Drift-diffusion modeling, analysis and simulation of organic semiconductor devices

Duy-Hai Doan, Annegret Glitzky, Matthias Liero

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Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: duyhai.doan@wias-berlin.de
        annegret.glitzky@wias-berlin.de
        matthias.liero@wias-berlin.de

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Abstract

We discuss drift-diffusion models for charge-carrier transport in organic semiconductor devices. The crucial feature in organic materials is the energetic disorder due to random alignment of molecules and the hopping transport of carriers between adjacent energetic sites. The former leads to so-called Gauss-Fermi statistics, which describe the occupation of energy levels by electrons and holes. The latter gives rise to complicated mobility models with a strongly nonlinear dependence on temperature, density of carriers, and electric field strength. We present the state-of-the-art modeling of the transport processes and provide a first existence result for the stationary drift-diffusion model taking all of the peculiarities of organic materials into account. The existence proof is based on Schauder's fixed-point theorem. Finally, we discuss the numerical discretization of the model using finite-volume methods and a generalized Scharfetter-Gummel scheme for the Gauss-Fermi statistics.

1 Introduction

The use of organic materials in electronic applications such as displays, photovoltaics, lighting, or transistors, has seen an substantial increase in the last decade. This is mainly due to the lower production cost, sustainability, and flexibility. The toolbox of organic chemistry opens an enormous potential for new device concepts. Since the optoelectronic properties of organic semiconductors are different from that of classical inorganic crystalline semiconductors, the knowledge of organic semiconductor physics is essential to further improve device applications. The most important problem hereby is the understanding of charge transport processes in the materials.

In contrast to classical semiconductors such as silicon or gallium-arsenide, charge-transport in organic materials happens via temperature activated hopping transport of electrons or holes between adjacent molecules. Here, the crucial feature is the random alignment of the molecule, which leads to a disordered system with Gaussian distributed energy levels. Consequently, the usual statistical description of the energetic distribution of charge carriers via Boltzmann or Fermi-Dirac statistics has to be replaced by so-called Gauss-Fermi statistics (see Subsection 2.1).

A common approach to simulate the transport of charge carriers in organic materials is based on a master equation description of the hopping transport and kinetic Monte-Carlo methods, see e.g. [KvdHAH+15, PCT+05, KBC+17]. However, the computational costs of this approach are typically very high and the treatment of complicated multi-dimensional device structures is very challenging. Moreover, the inclusion of multi-physics effects such as heat flow is out of scope. The latter, in particular, is of high importance as organic devices show a strong interplay between electrical current and heat flow, see [FPL+13, LKF+15]. Here, drift-diffusion models provide an immense advantage. Geometrically sophisticated organic devices, such as vertical organic field-effect transistors (VOFETs)

can be conveniently treated by drift-diffusion models. Let us mention that recently stable and efficient numerical discretization schemes for non-Boltzmann statistics have been developed [FRD+17].

However, from a mathematical point of view, drift-diffusion models for organic devices lead to complicated mobility laws and require the treatment of Gauss-Fermi statistics. In particular, for the latter classical results concerning Boltzmann statistics, e.g. in [Mar86] and references therein, or even extended results for non-Boltzmann statistics, see [GG89, Grö87], cannot be directly applied since they require monotone and unbounded statistical relations. Moreover, mobility laws, which arise from fitting to kinetic Monte Carlo simulations, exhibit strongly nonlinear dependences on the temperature, carrier density and the electric field strength, see Subsection 2.2. The dependence on the gradient of the electrostatic potential demands stronger convergence properties of the electrostatic potential within the iterative scheme of the Schauder mapping.

The aim of this text is to put the drift-diffusion description of charge-transport in organic materials on a sound mathematical basis. In particular, we will give a first existence result taking all of the features in the organic setting into account.

There is a very sparse amount of mathematical papers dealing with analytical investigations of drift-diffusion problems from organics. Most of them treat problems arising in organic photovoltaics and they completely ignore the Gauss-Fermi statistics, see [BFMW13, VPSS18] and the references therein.

The paper [BFMW13] discusses a model for organic solar cells including exciton dynamics. Here for the mobility functions μ_n and μ_p a Poole-Frenkel type law is incorporated, but still Boltzmann statistics (no Gauss-Fermi statistics) is used. There is an asymptotic analysis of the one-dimensional stationary system presented and a hybrid discontinuous Galerkin finite element method is applied to simulate a bilayer structure. The paper [VPSS18] investigates a reaction-drift-diffusion system containing besides electrons and holes polarons as well as excitons for the description of photo conversion mechanisms in organic solar cells. Under strong assumptions on the field dependence of the mobility functions μ_n and μ_p, the existence and uniqueness of weak solutions of the system, as well as the non-negativity of all species concentrations, are proven in the stationary regime. Moreover, a Galerkin finite element method stabilized by an exponential fitting technique was used for numerical simulations.

The outline of this text is as follows: In Section 2 we provide an overview of the physics that have to be properly represented in a mathematical model. More precisely, we discuss the carrier statistics, the form of the mobilities, the generalized Einstein relations, and the recombination. In Section 3 we prove the existence of solutions for the stationary drift-diffusion model. Finally, in Section 4 we present a discretization scheme for the model based on finite-volume methods and generalized Scharfetter-Gummel schemes and discuss the example of an organic n-doped/intrinsic/n-doped (n-i-n) resistor, where we demonstrate the difference of the modeling by classical Boltzmann statistics in comparison to Gauss-Fermi statistics.

2   Drift-diffusion modeling of electronic behavior

Organic semiconductor devices are based on organic molecules or polymers. Charge transport in such materials is realized by hopping of electrons (and holes) between discrete energy levels of molecular sites nearby, see Fig. 1. Organic molecules have two energy states, the Highest Occupied Molecul Orbital (HOMO, energy E_H) as well as the Lowest Unoccupied Molecul Orbital (LUMO, energy E_L). The LUMO-states describe delocalised electrons in the π-bindings, whereas the HOMO-states describe

the electrons in the localized electron pair-bindings between the atoms of the molecule.

By crossing the HOMO-LUMO-gap (e.g. by optical excitation) electrons in the molecule can change from the HOMO-state into the LUMO-state. Thereby a positively charged cavity in the charge cloud of the molecule arises which is called a hole. Electrons and holes can move by hopping transport between energy levels of neighboring molecules. Thus, in this respect organic semiconductor materials behave like amorphous semiconductors and the HOMO and LUMO energy have to be understood as valence and conduction band edge, respectively.
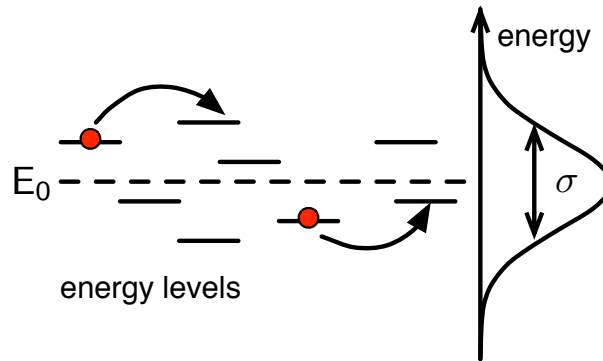

Figure 1: Hopping-transport between Gaussian distributed energy levels (centered at E_0 with variance σ) of neigboring molecules.

For the description of the charge transport in organic semiconductor devices neglecting thermal effects, generalized drift-diffusion models of van Roosbroeck-typ are used. The model consists of continuity equations for the densities n and p of electrons and holes, respectively, and of the Poisson equation for the electrostatic potential ψ considered on a domain Ω which comprises the semiconductor device:

$$
\begin{aligned}
-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \psi) &= q(C - n + p), \\
q\frac{\partial n}{\partial t} - \nabla \cdot j_n &= -qR, \qquad j_n = -qn\mu_n \nabla \varphi_n, \\
q\frac{\partial p}{\partial t} + \nabla \cdot j_p &= -qR, \qquad j_p = -qp\mu_p \nabla \varphi_p.
\end{aligned}
\tag{2.1}
$$

Here q is the elementary charge, ε_0 the dielectric constant, ε_r the relative permittivity, and R the recombination rate. φ_n and φ_p denote the quasi-Fermi potentials which are connected to the densities of the charge carrier by statistical relations and j_n and j_p are the electron- and hole current densities that are characterized by the electric mobilities μ_n, μ_p.

The principle form of (2.1) looks like the van Roosbroeck equations for classical inorganic semiconductors. But there are essential differences in statistical relations, mobility functions that here depend on the gradient of the electrostatic potential, and a generalized Einstein relation between mobility and diffusion coefficient. These cause additional difficulties in the mathematical analysis and numerical simulation for the model. The essential features are explained in the next subsections.

2.1 Statistical relation between densities and chemical potentials via the Gaussian Disorder Model (GDM)

In organic semiconductors, the energy positions are Gaussian distibuted, such that both, the electrons and holes, can be described by a Gaussian density of state, see Fig. 1

$$N_{\mathsf{Gauss}}(E) = \frac{N_0}{\sigma\sqrt{2\pi}} \exp\left[-\left(\frac{E - E_0}{\sqrt{2}\sigma}\right)^2\right],$$

where N_0 gives the total density of transport states. E_0 denotes the corresponding average HOMO- and LUMO-levels, respectively, and σ their variance. The constant σ is also called the disorder parameter which characterizes the disorder of the organic material. Then for semiconductors which are homogeneous and are not influenced by an externally applied electric field the density of electrons (and similarly also for holes) is given by the Gauss-Fermi integral

$$n = \int_{-\infty}^{\infty} N_{\mathsf{Gauss}}(E) \frac{1}{\exp\left(\frac{E-E_F}{k_{\mathrm{B}}T}\right) + 1} \, \mathrm{d}E$$

$$= \frac{N_{n0}}{\sigma_n\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{(E - E_L)^2}{2\sigma_n^2}\right) \frac{1}{\exp\left(\frac{E-E_F}{k_{\mathrm{B}}T}\right) + 1} \, \mathrm{d}E,$$

where E_L stands for the LUMO-energy, E_F denotes the Fermi energy and the Fermi function $f(E, T) = \left(\exp\left(\frac{E-E_F}{k_{\mathrm{B}}T}\right) + 1\right)^{-1}$ gives the probability that an electron is in the quantum state with energy E and k_{B} is the Boltzmann constant. Thus, using the variable $\xi = \frac{E-E_L}{\sigma_n}$ it follows

$$n = \frac{N_{n0}}{\sigma_n\sqrt{2\pi}} \sigma_n \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2}\right) \frac{1}{\exp\left(\frac{\sigma_n}{k_{\mathrm{B}}T}\xi - \frac{E_F-E_L}{k_{\mathrm{B}}T}\right) + 1} \, \mathrm{d}\xi$$

$$= \frac{N_{n0}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2}\right) \frac{1}{\exp\left(s_n\xi - \eta_n^0\right) + 1} \, \mathrm{d}\xi \qquad (2.2)$$

$$=: N_{n0}\mathcal{G}_{s_n}(\eta_n^0), \qquad \eta_n^0 := \frac{E_F - E_L}{k_{\mathrm{B}}T} \quad s_n := \frac{\sigma_n}{k_{\mathrm{B}}T}$$

with the dimensionless quantities s_n and η_n^0. The relation (2.2) is valid for homogeneous semiconductors in absence of an external field. It can be generalized to the case that in the semiconductor an electric field $-\nabla\psi$ is present with a weakly spatially varying potential ψ. Then the concept of bent bands can be applied and the energy level E_L has to be replaced by $E_L - q\psi$ and ξ by $\widetilde{\xi} = \frac{E-E_L+q\psi}{\sigma_n}$. Thus the electron density is given instead of (2.2) by

$$n = \frac{N_{n0}}{\sigma_n\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{(E - E_L + q\psi)^2}{2\sigma_n^2}\right) \frac{1}{\exp\left(\frac{E-E_F}{k_{\mathrm{B}}T}\right) + 1} \, \mathrm{d}E$$

$$= \frac{N_{n0}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\widetilde{\xi}^2}{2}\right) \frac{1}{\exp\left(s_n\widetilde{\xi} - \frac{E_F-E_L+q\psi}{k_{\mathrm{B}}T}\right) + 1} \, \mathrm{d}\widetilde{\xi} \qquad (2.3)$$

$$= N_{n0}\mathcal{G}_{s_n}(\eta_n), \qquad \eta_n := \frac{E_F - E_L + q\psi}{k_{\mathrm{B}}T} = \frac{q(\psi - \varphi_n) - E_L}{k_{\mathrm{B}}T}.$$

Similar to this representation of the electron density by means of the renormalized chemical potential of the electrons, the hole density p is given as function of the renormalized chemical potential of the

holes:

$$p = N_{p0}\mathcal{G}_{s_p}(\eta_p), \qquad \eta_p := \frac{E_H - q(\psi - \varphi_p)}{k_{\mathrm{B}}T}, \quad s_p := \frac{\sigma_p}{k_{\mathrm{B}}T},$$

where E_H denotes the HOMO energy.

Remark 2.1 *Since the Fermi function f takes only values between 0 and 1, from (2.3) it follows*

$$0 < n = n(\eta_n) < \frac{N_{n0}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2}\right) \mathrm{d}\xi = N_{n0} \quad \forall \eta_n \in \mathbb{R},$$

such that the carrier density in organic materials remains bounded for all values of η_n. Moreover, the mapping $\eta \mapsto \mathcal{G}_s(\eta)$ is strictly monotonously increasing, $\mathcal{G}_s$ is differentiable and

$$\frac{\mathrm{d}\mathcal{G}_s}{\mathrm{d}\eta}(\eta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2}\right) \frac{\exp\left(s\xi - \eta\right)}{\left(\exp(s\xi - \eta) + 1\right)^2} \mathrm{d}\xi.$$

Note that the fraction in the integrand takes only values between 0 and 1. Therefore

$$\frac{\mathrm{d}\mathcal{G}_s}{\mathrm{d}\eta}(\eta) \in (0,1) \quad \textit{and} \quad \lim_{\eta \to +\infty} \frac{\mathrm{d}\mathcal{G}_s}{\mathrm{d}\eta}(\eta) = \lim_{\eta \to -\infty} \frac{\mathrm{d}\mathcal{G}_s}{\mathrm{d}\eta}(\eta) = 0.$$

For infinite narrow distribution $\sigma \to 0$ the density of state converges to a Dirac distribution centered at E_0, i.e. $N_{\mathrm{Gauss}}(E) \to N_{n0}\delta(E - E_0)$. Let $\mathcal{G}_\delta$ denote the limiting statistical relation for the density of state $N_{n0}\delta(E - E_0)$, namely

$$\mathcal{G}_\delta(\eta) = \frac{1}{\exp\{-\eta\} + 1} \quad \left(= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{1}{\exp\{-\eta\} + 1} \mathrm{d}\xi\right).$$

Because of the identities

$$\int_{-\infty}^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \frac{1}{\exp\{s\xi\} + 1} \mathrm{d}\xi = \int_0^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \left(\frac{1}{\exp\{s\xi\} + 1} + \frac{1}{\exp\{-s\xi\} + 1}\right) \mathrm{d}\xi$$

$$= \int_0^{\infty} \exp\left\{-\frac{\xi^2}{2}\right\} \mathrm{d}\xi = \sqrt{\frac{\pi}{2}}$$

we find

$$\mathcal{G}_\delta(0) = \frac{1}{2}, \quad \mathcal{G}_s(0) = \frac{1}{2} \qquad \forall s > 0.$$

Following [PS10], for small carrier density and small disorder σ, the Boltzmann approximation can be applied

$$\mathcal{G}_s(\eta) \approx \exp\left(\frac{s^2}{2}\right) \exp(\eta), \qquad s = \frac{\sigma}{k_{\mathrm{B}}T}. \tag{2.4}$$

But in most applications s is too large. For further approximations and discussion of the Gauss-Fermi integral see [PS10].

2.2 Mobility function in the case of the Extended Gaussian Disorder Model (EGDM)

The mobility functions μ_n, μ_p for organic semiconductor materials with Gaussian density of state show a positive feedback with respect to temperature T, density n or p, and with respect to electrical field strength $F = |\nabla\psi|$. We summarize the results of [PCT$^+$05] obtained as extension of the Gaussian disorder model for the dependence of the charge carrier mobility. They used a numerical solution of the master equation for hopping transport in a disordered energy landscape with a Gaussian density of state to determine these dependencies. Written exemplarily for the electron mobility, [PCT$^+$05] ended up in the product form of the mobility

$$\mu_n(T, n, F) = \mu_{n0}(T) \times g_1(n, T) \times g_2(F, T). \tag{2.5}$$

The temperature dependence $\mu_{n0}(T)$ is described by

$$\mu_{n0}(T) = \mu_{n0}c_1 \exp\left\{-c_2 s_n^2\right\}, \quad s_n = \frac{\sigma_n}{k_B T} \tag{2.6}$$

with a reference mobility μ_{n0} and coefficients c_1, $c_2 > 0$. The function

$$(0, \infty) \ni T \mapsto \mu_{n0}(T) = \mu_{n0}c_1 \exp\left\{-c_2\left(\frac{\sigma_n}{k_B T}\right)^2\right\} \in (0, \mu_{n0}c_1)$$

is continuously increasing in T, but bounded. For $T \geq T_a > 0$ the function $\mu_{n0}(T)$ is positively bounded away from zero.

The density dependent enhancement of the mobility g_1 itself is influenced by the temperature and follows in the practical range of relevant values of s_n and densities the rule

$$g_1(n, T) = \exp\left\{\frac{1}{2}(s_n^2 - s_n)(2na^3)^\delta\right\}, \quad \delta = 2\frac{\ln(s_n^2 - s_n) - \ln(\ln 4)}{s_n^2}.$$

Here a denotes the average hopping distance. In [CPBM05, Appendix D] the validity of the given density dependence of the mobility $g_1(n, T)$ is stated for $2 < s_n < 6$ and for densities with na^3 between 10^{-6} and 10^{-2}. In particular, it fits well for the modeling of organic Field-Effect-Transistors (OFETs) where na^3 is close to 10^{-2}.

For applications in single layer LEDs, which typically operate at densities where na^3 is between 10^{-5} and 10^{-4}, and for PPV-based (Poly(p-Phenylen-Vinylen)) light-emitting polymers with s_n close to 4 at room temperature the following approximation is excellent (see [CPBM05, Appendix D])

$$g_1(n, T) = \exp\left\{\left(\frac{1}{2}s_n^2 + \ln 2\right)(2na^3)^\delta\right\}, \quad \delta = 2\frac{(\ln s_n^2 + \ln 4) - \ln(\ln 4)}{s_n^2}.$$

However, note that due to the Gauss-Fermi statistics in (2.3), the density is bounded by N_{n0} such that for such densities relevant in the drift-diffusion model the factor g_1 remains bounded by

$$0 < \underline{g_1}(T) \leq g_1(n, T) \leq \overline{g_1}(T).$$

The sensitivity of the mobility with respect to the field strength g_2 is also temperature dependent,

$$g_2(F, T) = \exp\left\{0.44(s_n^{3/2} - 2.2)\left(\sqrt{1 + 0.8\left(\frac{Fqa}{\sigma_n}\right)^2} - 1\right)\right\}. \tag{2.7}$$

In [PCT$^+$05, 206601-3/4] the following is stated: The parametrization for g_2 is optimized for the low density region, but it is rather accurate in the high-density region. g_2 shows a F^2 dependence at low field strength and describes the approximately linear dependence of $\ln(\mu_n/\mu_{n0})$ if the critical field strength of $\sigma_n/(qa)$ is passed. Further it is mentioned that at very high fields, where μ_n saturates and eventually decreases as a function of F, the parametrization g_2 breaks down. Although a field range could be given in which the so-called Poole-Frenkel model [Bäs93] with $\mu \sim \exp\left\{\gamma\sqrt{F}\right\}$ holds, the parametrization with g_2 is a more useful one in the range of the working regime of organic semiconductor devices.

Especially for the mathematical analysis, we should work with a saturating function g_2. However, the fundamental difficulty remains that there is a dependency of the mobility function μ_n on $F = |\nabla\psi|$.

For the further analysis we suppose for the electron and hole mobilities that $\mu_n : \Omega \times (0,\infty) \times [0, \text{ess sup } N_{n0}] \times \mathbb{R}_+ \to \mathbb{R}$, $\mu_p : \Omega \times (0,\infty) \times [0, \text{ess sup } N_{p0}] \times \mathbb{R}_+ \to \mathbb{R}$ are Caratheodory functions fulfilling

$$
\begin{aligned}
0 < \underline{\mu} \leq \mu_n(\cdot, T, n, F),\ \mu_p(\cdot, T, p, F) \leq \overline{\mu} < \infty \\
\forall (T, n, p, F) \in [T_a, \infty) \times [0, \text{ess sup } N_{n0}] \times [0, \text{ess sup } N_{p0}] \times \mathbb{R}_+ \text{ a.e. in } \Omega.
\end{aligned}
\tag{2.8}
$$

The boundedness assumption on the mobilities is reasonable since in real applications the model in (2.7) and the Poole-Frenkel law break down for too high field strengths.

2.3 Generalized Einstein relation

In drift-diffusion form, the carrier flux densities in (2.1) can also be written by

$$
j_n = -qn\mu_n\nabla\psi + qD_n\nabla n, \qquad j_p = -qp\mu_p\nabla\psi - qD_p\nabla p,
\tag{2.9}
$$

with diffusion coefficients D_n, D_p. In case of thermodynamic equilibrium (meaning that $j_n = 0$, $\varphi_n = \text{const}$, $T = \text{const}$), from the statistical relation (2.3) we find

$$
\nabla n = N_{n0}\mathcal{G}'_{s_n}(\eta_n)\nabla\eta_n = N_{n0}\mathcal{G}'_{s_n}(\eta_n)\frac{q}{k_B T}\nabla\psi.
$$

Inserting this in (2.9) we obtain

$$
j_n = 0 = -qn\mu_n\nabla\psi + qD_n N_{n0}\mathcal{G}'_{s_n}(\eta_n)\frac{q}{k_B T}\nabla\psi
$$

leading to a generalized Einstein relation of the form

$$
\frac{D_n}{\mu_n} = \frac{k_B T}{q}\frac{n}{N_{n0}}\frac{1}{\mathcal{G}'_{s_n}(\eta_n)} = \frac{k_B T}{q}\frac{n}{N_{n0}}\left(\mathcal{G}^{-1}_{s_n}\right)'\left(\frac{n}{N_{n0}}\right) =: \frac{k_B T}{q}g_3\left(T, \frac{n}{N_{n0}}\right).
\tag{2.10}
$$

Alternatively the generalized Einstein relation can also be written

$$
\frac{D_n}{\mu_n} = \frac{k_B T}{q}\frac{\mathcal{G}_{s_n}(\eta_n)}{\mathcal{G}'_{s_n}(\eta_n)} = \frac{k_B T}{q}\frac{1}{(\ln\mathcal{G}_{s_n}(\eta_n))'}.
\tag{2.11}
$$

Although the generalized Einstein relation was derived under the assumption of thermodynamic equilibrium, this relation can also be applied in the situation that a current is present and the current density is not such large that an essential perturbation of the distribution function for the charge carrier occurs (see [vMC08, BBK82, p. 196]).
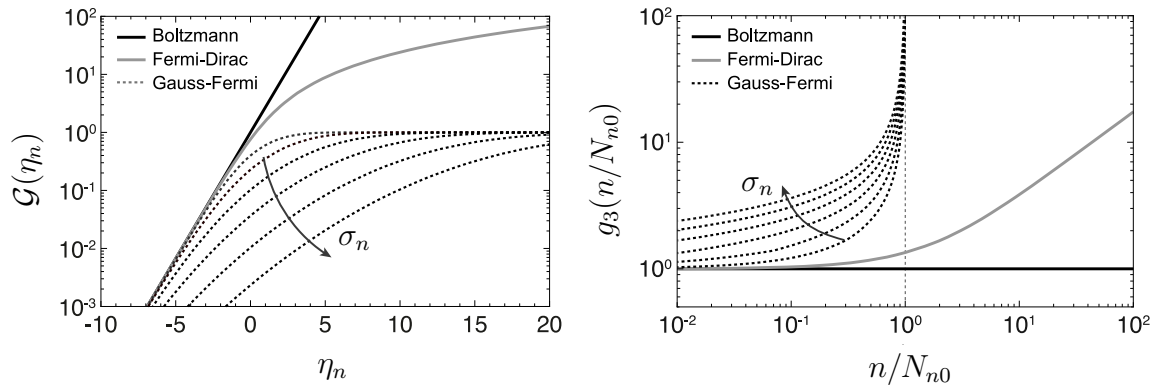
Figure 2: Statistical distribution function $\mathcal{G}$ (left) and so-called diffusion enhancement g_3 (right) for Gauss-Fermi statistics (see (2.3) and (2.10)) with different disorder parameters σ_n (dotted) in comparison to Boltzmann (black) and Fermi-Dirac statistics (gray).

This generalized Einstein relation is often interpreted as so-called diffusion enhancement in the literature on organic semiconductor materials, see [vMC08]. The function g_3 is depicted for different values of s_n in Fig. 2 and compared to Boltzmann (where $\mathcal{G}(\eta_n) = \exp(\eta_n)$ and $g_3(T, n/N_{n0}) \equiv 1$) and Fermi-Dirac statistics used in conventional semiconductors.

Note that due to the properties of $\mathcal{G}_{s_n}$, we have $g_3(T, n/N_{n0}) \geq 1$ and $\lim_{n \to N_{n0}} g_3(T, n/N_{n0}) = +\infty$.

The influence of the diffusion enhancement factor g_3 in numerical simulations of organic devices cannot be neglected. We refer to Section 4 for the simulation of a simple organic n-i-n (n-doped/intrinsic/n-doped) resistor, where also the spatial distribution of g_3 is shown.

2.4 Reaction term

In the literature [KSMB05, Wet14] the reaction term R in the drift-diffusion model (2.1) is written in the variables of n and p. In [KSMB05, vdHvOCB09] the expression for the Langevin recombination rate reads as

$$R_{\mathsf{L}} = \frac{q}{\varepsilon_0 \varepsilon_r} (\mu_n + \mu_p)(np - n_i^2)$$

with the permittivity $\varepsilon_0 \varepsilon_r$ and the electron and hole mobilities μ_n and μ_p, respectively. In [Wet14], besides Langevin recombination an additional trap assisted Shockley-Read-Hall (SRH) recombination mechanism known from classical (inorganic) semiconductor modeling is used with the recombination rate

$$R_{\mathsf{SRH}} = C_n C_p N_t \frac{np - n_1 p_1}{C_n(n + n_1) + C_p(p + p_1)},$$

with C_n and C_p the capture coefficients for electrons and holes, respectively, N_t the density of electron traps, and $n_1 p_1 = n_i^2$ the product under equilibrium conditions in the case that the Fermi level coincides with the position of the recombination centers, where n_i denotes the intrinsic carrier concentration in the sample. The sum of both recombination rates enters the continuity equations according to $R = R_{\mathsf{SRH}} + R_{\mathsf{L}}$.

We assume an expression of the form

$$R = r(\cdot, n, p, T)\Big(1 - \exp \frac{q(\varphi_n - \varphi_p)}{k_{\mathsf{B}} T}\Big), \quad r(\cdot, n, p, T) = r_0(\cdot, n, p, T)\, np, \qquad (2.12)$$

where $r(\cdot, n, p, T) : \Omega \times [0, \operatorname{ess\,sup} N_{n0}] \times [0, \operatorname{ess\,sup} N_{p0}] \times (0, \infty) \to \mathbb{R}$ is a Caratheodory function with

$$0 \le r_0(\cdot, n, p, T) \le \bar{r} \quad \forall (n, p, T) \in [0, \operatorname{ess\,sup} N_{n0}] \times [0, \operatorname{ess\,sup} N_{p0}] \times (0, \infty) \text{ and a.a. } x \in \Omega.$$

In case of Boltzmann statistics this is equivalent to the widely used form

$$R(n, p) = C(n, p)(np - n_i^2),$$

where n_i is the intrinsic carrier density. The expression for the rate in (2.12) is compatible with thermodynamic equilibrium. Especially, it reflects the fact, that in equilibrium the quasi-Fermi levels of electrons and holes have to coincide, leading to a vanishing recombination rate.

2.5 Initial and boundary conditions

The drift-diffusion model (2.1) is supplemented with initial and boundary conditions which we formulate in terms of the electrostatic and quasi-Fermi potentials,

$$\psi(0) = \psi^0, \quad \varphi_n(0) = \varphi_n^0, \quad \varphi_p(0) = \varphi_p^0 \quad \text{in } \Omega. \tag{2.13}$$

For the formulation of boundary conditions we decompose $\partial\Omega$ into Ohmic contacts $\Gamma_D = \cup_{i=1}^I \Gamma_{Di}$, gate contacts Γ_G, and Neumann boundaries Γ_N resulting from semiconductor-insulator interfaces or from "cutting off" regions of the device with insignificant action. Ohmic contacts like semiconductor-metal interfaces are modeled by Dirichlet boundary conditions

$$\psi = \psi_* + V_i, \quad \varphi_n = V_i, \quad \varphi_p = V_i \quad \text{on } \mathbb{R}_+ \times \Gamma_{Di},$$

where V_i denotes the corresponding externally applied contact voltage at Γ_{Di}. The value ψ_* (at the boundary) is defined by the local electroneutrality condition,

$$0 = C - N_{n0} \mathcal{G}_{s_n} \left(\frac{q\psi_* - E_L}{k_B T} \right) + N_{p0} \mathcal{G}_{s_p} \left(\frac{E_H - q\psi_*}{k_B T} \right). \tag{2.14}$$

The solvability of (2.14) gives a restriction on the range of the doping profile C, e.g., in the unipolar situation $|C| \le N_{i0}$ is needed. The semiconductor-insulator interface is realized by homogeneous Neumann boundary conditions

$$\varepsilon_0 \varepsilon_r \nabla \psi \cdot \nu = j_n \cdot \nu = j_p \cdot \nu = 0 \quad \text{on } \mathbb{R}_+ \times \Gamma_N,$$

where ν denotes the outer normal vector. Gate contacts are described by Robin boundary conditions for the electrostatic potential ψ and Neumann boundary conditions in the continuity equations

$$\varepsilon_0 \varepsilon_r \nabla \psi \cdot \nu + \alpha_{\text{ox}}(\psi - V_G) = 0, \quad j_n \cdot \nu = j_p \cdot \nu = 0 \quad \text{on } \mathbb{R}_+ \times \Gamma_G.$$

3 Analysis of the stationary drift-diffusion model

The classical (inorganic) stationary semiconductor device equations in the case of Boltzmann statistics are studied in [GG86, Sec. 4]. Therein, an existence result as well as the uniqueness of the

thermodynamic equilibrium is proven. In [Mar86, Chap. 3] again the case of Boltzmann statistics is investigated. Using Slotboom variables and Schauder's fixed point theorem (and Leray-Schauder for the subproblem of the non-linear Poisson equation) the existence of solutions to the stationary problem is verified. The paper [Grö87] admits a class of statistical relations including Boltzmann and Fermi-Dirac statistics assuming $n = N_{n0}e_n(\eta_n)$ where $e_n \in C^2(\mathbb{R}, \mathbb{R}_+)$ with the additional requirement that $\lim_{y \to +\infty} e_n(y) = +\infty$, which is definitely not fulfilled in the case of organic semiconductors, compare Fig. 2. Also here a-priori estimates are obtained by means of maximum principle arguments and an existence proof using Schauder's fixed point theorem.

In our setting, another additional difficulty arises from the dependence of the mobility functions μ_i on the gradient of the electrostatic potential. For this, special arguments in the proof of the continuity of the Schauder map are necessary, see Step 2 in the proof of Lemma 3.3.

3.1 Scaled model equations and assumptions on the data

We study in the bounded domain $\Omega \subset \mathbb{R}^d$ the stationary drift-diffusion problem

$$-\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \psi) = q(C - n + p),$$

$$-\nabla \cdot j_n = -qR, \qquad j_n = -qn\mu_n \nabla \varphi_n, \quad n = N_{n0}\mathcal{G}_{s_n}\left(\frac{q(\psi - \varphi_n) - E_L}{k_\mathrm{B}T}\right),$$

$$\nabla \cdot j_p = -qR, \qquad j_p = -qp\mu_p \nabla \varphi_p, \quad p = N_{p0}\mathcal{G}_{s_p}\left(\frac{E_H - q(\psi - \varphi_p)}{k_\mathrm{B}T}\right)$$

with

$$R = R(n, p, \varphi_n, \varphi_p, T) = r(n, p, T)\left(1 - \exp\frac{q(\varphi_n - \varphi_p)}{k_\mathrm{B}T}\right).$$

To simplify the notation, we introduce scaled quantities as follows

- ■ The potentials ψ, φ_n, φ_p, V_G and the applied voltage are scaled by the thermal voltage $U_T := \frac{k_\mathrm{B}T}{q}$.

- ■ The band edges E_L, E_H are divided by $k_\mathrm{B}T$.

Dividing the Poisson equation as well as the continuity equations by q and denoting the scaled quantities by the same symbol as the original ones, we obtain in Ω

$$-\nabla \cdot (\varepsilon \nabla \psi) = C - n + p,$$

$$-\nabla \cdot j_n = -R, \qquad j_n = -n\mu_n \nabla \varphi_n, \quad n = N_{n0}\mathcal{G}_{s_n}\left(\psi - \varphi_n - E_L\right), \qquad (3.1)$$

$$\nabla \cdot j_p = -R, \qquad j_p = -p\mu_p \nabla \varphi_p, \quad p = N_{p0}\mathcal{G}_{s_p}\left(E_H - (\psi - \varphi_p)\right)$$

with

$$R = R(n, p, \varphi_n, \varphi_p, T) = r(n, p, T)\left(1 - \mathrm{e}^{\varphi_n - \varphi_p}\right),$$

where electron and hole current densities j_i as well as the the generation-recombination rate result from the original ones by scaling with $k_\mathrm{B}T$. And the new coefficient in the Poisson equation is $\varepsilon = \frac{\varepsilon_0 \varepsilon_r k_\mathrm{B}T}{q^2}$.

We complete the system by the following boundary conditions

$$\psi = \psi^D, \quad \varphi_n = \varphi_n^D, \quad \varphi_p = \varphi_p^D \quad \text{on } \Gamma_D,$$
$$\varepsilon \nabla \psi \cdot \nu = j_n \cdot \nu = j_p \cdot \nu = 0 \quad \text{on } \Gamma_N, \tag{3.2}$$
$$\varepsilon \nabla \psi \cdot \nu + \alpha_{\text{ox}}(\psi - V_G) = 0, \quad j_n \cdot \nu = j_p \cdot \nu = 0 \quad \text{on } \Gamma_G.$$

We work with the Lebesgue spaces $L^p(\Omega)$ and the Sobolev spaces $W^{1,\infty}(\Omega)$ and $H^1(\Omega)$ as well as its closed subspace

$$H_D^1(\Omega) := \{ u \in H^1(\Omega) : u|_{\Gamma_D} = 0 \}.$$

(Note that $\text{mes}(\Gamma_D) > 0$ will be assumed.) 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 carry our analytical investigations of the stationary drift-diffusion model out under the following **Assumptions (A)**:

- $\Omega \subset \mathbb{R}^d$ bounded Lipschitz domain, $\Gamma_D, \Gamma_N, \Gamma_G \subset \Gamma := \partial\Omega$ disjoint subsets such that $\overline{\Gamma_D \cup \Gamma_N \cup \Gamma_G} = \Gamma$ and $\text{mes}(\Gamma_D) > 0$,

- $\psi^D \in W^{1,\infty}(\Omega), \varphi_n^D, \varphi_p^D \in H^1(\Omega) \cap L^\infty(\Omega), \|\varphi_n^D\|_{L^\infty}, \|\varphi_p^D\|_{L^\infty} \leq K$ with $K > 1$, $V_G \in L^\infty(\Gamma_G), \alpha_{\text{ox}} \in L_+^\infty(\Gamma_G)$,

- $N_{i0} \in L^\infty(\Omega), N_{i0} \geq c > 0$ a.e. in $\Omega, i = n, p, T = \text{const} > 0, \sigma_n, \sigma_p = \text{const} > 0$,

- $\varepsilon \in L^\infty(\Omega), 0 < c \leq \varepsilon$ a.e. in $\Omega, C \in L^\infty(\Omega)$,

- $\mu_i(\cdot, T, \cdot, \cdot) : \Omega \times [0, \text{ess sup } N_{i0}] \times \mathbb{R}_+ \to \mathbb{R}$, are Caratheodory functions, $i = n, p$, fulfilling

$$0 < \underline{\mu} \leq \mu_n(\cdot, T, n, F), \ \mu_p(\cdot, T, p, F) \leq \overline{\mu} < \infty$$
$$\forall (n, p, F) \in [0, \text{ess sup } N_{n0}] \times [0, \text{ess sup } N_{p0}] \times \mathbb{R}_+ \text{ a.e. in } \Omega. \tag{3.3}$$

- $R = r(\cdot, n, p, T)\left(1 - e^{\varphi_n - \varphi_p}\right), r(\cdot, n, p, T) = r_0(\cdot, n, p, T)np$, where $r_0(\cdot, n, p, T) : \Omega \times [0, \text{ess sup } N_{n0}] \times [0, \text{ess sup } N_{p0}] \times (0, \infty) \to \mathbb{R}$ is a Caratheodory function satisfying $0 \leq r_0(\cdot, n, p, T) \leq \overline{r}$ for all $(n, p, T) \in [0, \text{ess sup } N_{n0}] \times [0, \text{ess sup } N_{p0}] \times (0, \infty)$ and a.a. $x \in \Omega$.

In the following, we suppress in the writing the spatial position x and the argument T in the mobility functions μ_n, μ_p and in the reaction coefficient r.

3.2 Existence of weak solutions

The weak formulation of the van Roosbroeck system for organic semiconductor devices (3.1), (3.2) reads as follows: Find $(\psi, \varphi_n, \varphi_p) \in (\psi^D + H_D^1(\Omega)) \times (\varphi_n^D + H_D^1(\Omega)) \times (\varphi_p^D + H_D^1(\Omega))$ such that

$$\int_\Omega \varepsilon \nabla \psi \cdot \nabla \overline{\psi} \, dx + \int_{\Gamma_G} \alpha_{\text{ox}}(\psi - V_G)\overline{\psi} \, d\Gamma = \int_\Omega (C - n + p)\overline{\psi} \, dx,$$

$$\int_\Omega \big(n\mu_n(n, |\nabla\psi|)\nabla\varphi_n \cdot \nabla\overline{\varphi}_n + p\mu_p(p, |\nabla\psi|)\nabla\varphi_p \cdot \nabla\overline{\varphi}_p\big) \, dx \tag{3.4}$$

$$= \int_\Omega r(n,p)\big(1 - e^{\varphi_n - \varphi_p}\big)(\overline{\varphi}_n - \overline{\varphi}_p) \, dx \qquad \forall \overline{\psi}, \overline{\varphi}_n, \overline{\varphi}_p \in H_D^1(\Omega),$$

where the densities n and p have to be calculated pointwise by

$$n = N_{n0}\mathcal{G}_{s_n}\big(\psi - \varphi_n - E_L\big), \quad p = N_{p0}\mathcal{G}_{s_p}\big(E_H - (\psi - \varphi_p)\big). \tag{3.5}$$

Now we formulate the main result of our paper, which is proven in the subsequent subsections.

Theorem 3.1 *Under the assumption (A) there exists a weak solution $(\psi, \varphi_n, \varphi_p)$ to problem (3.4). Moreover, there are positive constants c_{ψ,L^∞}, c_{ψ,H^1}, c_{H^1}, $\underline{c_c}$, $\overline{c_c}$ such that*

$$\|\psi\|_{L^\infty} \leq c_{\psi,L^\infty}, \quad \|\psi\|_{H^1} \leq c_{\psi,H^1},$$

$$\|\varphi_n\|_{L^\infty}, \|\varphi_p\|_{L^\infty} \leq K, \quad \|\varphi_n\|_{H^1}, \|\varphi_p\|_{H^1} \leq c_{H^1},$$

and the by (3.5) related densities n and p are bounded by $\underline{c_c} \leq n, p \leq \overline{c_c}$ a.e. on Ω.

3.3 Iteration scheme

We introduce the non empty, convex, closed, precompact set

$$\mathcal{M} := \big\{(\varphi_n, \varphi_p) \in L^2(\Omega)^2 : -K \leq \varphi_n, \varphi_p \leq K, \|\varphi_n\|_{H^1}, \|\varphi_p\|_{H^1} \leq c_{H^1}\big\}.$$

The constant K is given in assumption (A) and $c_{H^1} > 0$ will be fixed in Lemma 3.2. We define a fixed point map $\mathcal{Q} : \mathcal{M} \to \mathcal{M}$, $(\varphi_n, \varphi_p) = \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p)$ by the following three steps:

1. For given $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ we solve the nonlinear Poisson equation

$$-\nabla \cdot (\varepsilon\nabla\psi) = C - N_{n0}\mathcal{G}_{s_n}\big(\psi - \widetilde{\varphi}_n - E_L\big) + N_{p0}\mathcal{G}_{s_p}\big(E_H - (\psi - \widetilde{\varphi}_p)\big) \quad \text{in } \Omega,$$
$$\psi = \psi^D \quad \text{on } \Gamma_D, \quad \varepsilon\nabla\psi \cdot \nu + \alpha_{\text{ox}}(\psi - V_G) = 0 \quad \text{on } \Gamma_G, \quad \varepsilon\nabla\psi \cdot \nu = 0 \quad \text{on } \Gamma_N. \tag{3.6}$$

The existence of a unique weak solution $\psi \in \psi^D + H_D^1(\Omega)$ to (3.6) and the estimate

$$\|\psi\|_{L^\infty} \leq c_{\psi,L^\infty}, \quad \|\psi\|_{H^1} \leq c_{\psi,H^1}$$

with constants c_{ψ,L^∞}, $c_{\psi,H^1} > 0$ independent of the special choice of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ will be guaranteed by Lemma 3.1.

2. With the solution ψ to (3.6), we set

$$\widetilde{n} := N_{n0}\mathcal{G}_{s_n}\big(\psi - \widetilde{\varphi}_n - E_L\big), \quad \widetilde{p} := N_{p0}\mathcal{G}_{s_p}\big(E_H - (\psi - \widetilde{\varphi}_p)\big). \tag{3.7}$$

Due to the uniform $L^\infty(\Omega)$-estimates for ψ in Lemma 3.1 and for $\widetilde{\varphi}_n$ and $\widetilde{\varphi}_p$ from the set $\mathcal{M}$ and the properties of N_{n0}, N_{p0}, and $\mathcal{G}_s$ from (A), the carrier densities $\widetilde{n}$ and $\widetilde{p}$ from (3.7) fulfil

$$0 < \underline{c_c} \le \widetilde{n},\, \widetilde{p} \le \overline{c_c} \quad \text{a.e. in } \Omega,$$

where the constants $\underline{c_c}$, $\overline{c_c} > 0$ are independent of the special choice of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$. Therefore, by (2.8)

$$\widetilde{n}\mu_n(\widetilde{n}, |\nabla\psi|),\ \widetilde{p}\mu_n(\widetilde{p}, |\nabla\psi|) \in [\underline{c_c}\,\underline{\mu}, \overline{c_c}\,\overline{\mu}] \quad \text{a.e. in } \Omega. \tag{3.8}$$

3. Finally, we solve the system of continuity equations with densities $\widetilde{n}$ and $\widetilde{p}$ and with mobilities $\mu_n(\cdot, \widetilde{n}, |\nabla\psi|)$ and $\mu_p(\cdot, \widetilde{p}, |\nabla\psi|)$ for a solution (φ_n, φ_p) of

$$
\begin{aligned}
&\nabla \cdot \big(\widetilde{n}\mu_n(\widetilde{n}, |\nabla\psi|)\nabla\varphi_n\big) + r(\widetilde{n}, \widetilde{p})\big(1 - e^{\varphi_n - \varphi_p}\big) = 0 \quad \text{on } \Omega, \\
&-\nabla \cdot \big(\widetilde{p}\mu_p(\widetilde{p}, |\nabla\psi|)\nabla\varphi_p\big) + r(\widetilde{n}, \widetilde{p})\big(1 - e^{\varphi_n - \varphi_p}\big) = 0 \quad \text{on } \Omega, \\
&\varphi_n = \varphi_n^D,\ \varphi_p = \varphi_p^D \quad \text{on } \Gamma_D, \\
&\widetilde{n}\mu_n(\widetilde{n}, |\nabla\psi|)\nabla\varphi_n \cdot \nu = \widetilde{p}\mu_p(\widetilde{p}, |\nabla\psi|)\nabla\varphi_p \cdot \nu = 0 \quad \text{on } \Gamma_N \cup \Gamma_G.
\end{aligned}
\tag{3.9}
$$

Lemma 3.2 ensures a unique weak solution of (3.9) and the bounds independent of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ (and the resulting $\widetilde{n}$ and $\widetilde{p}$)

$$-K \le \varphi_n,\, \varphi_p \le K \quad \text{a.e. on } \Omega, \quad \|\varphi_n\|_{H^1},\, \|\varphi_p\|_{H^1} \le c_{H^1}.$$

This guarantees that $(\varphi_n, \varphi_p) = \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$.

3.4 Results for subproblems

Lemma 3.1 *We assume (A). Let $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$. Then there exists a unique weak solution $\psi \in \psi^D + H_D^1(\Omega)$ to (3.6). It fulfils the estimates*

$$\|\psi\|_{L^\infty} \le c_{\psi, L^\infty}, \quad \|\psi\|_{H^1} \le c_{\psi, H^1}$$

with constants c_{ψ, L^∞}, $c_{\psi, H^1} > 0$ independent of the special choice of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$.

Proof. 1. Due to assumption (A) and the properties of the function $\mathcal{G}_s$, see Remark 2.1, for given $(\widetilde{\varphi}_n, \widetilde{\varphi}_p)$ the operator $\mathcal{B}_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)} : \psi^D + H_D^1(\Omega) \to (H_D^1(\Omega))^*$,

$$
\begin{aligned}
\langle \mathcal{B}_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}\psi, \overline{\psi}\rangle := &\int_\Omega \varepsilon\nabla\psi \cdot \nabla\overline{\psi}\,dx + \int_{\Gamma_G} \alpha_{\text{ox}}(\psi - V_G)\overline{\psi}\,d\Gamma \\
&+ \int_\Omega \big(N_{n0}\mathcal{G}_{s_n}(\psi - \widetilde{\varphi}_n - E_L) - N_{p0}\mathcal{G}_{s_p}(E_H - (\psi - \widetilde{\varphi}_p)) - C\big)\overline{\psi}\,dx,
\end{aligned}
$$

$\overline{\psi} \in H_D^1(\Omega)$, is strongly monotone and Lipschitz continuous. Thus, the unique solution $\psi \in \psi^D + H_D^1(\Omega)$ to $\mathcal{B}_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}\psi = 0$ is the unique weak solution to (3.6).

2. Since $\mathcal{G}_{s_n}(\psi - \widetilde{\varphi}_n - E_L) \in (0, 1)$ and $\mathcal{G}_{s_p}(E_H - (\psi - \widetilde{\varphi}_p)) \in (0, 1)$ the quantity $\|C\|_{L^\infty} + \|N_{n0}\|_{L^\infty} + \|N_{p0}\|_{L^\infty}$ is a uniform $L^\infty(\Omega)$-bound for

$$h := C - N_{n0}\mathcal{G}_{s_n}(\psi - \widetilde{\varphi}_n - E_L) + N_{p0}\mathcal{G}_{s_p}(E_H - (\psi - \widetilde{\varphi}_p)).$$

3. By Moser iteration, we prove a L^∞ bound independent of the chosen $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ for the weak solution ψ to (3.6). Since $\mathrm{mes}(\Gamma_D) > 0$ the term $\|\nabla \cdot \|_{L^2}$ is an equivalent norm on $H_D^1(\Omega)$ such that $\underline{\alpha}\|w\|_{H^1(\Omega)}^2 \le \|\nabla w\|_{L^2}^2$ for all $w \in H_D^1(\Omega)$. We test (3.6) by $m(\psi - \psi^D)^{m-1}$, $m = 2^k$, $k \in \mathbb{N}$, and use the notation $v := (\psi - \psi^D)^{\frac{m}{2}}$ to obtain

$$
\begin{aligned}
\underline{\alpha}&\|v\|_{H^1}^2 \\
&\le \int_\Omega c(m-1)|v|^{\frac{m-2}{m}}|\nabla v||\nabla \psi^D|\,\mathrm{d}x \\
&\quad + cm\|h\|_{L^\infty} \int_\Omega |\psi - \psi^D|^{m-1}\,\mathrm{d}x + cm\|V_G - \psi^D\|_{L^\infty(\Gamma_G)} \int_{\Gamma_G} |\psi - \psi^D|^{m-1}\,\mathrm{d}\Gamma \\
&\le \frac{\alpha}{2}\|v\|_{H^1}^2 + cm^2\|\psi^D\|_{W^{1,\infty}}^2 (1 + \|v\|_{L^2}^2) \\
&\quad + cm\|h\|_{L^\infty} \int_\Omega (1 + v^2)\,\mathrm{d}x + cm\|V_G - \psi^D\|_{L^\infty(\Gamma_G)} \int_{\Gamma_G} (1 + v^2)\,\mathrm{d}\Gamma.
\end{aligned}
\tag{3.10}
$$

By the Gagliardo-Nirenberg inequality, the trace inequality, and Young's inequality we find for all $\epsilon > 0$ a $c_\epsilon > 0$ such that

$$
m^2\|v\|_{L^2}^2 \le cm^2\|v\|_{L^1}^{\frac{4}{d+2}}\|v\|_{H^1}^{\frac{2d}{d+2}} \le \epsilon\|v\|_{H^1}^2 + c_\epsilon\, m^{d+2}\,\|v\|_{L^1}^2,
$$

$$
m\|v\|_{L^2(\Gamma)}^2 \le cm\|v\|_{L^2}\|v\|_{H^1} \le cm\|v\|_{L^1}^{\frac{2}{d+1}}\|v\|_{H^1}^{\frac{2d+2}{d+1}} \le \epsilon\|v\|_{H^1}^2 + c_\epsilon\, m^{d+2}\,\|v\|_{L^1}^2.
$$

From (3.10), the following the estimate results with the same constant $c_0(h, V_G, \psi^D) \ge 2$ for $m = 2^k$, $k \in \mathbb{N}$, and $\overline{c} := 2^{d+2}$

$$
\|v\|_{L^2}^2 \le \|v\|_{H^1}^2 \le \frac{1}{2}c_0(h, V_G, \psi^D)\,\overline{c}^k(1 + \|v\|_{L^1}^2),
$$

where c_0 only depends on the norms of h, V_G, and ψ^D. Setting $a_k := 1 + \|\psi - \psi^D\|_{L^{2^k}}^{2^k}$ the previous estimates ensure the recursion

$$
\begin{aligned}
a_k &\le c_0(h, V_G, \psi^D)\overline{c}^k a_{k-1}^2 \le c_0(h, V_G, \psi^D)^{1+2}\overline{c}^{k+2(k-1)}a_{k-2}^4 \\
&\le c_0(h, V_G, \psi^D)^{1+2+\cdots+2^{k-2}}\overline{c}^{k+2(k-1)+\cdots+2^{k-2}\cdot 2}a_1^{2^{k-1}} \le c_0(h, V_G, \psi^D)^{2^k}\overline{c}^{2^{k+1}}a_1^{2^k}.
\end{aligned}
\tag{3.11}
$$

Note that $\sum_{i=0}^{k-2} 2^i \le 2^k$ and $\sum_{i=0}^{k-2} 2^i(k - i) \le 2^{k+1}$ for $k \ge 2$. The starting estimate for a_1 is obtained by testing (3.6) by $\psi - \psi^D$. Applying embedding and trace inequality as well as Young's inequality gives

$$
\begin{aligned}
\underline{\alpha}\|\psi - \psi^D\|_{H^1}^2 &\le c \int_\Omega \big(|h||\psi - \psi^D| + |\nabla(\psi - \psi^D)||\nabla \psi^D|\big)\,\mathrm{d}x \\
&\quad + c \int_{\Gamma_G} |V_G - \psi^D||\psi - \psi^D|\,\mathrm{d}\Gamma \\
&\le \frac{\alpha}{2}\|\psi - \psi^D\|_{H^1}^2 + c_{\underline{\alpha}}\big(\|h\|_{L^2}^2 + \|V_G - \psi^D\|_{L^2(\Gamma_G)}^2 + \|\psi^D\|_{H^1}^2\big).
\end{aligned}
\tag{3.12}
$$

This ensures that $a_1 = 1 + \|\psi - \psi^D\|_{L^2}^2 \le c_1(h, V_G, \psi^D)$ which induces together with the recursion formula (3.11) the L^∞ bound for $\psi - \psi^D$, and since $\psi^D \in L^\infty(\Omega)$ we find the desired L^∞ estimate. From (3.12) and $\psi^D \in H^1(\Omega)$ the H^1 estimate for ψ follows. $\square$

Lemma 3.2 *We assume (A). Let $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ and let ψ be the weak solution to (3.6) and $\widetilde{n}$ and $\widetilde{p}$ be given by (3.7). Then there exists a unique weak solution $(\varphi_n, \varphi_p) \in (\varphi_n^D + H_D^1(\Omega)) \times (\varphi_p^D + H_D^1(\Omega))$ to (3.9). It fulfils the estimates*

$$-K \leq \varphi_n, \, \varphi_p \leq K \quad \text{a.e. on } \Omega, \quad \|\varphi_n\|_{H^1}, \, \|\varphi_p\|_{H^1} \leq c_{H^1}$$

with K from Assumption (A) and a constant $c_{H^1} > 0$ independent of the special choice of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ (and the resulting ψ, $\widetilde{n}$ and $\widetilde{p}$).

Proof. 1. For $M > 0$ let $\rho_M : \mathbb{R}^2 \to [0, 1]$ be a fixed Lipschitz continuous function with

$$\rho_M(y, z) := \begin{cases} 0 & \text{if } \max\{|y|, |z|\} \geq M, \\ 1 & \text{if } \max\{|y|, |z|\} \leq \frac{M}{2}. \end{cases}$$

Due to (3.8) the operator $A_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M : (\varphi_n^D + H_D^1(\Omega)) \times (\varphi_p^D + H_D^1(\Omega)) \to (H_D^1(\Omega)^*)^2$,

$$A_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M(\varphi_n, \varphi_p) = \widehat{A}_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M \big((\varphi_n, \varphi_p), (\varphi_n, \varphi_p)\big)$$

with the argument splitting

$$\langle \widehat{A}_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M \big((\varphi_n, \varphi_p), (\widehat{\varphi}_n, \widehat{\varphi}_p)\big), (\overline{\varphi}_n, \overline{\varphi}_p) \rangle :=$$

$$\int_\Omega \big(\widetilde{n} \mu_n(\widetilde{n}, |\nabla\psi|) \nabla\widehat{\varphi}_n \cdot \nabla\overline{\varphi}_n + \widetilde{p} \mu_p(\widetilde{p}, |\nabla\psi|) \nabla\widehat{\varphi}_p \cdot \nabla\overline{\varphi}_p \big) \, \mathrm{d}x$$

$$+ \int_\Omega \rho_M(\varphi_n, \varphi_p) r(\widetilde{n}, \widetilde{p}) \big(e^{\varphi_n - \varphi_p} - 1 \big) (\overline{\varphi}_n - \overline{\varphi}_p) \, \mathrm{d}x, \quad \overline{\varphi}_n, \overline{\varphi}_p \in H_D^1(\Omega),$$

is an operator of variational type (see [Lio69, p. 182]). Have in mind that the main part (in the arguments $\widehat{\varphi}_n$, $\widehat{\varphi}_p$) is monotone, continuous and bounded and the regularized reaction term is bounded and the mapping $(\varphi_n, \varphi_p) \mapsto \rho_M(\varphi_n, \varphi_p)(e^{\varphi_n - \varphi_p} - 1)$ is Lipschitz continuous. Since the operator $A_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M(\varphi_n, \varphi_p)$ additionally is coercive, the equation $A_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M(\varphi_n, \varphi_p) = 0$ has at least one solution $(\varphi_n^M, \varphi_p^M) \in (\varphi_n^D + H_D^1(\Omega)) \times (\varphi_p^D + H_D^1(\Omega))$.

2. Using the test function $((\varphi_n^M - K)^+, (\varphi_p^M - K)^+) \in H_D^1(\Omega)^2$ for $A_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M(\varphi_n^M, \varphi_p^M) = 0$ with K from assumption (A) we obtain

$$0 = \int_\Omega \big(\widetilde{n} \mu_n(\widetilde{n}, |\nabla\psi|) |\nabla(\varphi_n^M - K)^+|^2 + \widetilde{p} \mu_p(\widetilde{p}, |\nabla\psi|) |\nabla(\varphi_p^M - K)^+|^2 \big) \, \mathrm{d}x$$

$$+ \int_\Omega \rho_M(\varphi_n^M, \varphi_p^M) r(\widetilde{n}, \widetilde{p}) \big(e^{\varphi_n^M - \varphi_p^M} - 1 \big) \big((\varphi_n^M - K)^+ - (\varphi_p^M - K)^+ \big) \, \mathrm{d}x.$$

Discussing the four different cases $\varphi_n^M (\varphi_p^M) > K (\leq K)$ we find that the integrand in the last line is always non-negative (note that ρ_M and r are also non-negative), (3.8) ensures that $\varphi_n^M, \varphi_p^M \leq K$ a.e. in Ω. On the other hand, testing by $(-(\varphi_n^M + K)^-, -(\varphi_p^M + K)^-)$ gives the estimates $\varphi_n^M, \varphi_p^M \geq -K$ a.e. in Ω. Therefore, if we choose $M \geq 2K$, each solution to $A_{(\widetilde{\varphi}_n, \widetilde{\varphi}_p)}^M(\varphi_n, \varphi_p) = 0$ is a weak solution to (3.9), too. The estimates of Step 2 can be done in exactly the same way (now without the factor ρ_M) to obtain the upper and lower bounds for all weak solutions (φ_n, φ_p) to (3.9)

$$\|\varphi_n\|_{L^\infty}, \|\varphi_p\|_{L^\infty} \leq K.$$

3. Next, we show that there is at most one weak solution to (3.9). If there would be two different solutions (φ_n, φ_p) and $(\widehat{\varphi}_n, \widehat{\varphi}_p)$, the test function $(\varphi_n - \widehat{\varphi}_n, \varphi_p - \widehat{\varphi}_p) \in H^1_D(\Omega)^2$ for (3.9) yields

$$0 = \int_\Omega \left(\widetilde{n}\mu_n(\widetilde{n}, |\nabla\psi|)|\nabla(\varphi_n - \widehat{\varphi}_n)|^2 + \widetilde{p}\mu_p(\widetilde{p}, |\nabla\psi|)|\nabla(\varphi_p - \widehat{\varphi}_p)|^2 \right) \mathrm{d}x$$
$$+ \int_\Omega r(\widetilde{n}, \widetilde{p})\left(\mathrm{e}^{\varphi_n - \varphi_p} - \mathrm{e}^{\widehat{\varphi}_n - \widehat{\varphi}_p} \right)\left(\varphi_n - \varphi_p - (\widehat{\varphi}_n - \widehat{\varphi}_p) \right) \mathrm{d}x.$$

Because of $\mathrm{mes}(\Gamma_D) > 0$, (3.8), the monotonicity of the exponential function and $r(\widetilde{n}, \widetilde{p}) \geq 0$ we obtain $(\varphi_n, \varphi_p) = (\widehat{\varphi}_n, \widehat{\varphi}_p)$.

4. In the last step we verify the uniform H^1-estimate for the weak solution to (3.9) by testing with $(\varphi_n - \varphi_n^D, \varphi_p - \varphi_p^D) \in H^1_D(\Omega)^2$, using Hölder's inequality and the L^∞ bounds $\varphi_n, \varphi_p \in [-K, K]$ a.e. in Ω from Step 2. (Here we left out the arguments of μ_n and μ_p.)

$$\int_\Omega \left(\widetilde{n}\mu_n|\nabla(\varphi_n - \varphi_n^D)|^2 + \widetilde{p}\mu_p|\nabla(\varphi_p - \varphi_p^D)|^2 \, \mathrm{d}x + r(\widetilde{n}, \widetilde{p})\left(\mathrm{e}^{\varphi_n - \varphi_p} - 1 \right)\left(\varphi_n - \varphi_p \right) \right) \mathrm{d}x$$
$$\leq \int_\Omega \frac{1}{2} \left(\widetilde{n}\mu_n(|\nabla(\varphi_n - \varphi_n^D)|^2 + |\nabla\varphi_n^D|^2) + \widetilde{p}\mu_p(|\nabla(\varphi_p - \varphi_p^D)|^2 + |\nabla\varphi_p^D|^2) \right) \mathrm{d}x$$
$$+ 2\overline{r}\, K \exp\{2K\}\, \mathrm{mes}(\Omega).$$

Exploiting again (3.8), the non-negativity of the function r, the monotonicity of the exponential function, and that $\varphi_n^D, \varphi_p^D \in H^1(\Omega)$ are given functions, and using the constants $\overline{r}$ and K from assumption (A), we end up with the bounds $\|\varphi_n\|_{H^1}, \|\varphi_p\|_{H^1} \leq c_{H^1}$, where the constant c_{H^1} does not depend on the special choice of $(\widetilde{\varphi}_n, \widetilde{\varphi}_p) \in \mathcal{M}$ (and the resulting ψ, $\widetilde{n}$ and $\widetilde{p}$). $\quad\square$

3.5 Continuity of the fixed point map $\mathcal{Q}$ and proof of the main result

Lemma 3.3 *We assume (A). Then the map $\mathcal{Q} : \mathcal{M} \to \mathcal{M}$ is continuous.*

Proof. 1. Let $(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l)$, $(\widetilde{\varphi}_n, \widetilde{\varphi}_n) \in \mathcal{M}$ with $\widetilde{\varphi}_n^l \to \widetilde{\varphi}_n$ in $L^2(\Omega)$, $\widetilde{\varphi}_p^l \to \widetilde{\varphi}_p$ in $L^2(\Omega)$, let ψ^l and ψ denote the corresponding unique weak solutions to (3.6), $\widetilde{n}^l$ and $\widetilde{n}$ denote the corresponding quantities in (3.7), and $(\varphi_n^l, \varphi_p^l) = \mathcal{Q}(\widetilde{\varphi}_n^l, \widetilde{\varphi}_p^l)$, and $(\varphi_n, \varphi_p) = \mathcal{Q}(\widetilde{\varphi}_n, \widetilde{\varphi}_p)$. We test the problem (3.6) by $\psi^l - \psi \in H^1_D(\Omega)$ and obtain

$$c\|\psi^l - \psi\|_{H^1}^2 \leq -\int_\Omega N_{n0}\Big\{ \mathcal{G}_{s_n}\big(\psi^l - \widetilde{\varphi}_n^l - E_L\big) - \mathcal{G}_{s_n}\big(\psi - \widetilde{\varphi}_n - E_L\big) \Big\}(\psi^l - \psi)\,\mathrm{d}x$$
$$+ \int_\Omega N_{p0}\Big\{ \mathcal{G}_{s_p}\big(E_H - (\psi^l - \widetilde{\varphi}_p^l)\big) - \mathcal{G}_{s_p}\big(E_H - (\psi - \widetilde{\varphi}_p)\big) \Big\}(\psi^l - \psi)\,\mathrm{d}x$$
$$\leq -\int_\Omega N_{n0}\Big\{ \mathcal{G}_{s_n}\big(\psi^l - \widetilde{\varphi}_n^l - E_L\big) - \mathcal{G}_{s_n}\big(\psi - \widetilde{\varphi}_n^l - E_L\big) \Big\}(\psi^l - \psi)\,\mathrm{d}x$$
$$+ \int_\Omega N_{n0}\Big\{ \mathcal{G}_{s_n}\big(\psi - \widetilde{\varphi}_n - E_L\big) - \mathcal{G}_{s_n}\big(\psi - \widetilde{\varphi}_n^l - E_L\big) \Big\}(\psi^l - \psi)\,\mathrm{d}x$$
$$+ \int_\Omega N_{p0}\Big\{ \mathcal{G}_{s_p}\big(E_H - (\psi^l - \widetilde{\varphi}_p^l)\big) - \mathcal{G}_{s_p}\big(E_H - (\psi - \widetilde{\varphi}_p^l)\big) \Big\}(\psi^l - \psi)\,\mathrm{d}x$$
$$- \int_\Omega N_{p0}\Big\{ \mathcal{G}_{s_p}\big(E_H - (\psi - \widetilde{\varphi}_p)\big) - \mathcal{G}_{s_p}\big(E_H - (\psi - \widetilde{\varphi}_p^l)\big) \Big\}(\psi^l - \psi)\,\mathrm{d}x$$
$$\leq c\big(\max_{\theta\in\mathbb{R}} |\mathcal{G}_{s_n}'(\theta)| + \max_{\theta\in\mathbb{R}} |\mathcal{G}_{s_p}'(\theta)| \big)\big(\|\widetilde{\varphi}_n^l - \widetilde{\varphi}_n\|_{L^2} + \|\widetilde{\varphi}_p^l - \widetilde{\varphi}_p\|_{L^2} \big)\|\psi^l - \psi\|_{L^2}.$$

The last line results from the monotonicity of the function $\mathcal{G}_s$, see Remark 2.1. Since again by Remark 2.1, $|\mathcal{G}_s'(\theta)| \leq c$, we find that $\psi^l \to \psi$ in $H^1(\Omega)$.

2. By Lemma 3.2 we have $\|\varphi_n^l\|_{H^1}, \|\varphi_p^l\|_{H^1} \leq c_{H^1}$. We show that all weakly converging subsequences of $\{(\varphi_n^l, \varphi_p^l)\}$ in the reflexive Banach space $H^1(\Omega)^2$ converge weakly to (φ_n, φ_p). Then by [GGZ74, Lemma 5.4] the convergence $(\varphi_n^l, \varphi_p^l) \rightharpoonup (\varphi_n, \varphi_p)$ in $H^1(\Omega)^2$ holds for the whole sequence and therefore $(\varphi_n^l, \varphi_p^l) \to (\varphi_n, \varphi_p)$ in $L^2(\Omega)^2$ which we finally aim to prove.

Let for some subsequence $\{(\varphi_n^{l_k}, \varphi_p^{l_k})\}$ and some $(\varphi_n^*, \varphi_p^*) \in H^1(\Omega)^2$ hold true $(\varphi_n^{l_k}, \varphi_p^{l_k}) \rightharpoonup (\varphi_n^*, \varphi_p^*)$ in $H^1(\Omega)^2$. We have to verify that $\varphi_n^* = \varphi_n$ and $\varphi_p^* = \varphi_p$.

Since $(\widetilde{\varphi}_n^{l_k}, \widetilde{\varphi}_p^{l_k}) \to (\widetilde{\varphi}_n, \widetilde{\varphi}_p)$ in $L^2(\Omega)^2$ and $\psi^{l_k} \to \psi$ in $H^1(\Omega)$ we obtain for a non-relabeled subsubsequence that $\widetilde{\varphi}_n^{l_k} \to \widetilde{\varphi}_n, \widetilde{\varphi}_p^{l_k} \to \widetilde{\varphi}_p\ \psi^{l_k} \to \psi$, and $\nabla \psi^{l_k} \to \nabla \psi$ a.e. in Ω. Because of the continuity of the function $\mathcal{G}_s$ as well as the mobility functions μ_n, μ_p (with respect to n, p and $|\nabla \psi|$) we find for this subsequence that also $\widetilde{n}^{l_k} = N_{n0}\mathcal{G}_{s_n}(\psi^{l_k} - \widetilde{\varphi}_n^{l_k} - E_L) \to \widetilde{n} = N_{n0}\mathcal{G}_{s_n}(\psi - \widetilde{\varphi}_n - E_L)$ and $\mu_n(\widetilde{n}^{l_k}, |\nabla \psi^{l_k}|) \to \mu_n(\widetilde{n}, |\nabla \psi|)$ a.e. in Ω and correspondingly, $\widetilde{p}^{l_k} \to \widetilde{p}$ and $\mu_p(\widetilde{p}^{l_k}, |\nabla \psi^{l_k}|) \to \mu_p(\widetilde{p}, |\nabla \psi|)$ a.e. in Ω.

With the test function $(\varphi_n^{l_k} - \varphi_n, 0)$ for (3.9) we obtain that

$$
\begin{aligned}
0 &= \int_\Omega \left\{ \widetilde{n}^{l_k} \mu_n(\widetilde{n}^{l_k}, |\nabla \psi^{l_k}|) \nabla \varphi_n^{l_k} - \widetilde{n}\mu_n(\widetilde{n}, |\nabla \psi|)\nabla \varphi_n \right\} \cdot \nabla(\varphi_n^{l_k} - \varphi_n) \,\mathrm{d}x \\
&\quad + \int_\Omega \left\{ r(\widetilde{n}^{l_k}, \widetilde{p}^{l_k})\left(e^{\varphi_n^{l_k} - \varphi_p^{l_k}} - 1\right) - r(\widetilde{n}, \widetilde{p})\left(e^{\varphi_n - \varphi_p} - 1\right) \right\}(\varphi_n^{l_k} - \varphi_n)\,\mathrm{d}x \\
&= \int_\Omega \widetilde{n}^{l_k}\mu_n(\widetilde{n}^{l_k}, |\nabla \psi^{l_k}|)|\nabla(\varphi_n^{l_k} - \varphi_n)|^2 \,\mathrm{d}x \\
&\quad + \int_\Omega \left\{ \widetilde{n}^{l_k}\mu_n(\widetilde{n}^{l_k}, |\nabla \psi^{l_k}|) - \widetilde{n}\mu_n(\widetilde{n}, |\nabla \psi|) \right\}\nabla \varphi_n \cdot \nabla(\varphi_n^{l_k} - \varphi_n)\,\mathrm{d}x \\
&\quad + \int_\Omega \left\{ r(\widetilde{n}^{l_k}, \widetilde{p}^{l_k})\left(e^{\varphi_n^{l_k} - \varphi_p^{l_k}} - 1\right) - r(\widetilde{n}, \widetilde{p})\left(e^{\varphi_n - \varphi_p} - 1\right) \right\}(\varphi_n^{l_k} - \varphi_n)\,\mathrm{d}x.
\end{aligned}
$$

Because of (3.8), since $\varphi_n^{l_k} - \varphi_n \in H_D^1(\Omega)$ and $\mathrm{mes}(\Gamma_D) > 0$ we have

$$
\begin{aligned}
&\|\varphi_n^{l_k} - \varphi_n\|_{H^1}^2 \\
&\leq c \int_\Omega \left| \widetilde{n}^{l_k}\mu_n(\widetilde{n}^{l_k}, |\nabla \psi^{l_k}|) - \widetilde{n}\mu_n(\widetilde{n}, |\nabla \psi|) \right||\nabla \varphi_n||\nabla(\varphi_n^{l_k} - \varphi_n)|\,\mathrm{d}x \\
&\quad + c \int_\Omega \left| r(\widetilde{n}^{l_k}, \widetilde{p}^{l_k})\left(e^{\varphi_n^{l_k} - \varphi_p^{l_k}} - 1\right) - r(\widetilde{n}, \widetilde{p})\left(e^{\varphi_n - \varphi_p} - 1\right) \right||\varphi_n^{l_k} - \varphi_n|\,\mathrm{d}x \\
&\leq c\|\varphi_n^{l_k} - \varphi_n\|_{H^1}\left[\left(\int_\Omega \left| \widetilde{n}^{l_k}\mu_n(\widetilde{n}^{l_k}, |\nabla \psi^{l_k}|) - \widetilde{n}\mu_n(\widetilde{n}, |\nabla \psi|) \right|^2 |\nabla \varphi_n|^2 \,\mathrm{d}x \right)^{\frac{1}{2}} \right. \\
&\quad \left. + \left(\int_\Omega \left| r(\widetilde{n}^{l_k}, \widetilde{p}^{l_k})\left(e^{\varphi_n^{l_k} - \varphi_p^{l_k}} - 1\right) - r(\widetilde{n}, \widetilde{p})\left(e^{\varphi_n - \varphi_p} - 1\right) \right|^2 \,\mathrm{d}x \right)^{\frac{1}{2}} \right].
\end{aligned}
$$

Due to (3.8) and $\|\varphi_n\|_{H^1} \leq c_{H^1}$ the integral in the last but one line has an integrable majorant and we can apply Lebesgue's dominated convergence theorem to show that this integral tends to zero. For the last integrand we have the integrable majorant $4\overline{r}\exp(4K)$ such that the above mentioned pointwise convergences in Step 2 and Lebesgue's dominated convergence theorem ensure that this integral tends to zero, too. Therefore, it follows $\|\varphi_n^{l_k} - \varphi_n\|_{H^1} \to 0$ for this subsubsequence. Since by assumption this subsubsequence also weakly converges to φ_n^*, we find that $\varphi_n^* = \varphi_n$ and that the whole subsequence converges weakly to φ_n in $H^1(\Omega)$. By similar arguments one shows for the holes, that $\varphi_p^* = \varphi_p$ and that the whole subsequence converges weakly to φ_p in $H^1(\Omega)$.

Since we discussed here an arbitrary subsequence, we verified that all weakly converging subsequences of $\{(\varphi_n^l, \varphi_p^l)\}$ converge weakly to (φ_n, φ_p) in $H^1(\Omega)^2$. Thus by [GGZ74, Lemma 5.4] it results $(\varphi_n^l, \varphi_p^l) \rightharpoonup (\varphi_n, \varphi_p)$ in $H^1(\Omega)^2$ for the whole sequence and therefore $(\varphi_n^l, \varphi_p^l) \to (\varphi_n, \varphi_p)$ in $L^2(\Omega)^2$ which gives the continuity of the operator $\mathcal{Q}$ we had to prove.   □

Since Lemma 3.3 ensures the continuity of the map $\mathcal{Q}$ from the non-empty, convex, closed and precompact set $\mathcal{M}$ into itself, Schauder's fixed point theorem guarantees the existence of a fixed point $(\varphi_n, \varphi_p) \in \mathcal{M}$ of $\mathcal{Q}$. For a fixed point $(\varphi_n, \varphi_p) \in (\varphi^D + H_D^1(\Omega))^2$ of the mapping $\mathcal{Q}$ we uniquely solve $B_{(\varphi_n, \varphi_p)}\psi = 0$ and calculate according to (3.5)

$$n = N_{n0}\mathcal{G}_{s_n}(\psi - \varphi_n - E_L), \quad p = N_{p0}\mathcal{G}_{s_p}(E_H - (\psi - \varphi_p)).$$

Then $(\psi, \varphi_n, \varphi_p)$ is a solution to problem (3.4). Thus, Theorem 3.1 is proven.

3.6 Remarks on uniqueness

By physical reasons, the stationary solution of the van Roosbroeck system for an applied external voltage even in the case of classical (inorganic) semiconductors in general is not expected to be unique. Special cases in which there exist more than one solution are discussed in [BBK82]. In fact, some semiconductor devices (e.g. thyristors [SN07, Chap. 11]) are designed to have multiple steady states. Therefore, Schauder's fixed point theorem is adequate to prove the existence result in Theorem 3.1.

As in the inorganic situation, see [GG86, Sec. 4], we are able to prove the uniqueness of the stationary solution for Dirichlet data compatible with thermodynamic equilibrium.

Theorem 3.2 *Additionally to assumption (A) we suppose that $\varphi_n^D = \varphi_p^D = \varphi^D = const$ (meaning that the voltage at all Dirichlet contacts is the same and all driving forces for the fluxes vanish at the boundary). Then the solution $(\psi, \varphi_n, \varphi_p)$ to problem (3.4) is unique. In Ω it fulfills $\varphi_n = \varphi_p = \varphi^D$.*

Proof. If $\varphi^D = const$ and $(\psi, \varphi_n, \varphi_p)$ is a solution to (3.4) then the test by $(\varphi_n - \varphi^D, \varphi_p - \varphi^D) \in H_D^1(\Omega)^2$ leads to

$$\int_\Omega \left(n\mu_n(n, |\psi|)|\nabla\varphi_n|^2 + p\mu_p(p, |\psi|)|\nabla\varphi_p|^2 \right) \mathrm{d}x$$
$$+ \int_\Omega r(n, p)\left(\mathrm{e}^{\varphi_n - \varphi_p} - 1\right)\left(\varphi_n - \varphi_p\right) \mathrm{d}x = 0.$$

The strict monotonicity of the exponential function, $r \geq 0$, and the positive lower bound of $n\mu_n(n, |\psi|)$ and $p\mu_p(p, |\psi|)$ thus ensure $\varphi_n = \varphi_p = \varphi^D$ a.e. in Ω. Since $(\varphi^D, \varphi^D) \in \mathcal{M}$, the arguments in Step 1 in the proof of Lemma 3.1 ensure exactly one solution $\psi^* \in \psi^D + H_D^1(\Omega)$ to $\mathcal{B}_{(\varphi^D, \varphi^D)}\psi^* = 0$. Thus, $(\psi^*, \varphi^D, \varphi^D)$ is the unique solution to (3.4).   □

In the inorganic situation, for data nearly compatible with thermodynamic equilibrium, uniqueness can be verified by the implicit function theorem in a neighbourhood of the thermodynamic equilibrium, see e.g. [Mar86, Chap. 3] for the classical van Roosbroeck system and [GG10] for spin-polarized drift-diffusion systems, both assuming Boltzmann statistics. In [Mar86, Chap. 3], under additional assumptions on the coefficients, higher regularity of the solution is achieved and a uniqueness result for small applied voltages is obtained. Whereas [Mar86] uses Frechet differentiability in $H^2(\Omega)$, [GG10] works in a Sobolev-Campanato space setting. Note that, for mobilities depending on $|\nabla\psi|$, which have to be taken into account in organic electronics, the applicability of the implicit function theorem in a suitable functional analytic setting is not known.

4 Simulation

In this section, we briefly describe our discretization method applied to the scaled drift-diffusion system (3.1). Recently, a number of ideas was published how to modify the classical Scharfetter-Gummel scheme for the discretization of flux terms in the situation of non-Boltzmann statistical relation, see e.g. [BC12, FRD+17, Fuh15, Gär15, KRF+15]. In this paper we use a generalized Scharfetter-Gummel scheme related to inverse activities as proposed in [Fuh15].

Additionally, we present a simulation to demonstrate the effect of the Extended Gaussian Disorder Model (introduced in Section 2) in comparison to the Boltzmann model.

4.1 Discretization method

The discretization method we use here is a finite volume one where the computational domain Ω is supposed to be partitioned by a Voronoi mesh with several Voronoi volumes $\{V_l\}$ and accompanying collocation points $\{x_l\}$. The potentials ψ, φ_n, and φ_p are going to be evaluated at each node $\{x_l\}$. The discretized system corresponding to (3.1) is derived by integrating the equations over each Voronoi volume V_l, applying Gauss's theorem to get

$$\int_{\partial V_l} -\varepsilon \nabla \psi \cdot \nu \, d\Gamma = \sum_{V_r \in \mathcal{N}(V_l)} \int_{\partial V_l \cap \partial V_r} -\varepsilon \nabla \psi \cdot \nu \, d\Gamma + \int_{\partial V_l \cap \partial \Omega} -\varepsilon \nabla \psi \cdot \nu \, d\Gamma = \int_{V_l} (C - n + p) \, dx,$$

$$\int_{\partial V_l} -j_n \cdot \nu \, d\Gamma = \sum_{V_r \in \mathcal{N}(V_l)} \int_{\partial V_l \cap \partial V_r} -j_n \cdot \nu \, d\Gamma + \int_{\partial V_l \cap \partial \Omega} -j_n \cdot \nu \, d\Gamma = \int_{V_l} -R \, dx,$$

$$\int_{\partial V_l} j_p \cdot \nu \, d\Gamma = \sum_{V_r \in \mathcal{N}(V_l)} \int_{\partial V_l \cap \partial V_r} j_p \cdot \nu \, d\Gamma + \int_{\partial V_l \cap \partial \Omega} j_p \cdot \nu \, d\Gamma = \int_{V_l} -R \, dx$$

and then approximating these integrals suitably. Here $\mathcal{N}(V_l)$ stands for the set of Voronoi volumes V_r which are adjacent to the Voronoi volume V_l. We also add the subscript l in all quantities such as potentials, doping density and recombination-generation rate to denote their corresponding numerical values at the node x_l. In the following, we will assume that all material parameters, such as the permittivity ε, the reference mobilities μ_{i0}, and the densities of state N_{i0}, are constant, otherwise, suitable averages have to be used. While all the surface integrals on the boundary $\partial V_l \cap \partial \Omega$ can be evaluated by corresponding boundary conditions (3.2), integrals on interfaces $\partial V_l \cap \partial V_r$ must be treated specifically in order to maintain the consistency of the numerical solution.

More precisely, integrals of the charge density and the recombination-generation rate are approximated by the midpoint rule

$$\int_{V_l} (C - n + p) \, dx \approx \text{mes}(V_l) (C_l - n_l + p_l), \quad \int_{V_l} R \, dx \approx \text{mes}(V_l) R_l,$$

and the surface integral in the Poisson equation is approximated by the conventional central scheme

$$\int_{\partial V_l \cap \partial V_r} -\varepsilon \nabla \psi \cdot \nu \, d\Gamma \approx \frac{\text{mes}(\partial V_l \cap \partial V_r)}{|x_l - x_r|} \varepsilon (\psi_l - \psi_r).$$

The flux approximations in the continuity equations require a more careful treatment

$$\int_{\partial V_l \cap \partial V_r} j_i \cdot \nu \, d\Gamma \approx \frac{\text{mes}(\partial V_l \cap \partial V_r)}{|x_l - x_r|} J_i^{l;r}, \quad i = n, p,$$

where the numerical flux $J_i^{l;r}$ is determined by a generalized Scharfetter-Gummel scheme. For the simulations in this paper we choose the inverse activity scheme (see [Fuh15]) to get the explicit form of $J_n^{l;r}$ and $J_p^{l;r}$

$$J_n^{l,r} = -\overline{\mu}_n^{l,r}(\overline{n}^{l,r}, F^{l,r}) N_{n0} \frac{\mathcal{G}_{s_n}\left(\overline{\eta}_n^{l,r}\right)}{\exp\left(\overline{\eta}_n^{l,r}\right)} \Big(\exp\left(\eta_{n;l}\right) B\left(\psi_l - \psi_r\right) - \exp\left(\eta_{n;r}\right) B\left(\psi_r - \psi_l\right)\Big),$$

$$J_p^{l,r} = \overline{\mu}_p^{l,r}(\overline{p}^{l,r}, F^{l,r}) N_{p0} \frac{\mathcal{G}_{s_p}\left(\overline{\eta}_p^{l,r}\right)}{\exp\left(\overline{\eta}_p^{l,r}\right)} \Big(\exp\left(\eta_{p;l}\right) B\left(\psi_r - \psi_l\right) - \exp\left(\eta_{p;r}\right) B\left(\psi_l - \psi_r\right)\Big),$$

where $\eta_{n;l}$ and $\eta_{p;l}$ stand for (non-dimensionalized) $\psi_l - \varphi_{n;l} - E_L$, $E_H - \psi_l + \varphi_{p;l}$ respectively, and $\overline{\eta}_n^{l,r} = (\eta_{n;l} + \eta_{n;r})/2$ and $\overline{\eta}_p^{l,r} = (\eta_{p;l} + \eta_{p;r})/2$ are averaged quantities and B denotes the Bernoulli function $B(x) = \frac{x}{\exp(x)-1}$.

The mobilities $\overline{\mu}_i^{l,r}$ are evaluated at the averaged densities $\overline{n}^{l,r} = N_{n0}\mathcal{G}_{s_n}(\overline{\eta}_n^{l,r})$, $\overline{p}^{l,r} = N_{p0}\mathcal{G}_{s_p}(\overline{\eta}_p^{l,r})$, and at the field strength $F^{l,r}$ which is an approximation of $|\nabla\psi|$. In particular, it is important to include here also the tangential components of the electric field, not just the normal ones. This is achieved by using an average of the gradients of the P1 finite-element interpolant of the nodal values ψ_l as in [FGL17].
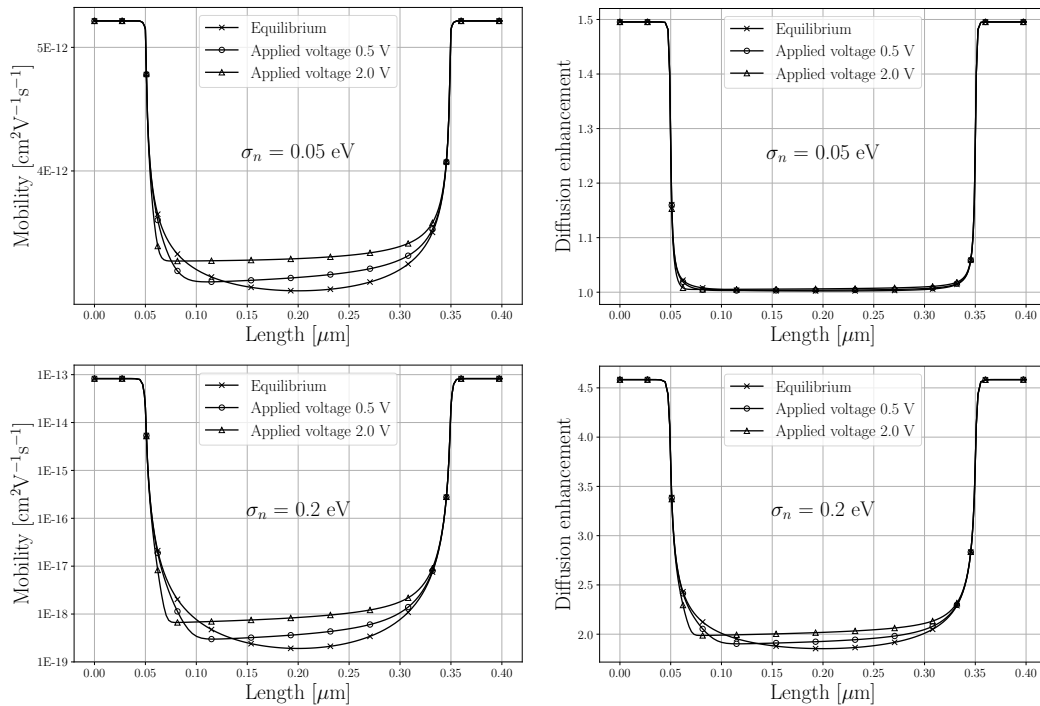

Figure 3: Mobility (left column) and so-called diffusion enhancement factor g_3 (right column) for an n-i-n resistor at the three biases: $0.0\,\text{V}$ (equilibrium), $0.5\,\text{V}$, $2.0\,\text{V}$ for small disorder parameter $\sigma_n = 0.05\,\text{eV}$ (first row) and large disorder $\sigma_n = 0.2\,\text{eV}$ (second row). See Subsection 2.2 and Subsection 2.3.

4.2 Numerical demonstration

We study the impact of the EGDM (see Section 2) in comparison to the conventional Boltzmann model by simulating an organic n-i-n resistor using the discretization scheme described in Subsection 4.1,

Temperature T	$300.0\,\text{K}$
Relative dielectric permittivity ε_r	3.0
HOMO-LUMO-gap $E_H - E_L$	$2.3\,\text{eV}$
Average hopping distance a	$1.8\,\text{nm}$
Total density of transport states N_{n0}	$1.0 \times 10^{20}\,\text{cm}^{-3}$
Doping C in n-doped region	$1.0 \times 10^{19}\,\text{cm}^{-3}$
Reference mobility μ_{n0}	$72.0\,\text{m}^2\,\text{V}^{-1}\,\text{s}^{-1}$
c_1 in formula for $\mu_0(T)$ in (2.6)	1.8×10^{-9}
c_2 in formula for $\mu_0(T)$ in (2.6)	0.42
Disorder parameter σ_n	$0.05\,\text{eV}$, $0.1\,\text{eV}$, or $0.2\,\text{eV}$

Table 1: Physical parameters used in simulations, compare [PCT⁺05].

which was implemented in the simulation tool `ddfermi` [DFF⁺16]. Our test structure consists of three regions: two doped regions at both ends of the resistor and one intrinsic region in the middle. The intrinsic region is $0.3\,\mu\text{m}$ in length while the length of each doped region is $0.05\,\mu\text{m}$. The donator doping density is set to $C = 1.0 \times 10^{19}\,\text{cm}^{-3}$ while there is no doping in the intrinsic region, i.e. $C = 0\,\text{cm}^{-3}$. Thus, the contacts at the two ends of the n-i-n resistor can be considered as Ohmic contacts. Since free electrons are the major transporting carriers in an n-i-n resistor, the holes are neglected in our simulation and therefore no generation-recombination rate has to be considered. The used organic semiconductor material is poly[{2-(4-(3',7'-dimethyloctyloxyphenyl))}-co-2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene] (NRS-PPV) whose material parameters can be found in Table 1, cf. also [PCT⁺05].

Simulations were done for both, the Boltzmann model and the EDGM. For the EDGM we applied the three different values of disorder parameter σ_n as given in Table 1. For all four cases we fixed the right contact to $0.0\,\text{V}$ and carried out a sweeping of the left one from $0.0\,\text{V}$ (equilibrium) to $2.0\,\text{V}$.

The spatially dependent mobility μ_n and the diffusion enhancement factor g_3 (see (2.10)) for the n-i-n resistor are plotted in the left and right column of Figure 3, respectively. The upper and lower row of figures compare the situation for small disorder parameter $\sigma_n = 0.05\,\text{eV}$ and larger disorder parameter $\sigma_n = 0.2\,\text{eV}$ (second row). For increasing disorder parameter globally the mobility decreases whereas the function g_3 is growing. The ratio of the mobility in the intrinsic region and the doped region is considerably decreasing (up to 5 orders of magnitude in case of $\sigma_n = 0.2\,\text{eV}$) and also the corresponding ratio for the diffusion enhancement decreases. For applied voltages the spatially symmetric situation of the equilibrium is destroyed, such that the smallest values for the mobility and the diffusion enhancement shift to the left side of the intrinsic layer.

In Figure 4, the resulting profiles of the electrostatic potential (pictures in the left column) and electron density (pictures in the right column) are shown. Without applied voltage (first line in Figure 4) the profiles of electrostatic potential and electron density are symmetric for both, Boltzmann model and EGDM.

In the equilibrium state (row (a) of Figure 4), EGDM results in a deeper built-in valley of the electrostatic potential in the intrinsic region than Boltzmann model does. The deepness increases for larger disorder parameter.

Moreover, in the intrinsic layer, the EDGM produces higher carrier densities in comparison to the Boltzmann approximation, which is more pronounced for higher values of the disorder parameter. For $\sigma_n \to 0$ the potential and electron density profile tend to the Boltzmann profile, compare (2.4), too.

When the external voltage is applied, in the intrinsic region the shifted to the right potential valley remains deeper for the EDGM than in the Boltzmann case and the electron density calculated by EGDM is also higher than in the Boltzmann model.
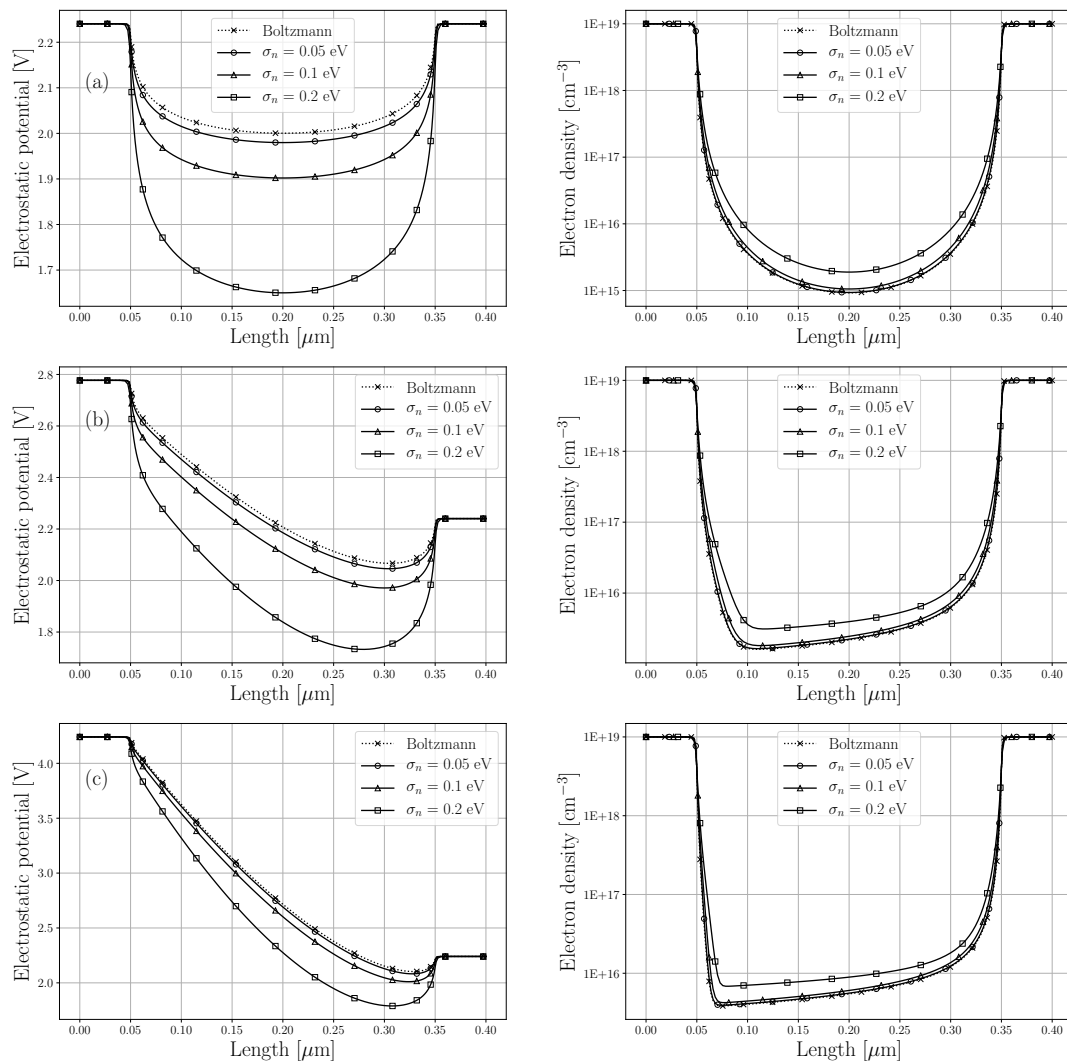

Figure 4: Electrostatic potential (left column) and electron density (right column) for an n-i-n resistor at three biases: row (a) $0.0\,\mathrm{V}$ also called equilibrium state, row (b) $0.5\,\mathrm{V}$, and row (c) $2.0\,\mathrm{V}$. For better comparison, the electrostatic potential is shifted by the corresponding built-in voltage for each of the four cases.

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