieved for electrochemical potentials from $W^{1,q}(\Omega_{\mathrm{D}})$ for suitable $q > 2$.

For the latter, available regularity results for elliptic equations in the 3D case (see, e.g., sect. 6 in Disser et al.[26]) do not provide uniform estimates of

$$\|(-\nabla \cdot d_n(\widetilde{n}_M, \widetilde{T}, |\nabla\psi|)\nabla\cdot)^{-1}\|_{\mathcal{L}(W^{-1,q}_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}), W^{1,q}_{\mathrm{Dn}}(\Omega_{\mathrm{Dn}}))},$$

$$\|(-\nabla \cdot d_p(\widetilde{p}_M, \widetilde{T}, |\nabla\psi|)\nabla\cdot)^{-1}\|_{\mathcal{L}(W^{-1,q}_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}), W^{1,q}_{\mathrm{Dp}}(\Omega_{\mathrm{Dp}}))}$$

for all $(\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T})$ in a corresponding fixed point set $\mathcal{N}$ (comp. Lemma 4.2) even if we knew that

$$\underline{d} \leq d_n(\widetilde{n}_M, \widetilde{T}, |\nabla\psi|),\ d_p(\widetilde{p}_M, \widetilde{T}, |\nabla\psi|) \leq \overline{d} \text{ for all } (\widetilde{\varphi}_n, \widetilde{\varphi}_p, \widetilde{T}) \in \mathcal{N}.$$

In the 2D case, the last estimate ensures these necessary uniform bounds for the inverses for the suitable exponent $q > 2$ by exploiting Gröger's regularity result Theorem 1 in Gröger.[22]

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CONFLICTS OF INTEREST

This work does not have any conflicts of interest.

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APPENDIX A: PROPERTIES OF THE GAUSS–FERMI INTEGRAL

Here we collect important properties of the statistical relation for organic semiconductors from sect. 2.1 in Doan et al.,[27] Lemma 2.1 in Glitzky et al.,[28] Lemma 2.1 in Glitzky et al[11] and derive some further relevant properties. The Gauss–Fermi integral is given by

$$\mathcal{G}(\eta, z) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2}\right) \frac{1}{\exp(z\xi - \eta) + 1} \, \mathrm{d}\xi. \tag{A1}$$

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

$$\begin{aligned}
\frac{\partial \mathcal{G}}{\partial \eta}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{\exp(z\xi - \eta)}{[\exp(z\xi - \eta) + 1]^2} \, \mathrm{d}\xi, \\
\frac{\partial}{\partial z} \mathcal{G}(\eta; z) &= -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{\exp(z\xi - \eta)\xi}{[\exp(z\xi - \eta) + 1]^2} \, \mathrm{d}\xi, \\
\frac{\partial^2 \mathcal{G}}{\partial \eta^2}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{\exp(z\xi - \eta)[\exp(z\xi - \eta) - 1]}{[\exp(z\xi - \eta) + 1]^3} \, \mathrm{d}\xi, \\
\frac{\partial^2 \mathcal{G}}{\partial z \partial \eta}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{\xi \exp(z\xi - \eta)[1 - \exp(z\xi - \eta)]}{[\exp(z\xi - \eta) + 1]^3} \, \mathrm{d}\xi, \\
\frac{\partial^2 \mathcal{G}}{\partial z^2}(\eta, z) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{\xi^2 \exp(z\xi - \eta)[\exp(z\xi - \eta) - 1]}{[\exp(z\xi - \eta) + 1]^3} \, \mathrm{d}\xi.
\end{aligned} \tag{A2}$$

They satisfy

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

and

$$\frac{\partial}{\partial z} \mathcal{G}(\eta; z) \begin{cases} > 0 & \text{if } \eta < 0 \\ = 0 & \text{if } \eta = 0 \\ < 0 & \text{if } \eta > 0 \end{cases} \text{ and } \left| \frac{\partial}{\partial z} \mathcal{G}(\eta; z) \right| \leq \frac{1}{z}(1 + \exp|\eta|) \ \forall z > 0, \forall \eta \in \mathbb{R} \tag{A3}$$

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

$$\frac{\partial \mathcal{G}}{\partial \eta}(\eta, z) \ge c_{k,\bar{z}} \ \text{ for all } \ \eta \in \mathbb{R} \ \text{ with } \ |\eta| \le k \ \text{ and all } \ z \ \text{ with } \ \bar{z} \ge z > 0. \tag{A4}$$

This estimate follows directly from the inequalities

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

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*

$$T\mathcal{G}^{-1}\left(\frac{\delta}{N_0}; \frac{\sigma}{T_l}\right) - E \le V(T) \le -E. \tag{A5}$$

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 Lemma 2.1 in[11] we find

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

Since $\mathcal{G}$ is monotone increasing in the first argument, it follows $\frac{V(T)+E}{T} \ge \mathcal{G}^{-1}\left(\frac{\delta}{N_0}; \frac{\sigma}{T_l}\right)$, 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 $\frac{\partial \mathcal{H}}{\partial v}(T, v) = \frac{N_0}{T}\frac{\partial \mathcal{G}}{\partial \eta}\left(\frac{v+E}{T}; \frac{\sigma}{T}\right) > 0$ 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

$$\begin{aligned}\frac{\mathrm{d}V}{\mathrm{d}T}(T) &= -\left[\frac{\partial \mathcal{H}}{\partial v}(T, V(T))\right]^{-1} \frac{\partial \mathcal{H}}{\partial T}(T, V(T)) \\ &= \left[\frac{\partial \mathcal{G}}{\partial \eta}(\eta(T); z)\right]^{-1} \left[\frac{\partial \mathcal{G}}{\partial \eta}(\eta(T); z)\,\eta(T) + \frac{\partial \mathcal{G}}{\partial z}(\eta(T); z)\,z\right] \\ &= \left[\frac{\partial \mathcal{G}}{\partial \eta}(\eta(T); z)\right]^{-1} \frac{\partial \mathcal{G}}{\partial z}(\eta(T); z)\,z + \mathcal{G}^{-1}\left(\frac{\delta}{N_0}; z\right)\end{aligned} \tag{A6}$$

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 (A3), (A4), and Lemma A.1. Therefore, using $|V(T) - V(T_1)| \leq |\frac{\mathrm{d}V}{\mathrm{d}T}(T_\theta)||T - T_1|$ 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)

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

and results in

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

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

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

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 (A2) that

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

In the expressions for $\frac{\partial^2\mathcal{G}}{\partial z^2}$ and $\frac{\partial^2\mathcal{G}}{\partial z\partial\eta}$, respectively, in (A2), 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

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

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

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

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

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

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 $\mathcal{G}$. □