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Classical solutions of drift–diffusion equations for semiconductor devices: the 2d case

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Abstract

We regard drift–diffusion equations for semiconductor devices in Lebesgue spaces. To that end we reformulate the (generalized) van Roosbroeck system as an evolution equation for the potentials to the driving forces of the currents of electrons and holes. This evolution equation falls into a class of quasi-linear parabolic systems which allow unique, local in time solution in certain Lebesgue spaces. In particular, it turns out that the divergence of the electron and hole current is an integrable function. Hence, Gauss' theorem applies, and gives the foundation for space discretization of the equations by means of finite volume schemes. Moreover, the strong differentiability of the electron and hole density in time is constitutive for the implicit time discretization scheme. Finite volume discretization of space, and implicit time discretization are accepted custom in engineering and scientific computing. — This investigation puts special emphasis on non-smooth spatial domains, mixed boundary conditions, and heterogeneous material compositions, as required in electronic device simulation.

1 Introduction

In 1950 van Roosbroeck [48] established a system of partial differential equations describing the motion of electrons and holes in a semiconductor device due to drift and diffusion within a self-consistent electrical field. In 1964 Gummel [28] published the first report on the numerical solution of these drift–diffusion equations for an operating semiconductor device. From that time on van Roosbroeck's system has been the backbone of many a model in semiconductor device simulation. The first papers devoted to the mathematical analysis of van Roosbroeck's system appeared in the early seventies of the previous century [38, 39]; for a historical synopsis and further references see [11]. In 1986 Gajewski and Gröger proved the global existence and uniqueness of weak solutions under realistic physical and geometrical conditions [13]. The key for proving these results and also for establishing stable numerical solving procedures is the existence of a Lyapunov function for the van Roosbroeck system. This solution theory entails restricting conditions on the models for the recombination of electron–hole pairs, see [11, 2.2.3], [14, Ch. 5], [15, Ch. 6], [18], and [19]. In this paper we relax the condition on the reaction terms in the equations considerably, up to the point that some external control to the generation or annihilation of electrons or holes can be applied individually. In particular, this aims at radiative recombination of electron-hole pairs in semiconductor lasers, and at the generation of electron-hole pairs in optoelectronic detectors. Notwithstanding this generalization, we continue to use the name van Roosbroeck system for the model equations.

Van Roosbroeck's system consists of current–continuity equations — one for electrons, another one for holes — which are coupled to a Poisson equation for the electrostatic potential, and comprise generative terms, first of all recombination of electron–hole pairs. The current–continuity equations can be viewed as quasi-linear parabolic equations. However, the natural formulation of balance laws is in integral form

$$\frac{\partial}{\partial t}\int_\omega u_k \,\mathrm{d}x = \int_{\partial\omega} \nu \cdot j_k \,\mathrm{d}\sigma_\omega + \int_\omega r_k \,\mathrm{d}x. \tag{1.1}$$

Here u_2 and u_1 is the density of electrons and holes, respectively, j_k is the corresponding flux, and r_k is a reaction term. ω is any (suitable) sub-domain of the whole domain under consideration, ν the outer unit normal to the boundary $\partial\omega$ of ω and σ_ω the arc measure on $\partial\omega$. In the weak formulation of the balance law the boundary integral of the normal component of the current is expressed as the volume integral of the divergence of the corresponding current. Very little is known about the question whether the weak solutions also satisfy the original balance law equations (1.1). Obviously, this depends on the applicability of Gauss' theorem. So, the problem is about the divergence of the currents in weak solutions being functions —

not only distributions. In particular, this comes to bear in the numerical treatment of van Roosbroeck's system. The choice for space discretization of drift–diffusion equations is the finite volume method, see [17], which rests on the original balance law formulation (1.1) of the equations.

In this paper we solve this problem for the spatially two-dimensional van Roosbroeck system by showing that it admits a classical solution in a suitably chosen Lebesgue space—at least locally in time. Aiming at the inclusion of rather general recombination and generation processes for electron-hole pairs we cannot expect global existence anymore, and we cannot rely on a Lyapunov function. Instead we apply local methods for quasi-linear evolution equations. To that end, we rewrite van Roosbroeck's system as an evolution equation for the electrochemical potentials of electrons and holes, and apply a recently obtained result on quasi-linear parabolic equations in Lebesgue spaces, see [31]. This yields a classical solution of van Roosbroeck system locally in time with currents the divergence of which is Lebesgue integrable to some exponent greater than one. The strong differentiability of the electron and hole density in time is constitutive for the implicit time discretization scheme which is accepted custom in engineering and scientific computing, see for instance [11].

Please note that in device simulation one is always confronted with contacted devices of heterogeneous material composition. That leads to mixed boundary conditions and jumping material coefficients in the model equations. Hence, standard theorems on existence, uniqueness and regularity do not apply.

2 Van Roosbroeck's system

Basic variables

In the following we investigate van Roosbroeck's model for a semiconductor device which describes the flow of electrons and holes in a self-consistent electrical field due to drift and diffusion. The physical quantities one is interested in are: the densities u_1 and u_2 of holes and electrons, the densities j_1 and j_2 of the hole and electron current, the electrostatic potential $\widetilde{\varphi}$ of the self-consistent electrical field, and the electrochemical potentials $\widetilde{\phi}_1$ and $\widetilde{\phi}_2$ of holes and electrons These unknowns have to satisfy Poisson's equation and the current–continuity equations for electrons and holes with some side conditions. The latter are given by the relations between the potentials and the densities.

Spatial domain

We study only semiconductor devices which are quasi translational invariant in one space direction or angular symmetric. In that case van Roosbroeck's system in real space can be reduced to a similar set of equations in the plane. That means, we regard a cut through the device perpendicular to the direction of invariance. Let $\widehat{\Omega}$ be the resulting two-dimensional (bounded) representative domain. Parts of the device may be insulating, for instance formed by an oxide. Then, electrons and holes can move only in a sub-domain Ω of $\widehat{\Omega}$. This also covers the case of charges which are artificially immobilized on a sub-domain $\widehat{\Omega} \setminus \Omega$. Furthermore, we mark out a part $\widehat{\Gamma}$ of the boundary of $\widehat{\Omega}$ where the device borders on an insulator. The remaining part of the boundary represents (possibly several) contacts of the device. We also mark out a part Γ of Ω's boundary. In the case of a stand alone drift–diffusion model of the semiconductor device again Γ represents areas of the device bordering to an insulator, whereas the remaining part is the contact area.

External control

In real–world modeling of semiconductor devices van Roosbroeck's system often serves as a component in a compound model of the device. Then the superordinated system — for instance a circuit model — may exercise a control on van Roosbroeck's system. Apart of a superordinated circuit model, compound models comprising in addition to van Roosbroeck's system equations for the lattice temperature or the power of lasing modes play an important role in device simulation, see for instance [11, 2, 4, 3]. But the concept of external control also comes to bear in segmentation of the simulation domain, in particular in connection with multiscale modeling, see for instance [32, 33, 30].

If van Roosbroeck's equations serve as a component of a compound model, then system parameters, state equations, boundary conditions, et alii, possibly bear a different physical meaning than in the stand-alone model.

We make assumptions about an external control from the initial time T_0 up to a time T_1.

2.1 Poisson equation

The solution of the Poisson equation with mixed boundary conditions,

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla \widetilde{\varphi}) &= \tilde{d}(t) + u_1 - u_2 && \text{on } \widehat{\Omega}, \\ \widetilde{\varphi} &= \varphi_{\widehat{\mathrm{D}}}(t) && \text{on } \widehat{\mathrm{D}} \stackrel{\text{def}}{=} \operatorname{interior}(\partial\widehat{\Omega} \setminus \widehat{\Gamma}), \\ \nu \cdot (\varepsilon \nabla \widetilde{\varphi}) + \varepsilon_{\widehat{\Gamma}} \widetilde{\varphi} &= \varphi_{\widehat{\Gamma}}(t) && \text{on } \widehat{\Gamma}, \end{aligned} \tag{2.1}$$

gives the electrostatic potential $\widetilde{\varphi}$ on $\widehat{\Omega}$ subject to the electron and hole density u_2 and u_1. Strictly speaking, the densities u_k, $k = 1, 2$, are only defined on Ω but, we extend them by zero to $\widehat{\Omega}$.

The parameters in (2.1) have the following meaning: ε is a bounded, measurable function on $\widehat{\Omega}$ with values in the set of real, symmetric, 2×2, positive definite matrices and corresponds to the spatially varying dielectric permittivity on the space region occupied by the device. Moreover, we assume

$$\|\varepsilon(x)\|_{\mathcal{B}(\mathbb{R}^2)} \le \varepsilon^\bullet \text{ and } (\varepsilon(x)\xi) \cdot \xi \ge \varepsilon_\bullet \|\xi\|^2_{\mathbb{R}^2} \quad \text{for almost all } x \in \widehat{\Omega} \text{ and all } \xi \in \mathbb{R}^2$$

with two strictly positive constants $\varepsilon_\bullet$ and $\varepsilon^\bullet$. Furthermore, $\varepsilon_{\widehat{\Gamma}}$ is a non-negative function on $\widehat{\Gamma}$, representing the capacity of the part of the device surface bordering on an insulator. We assume that $\widehat{\mathrm{D}}$ is not empty or $\varepsilon_{\widehat{\Gamma}}$ is positive on a subset of $\widehat{\Gamma}$ with positive arc measure. In other words, the device has a Dirichlet contact or part of its surface has a positive capacity. $\varphi_{\widehat{\mathrm{D}}}(t)$ and $\varphi_{\widehat{\Gamma}}(t)$ are the voltages applied at the contacts of the device, and $\tilde{d}(t)$ represents a charge. In the case of a stand alone drift–diffusion model $\varphi_{\widehat{\mathrm{D}}}$, $\varphi_{\widehat{\Gamma}}$, and $\tilde{d}$ are constant in time, and $\tilde{d}$ solely is the charge density of dopants in the semiconductor materials composing the device. In general, $\varphi_{\widehat{\mathrm{D}}}$, $\varphi_{\widehat{\Gamma}}$, and $\tilde{d}$ are function which are defined on the time interval $[T_0, T_1]$ where a possible control acts on the device.

2.2 Current–continuity equations

The current–continuity equations for holes and electrons ($k = 1, 2$, respectively)

$$u_k' - \nabla \cdot j_k = r_k(t, \widetilde{\varphi}, \widetilde{\phi}_1, \widetilde{\phi}_2) \qquad \text{on } \Omega \tag{2.2}$$

characterize the evolution of the electron and hole density under the action of the currents j_k and the reactions r_k subject to the mixed boundary conditions

$$\begin{aligned} \widetilde{\phi}_k(t) &= \phi_{\mathrm{D},k}(t) && \text{on } \mathrm{D} \stackrel{\text{def}}{=} \operatorname{interior}(\partial\Omega \setminus \Gamma), \\ \nu \cdot j_k &= 0 && \text{on } \Gamma, \end{aligned} \tag{2.3}$$

from the initial conditions

$$\widetilde{\phi}_k(T_0) = \Phi_k^0. \tag{2.4}$$

Each r_k, $k = 1, 2$ is a reaction term which models the generation and annihilation of electrons and holes. In particular, this term covers the recombination of electrons and holes in the semiconductor device. r_1 and r_2 can be rather general functions of the particle and current densities, see §2.4. We require that the set $\mathrm{D} = \operatorname{interior}(\partial\Omega \setminus \Gamma)$ is not empty. The boundary values $\phi_{\mathrm{D},1}$, $\phi_{\mathrm{D},2}$ in general depend on time. Moreover, the reactions r_k may explicitly depend on time. This dependence on time, again, allows for a control of the system by some other part of a superordinated compound model.

2.3 Carrier and current densities

Van Roosbroeck's system has to be complemented by a prescription relating the density of electrons and holes as well as the densities of the electron and hole current to the chemical potentials of these charge carriers. We assume

$$u_k(t,x) \stackrel{\text{def}}{=} \rho_k(t,x)\mathcal{F}_k\left(\chi_k(t,x)\right), \quad x \in \Omega, \qquad k = 1,2, \tag{2.5}$$

where χ_1 and χ_2 are the chemical potentials

$$\chi_k \stackrel{\text{def}}{=} \widetilde{\phi}_k + (-1)^k \widetilde{\varphi} + b_k, \qquad k = 1,2, \tag{2.6}$$

and $\widetilde{\phi}_2$, $\widetilde{\phi}_1$ are the electrochemical potentials of electrons and holes, respectively. b_k, ρ_k, $k = 1,2$ are positive, bounded functions on Ω. They describe the electronic properties of the materials composing the device. b_2 and b_1 are the band edge offsets for electrons and holes, and ρ_2, ρ_1 are the corresponding effective band edge densities of states. If the equations under consideration form part of a compound model for the semiconductor device, then b_k, ρ_k, $k = 1,2$, may depend on time. For instance, the ρ_k could be subject to an external control of the device temperature. Then they depend on time via the temperature. Mathematically, we assume the following.

2.1 Assumption. For every $t \in [T_0, T_1]$ the functions $\rho_k(t)$ are essentially bounded on Ω and admit positive lower bounds which are uniform in $t \in [T_0, T_1]$. The mappings

$$[T_0, T_1] \ni t \mapsto \rho_k(t) \in L^2(\Omega), \quad k = 1,2 \tag{2.7}$$

are differentiable on the interval $]T_0, T_1[$ with Hölder continuous derivatives ρ_k'.

The functions $\mathcal{F}_1$ and $\mathcal{F}_2$ represent the statistical distribution of the holes and electrons on the energy band. In general, Fermi–Dirac statistics applies, i.e.

$$\mathcal{F}_k(s) \stackrel{\text{def}}{=} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{t}}{1 + \mathrm{e}^{t-s}}\,\mathrm{d}t, \qquad s \in \mathbb{R}. \tag{2.8}$$

However, often Boltzmann statistics $\mathcal{F}_k(s) = \mathrm{e}^s$ is a good approximation.

As for the kinetic relations specifying the current–continuity equations we assume that the electron and hole current is driven by the negative gradient of the electrochemical potential of electrons and holes, respectively. More precisely, the current densities are given by

$$j_k(t,x) = -\mathcal{G}_k\left(\chi_k(t,x)\right)\mu_k(x)\,\nabla\widetilde{\phi}_k(t,x), \quad x \in \Omega, \qquad k = 1,2. \tag{2.9}$$

The mobilities μ_2 and μ_1 for the electrons and holes, respectively, are measurable, bounded function on Ω with values in the set of real, 2×2, positive definite matrices satisfying for almost all $x \in \widehat{\Omega}$ and all $\xi \in \mathbb{R}^2$

$$\|\mu_k(x)\|_{\mathcal{B}(\mathbb{R}^2)} \le \mu^\bullet \quad \text{and} \quad (\mu_k(x)\xi)\cdot\xi \ge \mu_\bullet \|\xi\|^2_{\mathbb{R}^2}, \qquad k = 1,2,$$

with two strictly positive constants $\mu_\bullet$ and $\mu^\bullet$. The mobilities are accounted for on the parts of the device where electrons and holes can move due to drift and diffusion.

2.2 Remark. In semiconductor device modeling, usually, the functions $\mathcal{G}_k$ and $\mathcal{F}_k$ coincide, see for instance [44] and the references there. However, a rigorous formulation as a minimal problem for the free energy reveals that $\mathcal{G}_k = \mathcal{F}_k'$ is appropriate. This topic has been thoroughly investigated for analogous phase separation problems, see [40, 41, 22, 23], see also [18] and [24]. In order to cover both cases we regard independent functions $\mathcal{G}_k$ and $\mathcal{F}_k$.

2.3 Assumption. Mathematically, we demand that the distribution functions $\mathcal{F}_k$, $\mathcal{G}_k$, $k = 1, 2$, are defined on the real line, take positive values, and are either exponentials, or twice continuously differentiable and polynomially bounded. Moreover, $\mathcal{F}_1'$, $\mathcal{F}_2'$ are strictly positive on $\mathbb{R}$. In the sequel we will call such distribution functions 'admissible.' This includes Boltzmann statistics, as well as Fermi–Dirac statistics (see (2.8)).

Let us comment on the (effective) band edges b_k and the (effective) densities of states ρ_k, see (2.5) and (2.6): Basically the band edge offsets b_k and the effective band edge densities of states ρ_k are material parameters. In a heterogeneous semiconductor device they are generically piecewise constant on the spatial domain Ω. As Assumption 3.7 reveals, we cannot cope with such a situation as far as the band edges b_k are concerned. However, in the case of Boltzmann statistics one can rewrite (2.5) and (2.6) as

$$u_k = \rho_k e^{b_k} e^{\left(\widetilde{\phi}_k + (-1)^k \widetilde{\varphi}\right)} \quad \text{on } \Omega, \qquad k = 1, 2,$$

with modified effective densities of states and identically vanishing band edge offsets. In the case of Fermi–Dirac statistics this reformulation is not possible and one has to recourse to some approximation of the b_k by functions confirming to Assumption 3.7. Discontinuities of the band edge offsets up to now seem to be an obstacle in whatever approach to solutions of van Roosbroeck's equations, if the statistical distribution function is not an exponential, see for instance [19].

There are compound multiscale models of semiconductor devices such that the effective band edges and the effective densities of states result by upscaling from quantum mechanical models for the electronic structure in heterogeneous semiconductor materials, see [2, 3, 35]. In view of an offline coupling to electronic structure calculations we allow for an explicit dependence of ρ_k, and b_k on time.

2.4 Reaction rates

The reaction terms on the right hand side of the current–continuity equations can be rather general functions of time, of the electrostatic potential, and of the vector of the electrochemical potentials. r_1 and r_2 describes the production of holes and electrons, respectively — generation or annihilation, depending on the sign of the reaction term. Usually van Roosbroeck's system comprises only recombination of electrons and holes: $r = r_1 = r_2$. We have formulated the equations in a more general way, in order to include also coupling terms to other equations of a superordinated compound model. That is why we also allow for an explicit time dependency of the reaction rates.

Our formulation of the reaction rates, in particular, includes a variety of models for the recombination and generation of electrons–hole pairs in semiconductors. This covers non-radiative recombination of electrons and holes like the Shockley–Read–Hall recombination due to phonon transition and Auger recombination. But, radiative recombination (photon transition), both spontaneous and stimulated, is also included. Mathematical models for stimulated optical recombination typically require the solution of additional equations for the optical field. Thus, the recombination rate may be a non-local operator. Moreover, by coupling van–Roosbroecks system to the optical field some additional control of this optical field may also interact with the internal electronics. For instance, in modeling and simulation of edge–emitting multiple–quantum–well lasers van–Roosbroeck's system augmented by some Helmholtz equation often serves as a transversal (to the light beam) model, and a control of the optical field is exercised by a master equation or some model for the longitudinal (on the axis of the light beam) behavior of the laser, see for instance [51, 2, 3].

Modeling recombination of electron–hole pairs in semiconductor material is an art in itself, see for instance [36]. However, for illustration, let us list some common recombination models, see for instance [44, 11] and the references cited there.

Shockley–Read–Hall recombination (phonon transitions):

$$r_1 = r_2 = r^{\mathrm{SRH}} = \frac{u_1 u_2 - n_i^2}{\tau_2(u_1 + n_1) + \tau_1(u_2 + n_2)},$$

where n_i is the intrinsic carrier density, n_1, n_2 are reference densities, and τ_1, τ_2 are the lifetimes of holes and electrons, respectively. n_i, n_1, n_2, and τ_1, τ_2 are parameters of the semiconductor material; thus, depend on the space variable, and ultimately, also on time.

Auger recombination (three particle transitions):

$$r_1 = r_2 = r^{\mathrm{Auger}} = (u_1 u_2 - n_i^2)(c_1^{\mathrm{Auger}} u_1 + c_2^{\mathrm{Auger}} u_2),$$

where c_1^{Auger} and c_2^{Auger} are the Auger capture coefficients of holes and electrons, respectively, in the semiconductor material.

Stimulated optical recombination:

$$r_1 = r_2 = r^{\mathrm{stim}} = \sum_j f(\sigma_j) \frac{|\psi_j|^2}{\int |\psi_j|^2},$$

where f additionally depends on the vector of the densities, and on the vector of the electrochemical potentials. σ_j, ψ_j are the eigenpairs of a scalar Helmholtz–operator:

$$\Delta\psi_j + \epsilon(u_1, u_2)\psi_j = \sigma_j \psi_j.$$

In laser modeling each eigenpair corresponds to an optical (TE) mode of the laser and $|\psi_j|^2$ is the intensity of the electrical field of the σ_j–mode. ϵ is the dielectric permittivity (for the optical field); it depends on the density of electrons and holes. The scalar Helmholtz–equation originates from the Maxwell equations for the optical field [50].

The functional analytic requirements on the reaction terms will be established in Assumption 3.6.

3 Mathematical prerequisites

In this section we introduce some mathematical terminology and make precise assumptions about the problem.

3.1 General Assumptions

For a Banach space X we denote its norm by $\|\cdot\|_X$ and the value of a bounded linear functional ψ^* on X in $\psi \in X$ by $\langle \psi^* \mid \psi \rangle_X$. If X is a Hilbert space, identified with its dual, then $\langle \cdot \mid \cdot \rangle_X$ is the scalar product in X. Just in case X is the space $\mathbb{R}^2$, the scalar product of $a, b \in \mathbb{R}^2$ is written as $a \cdot b$. Upright X denotes the direct sum $X \oplus X$ of slanted X with itself. $\mathcal{B}(X;Y)$ is the space of linear, bounded operators from X into Y, where X and Y are Banach spaces. We abbreviate $\mathcal{B}(X) = \mathcal{B}(X;X)$ and we denote by $\mathcal{B}_\infty(X)$ the space of linear, compact operators on the Banach space X. The notation $[X,Y]_\theta$ means the complex interpolation space of X and Y to the index $\theta \in [0,1]$. The (distributional) ∇–calculus applies. If ψ is a (differentiable) function on an interval taking its values in a Banach space, then ψ' always indicates its derivative.

3.2 Spatial Domains

Throughout this paper we assume that $\widehat{\Omega}$ as well as Ω are bounded Lipschitz domains in $\mathbb{R}^2$, see [25, Ch. 1]. By $^{\uparrow}$ we denote the operator which extends any function defined on Ω by zero to a function defined on $\widehat{\Omega}$. Conversely, $_\downarrow$ denotes the operator which restricts any function defined on $\widehat{\Omega}$ to Ω. The operators $^\uparrow$ and $_\downarrow$ are adjoint to each other with respect to the duality induced by the usual scalar product in spaces of square integrable functions.

With respect to the marked out Neumann boundary parts $\widehat{\Gamma} \subset \partial\widehat{\Omega}$ and $\Gamma \subset \partial\Omega$ of the boundary of $\widehat{\Omega}$ and Ω we assume each being the union of a finite set of open arc pieces such that no connected component of $\partial\widehat{\Omega} \setminus \widehat{\Gamma}$ and $\partial\Omega \setminus \Gamma$ consists only of a single point. We denote the parts of the boundary where Dirichlet boundary conditions are imposed by $\widehat{\mathrm{D}} \stackrel{\text{def}}{=} \text{interior}(\partial\widehat{\Omega} \setminus \widehat{\Gamma})$ and $\mathrm{D} \stackrel{\text{def}}{=} \text{interior}(\partial\Omega \setminus \Gamma)$.

3.3 Function spaces and linear elliptic operators

We exemplarily define spaces of real-valued functions on spatial domains with respect to the bounded domain $\Omega \subset \mathbb{R}^2$ and its boundary. Spaces of functions on $\widehat{\Omega}$ and parts of its boundary may be similarly defined and are denoted by hatted symbols.

If $r \in [1, \infty[$, then L^r is the space of real, Lebesgue measurable, r-integrable functions on Ω and L^∞ is the space of real, Lebesgue measurable, essentially bounded functions on Ω. $W^{1,r}$ is the usual Sobolev space $W^{1,r}(\Omega)$, see for instance [46]. $W^{1,r}_\Gamma$ is the closure in $W^{1,r}$ of

$$\left\{\psi|_\Omega \,:\, \psi \in C_0^\infty(\mathbb{R}^2),\ \operatorname{supp}\psi \cap (\partial\Omega \setminus \Gamma) = \emptyset\right\},$$

i.e. $W^{1,r}_\Gamma$ consists of all functions from $W^{1,r}$ with vanishing trace on D. $W^{-1,r}_\Gamma$ denotes the dual of $W^{1,r'}_\Gamma$, where $1/r + 1/r' = 1$. $\langle \cdot \,|\, \cdot \rangle_{W^{1,2}_\Gamma}$ is the dual pairing between $W^{1,2}_\Gamma$ and $W^{-1,2}_\Gamma$. Correspondingly, the divergence for a vector of square integrable functions is defined in the following way: If $j \in \mathrm{L}^2$, then $\nabla \cdot j \in W^{-1,2}_\Gamma$ is given by

$$\langle \nabla \cdot j \,|\, \psi \rangle_{W^{1,2}_\Gamma} = -\int_\Omega j \cdot \nabla\psi \,\mathrm{d}x, \qquad \psi \in W^{1,2}_\Gamma. \tag{3.1}$$

σ is the natural arc measure on the boundary of Ω. We denote by $L^\infty(\partial\Omega)$ and $L^r(\partial\Omega)$, the spaces of σ-measurable, essentially bounded, and r-integrable, $r \in [1, \infty[$, functions on $\partial\Omega$, respectively. Moreover, $W^{s,r}(\partial\Omega)$ denotes the Sobolev space of fractional order $s \in]0, 1]$ and integrability exponent $r \in [1, \infty[$ on $\partial\Omega$, see [25, Ch. 1]. Mutatis mutandis for functions on σ-measurable, relatively open parts of $\partial\Omega$.

Let us now define in a strict sense the (linear) Poisson operator and the elliptic operators governing the current continuity equations.

3.1 Definition. We define the Poisson operator $-\nabla \cdot \varepsilon\nabla : \widehat{W}^{1,2} \to \widehat{W}^{-1,2}_{\widehat{\Gamma}}$ by

$$\langle -\nabla \cdot \varepsilon\nabla\psi_1 \,|\, \psi_2 \rangle_{\widehat{W}^{1,2}_{\widehat{\Gamma}}} \stackrel{\text{def}}{=} \int_{\widehat{\Omega}} \varepsilon\nabla\psi_1 \cdot \nabla\psi_2 \,\mathrm{d}x + \int_{\widehat{\Gamma}} \varepsilon_{\widehat{\Gamma}}\psi_1\psi_2 \,\mathrm{d}\widehat{\sigma}, \tag{3.2}$$

for $\psi_1 \in \widehat{W}^{1,2}$ and $\psi_2 \in \widehat{W}^{1,2}_{\widehat{\Gamma}}$. $\mathcal{P}_0$ denotes the restriction of $-\nabla \cdot \varepsilon \nabla$ to $\widehat{W}^{1,2}_{\widehat{\Gamma}}$; we denote the maximal restriction of $\mathcal{P}_0$ to any range space which continuously embeds into $\widehat{W}^{-1,2}_{\widehat{\Gamma}}$ by the same symbol $\mathcal{P}_0$.

3.2 Definition. With respect to a function $\varsigma \in L^\infty$ we define the operators

$$-\nabla \cdot \varsigma\mu_k \nabla : W^{1,2} \to W^{-1,2}_{\Gamma}, \quad k = 1,2, \quad \text{by}$$

$$\langle -\nabla \cdot \varsigma\mu_k \nabla \psi_1 \,|\, \psi_2 \rangle_{W^{1,2}_{\Gamma}} \overset{\text{def}}{=} \int_\Omega \varsigma\, \mu_k \nabla \psi_1 \cdot \nabla \psi_2 \,\mathrm{d}x, \qquad \psi_1 \in W^{1,2},\ \psi_2 \in W^{1,2}_{\Gamma}.$$

If, in particular, $\varsigma \equiv 1$, then we simply write $\breve{a}_k$ for $-\nabla \cdot \mu_k \nabla$. Moreover, we denote the restriction of $\breve{a}_k$ to the space $W^{1,2}_{\Gamma}$ by a_k, i.e. $a_k : W^{1,2}_{\Gamma} \to W^{-1,2}_{\Gamma}$.

3.3 Proposition. (see [26] and [27]) *There is a number $\hat{q} > 2$ (depending on $\widehat{\Omega}$, ε and $\widehat{\Gamma}$) such that for all $q \in [2, \hat{q}]$ the operator $\mathcal{P}_0 : \widehat{W}^{1,q}_{\widehat{\Gamma}} \to \widehat{W}^{-1,q}_{\widehat{\Gamma}}$ is a topological isomorphism. Moreover, there is a $\check{q} > 2$ (depending on Ω, μ_1, μ_2 and Γ) such that for all $q \in [2, \check{q}]$ the operators $a_k : W^{1,q}_{\Gamma} \to W^{-1,q}_{\Gamma}$ provide topological isomorphisms, and additionally, generate analytic semigroups on $W^{-1,q}_{\Gamma}$.*

3.4 Definition. From now on we fix a number $q \in]2, \min(4, \hat{q}, \check{q})[$ and define $p \overset{\text{def}}{=} \frac{q}{2}$. With respect to this p we define the operators

$$A_k : \psi \mapsto a_k \psi, \quad \psi \in \mathcal{D}_k \overset{\text{def}}{=} \operatorname{dom}(A_k) \overset{\text{def}}{=} \left\{ \psi \in W^{1,2}_{\Gamma} \,:\, a_k \psi \in L^p \right\}, \quad k = 1,2,$$

$$\mathrm{A} : \mathcal{D} \to \mathrm{L}^p, \quad \mathrm{A} \overset{\text{def}}{=} \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}, \quad \mathcal{D} \overset{\text{def}}{=} \operatorname{dom}(\mathrm{A}) = \mathcal{D}_1 \oplus \mathcal{D}_2 \hookrightarrow \mathrm{L}^p.$$

3.5 Remark. If $\psi \in \mathcal{D}_k$, $k = 1,2$, then $\nu \cdot (\mu_k \nabla \psi)|_\Gamma = 0$ in the sense of distributions, see for instance [5, Ch. 1.2] or [16, Ch.1.2].

After having fixed the number q and, correspondingly, the space L^p, we will now formulate our mathematical requirements on the reaction terms:

3.6 Assumption. The reaction terms r_k, $k = 1,2$, are mappings

$$r_k : [T_0, T_1] \times \widehat{W}^{1,q} \times \mathrm{W}^{1,q} \to L^p.$$

Moreover, we assume that there is a real number $\eta \in]0,1]$ and for any bounded subset $M \subset \widehat{W}^{1,q} \oplus \mathrm{W}^{1,q}$ a constant r_M such that

$$\begin{aligned} &\left\| r_k(t, v, \psi) - r_k(\check{t}, \check{v}, \check{\psi}) \right\|_{L^p} \\ &\qquad \le r_M \left(|t - \check{t}|^\eta + \|v - \check{v}\|_{\widehat{W}^{1,q}} + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}} \right), \\ &\qquad\qquad t, \check{t} \in [T_0, T_1], \quad (v, \psi), (\check{v}, \check{\psi}) \in M. \end{aligned}$$

3.7 Assumption. The functions $b_k : [T_0, T_1] \to W^{1,q}$, $k = 1,2$, are Hölder continuous. Moreover, they are Hölder continuously differentiable when considered as L^p valued.

3.4 Representation of Dirichlet boundary values

For setting up the Poisson and current–continuity equations in appropriate function spaces we must split up the solution into parts, where one part represents the inhomogeneous Dirichlet boundary values $\varphi_{\widehat{\mathrm{D}}}$ and $\phi_{\mathrm{D},k}$, $k = 1, 2$. In this section we treat of just this representation. We make the following assumptions about the Dirichlet boundary values of the electrochemical potentials ϕ_k, $k = 1, 2$, and for their initial values, see (2.3), (2.4).

3.8 Assumption. There is a Hölder continuous function

$$\Phi = (\Phi_1, \Phi_2) : [T_0, T_1] \to \mathrm{W}^{1,q}, \quad k = 1, 2,$$

such that for all $t \in [T_0, T_1]$

$$\breve{a}_k \Phi_k(t) = 0 \tag{3.3}$$

$$\operatorname{tr}\left(\Phi_k(t)\right)\Big|_{\mathrm{D}} = \phi_{\mathrm{D},k}(t) \tag{3.4}$$

Moreover, we assume, that each Φ_k, $k = 1, 2$, — as a function with values in L^p — is differentiable and its derivative is Hölder continuous.

3.9 Remark. It should be noted that (3.3) and the definition of the operators $\breve{a}_k$ imply $\nu \cdot \mu_k \nabla \Phi_k = 0$ on Γ in the distributional sense, see for instance [5, Ch. 1.2] or [16, Ch. II.2]. This implies for the current densities (2.9) that $\nu \cdot j_k = 0$ on Γ in the distributional sense, provided that $\chi_k \in W^{1,q}$.

We will now give a sufficient condition on $\phi_{\mathrm{D},k}$ for the existence of a Φ_k with the assumed properties.

3.10 Lemma. *1. If $\psi \in W^{1-1/q,q}(\mathrm{D})$, then there is a unique function $\Psi \in W^{1,q}$ fulfilling*

$$\breve{a}_k \Psi = 0, \quad \textit{and} \quad \operatorname{tr}(\Psi)\Big|_{\mathrm{D}} = \psi.$$

2. If $\psi : [T_0, T_1] \to W^{1-1/q,q}(\mathrm{D})$ is Hölder continuous with index η, then the function $\Psi : [T_0, T_1] \to W^{1,q}$ which is given for each $t \in [T_0, T_1]$ by item 1 is also Hölder continuous with index η. Moreover, if ψ — as a function with values in $W^{1/2,2}(\mathrm{D})$ — is Hölder continuously differentiable with Hölder index η, then Ψ is Hölder continuously differentiable with Hölder index η.

Proof. Let $\operatorname{ex} : W^{1-1/q,q}(\mathrm{D}) \to W^{1-1/q,q}(\partial\Omega)$ be a linear and continuous extension operator, and let tr^{-1} be a linear and continuous right inverse of the trace operator $\operatorname{tr} : W^{1,q}(\Omega) \to W^{1-1/q,q}(\partial\Omega)$. Such operators exist according to [25, Thm 1.4.3.1] and [25, Thm 1.5.1.3], respectively. Thus, $\operatorname{tr}^{-1} \circ \operatorname{ex} \psi \in W^{1,q}$. Moreover, let $\breve{\psi}$ be the solution of the differential equation

$$a_k \breve{\psi} = \breve{a}_k \circ \operatorname{tr}^{-1} \circ \operatorname{ex} \psi \tag{3.5}$$

in $W^{1,q}_\Gamma$. This solution exists and is unique because the right hand side of (3.5) is from $W^{-1,q}_\Gamma$ and the operators a_k are isomorphisms from $W^{1,q}_\Gamma$ onto $W^{-1,q}_\Gamma$. We now define

$$\Psi \stackrel{\text{def}}{=} \operatorname{tr}^{-1} \circ \operatorname{ex} \psi - \breve{\psi}. \tag{3.6}$$

The asserted properties of Ψ follow directly from the construction.

The second assertion is proved by observing that all steps in the first part of the proof depend linearly on the datum. □

3.11 Assumption. We assume that the initial values Φ_k^0 belong to $W^{1,q}$, $k = 1, 2$. Moreover, there is a $\theta \in]1/2 + 1/q, 1[$ such that for each of the initial values Φ_k^0 the difference $\Phi_k^0 - \Phi_k(T_0)$ belongs to the complex interpolation space $[L^p, \mathcal{D}_k]_\theta$.

3.12 Remark. For all $\theta \in]1/2 + 1/q, 1[$ the space $[L^p, \mathcal{D}_k]_\theta$ compactly embeds into $W^{1,q}_\Gamma \hookrightarrow L^\infty$, see [31, Thm. 5.2].

With respect to the inhomogeneous terms $\varphi_{\widehat{\mathrm{D}}}$ and $\varphi_{\widehat{\Gamma}}$ in the boundary conditions of Poisson's equation (2.1) we make the following assumptions.

3.13 Assumption. There is a Hölder continuous function $\varphi_\circ : [T_0, T_1] \to \widehat{W}^{1,q}$ such that $\varphi_\circ$ — as a function from $[T_0, T_1]$ into $\widehat{L}^p$ — is Hölder continuously differentiable. For all $t \in [T_0, T_1]$ it holds true

$$-\nabla \cdot \varepsilon \nabla \varphi_\circ(t) = 0, \tag{3.7}$$

$$\operatorname{tr}\big(\varphi_\circ(t)\big)\big|_{\widehat{\mathrm{D}}} = \varphi_{\widehat{\mathrm{D}}}(t). \tag{3.8}$$

The function

$$[T_0, T_1] \ni t \mapsto \varphi_{\widehat{\Gamma}}(t) \in L^\infty(\widehat{\Gamma})$$

is differentiable and possesses a Hölder continuous derivative.

3.14 Remark. Similar to Lemma 3.10 it is possible to give a sufficient condition on the existence of a representing function $t \mapsto \varphi_\circ(t)$ which only rests on the function $t \mapsto \varphi_{\widehat{\mathrm{D}}}(t)$. We do not carry out this here.

3.15 Remark. For all $t \in [T_0, T_1]$ we extend $\varphi_{\widehat{\Gamma}}(t)$ by zero to a $\widehat{\sigma}$–measurable, essentially bounded function on $\partial\widehat{\Omega}$. Due to the continuous embedding

$$\widehat{W}^{1,q'}_{\widehat{\Gamma}} \hookrightarrow \widehat{W}^{1,q'} \hookrightarrow W^{1-1/q',q'}(\partial\widehat{\Omega}) \hookrightarrow L^{q'}(\partial\widehat{\Omega}),$$

see [25, Thm 1.5.1.3], there is a continuous embedding

$$L^\infty(\partial\widehat{\Omega}) \hookrightarrow L^q(\partial\widehat{\Omega}) \hookrightarrow \widehat{W}^{-1,q}_{\widehat{\Gamma}}.$$

Thus, $\varphi_{\widehat{\Gamma}}(t)$, $t \in [T_0, T_1]$ can be regarded as an element of $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$. We denote $\varphi_{\widehat{\Gamma}}$ as a function from $[T_0, T_1]$ into $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$ by $\varphi_\bullet$. The Hölder continuous differentiability of $\varphi_{\widehat{\Gamma}}$ entails the Hölder continuous differentiability of $\varphi_\bullet : [T_0, T_1] \to \widehat{W}^{-1,q}_{\widehat{\Gamma}}$ with the same Hölder exponent.

3.5 The linear Poisson equation

Let us assume the following about $\tilde{d}$ — the doping profile (or control parameter) on the right hand side of Poisson's equation (2.1).

3.16 Assumption. The function $\tilde{d} : [T_0, T_1] \to \widehat{W}^{-1,q}_{\widehat{\Gamma}}$ is continuously differentiable with Hölder continuous derivative. We define a "generalized doping"

$$d : [T_0, T_1] \to \widehat{W}^{-1,q}_{\widehat{\Gamma}} \qquad \text{by} \qquad d(t) \stackrel{\text{def}}{=} \tilde{d}(t) + \varphi_\bullet(t), \quad t \in [T_0, T_1]. \tag{3.9}$$

We now define what is a solution of Poisson's equation (2.1).

3.17 Definition. Let $u_k \in \widehat{W}^{-1,q}_{\widehat{\Gamma}}$, $k = 1, 2$ be given. We say that $\widetilde{\varphi}$ is a solution of Poisson's equation (2.1) at $t \in [T_0, T_1]$, if

$$\widetilde{\varphi} = \varphi + \varphi_\circ(t), \tag{3.10}$$

and $\varphi \in \widehat{W}^{1,q}_{\widehat{\Gamma}}$ is the unique solution of

$$\mathcal{P}_0 \varphi = d(t) + u_1 - u_2. \tag{3.11}$$

φ and $\widetilde{\varphi}$ depend parametrically on t, u_1, and u_2. If convenient, we indicate the dependence on t by writing $\varphi(t)$ and $\widetilde{\varphi}(t)$, respectively.

3.18 Remark. With respect to the boundary conditions in (2.1) it should be noted that (3.8) and the property $\varphi \in \widehat{W}^{1,q}_{\widehat{\Gamma}}$ give $\widetilde{\varphi}|_{\widehat{\mathrm{D}}} = \varphi_{\widehat{\mathrm{D}}}$. Additionally, if $\tilde{d}$, u_1, and u_2 belong to the space $\widehat{L}^1$, then (3.9), (3.10) and (3.11) together with (3.7) imply $\nu \cdot (\varepsilon \nabla \widetilde{\varphi}) + \varepsilon_{\widehat{\Gamma}} \widetilde{\varphi} = \varphi_{\widehat{\Gamma}}(t)$, see for instance [5, Ch. 1.2] or [16, Ch. II.2].

Throughout this section we demand several times Hölder continuity of functions and/or their derivatives. Clearly, there is a common Hölder exponent which we will denote from now on by η.

4 Precise Formulation of the Problem

We are now going to define the problem outlined in §2.

4.1 Definition. We say the van Roosbroeck system admits a local in time solution, if there is a time $T \in]T_0, T_1]$ and $(\widetilde{\varphi}, \widetilde{\phi}) = (\widetilde{\varphi}, \widetilde{\phi}_1, \widetilde{\phi}_2)$ such that

$$\widetilde{\phi}(T_0) = (\widetilde{\phi}_1(T_0), \widetilde{\phi}_2(T_0)) = (\Phi_1^0, \Phi_2^0) \in \mathrm{W}^{1,q}, \tag{4.1}$$

$$\varphi \stackrel{\text{def}}{=} \widetilde{\varphi} - \varphi_\circ \in C([T_0, T]; \widehat{W}^{1,q}_{\widehat{\Gamma}}) \cap C^1(]T_0, T[; \widehat{W}^{1,q}_{\widehat{\Gamma}}) \tag{4.2}$$

$$\phi \stackrel{\text{def}}{=} \widetilde{\phi} - \Phi \in C^1(]T_0, T[, \mathrm{L}^p) \cap C(]T_0, T], \mathcal{D}) \cap C([T_0, T], [\mathrm{L}^p, \mathcal{D}]_\theta), \tag{4.3}$$

fulfill the Poisson equation and the current continuity equations:

$$\mathcal{P}_0(\varphi(t)) = d(t) + {}^{\uparrow}u_1(t) - {}^{\uparrow}u_2(t) \quad t \in [T_0, T], \tag{4.4}$$

$$u_k'(t) - \nabla \cdot j_k(t) = r_k(t, \widetilde{\varphi}(t), \widetilde{\phi}(t)), \quad k = 1, 2, \quad t \in]T_0, T[. \tag{4.5}$$

The carrier densities and the current densities are given by

$$u_k(t) \stackrel{\text{def}}{=} \rho_k(t) \mathcal{F}_k\big(\chi_k(t)\big), \tag{4.6}$$

$$j_k(t) \stackrel{\text{def}}{=} \mathcal{G}_k\big(\chi_k(t)\big) \mu_k \nabla \widetilde{\phi}_k(t), \tag{4.7}$$

$$\chi_k(t) \stackrel{\text{def}}{=} \widetilde{\phi}_k(t) + (-1)^k {}_{\downarrow}\widetilde{\varphi}(t) + b_k(t). \tag{4.8}$$

and satisfy

$$u_k \in C([T_0, T], L^\infty) \cap C^1(]T_0, T[, L^p), \tag{4.9}$$

$$j_k \in C([T_0, T], L^q), \tag{4.10}$$

$$\nabla \cdot j_k \in C(]T_0, T], L^p) \tag{4.11}$$

for $k = 1, 2$.

5 Reformulation as a quasi-linear parabolic system

In this section we provide the tools to rewrite the problem from Definition 4.1 as a quasi-linear system for the continuity equations. To that end we eliminate the electrostatic potential from the continuity equations. Replacing the carrier densities u_1 and u_2 on the right hand side of (4.4) by (4.6) making use of (4.8) and (3.10) one obtains a nonlinear Poisson equation for φ. We solve this equation with respect to prescribed parameters b_k and $\widetilde{\phi}_k$, $k = 1, 2$, which we will assume here to be from L^∞. This way to decouple van Roosbroeck's equations into a nonlinear Poisson equation and a system of parabolic equations is also one of the fundamental approaches to the numerical solution of the van Roosbroeck system. It is due to Gummel [28] and was the first reliable numerical technique to solve these equations for carriers in an operating semiconductor device structure.

5.1 The nonlinear Poisson equation

We are now going to prove the unique solvability of the nonlinear Poisson equation and some properties of its solution. First we show that the supposed admissibility of the carrier distribution functions $\mathcal{F}_k$ ensures that the relation between a potential and its corresponding carrier density is monotone and even continuously differentiable when considered between adequate spaces.

5.1 Lemma. *Let ρ and g be from L^∞ and $\mathcal{F} = \mathcal{F}_k$ be an admissible carrier distribution function, see Assumption 2.3.*

1. The operator

$$\widehat{W}^{1,2}_{\widehat{\Gamma}} \ni h \longmapsto {}^{\uparrow}\rho\mathcal{F}(g + {}_{\downarrow}h) \in \widehat{L}^2 \tag{5.1}$$

is well defined, continuous and bounded. Its composition with the embedding $\widehat{L}^2 \hookrightarrow \widehat{W}^{-1,2}_{\widehat{\Gamma}}$ is monotone.

2. The Nemyckii operator

$$L^\infty \ni h \longmapsto \rho\mathcal{F}(g + {}_{\downarrow}h)$$

induced by the function

$$\Omega \times \mathbb{R} \ni (x, s) \longmapsto \rho(x)\mathcal{F}(g(x) + s),$$

maps L^∞ continuously into itself and is even continuously differentiable. Its Fréchet derivative at $h \in L^\infty$ is the multiplication operator given by the essentially bounded function

$$\Omega \ni x \longmapsto \rho(x)\mathcal{F}'(g(x) + h(x)). \tag{5.2}$$

Proof. Indeed, the assumption that the carrier distribution functions should be admissible assures that the operator (5.1) is well defined, continuous and bounded, see [47] for the case of an exponential, and see [1, Chapter 3] for the case of a polynomially bounded function. The asserted monotonicity follows from the monotonicity of the function $\mathcal{F}$ and the fact that the duality between $\widehat{W}^{1,2}_{\widehat{\Gamma}}$ and $\widehat{W}^{-1,2}_{\widehat{\Gamma}}$ is the extension of the $\widehat{L}^2$ duality:

$$\begin{aligned}\langle {}^{\uparrow}\rho\mathcal{F}(g + {}_{\downarrow}h_1) - {}^{\uparrow}\rho\mathcal{F}(g + {}_{\downarrow}h_2) \mid h_1 - h_2\rangle_{\widehat{W}^{1,2}_{\widehat{\Gamma}}} \\ = \int_{\widehat{\Omega}} \left({}^{\uparrow}\rho\mathcal{F}(g + {}_{\downarrow}h_1) - {}^{\uparrow}\rho\mathcal{F}(g + {}_{\downarrow}h_2)\right)(h_1 - h_2)\,\mathrm{d}x \\ = \int_{\Omega} (\rho\mathcal{F}(g + {}_{\downarrow}h_1) - \rho\mathcal{F}(g + {}_{\downarrow}h_2))\,({}_{\downarrow}h_1 - {}_{\downarrow}h_2)\,\mathrm{d}x \geq 0 \quad \text{for all } h_1, h_2 \in \widehat{W}^{1,2}_{\widehat{\Gamma}}.\end{aligned}$$

The second assertion follows from a result by Gröger and Recke, see [42, Thm 5.1]. □

5.2 Corollary. *The mapping*

$$\widehat{W}^{1,q} \ni h \longmapsto {}^{\uparrow}\rho\mathcal{F}(g + {}_{\downarrow}h)$$

takes its values in $\widehat{L}^\infty$ and is also continuously differentiable. Its derivative at a point $h \in \widehat{W}^{1,q}$ equals the multiplication operator which is induced by the function ${}^{\uparrow}\rho\mathcal{F}'(g + {}_{\downarrow}h)$.

5.3 Theorem. *Under Assumption 2.3 on the distribution functions $\mathcal{F}_1$, $\mathcal{F}_2$ and Assumption 2.1 the following statements are true:*

1. For any pair of functions $z = (z_1, z_2) \in \mathrm{L}^\infty$ the operator

$$\varphi \longmapsto \mathcal{P}_0\varphi - {}^\uparrow\rho_1\mathcal{F}_1(z_1 - {}_\downarrow\varphi) + {}^\uparrow\rho_2\mathcal{F}_2(z_2 + {}_\downarrow\varphi) \tag{5.3}$$

is strongly monotone and continuous from $\widehat{W}^{1,2}_{\widehat{\Gamma}}$ to $\widehat{W}^{-1,2}_{\widehat{\Gamma}}$, where the operator $\mathcal{P}_0$ is according to Definition 3.1. The monotonicity constant of (5.3) is a least that of $\mathcal{P}_0$.

2. For all $f \in \widehat{W}^{-1,2}_{\widehat{\Gamma}}$ and $z = (z_1, z_2) \in \mathrm{L}^\infty$ the nonlinear Poisson equation

$$\mathcal{P}_0\varphi - {}^\uparrow\rho_1\mathcal{F}_1(z_1 - {}_\downarrow\varphi) + {}^\uparrow\rho_2\mathcal{F}_2(z_2 + {}_\downarrow\varphi) = f \tag{5.4}$$

admits exactly one solution φ which we denote by $\mathcal{L}(f, z)$. This solution belongs to $\widehat{W}^{1,2}_{\widehat{\Gamma}}$ and satisfies the estimate

$$\|\varphi\|_{\widehat{W}^{1,2}_{\widehat{\Gamma}}} \le \frac{1}{m} \left\|{}^\uparrow\rho_1\mathcal{F}_1(z_1) - {}^\uparrow\rho_2\mathcal{F}_2(z_2) + f\right\|_{\widehat{W}^{-1,2}_{\widehat{\Gamma}}},$$

where m is the monotonicity constant of $\mathcal{P}_0$.

3. The maximal restriction of the operator (5.3) to the range space $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$ has the domain $\widehat{W}^{1,q}_{\widehat{\Gamma}}$. Moreover, if M is a bounded subset of $\widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty$, then the set $\{\mathcal{L}(f, z) : (f, z) \in M\}$ is bounded in $\widehat{W}^{1,q}_{\widehat{\Gamma}}$.

4. The mapping $\mathcal{L} : \widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty \to \widehat{W}^{1,q}_{\widehat{\Gamma}}$ is continuously differentiable. Let $(F, Z) = (F, Z_1, Z_2)$ be from $\widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty$; we define the function

$$\mathcal{N}_k \stackrel{\text{def}}{=} {}^\uparrow\rho_k\mathcal{F}'_k(Z_k + (-1)^k{}_\downarrow\mathcal{L}(F, Z)), \tag{5.5}$$

and we also denote the corresponding multiplication operator on $\widehat{\Omega}$ by $\mathcal{N}_k$. Then the Fréchet derivative $\partial\mathcal{L}$ at a point $(F, Z) = (F, Z_1, Z_2)$ is the bounded linear mapping given by

$$[\partial\mathcal{L}(F, Z)]\,(f, z) = (\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1}\left(f + \mathcal{N}_1{}^\uparrow z_1 - \mathcal{N}_2{}^\uparrow z_2\right), \quad k = 1, 2 \tag{5.6}$$

for all $(f, z) = (f, (z_1, z_2)) \in \widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty$.

5. The norm of $\partial\mathcal{L}(F, Z) \in \mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty; \widehat{W}^{1,q}_{\widehat{\Gamma}})$ can be estimated as follows:

$$\begin{aligned}
&\|\partial\mathcal{L}(F, Z)\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty; \widehat{W}^{1,q}_{\widehat{\Gamma}})} \\
&\quad\le 2\|\mathcal{P}_0^{-1}\|_{\mathcal{B}(L^2; \widehat{W}^{1,q}_{\widehat{\Gamma}})}\sqrt{\|\mathcal{N}_1 + \mathcal{N}_2\|_{L^\infty}\|\mathcal{N}_1 + \mathcal{N}_2\|_{L^1}} + \|\mathcal{P}_0^{-1}\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}}; \widehat{W}^{1,q}_{\widehat{\Gamma}})} \\
&\qquad + \|\mathcal{P}_0^{-1}\|_{\mathcal{B}(\widehat{L}^2; \widehat{W}^{1,q}_{\widehat{\Gamma}})}\sqrt{\|\mathcal{N}_1 + \mathcal{N}_2\|_{L^\infty}}\|\mathcal{P}_0^{-1/2}\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}}; \widehat{L}^2)}
\end{aligned}$$

Proof. 1. The assumption that $\widehat{\mathrm{D}}$ is not empty or $\varepsilon_{\widehat{\Gamma}}$ is positive on a set of positive arc measure ensures that the operator $\mathcal{P}_0$ is strongly monotone. Thus, taking into account Lemma 5.1, the mapping (5.3) is strongly monotone and continuous from $\widehat{W}^{1,2}_{\widehat{\Gamma}}$ to $\widehat{W}^{-1,2}_{\widehat{\Gamma}}$.

2. The second assertion follows from the first one by standard results on monotone operators, see for instance [16].

3. For $f \in \widehat{W}^{-1,2}_{\widehat{\Gamma}}$ the solution $\mathcal{L}(f,z)$ is from $\widehat{W}^{1,2}_{\widehat{\Gamma}}$ and hence,

$$-{}^{\uparrow}\rho_1 \mathcal{F}_1\big(z_1 - {}_{\downarrow}\mathcal{L}(f,z)\big) + {}^{\uparrow}\rho_2 \mathcal{F}_2\big(z_2 + {}_{\downarrow}\mathcal{L}(f,z)\big) \in \widehat{L}^2 \hookrightarrow \widehat{W}^{-1,q}_{\widehat{\Gamma}},$$

see Lemma 5.1. By the second assertion of the theorem, the set

$$\{\mathcal{L}(f,z) : (f,z) \in M\} \quad \text{is bounded in } \widehat{W}^{1,2}_{\widehat{\Gamma}}.$$

From this we conclude again by Lemma 5.1 that the set

$$\left\{{}^{\uparrow}\rho_1 \mathcal{F}_1\big(z_1 - {}_{\downarrow}\mathcal{L}(f,z)\big) - {}^{\uparrow}\rho_2 \mathcal{F}_2\big(z_2 + {}_{\downarrow}\mathcal{L}(f,z)\big) \;:\; (f,z) \in M\right\}$$

is bounded in $\widehat{L}^2$, and hence, is bounded in $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$. Thus, the set

$$\left\{{}^{\uparrow}\rho_1 \mathcal{F}_1\big(z_1 - {}_{\downarrow}\mathcal{L}(f,z)\big) - {}^{\uparrow}\rho_2 \mathcal{F}_2\big(z_2 + {}_{\downarrow}\mathcal{L}(f,z)\big) + f \;:\; (f,z) \in M\right\}$$

is also bounded in $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$. Consequently, the image of this set under $\mathcal{P}_0^{-1}$ is bounded in $\widehat{W}^{1,q}_{\widehat{\Gamma}}$.

4. We define an auxiliary mapping $\mathcal{K} : \widehat{W}^{1,q}_{\widehat{\Gamma}} \oplus \widehat{W}^{-1,q}_{\widehat{\Gamma}} \oplus \mathrm{L}^\infty \to \widehat{W}^{-1,q}_{\widehat{\Gamma}}$ by

$$\mathcal{K}(\varphi, f, z) \stackrel{\text{def}}{=} \mathcal{P}_0\varphi - {}^{\uparrow}\rho_1 \mathcal{F}_1(z_1 - {}_{\downarrow}\varphi) + {}^{\uparrow}\rho_2 \mathcal{F}_2(z_2 + {}_{\downarrow}\varphi) - f$$

such that $\mathcal{K}\big(\mathcal{L}(f,z), f, z\big) = 0$ for all $f \in \widehat{W}^{-1,q}_{\widehat{\Gamma}}$ and all $z \in \mathrm{L}^\infty$. The assertion follows from the *Implicit Function Theorem* if we can prove that $\mathcal{K}$ is continuously differentiable and the partial derivative with respect to φ is a topological isomorphism between $\widehat{W}^{1,q}_{\widehat{\Gamma}}$ and $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$. For any $\varphi \in \widehat{W}^{1,q}_{\widehat{\Gamma}}$, $f \in \widehat{W}^{-1,q}_{\widehat{\Gamma}}$, and $z \in \mathrm{L}^\infty$ the partial derivatives of $\mathcal{K}$ are given by

$$\partial_\varphi \mathcal{K}(\varphi, f, z) = \mathcal{P}_0 + \sum_{k=1}^{2} {}^{\uparrow}\rho_k \mathcal{F}_k'(z_k + (-1)^k {}_{\downarrow}\varphi) \in \mathcal{B}(\widehat{W}^{1,q}_{\widehat{\Gamma}}; \widehat{W}^{-1,q}_{\widehat{\Gamma}}), \tag{5.7}$$

$$\partial_f \mathcal{K}(\varphi, f, z) = -\mathbb{I} \in \mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}}; \widehat{W}^{-1,q}_{\widehat{\Gamma}}), \tag{5.8}$$

$$\partial_{z_k} \mathcal{K}(\varphi, f, z) = (-1)^{k\uparrow}\rho_k \mathcal{F}_k'(z_k + (-1)^k {}_{\downarrow}\varphi) \in \widehat{L}^\infty \hookrightarrow \mathcal{B}(\mathrm{L}^\infty; \widehat{W}^{-1,q}_{\widehat{\Gamma}}) \tag{5.9}$$

and they are continuous, see Lemma 5.1 and [42, §5].

Now we consider the equation

$$\mathcal{P}_0\psi + \sum_{k=1}^{2} {}^{\uparrow}\rho_k \mathcal{F}_k'(z_k + (-1)^k {}_{\downarrow}\varphi)\psi = f \in \widehat{W}_{\widehat{\Gamma}}^{-1,q} \tag{5.10}$$

Because $\sum_{k=1}^{2} {}^{\uparrow}\rho_k \mathcal{F}_k'(z_k+(-1)^k {}_{\downarrow}\varphi)$ is a positive function from $\widehat{L}^\infty$, (5.10) has exactly one solution $\psi \in \widehat{W}_{\widehat{\Gamma}}^{1,2}$ by the *Lax-Milgram-Lemma*. Moreover,

$$\sum_{k=1}^{2} {}^{\uparrow}\rho_k \mathcal{F}_k'(z_k + (-1)^k {}_{\downarrow}\varphi)\psi \in \widehat{L}^2 \hookrightarrow \widehat{W}_{\widehat{\Gamma}}^{-1,q},$$

and $\mathcal{P}_0 : \widehat{W}_{\widehat{\Gamma}}^{1,q} \to \widehat{W}_{\widehat{\Gamma}}^{-1,q}$ is a topological isomorphism. Thus, a rearrangement of terms in (5.10) gives $\psi \in \widehat{W}_{\widehat{\Gamma}}^{1,q}$.

5. We now estimate the Fréchet derivative (5.6):

$$\begin{aligned} &\left\|(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1}(f + \mathcal{N}_1{}^{\uparrow}z_1 - \mathcal{N}_2{}^{\uparrow}z_2)\right\|_{\widehat{W}_{\widehat{\Gamma}}^{1,q}} \\ &\qquad \le \left\|(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1} f\right\|_{\widehat{W}_{\widehat{\Gamma}}^{1,q}} \\ &\qquad\quad + \left\|(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1}(\mathcal{N}_1{}^{\uparrow}z_1 - \mathcal{N}_2{}^{\uparrow}z_2)\right\|_{\widehat{W}_{\widehat{\Gamma}}^{1,q}} . \end{aligned} \tag{5.11}$$

We treat the right hand side terms separately; for the second addend one obtains

$$\begin{aligned} &\left\|(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1}(\mathcal{N}_1{}^{\uparrow}z_1 - \mathcal{N}_2{}^{\uparrow}z_2)\right\|_{\widehat{W}_{\widehat{\Gamma}}^{1,q}} \\ &\qquad \le \left\|(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1}\sqrt{\mathcal{N}_1 + \mathcal{N}_2}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}_{\widehat{\Gamma}}^{1,q})} \|g\|_{L^2} , \end{aligned} \tag{5.12}$$

where the function $g \in L^2$ is defined by

$$g(x) \stackrel{\text{def}}{=} \frac{\mathcal{N}_1(x)z_1(x) - \mathcal{N}_2(x)z_2(x)}{\sqrt{\mathcal{N}_1(x) + \mathcal{N}_2(x)}} \quad \text{for } x \in \Omega. \tag{5.13}$$

Please note that the functions $\mathcal{N}_k$ are strictly positive almost everywhere in Ω due to the positivity of the distribution functions and Assumption 2.1. For the function g in (5.13) one has the following bound:

$$\|g\|_{L^2} \le \sqrt{\|\mathcal{N}_1 + \mathcal{N}_2\|_{\widehat{L}^1}} \left(\|z_1\|_{L^\infty} + \|z_2\|_{L^\infty}\right).$$

Making use of the operator identity

$$(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1} = \mathcal{P}_0^{-1} - \mathcal{P}_0^{-1}(\mathcal{N}_1 + \mathcal{N}_2)(\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1} \tag{5.14}$$

one obtains

$$\begin{aligned}\left\|(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}\sqrt{\mathcal{N}_1+\mathcal{N}_2}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})} &\le \left\|\mathcal{P}_0^{-1}\sqrt{\mathcal{N}_1+\mathcal{N}_2}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}\\ &+\left\|\mathcal{P}_0^{-1}\sqrt{\mathcal{N}_1+\mathcal{N}_2}\sqrt{\mathcal{N}_1+\mathcal{N}_2}(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}\sqrt{\mathcal{N}_1+\mathcal{N}_2}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}\\ &\le \left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}\sqrt{\|\mathcal{N}_1+\mathcal{N}_2\|_{\widehat{L}^\infty}}\,\times\\ &\times\left(1+\left\|\sqrt{\mathcal{N}_1+\mathcal{N}_2}(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1/2}\right\|^2_{\mathcal{B}(\widehat{L}^2)}\right)\end{aligned}$$

We note that

$$\left\|\sqrt{\mathcal{N}_1+\mathcal{N}_2}(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1/2}\right\|_{\mathcal{B}(\widehat{L}^2)}\le 1 \tag{5.15}$$

because the bounded multiplication operator $\mathcal{N}_1+\mathcal{N}_2$ is form subordinated to $\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2$, see for instance [34, VI.2.6]. Thus, we get for the second addend of (5.11):

$$\begin{aligned}&\left\|(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}(\mathcal{N}_1{}^{\uparrow}z_1-\mathcal{N}_2{}^{\uparrow}z_2)\right\|_{\widehat{W}^{1,q}_{\widehat{\Gamma}}}\\ &\le 2\left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}\sqrt{\|\mathcal{N}_1+\mathcal{N}_2\|_{\widehat{L}^\infty}}\sqrt{\|\mathcal{N}_1+\mathcal{N}_2\|_{\widehat{L}^1}}\left(\|z_1\|_{L^\infty}+\|z_2\|_{L^\infty}\right)\end{aligned} \tag{5.16}$$

Applying (5.14) to the first term on the right hand side of (5.11) we find

$$\begin{aligned}\left\|(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}f\right\|_{\widehat{W}^{1,q}_{\widehat{\Gamma}}} &\le \left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{W}^{1,q}_{\widehat{\Gamma}})}\|f\|_{\widehat{W}^{-1,q}_{\widehat{\Gamma}}}\\ &+\left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}\left\|(\mathcal{N}_1+\mathcal{N}_2)(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{L}^2)}\|f\|_{\widehat{W}^{-1,q}_{\widehat{\Gamma}}}.\end{aligned} \tag{5.17}$$

The terms $\left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{W}^{1,q}_{\widehat{\Gamma}})}$ and $\left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}$ are finite. As for the remaining term

$$\begin{aligned}&\left\|(\mathcal{N}_1+\mathcal{N}_2)(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{L}^2)}\\ &\le\sqrt{\|\mathcal{N}_1+\mathcal{N}_2\|_{\widehat{L}^\infty}}\left\|\sqrt{\mathcal{N}_1+\mathcal{N}_2}(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1/2}\right\|_{\mathcal{B}(\widehat{L}^2)}\\ &\qquad\left\|(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1/2}\mathcal{P}_0^{1/2}\right\|_{\mathcal{B}(\widehat{L}^2)}\left\|\mathcal{P}_0^{-1/2}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{L}^2)}\end{aligned}$$

we note that $\left\|\mathcal{P}_0^{-1/2}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{L}^2)}$ is finite, since $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$ embeds continuously into $\widehat{W}^{-1,2}_{\widehat{\Gamma}}$ and $\mathcal{P}_0^{1/2}:\widehat{L}^2\to\widehat{W}^{-1,2}_{\widehat{\Gamma}}$ is a topological isomorphism. Again, $\mathcal{P}_0$ is form subordinated to $\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2$. Hence, besides (5.15) one has

$$\|(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1/2}\mathcal{P}_0^{1/2}\|_{\mathcal{B}(\widehat{L}^2)}\le 1.$$

Thus, we get from (5.17):

$$\begin{aligned}\left\|(\mathcal{P}_0+\mathcal{N}_1+\mathcal{N}_2)^{-1}f\right\|_{\widehat{W}^{1,q}_{\widehat{\Gamma}}} &\le \left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{W}^{1,q}_{\widehat{\Gamma}})}\|f\|_{\widehat{W}^{-1,q}_{\widehat{\Gamma}}}\\ &+\left\|\mathcal{P}_0^{-1}\right\|_{\mathcal{B}(\widehat{L}^2;\widehat{W}^{1,q}_{\widehat{\Gamma}})}\sqrt{\|\mathcal{N}_1+\mathcal{N}_2\|_{\widehat{L}^\infty}}\left\|\mathcal{P}_0^{-1/2}\right\|_{\mathcal{B}(\widehat{W}^{-1,q}_{\widehat{\Gamma}};\widehat{L}^2)}\|f\|_{\widehat{W}^{-1,q}_{\widehat{\Gamma}}}.\end{aligned} \tag{5.18}$$

Inserting (5.16) and (5.18) into (5.11) finishes the proof. □

5.4 Corollary. *Let the assumptions of Theorem 5.3 be satisfied. Then holds true:*

1. The mapping $\mathcal{L} : \widehat{W}_{\widehat{\Gamma}}^{-1,q} \oplus \mathrm{L}^\infty \to \widehat{W}_{\widehat{\Gamma}}^{1,q}$ *is boundedly Lipschitzian, i.e. for any bounded subset* $M \subset \widehat{W}_{\widehat{\Gamma}}^{-1,q} \oplus \mathrm{L}^\infty$ *there is a constant* $\mathcal{L}_M$ *such that*

$$\left\|\mathcal{L}(f,z) - \mathcal{L}(\check{f},\check{z})\right\|_{W^{1,q}} \le \mathcal{L}_M \left(\|f - \check{f}\|_{\widehat{W}_{\widehat{\Gamma}}^{-1,q}} + \|z - \check{z}\|_{\mathrm{L}^\infty} \right)$$

for all (f,z), $(\check{f},\check{z}) \in M$.

2. Let additionally Assumption 3.16 be satisfied. If

$$z = (z_1, z_2) \in C([T_0,T],\mathrm{L}^\infty) \cap C^1(]T_0,T[,\mathrm{L}^p),$$

then the function $[T_0,T] \ni t \mapsto \varphi(t) \in \widehat{W}_{\widehat{\Gamma}}^{1,q}$ *given by* $\varphi(t) \stackrel{\text{def}}{=} \mathcal{L}(d(t), z(t)) \in \widehat{W}_{\widehat{\Gamma}}^{1,q}$ *is continuous, and continuously differentiable on* $]T_0,T[$. *Its derivative is*

$$\begin{aligned}\varphi'(t) = \left[\partial\mathcal{L}\big(d(t), z(t)\big)\right] \big(d'(t), z'(t)\big)& \\ = (\mathcal{P}_0 + \mathcal{N}_1 + \mathcal{N}_2)^{-1} \left(d'(t) + \mathcal{N}_1{}^{\uparrow} z_1' - \mathcal{N}_2{}^{\uparrow} z_2'\right),&\end{aligned}$$

where $\mathcal{N}_k$ *is again defined by* (5.5) *— there* (F,Z) *specified as* $\big(d(t), z(t)\big)$.

5.2 Derivation of the quasi-linear system

We start now with the reformulation of the van Roosbroeck system as defined in Definition 4.1 as a quasi-linear parabolic system for the continuity equations. The aim of eliminating the electrostatic potential in mind, we first look for a substitute for its time derivative. In order to achieve this, we formally differentiate Poisson's equation (4.4) with respect to time. This gives

$$\mathcal{P}_0\varphi' = d' + {}^{\uparrow}(u_1' - u_2'). \tag{5.19}$$

From (4.5) one obtains

$$u_1' - u_2' = \nabla \cdot j_1 - \nabla \cdot j_2 + r_1(t, \widetilde{\varphi}, \widetilde{\phi}) - r_2(t, \widetilde{\varphi}, \widetilde{\phi}). \tag{5.20}$$

Inserting (5.20) into (5.19), one gets

$$\mathcal{P}_0\varphi' = d' + {}^{\uparrow}\big(\nabla \cdot j_1 - \nabla \cdot j_2 + r_1(t, \widetilde{\varphi}, \widetilde{\phi}) - r_2(t, \widetilde{\varphi}, \widetilde{\phi})\big). \tag{5.21}$$

Just in case, $r = r_1 = r_2$ is only recombination, this is precisely the well known conservation law for the total current, see [11]. Clearly, (5.21) leads to

$$_{\downarrow}\varphi' = {}_{\downarrow}\mathcal{P}_0^{-1} \Big(d' + {}^{\uparrow}\big(\nabla \cdot j_1 - \nabla \cdot j_2 + r_1(t, \widetilde{\varphi}, \widetilde{\phi}) - r_2(t, \widetilde{\varphi}, \widetilde{\phi})\big)\Big). \tag{5.22}$$

Now we differentiate (4.6) (with (4.8)) with respect to time and obtain

$$u_k' = \rho_k \mathcal{F}_k'(\widetilde{\phi}_k + (-1)^k{}_\downarrow\widetilde{\varphi} + b_k)\big[\widetilde{\phi}_k' + (-1)^k{}_\downarrow\widetilde{\varphi}' + b_k'\big] + \rho_k' \mathcal{F}_k(\widetilde{\phi}_k + (-1)^k{}_\downarrow\widetilde{\varphi} + b_k), \quad k = 1, 2, \tag{5.23}$$

Pending further notice we do not write out the argument $\widetilde{\phi}_k + (-1)^k{}_\downarrow\widetilde{\varphi} + b_k$ of the distribution function $\mathcal{F}_k$ and its derivative. We also abstain from drawing out the argument of the reaction terms r_k. According to (3.10) we split $\widetilde{\varphi}' = \varphi' + \varphi_\circ'$ and insert (5.23) into the current continuity equation (4.5). Thus, we find

$$\big[\widetilde{\phi}_k' + (-1)^k{}_\downarrow\varphi'\big]\rho_k\mathcal{F}_k' - \nabla\cdot j_k = r_k - \big[(-1)^k{}_\downarrow\varphi_\circ' + b_k'\big]\rho_k\mathcal{F}_k' - \rho_k'\mathcal{F}_k, \quad k = 1, 2.$$

Using (5.22) we get further

$$\rho_k\mathcal{F}_k'\widetilde{\phi}_k' - \nabla\cdot j_k + (-1)^k\rho_k\mathcal{F}_{k\downarrow}'\mathcal{P}_0^{-1}\big(d' + {}^\uparrow(\nabla\cdot j_1 - \nabla\cdot j_2 + r_1 - r_2)\big) = r_k - \big[(-1)^k{}_\downarrow\varphi_\circ' + b_k'\big]\rho_k\mathcal{F}_k' - \rho_k'\mathcal{F}_k, \quad k = 1, 2.$$

Dividing this by $\rho_k\mathcal{F}_k'$ we obtain

$$\begin{pmatrix} \widetilde{\phi}_1' \\ \widetilde{\phi}_2' \end{pmatrix} - \begin{pmatrix} 1 + {}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_1'\rho_1 & -{}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_2'\rho_2 \\ -{}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_1'\rho_1 & 1 + {}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_2'\rho_2 \end{pmatrix} \begin{pmatrix} \frac{1}{\rho_1\mathcal{F}_1'} & 0 \\ 0 & \frac{1}{\rho_2\mathcal{F}_2'} \end{pmatrix} \begin{pmatrix} \nabla\cdot j_1 \\ \nabla\cdot j_2 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{r_1}{\rho_1\mathcal{F}_1'} + r_{1\downarrow}\mathcal{P}_0^{-1\uparrow} - r_{2\downarrow}\mathcal{P}_0^{-1\uparrow} \\ -r_{1\downarrow}\mathcal{P}_0^{-1\uparrow} + \frac{r_2}{\rho_2\mathcal{F}_2'} + r_{2\downarrow}\mathcal{P}_0^{-1\uparrow} \end{pmatrix} + \begin{pmatrix} {}_\downarrow\mathcal{P}_0^{-1}d' + {}_\downarrow\varphi_\circ' - b_1' - \frac{\rho_1'}{\rho_1}\frac{\mathcal{F}_1}{\mathcal{F}_1'} \\ -{}_\downarrow\mathcal{P}_0^{-1}d' - {}_\downarrow\varphi_\circ' - b_2' - \frac{\rho_2'}{\rho_2}\frac{\mathcal{F}_2}{\mathcal{F}_2'} \end{pmatrix}$$

This evolution equation can be written in the condensed form

$$\widetilde{\phi}' - [I + Z(t,\widetilde{\phi})]E(t,\widetilde{\phi})\nabla\cdot j = Y(t,\widetilde{\phi}) \tag{5.24}$$

where $\widetilde{\phi} = (\widetilde{\phi}_1, \widetilde{\phi}_2)$ and $\nabla\cdot j \stackrel{\text{def}}{=} (\nabla\cdot j_1, \nabla\cdot j_2)$. Moreover, I denotes the identity. The coefficients Z, E, and Y are given in the following way: First we split off the Dirichlet inhomogeneities of $\widetilde{\varphi}$ in the sense of §3.4 and we replace φ by the solution of the nonlinear Poisson equation, see Theorem 5.3. With respect to an arbitrary $\psi = (\psi_1, \psi_2) \in \mathrm{W}^{1,q}$ we set

$$Q_k(t,\psi) \stackrel{\text{def}}{=} \psi_k + (-1)^k{}_\downarrow\mathcal{L}\big(d(t), z(t)\big) + (-1)^k{}_\downarrow\varphi_\circ(t) + b_k(t), \quad k = 1, 2, \tag{5.25}$$

where $z \stackrel{\text{def}}{=} (z_1, z_2)$ with

$$z_k(t) \stackrel{\text{def}}{=} \psi_k + (-1)^k{}_\downarrow\varphi_\circ(t) + b_k(t), \quad k = 1, 2. \tag{5.26}$$

Now we define

$$Z(t,\psi) \stackrel{\text{def}}{=} \begin{pmatrix} {}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_1'(Q_1(t,\psi))\rho_1(t) & -{}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_2'(Q_2(t,\psi))\rho_2(t) \\ -{}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_1'(Q_1(t,\psi))\rho_1(t) & {}_\downarrow\mathcal{P}_0^{-1\uparrow}\mathcal{F}_2'(Q_2(t,\psi))\rho_2(t) \end{pmatrix} \tag{5.27}$$

$$E(t,\psi) \stackrel{\text{def}}{=} \begin{pmatrix} E_1(t,\psi) & 0 \\ 0 & E_2(t,\psi) \end{pmatrix}, \quad E_k(t,\psi) \stackrel{\text{def}}{=} \frac{1}{\rho_k(t)\mathcal{F}_k'(Q_k(t,\psi))} \tag{5.28}$$

$$R(t,\psi) \stackrel{\text{def}}{=} \begin{pmatrix} r_1(t, \mathcal{L}(d(t), z(t)) + \varphi_\circ(t), \psi) \\ r_2(t, \mathcal{L}(d(t), z(t)) + \varphi_\circ(t), \psi) \end{pmatrix}, \tag{5.29}$$

and finally

$$Y(t,\psi) \stackrel{\text{def}}{=} \big[I + Z(t,\psi)\big]E(t,\psi)R(t,\psi) - X(t,\psi), \tag{5.30}$$

where $X(t,\psi) = \big(X_1(t,\psi), X_2(t,\psi)\big)$ with

$$X_k(t,\psi) \stackrel{\text{def}}{=} (-1)^k{}_\downarrow\big(\mathcal{P}_0^{-1}d'(t) + \varphi_\circ'(t)\big) + b_k'(t) + \frac{\rho_k'(t)}{\rho_k(t)}\frac{\mathcal{F}_k(Q_k(t,\psi))}{\mathcal{F}_k'(Q_k(t,\psi))}, \tag{5.31}$$

$k = 1, 2$. Please note

$$Z(t,\psi)E(t,\psi) = \begin{pmatrix} {}_\downarrow\mathcal{P}_0^{-1\uparrow} & -{}_\downarrow\mathcal{P}_0^{-1\uparrow} \\ -{}_\downarrow\mathcal{P}_0^{-1\uparrow} & {}_\downarrow\mathcal{P}_0^{-1\uparrow} \end{pmatrix}. \tag{5.32}$$

Next we apply the definition (2.9) of the currents j_k and get

$$\nabla\cdot j_k = \nabla\cdot\big(\mathcal{G}_k(\widetilde{\phi}_k + (-1)^k{}_\downarrow\varphi + (-1)^k{}_\downarrow\varphi_\circ + b_k)\mu_k\nabla\widetilde{\phi}_k\big), \quad k = 1, 2,$$

or in shorter notation

$$\nabla\cdot j = \nabla\cdot G(t,\widetilde{\phi})\mu\nabla\widetilde{\phi}, \tag{5.33}$$

where — see also (5.25) and (2.9) —

$$G(t,\psi) \stackrel{\text{def}}{=} \begin{pmatrix} G_1(t,\psi) & 0 \\ 0 & G_2(t,\psi) \end{pmatrix}, \quad G_k(t,\psi) \stackrel{\text{def}}{=} \mathcal{G}_k\big(Q_k(t,\psi)\big). \tag{5.34}$$

Now, putting together (5.33) and (5.24) we obtain in conclusion the evolution equation

$$\widetilde{\phi}' - \big[I + Z(t,\widetilde{\phi})\big]E(t,\widetilde{\phi})\nabla\cdot G(t,\widetilde{\phi})\mu\nabla\widetilde{\phi} = Y(t,\widetilde{\phi}) \tag{5.35}$$

which has to be complemented by the boundary conditions (2.3) and the initial condition (2.4), see also Remark 3.9.

6 The quasi-linear parabolic equation

Evolution equations of the type (5.35) were investigated in [31]: (5.35) has a unique, local in time solution, if the functions E, G, Z and Y defined by (5.28), (5.34), (5.27) and (5.30), respectively, satisfy the following conditions.

6.1 Assumption. With respect to $q \in]2,\infty[$ and $p = q/2$, as specified in Definition 3.4, there is an $\eta \in]0,1]$ and further for any bounded set $M \subset \mathrm{W}^{1,q}$ exist positive constants E_M, G_M, Y_M, and Z_M such that the mappings

$$E : [T_0,T_1]\times\mathrm{W}^{1,q} \longrightarrow \mathrm{L}^\infty, \tag{6.1}$$
$$G : [T_0,T_1]\times\mathrm{W}^{1,q} \longrightarrow \mathrm{W}^{1,q}, \tag{6.2}$$
$$Z : [T_0,T_1]\times\mathrm{W}^{1,q} \longrightarrow \mathcal{B}_\infty(\mathrm{L}^p), \tag{6.3}$$
$$Y : [T_0,T_1]\times\mathrm{W}^{1,q} \longrightarrow \mathrm{L}^p \tag{6.4}$$

satisfy the conditions

$$\min_{k=1,2} \inf_{\substack{t\in[T_0,T_1]\\ \psi\in M}} \operatorname*{vraimin}_{x\in\Omega} E_k(t,\psi)(x) \quad > \quad 0 \tag{6.5}$$

$$\min_{k=1,2} \inf_{\substack{t\in[T_0,T_1]\\ \psi\in M}} \operatorname*{vraimin}_{x\in\Omega} G_k(t,\psi)(x) \quad > \quad 0 \tag{6.6}$$

and for all t, $\check{t} \in [T_0, T_1]$ and all $\psi, \check{\psi} \in M$:

$$\|E(t,\psi) - E(\check{t},\check{\psi})\|_{\mathrm{L}^\infty} \leq E_M \left(|t-\check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}}\right), \tag{6.7}$$

$$\|G(t,\psi) - G(\check{t},\check{\psi})\|_{\mathrm{W}^{1,q}} \leq G_M \left(|t-\check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}}\right), \tag{6.8}$$

$$\|Z(t,\psi) - Z(\check{t},\check{\psi})\|_{\mathcal{B}(\mathrm{L}^p)} \leq Z_M \left(|t-\check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}}\right), \tag{6.9}$$

$$\|Y(t,\psi) - Y(\check{t},\check{\psi})\|_{\mathrm{L}^p} \leq Y_M \left(|t-\check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}}\right). \tag{6.10}$$

6.2 Definition. Let the Assumptions 3.8 and 6.1 be satisfied. Further, let $\mathrm{A} : \mathcal{D} \to \mathrm{L}^p$ be the operator from Definition 3.4 and let V be a Banach space such that $\mathcal{D} \hookrightarrow V \hookrightarrow \mathrm{W}^{1,q}$. We say the evolution equation (5.35) with initial condition $\widetilde{\phi}(T_0) = \Phi^0 \in \mathrm{W}^{1,q}$ has a unique local solution $\widetilde{\phi} = \phi + \Phi$ with respect to V if $\Phi^0 - \Phi(T_0) \in V$ implies the existence of a number $T \in]T_0, T_1]$ such that the initial value problem

$$\begin{aligned} \phi'(t) &+ \left[I + Z\big(t, \phi(t) + \Phi(t)\big)\right] E\big(t, \phi + \Phi(t)\big) G\big(t, \phi(t) + \Phi(t)\big) \,\mathrm{A}\,\phi(t) \\ &= Y\big(t, \phi(t) + \Phi(t)\big) - \Phi'(t) + J\big(t, \phi(t)\big), \quad \phi(T_0) = \Phi^0 - \Phi(T_0) \end{aligned} \tag{6.11}$$

admits a unique solution

$$\phi \in C^1(]T_0, T[, \mathrm{L}^p) \cap C(]T_0, T], \mathcal{D}) \cap C([T_0, T], V). \tag{6.12}$$

For $(t, \psi) \in [T_0, T_1] \times \mathrm{W}^{1,q}_\Gamma$ the term J in (6.11) is given by

$$J(t,\psi) \stackrel{\text{def}}{=} \left[I + Z\big(t, \psi + \Phi(t)\big)\right] E\big(t, \psi + \Phi(t)\big) \nabla G\big(t, \psi + \Phi(t)\big) \cdot \mu \nabla\big(\psi + \Phi(t)\big).$$

6.3 Remark. We have to clarify the relation between (5.35) and (6.11). If $\widetilde{\phi} = \phi + \Phi$ is a solution in the sense of Definition 6.2, then

$$\nabla \cdot G(t, \widetilde{\phi}) \mu \nabla \widetilde{\phi} = G(t, \widetilde{\phi}) \,\mathrm{A}\,\phi + \nabla G(t, \widetilde{\phi}) \cdot \mu \nabla \widetilde{\phi} \tag{6.13}$$

is satisfied, which allows to rewrite (6.11) in the form (5.35).

6.4 Remark. If $\widetilde{\phi} = (\widetilde{\phi}_1, \widetilde{\phi}_2)$ is a solution of (5.35) in the sense of Definition 6.2, then

$$\operatorname{tr}\left(\widetilde{\phi}_k(t)\right)\big|_{\mathrm{D}} = \operatorname{tr}\left(\Phi_k(t)\right)\big|_{\mathrm{D}} = \phi_{\mathrm{D},k}(t), \quad k = 1, 2, \quad t \in [T_0, T].$$

The Neumann boundary condition

$$0 = \nu \cdot \mu_k \nabla \widetilde{\phi}_k(t)\big|_\Gamma = \nu \cdot \mu_k \nabla \Phi_k(t)\big|_\Gamma, \quad k = 1, 2, \quad t \in [T_0, T],$$

holds in the distributional sense, see Remark 3.9.

6.5 Proposition. (See [31].) *Let the Assumptions 3.8 and 6.1 be satisfied. For each* $\gamma \in \left]\frac{1}{2}+\frac{1}{q},1\right[$ *the initial value problem* (5.35) *with initial value* $\Phi^0 \in \mathrm{W}^{1,q}$ *has a unique local solution* ϕ *with respect to the complex interpolation spaces* $V \overset{\text{def}}{=} \left[\mathrm{L}^p,\mathcal{D}\right]_\gamma$.

We are now going to show that the mappings E, G, Y and Z satisfy Assumption 6.1. To that end we need the following preparatory lemma.

6.6 Lemma. *If* $\xi:\mathbb{R}\to\mathbb{R}$ *is continuously differentiable, then* ξ *induces a Nemyckii operator from* L^∞ *into itself which is boundedly Lipschitzian. If* $\xi:\mathbb{R}\to\mathbb{R}$ *is twice continuously differentiable, then it induces a Nemyckii operator from* $W^{1,q}$ *into itself which is boundedly Lipschitzian.*

The proof is straightforward. Recall that, according to Definition 3.4, q is fixed and larger than two.

6.7 Lemma. *Let the Assumptions 3.7, 3.13 and 3.16 be satisfied. Then the equation* (5.25) *defines mappings* $Q_k : [T_0,T_1]\times \mathrm{L}^\infty \to L^\infty$, $k=1,2$, *and the restriction of each* Q_k *to* $[T_0,T_1]\times \mathrm{W}^{1,q}$ *takes its values in* $W^{1,q}$. *Moreover, there is a number* $\eta \in]0,1]$ *and then for any bounded subset* $M\subset \mathrm{L}^\infty$ *a positive number* Q_M *exists such that for all* t, $\check{t}\in[T_0,T_1]$ *and all* ψ, $\check{\psi}\in M$:

$$\|Q_k(t,\psi)-Q_k(\check{t},\check{\psi})\|_{L^\infty} \le Q_M\big(|t-\check{t}|^\eta + \|\psi-\check{\psi}\|_{\mathrm{L}^\infty}\big), \quad k=1,2.$$

Analogously, for each bounded subset $M\subset \mathrm{W}^{1,q}$ *there is a positive number* Q_M *such that for all* t, $\check{t}\in[T_0,T_1]$ *and all* ψ, $\check{\psi}\in M$:

$$\|Q_k(t,\psi)-Q_k(\check{t},\check{\psi})\|_{W^{1,q}} \le Q_M\big(|t-\check{t}|^\eta + \|\psi-\check{\psi}\|_{\mathrm{W}^{1,q}}\big), \quad k=1,2.$$

The proof is obtained from Corollary 5.4.

6.8 Lemma. *Let the Assumptions 3.7, 3.13 and 3.16 be satisfied. If* $\xi:\mathbb{R}\to\mathbb{R}$ *is continuously differentiable, then* ξ *induces operators*

$$[T_0,T_1]\times \mathrm{L}^\infty \ni (t,\psi)\longmapsto \xi(Q_k(t,\psi))\in L^\infty, \quad k=1,2.$$

Moreover, there is a constant $\eta\in]0,1]$ *and for any bounded set* $M\subset \mathrm{L}^\infty$ *a constant* ξ_M *such that for all* t, $\check{t}\in[T_0,T_1]$ *and all* ψ, $\check{\psi}\in M$:

$$\|\xi\big(Q_k(t,\psi)\big)-\xi\big(Q_k(\check{t},\check{\psi})\big)\|_{L^\infty} \le \xi_M\big(|t-\check{t}|^\eta + \|\psi-\check{\psi}\|_{\mathrm{L}^\infty}\big), \quad k=1,2.$$

If ξ *is twice continuously differentiable, then the restriction of* $\xi\circ Q_k$ *to* $[T_0,T_1]\times \mathrm{W}^{1,q}$ *maps into* $W^{1,q}$, $k=1,2$. *Moreover, there is a number* $\eta\in]0,1]$ *and for any bounded subset* $M\subset \mathrm{W}^{1,q}$ *a constant* ξ_M *such that for all* t, $\check{t}\in[T_0,T_1]$ *and all* ψ, $\check{\psi}\in M$:

$$\|\xi\big(Q_k(t,\psi)\big)-\xi\big(Q_k(\check{t},\check{\psi})\big)\|_{W^{1,q}} \le \xi_M\big(|t-\check{t}|^\eta + \|\psi-\check{\psi}\|_{\mathrm{W}^{1,q}}\big), \quad k=1,2.$$

The proof follows from Lemma 6.6 and Lemma 6.7.

6.9 Lemma. *Let the Assumptions 3.7, 3.13 and 3.16 be satisfied. Then there is a number* $\eta \in]0,1]$ *such that the mappings* E *and* G *defined by* (5.28) *and* (5.34) *satisfy the conditions* (6.1), (6.5), (6.7), *and* (6.2), (6.6), (6.8), *respectively.*

Proof. The functions $\frac{1}{\mathcal{F}_k'}$ are continuously differentiable by Assumption 2.3. Consequently, by Lemma 6.8 the mappings $\widetilde{E}_k$, given by

$$[T_0, T_1] \times \mathrm{L}^\infty \ni (t, \psi) \longmapsto \frac{1}{\mathcal{F}_k'\big(Q_k(t,\psi)\big)} \in L^\infty, \quad k = 1, 2,$$

are well defined. Moreover, Lemma 6.8 provides a constant $\eta \in]0,1]$ such that for any bounded set $M \subset \mathrm{L}^\infty$ a constant C_M exists such that for all t, $\check{t} \in [T_0, T_1]$ and all ψ, $\check{\psi} \in M$:

$$\|\widetilde{E}_k(t,\psi) - \widetilde{E}_k(\check{t},\check{\psi})\|_{\mathrm{L}^\infty} \le C_M\big(|t-\check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{L}^\infty}\big), \quad k = 1, 2.$$

Since $\mathrm{W}^{1,q}$ embeds continuously into L^∞ for any bounded set $M \subset \mathrm{W}^{1,q}$ there is a constant, again named C_M, such that for all t, $\check{t} \in [T_0, T_1]$ and all ψ, $\check{\psi} \in M$:

$$\|\widetilde{E}_k(t,\psi) - \widetilde{E}_k(\check{t},\check{\psi})\|_{\mathrm{L}^\infty} \le C_M\big(|t-\check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}}\big), \quad k = 1, 2.$$

The identity $E_k = \frac{1}{\rho_k}\widetilde{E}_k$ and Assumption 2.1 now imply (6.1) and (6.7). According to Lemma 6.7 the sets

$$\{Q_k(t,\phi) \,:\, (t,\phi) \in [T_0, T_1] \times M\}, \quad k = 1, 2,$$

are bounded in L^∞. Since the derivative of the carrier distribution functions $\mathcal{F}_k$, $k = 1, 2$, are continuous and positive, (6.5) immediately follows.

Using the second assertion of Lemma 6.8 we verify (6.2), (6.6), and (6.8) in a similar manner. □

6.10 Lemma. *Let the Assumptions 3.7, 3.13, and 3.16 be satisfied. Then the mapping* Z *given by* (5.27) *defines a family* $\{Z(t,\psi)\}_{(t,\psi)\in[T_0,T_1]\times \mathrm{W}^{1,q}}$ *of linear, compact operators* $Z(t,\phi) : \mathrm{L}^p \to \mathrm{L}^p$*. Additionally, there is a Hölder exponent* $\eta \in]0,1]$ *and constants* Z_M *such that* (6.3) *and* (6.9) *are satisfied.*

Proof. It suffices to show the analogous assertions for the entries of the operator matrices $Z(t,\psi)$. Firstly, Lemma 6.8 gives us the estimate

$$\begin{aligned}\|\mathcal{F}_k'\big(Q_k(t,\psi)\big) &- \mathcal{F}_k'\big(Q_k(\check{t},\check{\psi})\big)\|_{\mathcal{B}(L^p)} \\ &\le \|\mathcal{F}_k'\big(Q_k(t,\psi)\big) - \mathcal{F}_k'\big(Q_k(\check{t},\check{\psi})\big)\|_{L^\infty} \\ &\le C_M\big(|t-\check{t}|^\eta + \|\psi-\check{\psi}\|_{\mathrm{W}^{1,q}}\big), \quad k = 1, 2,\end{aligned}$$

where the constant C_M can be taken uniformly with respect to t, $\check{t} \in [T_0, T_1]$ and ψ, $\check{\psi}$ from any bounded set $M \subset \mathrm{W}^{1,q}$. This estimate together with Assumption 2.1 implies (6.9). As ${}_{\downarrow}\mathcal{P}_0^{-1\uparrow}$ is a linear and even compact operator from L^p into itself, this gives (6.3). ☐

6.11 Lemma. *Let the Assumptions 3.6, 3.7, 3.13, and 3.16 be satisfied. Then the mapping Y defined by* (5.30) *meets the conditions* (6.4) *and* (6.10).

Proof. At first one deduces from the assumptions and Corollary 5.4 that (5.29) defines a mapping $R : [T_0, T_1] \times \mathrm{W}^{1,q} \to \mathrm{L}^p$ for which there is a Hölder exponent $\eta \in]0, 1]$. Moreover, for any bounded set $M \subset \mathrm{W}^{1,q}$ exists a constant C_M such that for all t, $\check{t} \in [T_0, T_1]$ and all ψ, $\check{\psi} \in M$:

$$\|R(t, \psi) - R(\check{t}, \check{\psi})\|_{\mathrm{L}^p} \leq C_M\big(|t - \check{t}|^\eta + \|\psi - \check{\psi}\|_{\mathrm{W}^{1,q}}\big).$$

Applying Lemma 6.9 and Lemma 6.10 one obtains (6.4) and (6.10) for the mapping

$$[T_0, T_1] \times \mathrm{W}^{1,q} \ni (t, \psi) \longmapsto \big[I + Z(t, \psi)\big]E(t, \psi)R(t, \psi).$$

The addends b_k' and ${}_{\downarrow}\varphi_\circ'$ of (5.31) have the required properties due to Assumption 3.7 and Assumption 3.13, respectively. For $\mathcal{P}_0^{-1}d'$ they follow from Assumption 3.13 (see also Remark 3.15), Assumption 3.16 and the fact that $\mathcal{P}_0$ is an isomorphism from $\widehat{W}^{1,q}_{\widehat{\Gamma}}$ onto $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$. The addend $\frac{\rho_k'(t)}{\rho_k(t)} \frac{\mathcal{F}_k(Q_k(t,\psi))}{\mathcal{F}_k'(Q_k(t,\psi))}$ of (5.31) can be treated by means of Lemma 6.8 and Assumption 2.1. ☐

We are now going to establish existence and uniqueness of a local solution to the evolution equation (5.35).

6.12 Theorem. *Under the Assumptions 3.6, 3.7, 3.8, 3.11, 3.13 and 3.16 the quasi-linear parabolic equation* (5.35) *with the initial condition $\widetilde{\phi}(T_0) = \Phi^0$ admits a unique local solution in the sense of Definition 6.2 with respect to the interpolation space $V = [\mathrm{L}^p, \mathcal{D}]_\theta$.*

Proof. According to the Lemmas 6.9, 6.10, 6.11 the mappings E, G, Z, and Y, defined by (5.28), (5.34), (5.27), and (5.30), respectively, fulfill Assumption 6.1. Hence, the result follows from Proposition 6.5, see also Remarks 6.3 and 6.4. ☐

7 Main result

We are going to show that a solution of the evolution equation (5.35) in the sense of Definition 6.2 provides a solution of the van Roosbroeck system in the sense of Definition 4.1.

We start with a technical lemma.

7.1 Lemma. *Let $\xi : \mathbb{R} \to \mathbb{R}$ be twice continuously differentiable. The composition $\xi \circ \psi$ is from $C([T_0, T], L^\infty)$, if $\psi \in C([T_0, T], L^\infty)$. If ψ composed with the embedding $L^\infty \hookrightarrow L^p$, $p \geq 1$, is continuously differentiable in L^p on $]T_0, T[$, then $\xi \circ \psi$ composed with the same embedding is continuously differentiable in L^p on $]T_0, T[$ and its derivative is given by*

$$\frac{d\xi \circ \psi}{dt}(t) = \xi'\big(\psi(t)\big)\psi'(t) \in L^p, \quad t \in]T_0, T[.$$

Proof. If $h_1,\ h_2 \in L^\infty$, then, by Lemma 5.1 — see also Assumption 2.3, we may write

$$\xi(h_1) - \xi(h_2) = \xi'(h_1)(h_1 - h_2) + T(h_1, h_2)((h_1 - h_2)$$

where $T(h_1, h_2)$ converges to zero in L^∞ if $h_1 \in L^\infty$ is fixed and h_2 approaches h_1 in the L^∞-norm. Now we set $h_1 = \psi(t)$ and $h_2 = \psi(\check{t})$ and divide both sides by $t - \check{t}$. In the limit $\check{t} \to t$ there is $\lim_{\check{t} \to t} T(\psi(t), \psi(\check{t})) = 0$ in L^∞, while $\lim_{\check{t} \to t} \frac{\psi(t) - \psi(\check{t})}{t - \check{t}} = \psi'(t)$ in L^p by supposition. □

Our next aim is to justify formula (5.23).

7.2 Lemma. *Let the Assumptions 3.7, 3.8, 3.13, and 3.16 be satisfied and assume that $\widetilde{\phi}$ is a solution of (5.35). We define*

$$z \stackrel{\text{def}}{=} (z_1, z_2) \quad \textit{with} \quad z_k(t) \stackrel{\text{def}}{=} \widetilde{\phi}_k(t) + b_k(t) + (-1)^k{}_{\downarrow}\varphi_\circ(t), \quad k = 1, 2,\ t \in [T_0, T], \tag{7.1}$$

and $\varphi(t) \stackrel{\text{def}}{=} \mathcal{L}\big(d(t), z(t)\big)$. Then $Q_k(t, \widetilde{\phi}(t)) = z_k(t) + (-1)^k{}_{\downarrow}\varphi(t)$, and the functions

$$[T_0, T] \ni t \longmapsto G_k(t, \widetilde{\phi}(t)) = \mathcal{G}_k\big(Q_k(t, \widetilde{\phi}(t))\big) \in L^\infty,$$

and

$$[T_0, T] \ni t \longmapsto u_k(t) \stackrel{\text{def}}{=} \rho_k(t)\mathcal{F}_k\big(Q_k(t, \widetilde{\phi}(t))\big) \in L^\infty$$

are continuous and concatenated with the embedding $L^\infty \hookrightarrow L^p$ they are continuously differentiable on $]T_0, T[$. The time derivative of u_k is given by

$$\begin{aligned} u_k'(t) = {} & \rho_k'(t)\mathcal{F}_k\big(Q_k(t, \widetilde{\phi}(t))\big) \\ & + \rho_k(t)\mathcal{F}_k'\big(Q_k(t, \widetilde{\phi}(t))\big)\big[\widetilde{\phi}_k'(t) + b_k'(t) + (-1)^k{}_{\downarrow}\varphi_\circ'(t) + (-1)^k{}_{\downarrow}\varphi'(t)\big] \end{aligned} \tag{7.2}$$

$k = 1, 2,\ t \in]T_0, T]$.

Proof. Due to Assumption 3.8 and Definition 6.2 the function $\widetilde{\phi}$ belongs to the space

$$C([T_0, T], \mathrm{L}^\infty) \cap C^1(]T_0, T[, \mathrm{L}^p) \tag{7.3}$$

see also Remark 3.12. Hence, the Assumptions 3.7 and 3.13 ensure that the function z also belongs to this space, and by Corollary 5.4, so does the function $\varphi = \mathcal{L}\big(d(t), z(t)\big)$. Thus, we may apply Lemma 7.1. □

7.3 Remark. Lemma 7.2 justifies the formal manipulations in §5.2. First, (5.23) is given a strict sense. Furthermore, the differentiation of Poisson's equation (5.19) has the following precise meaning: since $\widetilde{\phi}$ is from the space (7.3), the function $t \mapsto \varphi(t)$ is differentiable — even in a much 'better' space than $\widetilde{\phi}$ — see Corollary 5.4. Hence, the right hand side of (4.4) is differentiable with respect to time in the space $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$ and (5.19) is an equation in the space $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$.

We come now to the main results of this paper.

7.4 Theorem. *Under the Assumptions 3.6, 3.7, 3.8, 3.11, 3.13, and 3.16 van Roosbroeck's system with initial condition $\widetilde{\phi}(T_0) = \Phi^0 \in \mathrm{W}^{1,q}$ admits a unique local in time solution in the sense of Definition 4.1.*

Proof. By Theorem 6.12 the auxiliary evolution equation (5.35) admits — in the sense of Definition 6.2 — a unique local solution $\widetilde{\phi}$ satisfying the initial condition $\widetilde{\phi}(T_0) = \Phi^0$. Let us show that — in the sense of Definition 4.1 — the pair $\{\widetilde{\varphi}, \widetilde{\phi}\}$, with $\widetilde{\varphi}$ given by

$$\widetilde{\varphi}(t) \stackrel{\text{def}}{=} \varphi_\circ(t) + \mathcal{L}\big(d(t), z(t)\big), \quad t \in [T_0, T], \tag{7.4}$$

and z according to (7.1), is a local solution of van Roosbroeck's system. First, (4.3) is identical with (6.12). By the embedding $V \hookrightarrow \mathrm{W}^{1,q}_\Gamma \hookrightarrow \mathrm{L}^\infty$ (see Remark 3.12) the function $[T_0, T] \ni t \mapsto \phi(t) \in \mathrm{L}^\infty$ is continuous, and so is the function $[T_0, T] \ni t \mapsto \Phi(t) \in \mathrm{L}^\infty$ in view of Assumption 3.8. Thus, $\widetilde{\phi} \in C([T_0, T], \mathrm{L}^\infty) \cap C^1(]T_0, T[, \mathrm{L}^p)$. Moreover, for z, see (7.1), one obtains from the Assumptions 3.7 and 3.13 that $z \in C([T_0, T], \mathrm{L}^\infty) \cap C^1(]T_0, T[, \mathrm{L}^p)$. Consequently, property (4.2) follows by Corollary 5.4, while (4.9) results from Lemma 7.2. The Poisson equation (4.4) with densities (4.6) is obviously satisfied by (7.4) due to the definition of $\mathcal{L}$. (4.10) follows from $\nabla\widetilde{\phi}_k \in C(]T_0, T], \mathrm{L}^q)$, $k = 1, 2$, and Lemma 7.2. (4.11) is implied by (6.12) and (6.13). It remains to show that the continuity equations (4.5) are satisfied. For this, one first notes the relations

$$Q_k(t, \widetilde{\phi}(t)) = \widetilde{\phi}_k(t) + (-1)^k{}_\downarrow\widetilde{\varphi}(t) + b_k(t) = z_k(t) + (-1)^k{}_\downarrow\varphi(t), \quad k = 1, 2, \tag{7.5}$$

and

$$R(t, \widetilde{\phi}(t)) = \begin{pmatrix} r_1(t, \widetilde{\varphi}(t), \widetilde{\phi}(t)) \\ r_2(t, \widetilde{\varphi}(t), \widetilde{\phi}(t)) \end{pmatrix}, \tag{7.6}$$

which follows from the definitions (5.25) and (5.29) of R and Q, and (7.1), (7.4). Further, in Assumption 3.6 we demand that the mappings r_k, $k = 1, 2$, take their values in L^p — consequently, R takes its values in L^p. From (7.2) and (5.28) one gets

$$E_k(t, \widetilde{\phi}(t))u_k'(t) = \widetilde{\phi}_k'(t) + b_k'(t) + (-1)^k{}_\downarrow\widetilde{\varphi}'(t) + \frac{\rho_k'(t)}{\rho_k(t)} \frac{\mathcal{F}_k(Q_k(t, \widetilde{\phi}(t)))}{\mathcal{F}_k'(Q_k(t, \widetilde{\phi}(t)))},$$

and by means of the evolution equation (5.35) we obtain

$$E(t,\widetilde{\phi}(t))u'(t) = \big[I + Z(t,\widetilde{\phi}(t))\big]E(t,\widetilde{\phi}(t))\nabla\cdot G(t,\widetilde{\phi}(t))\mu\nabla\widetilde{\phi}(t) + \big[I + Z(t,\widetilde{\phi}(t))\big]E(t,\widetilde{\phi}(t))R(t,\widetilde{\phi}(t)) + \left(\begin{smallmatrix} {}_\downarrow\mathcal{P}_0^{-1}d'(t) - {}_\downarrow\varphi'(t) \\ {}_\downarrow\varphi'(t) - {}_\downarrow\mathcal{P}_0^{-1}d'(t)\end{smallmatrix}\right).$$

We now make use of the representation (4.7) of the currents $j = (j_1, j_2)$, and get

$$E(t,\widetilde{\phi}(t))\left[u'(t) - \nabla\cdot j(t) - R(t,\widetilde{\phi}(t))\right] = Z(t,\widetilde{\phi}(t))E(t,\widetilde{\phi}(t))\left[\nabla\cdot j(t) + R(t,\widetilde{\phi}(t))\right] + \left(\begin{smallmatrix} {}_\downarrow\mathcal{P}_0^{-1}d'(t) - {}_\downarrow\varphi'(t) \\ {}_\downarrow\varphi'(t) - {}_\downarrow\mathcal{P}_0^{-1}d'(t)\end{smallmatrix}\right).$$

We already know that the formal differentiation of Poisson's equation is justified, see Remark 7.3. Thus, (5.19) yields

$$E(t,\widetilde{\phi}(t))\left[u'(t) - \nabla\cdot j(t) - R(t,\widetilde{\phi}(t))\right] = Z(t,\widetilde{\phi}(t))E(t,\widetilde{\phi}(t))\left[\nabla\cdot j(t) + R(t,\widetilde{\phi}(t))\right] + \left(\begin{smallmatrix} {}_\downarrow\mathcal{P}_0^{-1\uparrow}(u_2'(t) - u_1'(t)) \\ {}_\downarrow\mathcal{P}_0^{-1\uparrow}(u_1'(t) - u_2'(t))\end{smallmatrix}\right),$$

and, observing (5.32) and (7.6), we get

$$\left[E(t,\widetilde{\phi}(t)) + \left(\begin{smallmatrix} {}_\downarrow\mathcal{P}_0^{-1\uparrow} & -{}_\downarrow\mathcal{P}_0^{-1\uparrow} \\ -{}_\downarrow\mathcal{P}_0^{-1\uparrow} & {}_\downarrow\mathcal{P}_0^{-1\uparrow}\end{smallmatrix}\right)\right]\left(\begin{smallmatrix} u_1'(t) - \nabla\cdot j_1(t) - r_1(t,\widetilde{\varphi}(t),\widetilde{\phi}(t)) \\ u_2'(t) - \nabla\cdot j_2(t) - r_2(t,\widetilde{\varphi}(t),\widetilde{\phi}(t))\end{smallmatrix}\right) = 0. \tag{7.7}$$

The operator on the left is continuous on L^p; we show now that its kernel is trivial. Let $f_1,\ f_2 \in L^p$ be such that

$$\left[E(t,\widetilde{\phi}(t)) + \left(\begin{smallmatrix} {}_\downarrow\mathcal{P}_0^{-1\uparrow} & -{}_\downarrow\mathcal{P}_0^{-1\uparrow} \\ -{}_\downarrow\mathcal{P}_0^{-1\uparrow} & {}_\downarrow\mathcal{P}_0^{-1\uparrow}\end{smallmatrix}\right)\right]\left(\begin{smallmatrix} f_1 \\ f_2\end{smallmatrix}\right) = 0.$$

This is equivalent to the relations

$$f_2 = -\tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}f_1 \quad\text{and}\quad {}_\downarrow\mathcal{P}_0^{-1\uparrow}\left(\left(1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}\right)f_1\right) = -E_1(t,\widetilde{\phi}(t))f_1.$$

$\mathcal{P}_0^{-1\uparrow}\big((1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))})f_1\big)$ is a continuous mapping from $W_\Gamma^{1,q}$ into $\widehat{L}^\infty$. Indeed, the embedding $\widehat{L}^p \hookrightarrow \widehat{W}_{\widehat{\Gamma}}^{-1,q}$ is continuous, and $\mathcal{P}_0$ is an isomorphism between $\widehat{W}_{\widehat{\Gamma}}^{1,q}$ and $\widehat{W}_{\widehat{\Gamma}}^{-1,q}$, see Proposition 3.3. Hence, we may multiply both sides with $f_1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}f_1$ and integrate over Ω; this yields

$$\int_\Omega {}_\downarrow\mathcal{P}_0^{-1\uparrow}\left(f_1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}f_1\right)\left(f_1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}f_1\right)\mathrm{d}x = \int_{\widehat{\Omega}} \mathcal{P}_0^{-1\uparrow}\left(f_1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}f_1\right)^{\uparrow}\left(f_1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}f_1\right)\mathrm{d}x = -\int_\Omega E_1(t,\widetilde{\phi}(t))\left(1 + \tfrac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}\right)f_1^2\,\mathrm{d}x \tag{7.8}$$

The quadratic form $\psi \mapsto \int_{\widehat{\Omega}} (\mathcal{P}_0^{-1}\psi)\psi \,\mathrm{d}x$ is non-negative on $\widehat{L}^2$ and extends by continuity to $\widehat{L}^p$, where it is also non-negative. On the other hand, the function $E_1(t,\widetilde{\phi}(t)) \left(1 + \frac{E_1(t,\widetilde{\phi}(t))}{E_2(t,\widetilde{\phi}(t))}\right)$ is almost everywhere on Ω strictly positive. Therefore, the right hand side of (7.8) can only be non-negative if f_1 is zero almost everywhere on Ω. Hence, (7.7) establishes the continuity equations (4.5).

To prove uniqueness of a solution of van Roosbroeck's system in the sense of Definition 4.1 one assures that any solution in the sense of Definition 4.1 procures a solution in the sense of Definition 6.2. Indeed this has been done on a formal stage by the reformulation of van Roosbroeck's system as a quasi-linear parabolic system in §5. In fact, all formal steps can be carried out in the underlying function spaces. We accomplish this in the sequel for the crucial points. (4.4) and (4.6) ensure, that φ is a solution of (5.4). Hence, Corollary 5.4 implies that φ indeed is continuously differentiable in $\widehat{W}^{1,q}_{\widehat{\Gamma}}$, and, consequently, (5.21) makes sense in $\widehat{W}^{-1,q}_{\widehat{\Gamma}}$. The derivation of (4.6), see also (4.8), is justified by Lemma 7.1. Thus, (5.23) holds in a strict sense. The division by $\rho_k \mathcal{F}_k'$ is allowed because both factors have (uniform) upper and lower bounds. The rest of the manipulations up to (5.35) is straight forward to justify. □

Next we want to establish the natural formulation of the balance laws in van Roosbroeck's system in integral form, see (1.1), which is one of the central goals of this paper. At first, one realizes that the boundary integral has to be understood in the distributional sense — as is well known from Navier-Stokes theory, see [45] — if one only knows that the current is a q–summable function and that its divergence is p–summable. More precisely, the following proposition holds.

7.5 Proposition. *Let $\omega \subset \mathbb{R}^2$ be any bounded Lipschitz domain. Assume $j : \omega \to \mathbb{R}^2$ to be from $L^q(\omega;\mathbb{R}^2)$ and let the divergence (in the sense of distributions) $\nabla \cdot j$ of j be p–integrable on ω. If $q > 2$ and $p = \frac{q}{2}$, then there is a uniquely determined linear continuous functional $j_\nu \in W^{-1+\frac{1}{q'},q}(\partial\omega)$ such that*

$$\int_\omega j \cdot \nabla\psi \,\mathrm{d}x + \int_\omega \psi \nabla \cdot j \,\mathrm{d}x = \langle j_\nu \,|\, \psi|_{\partial\omega} \rangle \quad \textit{for all } \psi \in W^{1,q'}(\omega), \tag{7.9}$$

where $\langle \cdot \,|\, \cdot \rangle$ on the right hand side denotes the duality between $W^{1-\frac{1}{q'},q'}(\partial\omega)$ and $W^{-1+\frac{1}{q'},q}(\partial\omega)$. If, in addition, the function j is continuously differentiable on ω and the partial derivatives have continuous extensions to $\overline{\omega}$, then

$$\int_\omega j \cdot \nabla\psi \,\mathrm{d}x + \int_\omega \psi \nabla \cdot j \,\mathrm{d}x = \int_{\partial\omega} \psi|_{\partial\omega} \nu \cdot j \,\mathrm{d}\sigma_\omega \quad \textit{for all } \psi \in W^{1,q'}(\omega),$$

where ν is the outer unit normal of $\partial\omega$, and σ_ω is the arc–measure on $\partial\omega$.

Proof. The first statement is a slight generalization, see [30, Lemma 2.4], of well known results from [45, Ch. 1]. The second assertion has been proved in [8, Ch. 5.8]. □

7.6 Theorem. *If $(\widetilde{\varphi}, \widetilde{\phi})$ is a solution of van Roosbroeck's system in the sense of Definition 4.1, and $\omega \subset \Omega$ is an open Lipschitz domain, then there are unique continuous functions $j_{k\nu} :]T_0, T] \to W^{-1+\frac{1}{q'},q}(\partial\omega)$, $k = 1, 2$, such that*

$$\frac{\partial}{\partial t} \int_\omega u_k(t)\,\mathrm{d}x = \langle j_{k\nu}(t) \,|\, 1\rangle + \int_\omega r_k(t, \widetilde{\varphi}(t), \widetilde{\phi}(t))\,\mathrm{d}x, \quad k = 1, 2, \tag{7.10}$$

where $\langle \cdot \,|\, \cdot \rangle$ again denotes the duality between $W^{1-\frac{1}{q'},q'}(\partial\omega)$ and $W^{-1+\frac{1}{q'},q}(\partial\omega)$.

Proof. From (4.5) we obtain for any open Lipschitz domain $\omega \subset \Omega$

$$\int_\omega u_k'(t) - \nabla \cdot j_k(t)\,\mathrm{d}x = \frac{\partial}{\partial t}\int_\omega u_k(t)\,\mathrm{d}x - \int_\omega \nabla \cdot j_k(t)\,\mathrm{d}x = \int_\omega r_k(t, \widetilde{\varphi}(t), \widetilde{\phi}(t))\,\mathrm{d}x,$$

where j_k is defined by (4.7). Using Proposition 7.5 we find for every $t \in]T_0, T]$ a unique element $j_{k\nu}(t) \in W^{-1+\frac{1}{q'},q}(\partial\omega)$ such that (7.10) holds. Moreover, continuity passes over from the functions (4.10) to the mappings $]T_0, T] \ni t \mapsto j_{k\nu}(t) \in W^{-1+\frac{1}{q'},q}(\partial\omega)$. □

If the currents $j_k(t)$ are continuously differentiable on ω and the partial derivatives have continuous extensions to $\overline{\omega}$, then by the second part of Proposition 7.5 the formula (7.10) takes the form (1.1).

8 Numerics

Theorem 7.6 is the basis for space discretization of drift–diffusion equations by means of the finite volume method (FVM). The FVM was adopted for the numerical solution of van Roosbroeck's equations by Gajewski, and this approach has been further investigated in [12, 10, 17, 9]. To discretise the spatial domain one uses a partition into simplex elements. Let $\mathcal{E}$ be the set of all edges $e_{il} = x_i - x_l$ of this triangulation, where x_1, x_2,... are the vertices. Moreover, we define the Voronoi cell assigned to a vertex x_i by

$$V_i \stackrel{\text{def}}{=} \{x \text{ in the spatial simulation domain, such that} \\ \|x - x_i\| \le \|x - x_l\| \quad \text{for all vertices } x_l \text{ of the triangulation}\},$$

where $\|\cdot\|$ refers to the norm in the spatial simulation space $\mathbb{R}^2$. Now, to get a space discrete version of the current–continuity equation, we specify (7.10) with $\omega = V_i$, and approximate $\langle j_{k\nu}(t) \,|\, 1\rangle$ piecewise by $j_{kil}\sigma(\partial V_i \cap \partial V_l)$, σ being the arc measure on the boundary of $\omega = V_i$. The intermediate value j_{kil} can be obtained as follows: The main hypothesis with respect to the discretization of the currents — due to Scharfetter and Gummel [49] — is that the electron and hole current density j_2 and j_1 are constant along simplex edges. This assumption allows to calculate j_{1il} and j_{2il} — the constant values on the edge e_{il} — in terms of the node values of the electrostatic potential and the particle densities, see for instance [17]. Thus, one ends up with the following FVM discretization of van Roosbroeck's system for all interior Voronoi cells V_i:

$$\varepsilon(x_i) \sum_{l\,:\,e_{il}\in\mathcal{E}} (\nabla\varphi)_{il}\sigma(\partial V_k \cap \partial V_l) = \Big(\tilde{d}(x_i) + u_1(x_i) - u_2(x_i)\Big)\,|V_i|,$$
$$\frac{\partial u_k}{\partial t}(x_i)|V_i| - j_{kil}\sigma(\partial V_i \cap \partial V_l) = r_k(t,\widetilde{\varphi},\widetilde{\phi}_1,\widetilde{\phi}_2)(x_i)|V_i|,$$

where $|V_i|$ is the volume of the Voronoi cells V_i. Here we have tested the Poisson equation also with the characteristic function 1_{V_i} of the Voronoi cell V_i, and we have applied Gauss' theorem. In view of Proposition 7.5 we assume, additional to Assumption 3.16, $\tilde{d} : [T_0, T_1] \to \widehat{L}^p$, and observe that $\varphi_\bullet$ can be choosen such that $\langle \varphi_\bullet \,|\, 1_{V_i}\rangle = 0$ for interior Voronoi cells V_i, see Remark 3.15. Again, we approximate the right hand side of (7.9) piecewise by $(\nabla\varphi)_{il}\sigma(\partial V_i \cap \partial V_l)$, and we assume — in consonance with the hypothesis about currents — that the gradient of the electrostatic potential is constant on the edges of the triangulation, that means $(\nabla\varphi)_{il} = (\varphi(x_i) - \varphi(x_l))/\|x_i - x_l\|$.

Usually, this finite volume discretization of space has been combined with implicit time discretization, see for instance [11]. Please note that the strong differentiability of the electron and hole density in time is constitutive for this approach.

9 Outlook to three spatial dimensions

Much of semiconductor device simulation relies on spatially two-dimensional models. However, with increasing complexity of electronic device design spatially three-dimensional simulations become ever more important, see for instance [17, 21, 20]. This raises the question which of the results for the two-dimensional case carry over to the three-dimensional case. In particular, can one expect that in three spatial dimensions the divergence of the currents belongs to a Lebesgue space, and is it possible to establish strong differentiability of the carrier densities under the rather weak assumptions about the reaction terms of this paper.

Conditio sine qua non for a modus operandi as in this paper is that in the three-dimensional case the operators

$$-\nabla \cdot \varepsilon \nabla : \widehat{W}^{1,q}_{\widehat{\Gamma}} \to \widehat{W}^{-1,q}_{\widehat{\Gamma}} \quad \text{and} \quad -\nabla \cdot \mu_k \nabla : W^{1,q}_{\Gamma} \to W^{-1,q}_{\Gamma}$$

provide isomorphisms for a summability index $q > 3$. Unfortunately, this is not so for arbitrary three-dimensional spatial domains, see [37]. However, one can proof such a result for certain classes of three-dimensional material structures and boundary conditions, see [7], for instance for layered media and Dirichlet boundary conditions. Dauge proved the result in [6] for the Dirichlet Laplacian on a convex polyhedron, provided the Dirichlet boundary part is separated from its complement by a finite union of line segments. It would be satisfactory to combine this conclusion with a heterogeneous material composition.

Under the hypothesis the afore mentioned isomorphisms exist there are results on quasilinear parabolic systems — analogous to Proposition 6.5 — see [43] and [29], such that one can obtain classical solutions of the spatially three-dimensional drift–diffusion equations very much in the same way as here in the two-dimensional case.

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