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EXISTENCE AND LOCAL UNIQUENESS FOR THE STOKES-NERNST-PLANCK-DRIFT-DIFFUSION-POISSON SYSTEM MODELING NANOPORE AND NANOWIRE SENSORS*

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Abstract. This work gives analytical results for a system of transport equations which is the underlying mathematical model for nanopore sensors and for all types of affinity-based nanowire sensors. This model consists of the Poisson equation for the electrostatic potential ensuring self-consistency and including interface conditions stemming from a homogenized boundary layer, the drift-diffusion equations describing the transport of charge carriers in the sensor, the Nernst-Planck equations describing the transport of ions, and the Stokes equations describing the flow of the background medium water. We present existence and local uniqueness theorems for this stationary, nonlinear, and fully coupled system. The existence proof is based on the Schauder fixed-point theorem and local uniqueness around equilibrium is obtained from the implicit-function theorem. The maximum principle is used to obtain a-priori estimates for the solution. Due to the multiscale problem inherent in affinity-based field-effect sensors, a homogenized equation for the potential with interface conditions at a surface is used.

Keywords. Stokes-Nernst-Planck-drift-diffusion-Poisson system; nanowire sensors; nanopore sensors; existence; local uniqueness.

AMS subject classifications. 82D80; 76R50; 35Q20; 82D37; 62P30.

1. Introduction

The objective of this work is to prove existence and local uniqueness of the solution of a system of partial differential equations that is fundamental for the mathematical modeling of field-effect sensors and for nanopore sensors in a self-consistent manner. We start with a short description of the applications covered by the system of equations in order to describe the physical system and to explain the root of the model equations.

Field-effect biosensors based on silicon nanowires have been realized in experiments in recent years [39, 40, 48], and field-effect gas sensors based on metal-oxide nanowires have been demonstrated as well [15, 26, 27]. The common working principle of these affinity-based sensors is that the target molecules to be detected change the charge concentration at the sensor surface, which in turn modulates the conductance of the semiconducting nanowire. The currents through the nanowires are recorded and indicate the amount of target molecules present.

A schematic diagram of a nanowire field-effect biosensor is shown in Figure 1.1. The main advantage of this type of affinity-based sensor compared to currently employed technology is its label-free operation; no fluorescent or radioactive markers are required. Further advantages are high sensitivity, real-time operation, and high selectivity. The concept is a very general one, since any DNA oligomers, RNA oligomers, and antigens with known antibodies can be detected. Therefore there is a wide range of applications including biomedicine, biotechnology, and the food and drug industries.

In the case of gas sensors, reducing or oxidizing gases react with the surface of the nanowire in reactions that are not yet fully understood. These reactions result in charge

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transfer from or to the surface of the nanowire. Again, this change in charge concentration modulates the current through the nanowire. Applications include the detection of toxic gases such as carbon monoxide and hydrogen sulfide, which are important, e.g., in environmental monitoring and process technology. Despite the experimental progress in recent years, the detection mechanisms are not completely understood and quantitative models are necessary in order to gain insight into the physical processes.

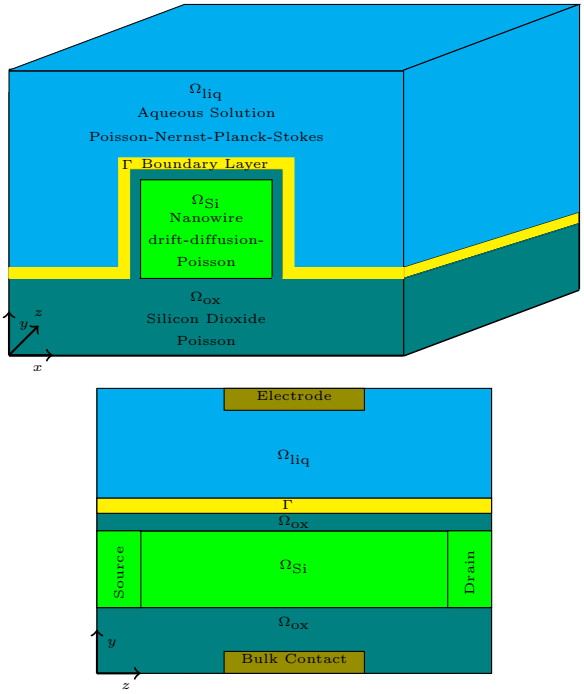

FIG. 1.1. *Schematic diagram of a nanowire field-effect sensor (top) and a z-y cross section (bottom), displaying the different subdomains as well as the source and drain contacts.*

The third application governed by the system of equations investigated here are nanopore sensors. The main application areas of nanopore sensors are DNA sequencing, protein sequencing, and single-molecule detection following the principle of a Coulter counter. Notable experimental progress towards the repeatable fabrication of well-defined nanopores has been made [7, 11–13, 17, 23, 24, 28–30, 33, 38, 45]. Overviews of this field can be found in [8, 25, 46].

A schematic diagram of a nanopore device is shown in Figure 1.2. The aqueous solution on both sides of the membrane with the nanopore contains anions and cations. An electric potential is applied across the membrane and results in ionic currents through the nanopore. The ionic currents are measured. When a target molecule translocates the nanopore, the ionic currents are reduced as in the detection mechanism of a Coulter counter. In order to quantify the on- and off-currents as well as the forces on the target molecules, it is therefore necessary to understand the transport of the ions and of the background medium, i.e., water.

Mathematical models relevant to the quantitative understanding of field-effect sensors have already been studied, e.g., in [1, 20, 22, 34, 47]. Mathematical problems stemming from the modeling and simulation of nanowire field-effect sensors have been solved

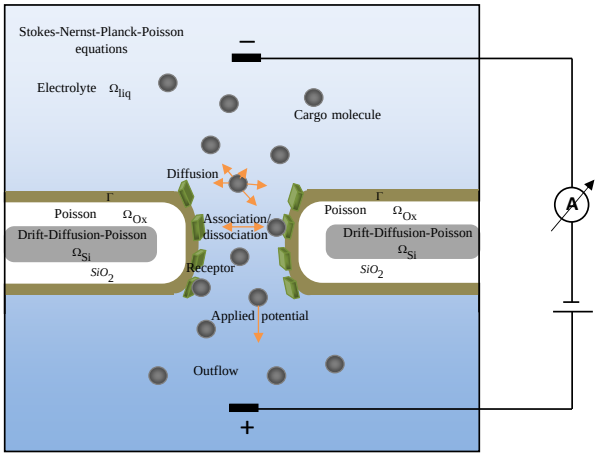

FIG. 1.2. *Schematic of a nanopore sensor with typical contacts for measuring currents. The ionic current between two compartments is measured in this manner.*

recently. The multiscale problem inherent to this sensor type was solved in [19], and existence and uniqueness for the stationary homogenized model, excluding the Stokes equation, was shown in [2]. A stochastic version of the multiscale problem was solved in [21]. A parallel numerical algorithm was developed in [3]. Based on these results, realistic nanowire biosensors were simulated and optimized [4, 5, 10, 35]. The surface reactions at gas sensors were investigated in [41–43], and noise and fluctuations due to surface processes were modeled and simulated in [44]. In the present work, we extend the drift-diffusion-Poisson system with interface conditions [2] stemming from homogenization [19] by a model for the liquid, i.e., the Stokes-Nernst-Planck equations.

The predominant model for nanopores is still the drift-diffusion-Poisson system, which does not take into account the flow of the background medium. The drift-diffusion-(Navier-)Stokes-Poisson system was theoretically investigated in [37]. The main difference to the present results is that the present ones are more general, holding for nanowire sensors and nanopores, and that they include interface conditions at material interfaces due to homogenized surface layers. The present results also include a third subdomain to cover realistic devices, and the uniqueness proofs here are based on the implicit-function theorem.

The rest of this paper is organized as follows. In Section 2, the model equations are described in detail. In Section 3, necessary assumptions are presented and weak solutions of the system are analyzed. In Section 4, our main results are presented and existence and local uniqueness of the weak solution are proved. Finally, the conclusions are drawn in Section 5.

2. The model equations

In this section, we present the system of equations which models nanoscale devices including nanowire and nanopore sensors. First, we describe the geometry of the devices including the subdomains, their equations, and the boundary conditions in each subdomain. Then the system of equations is summarized in the last subsection of this section.

2.1. The subdomains. We begin by describing the geometry of the devices (see Figures 1.1 and 1.2). The domain is $\Omega \subset \mathbb{R}^3$ and consists of three subdomains: the semiconductor (silicon) Ω_{Si}, the dielectric (silicon dioxide) Ω_{ox}, and the electrolyte Ω_{liq}.

These subdomains contain different types of charge carriers and have different physical properties, and hence they are governed by different equations. The Poisson equation for the electrostatic potential V provides self-consistency and is solved on the whole domain Ω. In the first subdomain Ω_{Si}, the drift-diffusion equations are used to model charge transport. In the second subdomain Ω_{ox}, there are no charge carriers, so that only the Poisson equation holds. In the third domain Ω_{liq} – the aqueous solution containing cations and anions – we consider an isothermal, incompressible, and viscous Newtonian fluid of uniform and homogeneous composition with cations and anions. In this subdomain, the Stokes-Nernst-Planck-Poisson system holds. (In the biological literature, it is customary to call the Fokker-Planck or drift-diffusion equations without recombination the Nernst-Planck equations.)

The boundary layer at the sensor surface is responsible for recognition of the analyte molecules and therefore of great importance. In the case of biosensors, solving a homogenization problem gives rise to two interface conditions for the Poisson equation [19]. These interface conditions depend on the surface-charge density and the dipole-moment density of the boundary layer. In the case of gas sensors, the model for the surface charge is a system of ODE that models surface reactions [14, 41]. Both of these surface models are included in the following and consequently the results hold for both bio- and gas sensors.

In the case of nanopores, there are charging effects of the surface. They result in a constant charge concentration at the manifold between Ω_{ox} and Ω_{liq}. Some nanopore sensors contain a recognition element (see Figure 1.2) that is also governed by the drift-diffusion equations.

Throughout the rest of the paper, we assume that the domain $\Omega \subset \mathbb{R}^3$ is bounded and convex. In summary, the domain $\Omega \subset \mathbb{R}^d$ is partitioned into three subdomains Ω_{Si}, Ω_{ox}, and Ω_{liq}, and the manifold Γ between Ω_{ox} and Ω_{liq} either in nanowire or nanopore sensors. The subdomains and corresponding equations are shown in Figures 1.1 and 1.2. Furthermore, Dirichlet boundary conditions are applied at the contacts, and no-flux (Neumann) conditions are used on the other boundaries.

2.2. The domain Ω_{Si} (semiconductor). The first subdomain Ω_{Si} consists of the nanowire, a semiconductor. Here the drift-diffusion-Poisson equations

$$-\nabla \cdot (A \nabla V) = C_{\mathrm{dop}} + p - n, \tag{2.1a}$$

$$\nabla \cdot J_n = R(n,p), \tag{2.1b}$$

$$\nabla \cdot J_p = -R(n,p), \tag{2.1c}$$

$$J_n = D_n \nabla n - \mu_n n \nabla V, \tag{2.1d}$$

$$J_p = -D_p \nabla p - \mu_p p \nabla V, \tag{2.1e}$$

are used to model the transport of electrons and holes, where V is the electrostatic potential, A is the permittivity, and C_{dop} is the doping concentration. The variables n and p are the concentrations of electrons and holes, respectively, J_n and J_p are their current densities, D_n and D_p are the diffusion coefficients, μ_n and μ_p are the mobilities of electrons and holes, and R is the recombination rate. We use the Shockley-Read-Hall recombination rate

$$R(n,p) := \frac{np - n_i^2}{\tau_p(n+n_i) + \tau_n(p+n_i)},$$

where n_i is the intrinsic charge density and τ_n and τ_p are the lifetimes of the free carriers. Under reasonable assumptions, the results here also hold for other choices of the recombination model.

Furthermore, we assume that the Einstein relations $D_n = U_T \mu_n$ and $D_p = U_T \mu_p$ hold, where U_T is the thermal voltage $U_T := k_B T/q$ with a value of $\approx 0.025V$ for silicon at room temperature ($q > 0$ is the elementary charge).

In the Slotboom variables u and v, which are defined by

$$n =: n_i e^{V/U_T} u, \tag{2.2a}$$

$$p =: n_i e^{-V/U_T} v, \tag{2.2b}$$

the recombination rate becomes

$$R := n_i \frac{uv-1}{\tau_p(e^{V/U_T}u+1)+\tau_n(e^{-V/U_T}v+1)}.$$

Then, using the Einstein relations, the system (2.1) becomes

$$\begin{aligned} -\nabla\cdot(A\nabla V) &= n_i(e^{-V/U_T}v - e^{V/U_T}u) + C_{\mathrm{dop}}, \\ U_T\nabla\cdot(\mu_n e^{V/U_T}\nabla u) &= \frac{uv-1}{\tau_p(e^{V/U_T}u+1)+\tau_n(e^{-V/U_T}v+1)}, \\ U_T\nabla\cdot(\mu_p e^{-V/U_T}\nabla v) &= \frac{uv-1}{\tau_p(e^{V/U_T}u+1)+\tau_n(e^{-V/U_T}v+1)}. \end{aligned}$$

The boundary $\partial\Omega$ is partitioned into Dirichlet and Neumann boundaries. The Dirichlet boundary conditions

$$V|_{\partial\Omega_D} = V_D, \quad u|_{\partial\Omega_{\mathrm{Si},D}} = u_D, \quad \text{and} \quad v|_{\partial\Omega_{\mathrm{Si},D}} = v_D \tag{2.3}$$

hold on the Dirichlet boundary $\partial\Omega_D$ and are chosen such that the Ohmic contacts are charge neutral.

To determine the potential and the concentrations on the boundary $\partial\Omega_{\mathrm{Si},D}$, we make these assumptions.

(1) The total space charge vanishes on $\partial\Omega_{\mathrm{Si,D}}$, i.e.,

$$p_D - n_D + C_{\mathrm{dop}} = 0. \tag{2.4}$$

(2) The densities are in equilibrium on $\partial\Omega_{\mathrm{Si,D}}$, i.e.,

$$p_D n_D = n_i^2. \tag{2.5}$$

(3) The boundary values for the potential are the combination of the built-in potential V_{bi} and the applied potential U, i.e.,

$$V_{\mathrm{Si,D}} = U(x) + V_{\mathrm{bi}}(x).$$

Clearly, in thermal equilibrium, we have $U = 0$. Furthermore, using (2.2), we define

$$u_D(x) = n_i^{-1} e^{-V_{\mathrm{bi}}(x)/U_T} n_D(x), \tag{2.6a}$$

$$v_D(x) = n_i^{-1} e^{V_{\mathrm{bi}}(x)/U_T} p_D(x), \tag{2.6b}$$

where

$$n_D(x) = \frac{1}{2}\left(C_{\mathrm{dop}}(x) + \sqrt{C_{\mathrm{dop}}^2(x) + 4n_i^2}\right),$$
$$p_D(x) = \frac{1}{2}\left(-C_{\mathrm{dop}}(x) + \sqrt{C_{\mathrm{dop}}^2(x) + 4n_i^2}\right).$$

These expressions can be found by substituting (2.5) into (2.4) so that charge neutrality at the contacts is ensured.
Therefore, the built-in potential is given by

$$V_{\mathrm{bi}}(x) = U_T \ln\left(\frac{n_D(x)}{n_i u_D(x)}\right) = U_T \ln\left(\frac{1}{u_D(x)}\left(\frac{C_{\mathrm{dop}}(x)}{2n_i} + \sqrt{\frac{C_{\mathrm{dop}}^2(x)}{4n_i^2} + 1}\right)\right)$$

using (2.6).

The zero Neumann conditions

$$\nabla V \cdot \mathbf{n} = 0, \qquad \nabla u \cdot \mathbf{n} = 0, \quad \text{and} \quad \nabla v \cdot \mathbf{n} = 0 \qquad \text{on } \partial\Omega_{\mathrm{Si},N}, \tag{2.7}$$

hold on the Neumann part $\partial\Omega_{N,\mathrm{Si}}$ of the boundary as well.

2.3. The surface (interface conditions). The fast varying spatial structure of the charge concentration in the boundary layer between the liquid and the surface gives rise to a multiscale problem, whose deterministic version was solved by homogenization [19]. For the sake of notational simplicity, we introduce a local coordinate system such that the normal vector of the manifold Γ, i.e., the interface between Ω_{liq} and Ω_{ox}, points in the positive x-direction and is located at $x = 0$. The rest of the coordinates are parallel to the interface and are denoted by y.

The main result in [19] states that the fast varying charge concentration at the manifold Γ can be replaced by two interface conditions that depend only on the slow variable. Even in the absence of a homogenization problem, the jump in the permittivity A gives rise to two continuity conditions because of physical reasons: The continuity of the potential and the continuity of the electric displacement field must hold. In summary, we can replace the fast oscillating charge in the boundary layer at the manifold Γ between Ω_{liq} and Ω_{ox} by the two interface conditions

$$V(0+,y) - V(0-,y) = \alpha(y), \tag{2.8a}$$
$$A(0+)\partial_x V(0+,y) - A(0-)\partial_x V(0-,y) = \gamma(y) \tag{2.8b}$$

after homogenization, where α and γ are given by the dipole-moment and the surface-charge densities of the boundary layer. The functions α and γ in the interface conditions are given by the microscopic models $M_\alpha(V)$ and $M_\gamma(V)$ for the dipole-moment density and the surface-charge density of the boundary layer as functions of the potential V. The microscopic models M_α and M_γ have been realized, e.g., by Metropolis Monte-Carlo simulations [10], by Poisson-Boltzmann calculations [18], and by systems of ordinary differential equations for surface reactions [14, 41].

As mentioned above, in [10] a Metropolis Monte-Carlo (MMC) algorithm was developed for the simulation of biomolecules and free ions in the constant-voltage ensemble. In this method, a simulation box is considered including an electrolyte and target (bio-)molecules fixed at the charged bottom of the box as well as free ions. A simulation in the MMC constant-voltage ensemble starts with a random state of the system, i.e., the

locations of all ions are random. A new state of the system is generated by randomly adding or deleting a pair of ions, changing the position of an ion while avoiding overlaps, and by transferring a random amount of charge between the walls. Then the potential energy is calculated for each state of the system. The interactions between all pairs of charge types, i.e., the ion-ion, the ion-biomolecule, the ion-plate, the biomolecule-plate, and the plate-plate interactions, are included in this calculation and the long-range contributions of the Coulomb forces are taken into account via integration over infinitely many periodically repeated cells. If the movement of a charge reduces the energy of the system, the new state is unconditionally accepted, while otherwise the movement is allowed only with a certain probability that depends exponentially on the energy difference. Finally, the surface-charge density γ and the dipole-moment density α are calculated as integrals over the charge concentration in the simulation cell [6].

2.4. The domain Ω_{ox} (oxide). In Ω_{ox}, there are no charges and the Poisson equation is simply

$$-\nabla\cdot(A\nabla V)=0.$$

No other equations are solved on Ω_{ox}.

2.5. The domain Ω_{liq} (liquid). In the domain Ω_{liq} of the liquid, we consider two types of charge carriers, namely positively and negatively charged ions, which are modeled by their number densities c^+ and c^-. In the remainder of the paper, the notation $c^\pm$ is used to refer to both of them simultaneously.

Their spatially inhomogeneous concentrations generate an electric field and an electric force in the liquid. An electroosmotic flow develops which, on the other hand, feeds back on the particles. This leads to a complicated interplay between electrophoretic movement and electroosmotic flow in a varying electric field. The drift-diffusion-Stokes-Poisson system models such phenomena in a self-consistent manner based on these three conservation laws.

- The electric field E satisfies Gauss's law with the moving particles as the free charge density. This couples the electric field to the number densities $c^\pm$ yielding the Poisson equation.
- The velocity field $\mathbf{u}$ of the fluid conserves mass and momentum (Stokes equations), which relates the liquid flux to the gradient of the pressure P. In the momentum balance, an electric body force enters, which couples the fluid flow to the electrostatic field and the number densities $c^\pm$.
- The evolution of the number densities $c^\pm$ of the charged particles are governed by transport equations such as the drift-diffusion or Nernst-Planck equations, which can be viewed as the mass-balance equations for the respective particle species. In the mass flux, a convective and an electric drift term are present. This couples the number densities $c^\pm$ to the fluid flow and the electric field.

The Poisson-Nernst-Planck part for our model equations are the system

$$-\nabla\cdot(A\nabla V)=c^+-c^-, \tag{2.9a}$$
$$-\nabla\cdot J^-=0, \tag{2.9b}$$
$$\nabla\cdot J^+=0, \tag{2.9c}$$
$$J^-=D^-\nabla c^--\mu^-c^-\nabla V-c^-\mathbf{u}, \tag{2.9d}$$
$$J^+=-D^+\nabla c^+-\mu^+c^+\nabla V+c^+\mathbf{u}, \tag{2.9e}$$

where A is the permittivity, V is the electrostatic potential, c^- and c^+ are the concentrations of anions and cations, respectively, D^- and D^+ are their diffusion coefficients, μ^- and μ^+ are their mobilities, and $\mathbf{u}$ is the velocity field of the liquid. The two terms $c^-\mathbf{u}$ and $c^+\mathbf{u}$ in (2.9d) and (2.9e) are nonstandard and provide the link to the Stokes equation.

The boundary conditions

$$c^\pm = c_D^\pm \quad \text{on } \partial\Omega_{D,\text{liq}} \qquad \text{and} \qquad J^\pm \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega_{N,\text{liq}} \tag{2.10}$$

hold, where $\mathbf{n}$ is the normal vector and

$$J^\pm := \mp D^\pm \nabla c^\pm - \mu^\pm c^\pm \nabla V \pm \mathbf{u} c^\pm \tag{2.11}$$

are the current densities.

The Stokes equations in the present model are

$$-\rho\Delta\mathbf{u} + \nabla P = -q(c^+ - c^-)\nabla V, \tag{2.12a}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{2.12b}$$

where ρ is the viscosity and P is the pressure of the liquid. The Stokes equations treat the liquid as an incompressible flow of a Newtonian fluid which flows slowly. Equation (2.12b) is the mass-continuity equation.

The Dirichlet boundary condition is the no-slip condition

$$\mathbf{u} = 0 \qquad \text{on } \partial\Omega_{D,\text{liq}} \tag{2.13}$$

on fluid-solid interfaces. This implies that the flow vanishes at the boundary. No boundary condition is given for P. Since both pairs $(\mathbf{u}, P)$ and $(\mathbf{u}, P + \text{const.})$ satisfy the Stokes Equations (2.12)–(2.13), P is determined only up to a constant by the Stokes Equations (2.12) and the boundary condition (2.13) [16].

2.6. The system of equations. In summary, the system of equations considered here are what we call the drift-diffusion-Nernst-Planck-Stokes-Poisson system with interface conditions, i.e., the drift-diffusion system (2.1) with the interface conditions (2.8), the Nernst-Planck system (2.9), and the Stokes Equations (2.12), all of which are coupled self-consistently by the Poisson equation. This system describes general nanowire sensors (see Figure 1.1) as well as general nanopore sensors (see Figure 1.2) even including transducers around the nanopore.

The model equations hence are the system

$$-\nabla\cdot(A\nabla V) = C_{\text{dop}} - n_i(e^{V/U_T}u - e^{-V/U_T}v) \qquad \forall x \in \Omega_{\text{Si}}, \tag{2.14a}$$

$$-\nabla\cdot(A\nabla V) = 0 \qquad \forall x \in \Omega_{\text{ox}}, \tag{2.14b}$$

$$-\nabla\cdot(A\nabla V) = c^+ - c^- \qquad \forall x \in \Omega_{\text{liq}}, \tag{2.14c}$$

$$-\rho\Delta\mathbf{u} + \nabla P = -(c^+ - c^-)\nabla V \qquad \forall x \in \Omega_{\text{liq}}, \tag{2.14d}$$

$$\nabla\cdot\mathbf{u} = 0 \qquad \forall x \in \Omega_{\text{liq}}, \tag{2.14e}$$

$$-\nabla\cdot(D^\pm\nabla c^\pm) \mp \mu^\pm\nabla\cdot(c^\pm\nabla V) + (\mathbf{u}\cdot\nabla)c^\pm = 0 \qquad \forall x \in \Omega_{\text{liq}}, \tag{2.14f}$$

$$U_T n_i \nabla\cdot(\mu_n e^{V/U_T}\nabla u) = n_i \frac{uv-1}{\tau_p(e^{V/U_T}u+1) + \tau_n(e^{-V/U_T}v+1)} \qquad \forall x \in \Omega_{\text{Si}}, \tag{2.14g}$$

$$U_T n_i \nabla\cdot(\mu_p e^{-V/U_T}\nabla v) = n_i \frac{uv-1}{\tau_p(e^{V/U_T}u+1) + \tau_n(e^{-V/U_T}v+1)} \qquad \forall x \in \Omega_{\text{Si}}, \tag{2.14h}$$

$$V(0+,y)-V(0-,y)=\alpha(y) \qquad \forall x\in\Gamma, \tag{2.14i}$$
$$A(0+)\partial_x V(0+,y)-A(0-)\partial_x V(0-,y)=\gamma(y) \qquad \forall x\in\Gamma, \tag{2.14j}$$
$$\alpha=M_\alpha(V) \qquad \forall x\in\Gamma, \tag{2.14k}$$
$$\gamma=M_\gamma(V) \qquad \forall x\in\Gamma, \tag{2.14l}$$
$$V=V_D \qquad \forall x\in\partial\Omega_D, \tag{2.14m}$$
$$\mathbf{n}\cdot\nabla V=0 \qquad \forall x\in\partial\Omega_N, \tag{2.14n}$$
$$u=u_D,\quad v=v_D \qquad \forall x\in\partial\Omega_{D,\mathrm{Si}}, \tag{2.14o}$$
$$\mathbf{n}\cdot\nabla u=0=\mathbf{n}\cdot\nabla v \qquad \forall x\in\partial\Omega_{N,\mathrm{Si}}, \tag{2.14p}$$
$$\mathbf{u}=0 \qquad \forall x\in\partial\Omega_{\mathrm{liq}}, \tag{2.14q}$$
$$c^\pm=c_D^\pm \qquad \forall x\in\partial\Omega_{D,\mathrm{liq}}, \tag{2.14r}$$
$$J^\pm\cdot\mathbf{n}=0 \qquad \forall x\in\partial\Omega_{N,\mathrm{liq}}. \tag{2.14s}$$

3. Assumptions and weak solutions

The coefficients and boundary conditions in (2.14) must satisfy the following assumptions.

Assumptions 3.1.

(1) *The bounded domain $\Omega\subset\mathbb{R}^3$ has a C^2 Dirichlet boundary $\partial\Omega_D$, where $|\partial\Omega_D|>0$. The Neumann boundary $\partial\Omega_N$, where $|\partial\Omega_N|>0$, consists of C^2 segments. The Lebesgue measure of the Dirichlet boundary $\partial\Omega_D$ is nonzero. The C^2-manifold $\Gamma\subset\Omega$ splits the domain Ω into two nonempty domains $\Omega^+=\Omega_{\mathrm{ox}}\cup\Omega_{\mathrm{Si}}$ and $\Omega^-=\Omega_{\mathrm{liq}}$ so that* $\mathrm{meas}(\Gamma\cap\partial\Omega)=0$ *and $\Gamma\cap\partial\Omega\subset\partial\Omega_N$ hold.*

(2) *The coefficient functions $A(x)$, $\mu_n(x)$, and $\mu_p(x)$ are uniformly elliptic and bounded functions of position x with the properties that*

$$0<A^-\le\operatorname{essinf}_{x\in\Omega}A(x)\le\|A(x)\|_{L^\infty(\Omega)}\le A^+<\infty \quad \text{a.e. in } \Omega$$

and

$$0<\mu_n^-\le\mu_n(x)\le\mu_n^+<\infty,$$
$$0<\mu_p^-\le\mu_p(x)\le\mu_p^+<\infty$$

a.e. in Ω_{Si}. Furthermore, $A(x)|_{\Omega^+}\in C^1(\Omega^+,\mathbb{R}^{3\times3})$, $A(x)|_{\Omega^-}\in C^1(\Omega^-,\mathbb{R}^{3\times3})$, and $\mu_p(x),\mu_n(x)\in C^1(\Omega_{\mathrm{Si}},\mathbb{R}^{3\times3})$ hold. For the data, the inclusions $f(x)\in L^\infty(\Omega)$, $V_D(x)\in H^{1/2}(\partial\Omega)\cap L^\infty(\Gamma)$, $c_D^\pm(x)\in H^{1/2}(\partial\Omega_{\mathrm{liq}})$ and $u_D,v_D(x)\in H^{1/2}(\partial\Omega_{\mathrm{Si}})$ hold. Similar assumptions hold for coefficients in Ω_{liq}: the coefficients ρ, μ^+ and μ^- are uniformly elliptic and bounded.

(3) *The doping concentration $C_{\mathrm{dop}}(x)$ is bounded above and below and we define*

$$\underline{C}:=\inf_{x\in\Omega}C_{\mathrm{dop}}(x)\le C(x)\le\sup_{x\in\Omega}C_{\mathrm{dop}}(x)=:\overline{C}.$$

(4) *There are constants $K\ge1$, C^+, and C^- in $\mathbb{R}^+$ satisfying*

$$\frac{1}{K}\le u_D(x)\le K \qquad \forall x\in\partial\Omega_{\mathrm{Si},D},$$
$$\frac{1}{K}\le v_D(x)\le K \qquad \forall x\in\partial\Omega_{\mathrm{Si},D},$$
$$C^-\le c_D^+(x)\le C^+ \qquad \forall x\in\partial\Omega_{\mathrm{liq},D},$$
$$C^-\le c_D^-(x)\le C^+ \qquad \forall x\in\partial\Omega_{\mathrm{liq},D}.$$

(5) *The microscopic models M_α and M_γ depend continuously in $H^1(\Omega)$ on the potential $V(x)$. For every potential $V(x)$ in $H^1(\Omega)\cap L^\infty(\Omega)$, the inclusions $\alpha(y)=M_\alpha(V(y))\in H^{1/2}(\Gamma)\cap L^\infty(\Gamma)$ and $\gamma(y)=M_\gamma(V(y))\in L^\infty(\Gamma)$ hold.*

To write the weak formulation of the boundary-value problem (2.14), we consider the more general form

$$-\nabla\cdot(A^*(x)\nabla w)+g(x,w)=f \qquad \forall x\in\Omega\setminus\Gamma, \tag{3.1a}$$
$$w=w_D \qquad \forall x\in\partial\Omega_D, \tag{3.1b}$$
$$\mathbf{n}\cdot\nabla w=0 \qquad \forall x\in\partial\Omega_N, \tag{3.1c}$$
$$w(0+,y)-w(0-,y)=\alpha(y) \qquad \forall x\in\Gamma, \tag{3.1d}$$
$$A^*(0+)\partial_x w(0+,y)-A^*(0-)\partial_x w(0-,y)=\gamma(y) \qquad \forall x\in\Gamma. \tag{3.1e}$$

The system (3.1) is a generalization of the Poisson equation with interface conditions. Here (3.1a) includes (2.14a)–(2.14c) if A^* and w are replaced by the permittivity A and potential V, respectively, and it includes (2.14g) and (2.14h) if A^* and w are replaced by $\mu_n e^{V/UT}$ and u, or $\mu_p e^{-V/UT}$ and v, respectively. Uniform ellipticity holds in each of these cases per Assumptions 3.1. In both cases, g and f denote the nonlinear and linear zero-order terms in these equations.

In order to give the weak formulations and to define weak solutions, we introduce the underlying function spaces. We suppose $1\le p\le\infty$ and denote the standard Lebesgue spaces for $\mathbb{R}^d$-valued functions by $L^p(\Omega;\mathbb{R}^d)$, in particular $L^p(\Omega):=L^p(\Omega;\mathbb{R})$ and the standard Sobolev space by $W^{1,p}(\Omega;\mathbb{R}^d)$, in particular $H^1(\Omega;\mathbb{R}^d):=W^{1,2}(\Omega;\mathbb{R}^d)$. Moreover $W^{1,p}(\Omega):=W^{1,p}(\Omega;\mathbb{R})$, in particular $H^1(\Omega):=W^{1,2}(\Omega;\mathbb{R})$. We use the Hilbert space $H^1_0(\Omega):=W^{1,2}_0(\Omega)$, where the subscript 0 denotes functions with vanishing traces. We define the Hilbert space

$$H^1_g(\Omega):=\{w\in H^1(\Omega)\,|\,Tw=g\} \tag{3.2}$$

as the solution space of admissible V, u, v, c^+, and c^-. The trace operator T is well-defined and continuous from $H^1(\Omega)$ onto $H^{1/2}(\partial\Omega)$ for the Lipschitz domain Ω. It is defined such that $Tw=g$, where g is Dirichlet lift of $w_D:=w|_{\partial\Omega_D}$. If g vanishes everywhere, we obtain the test space

$$H^1_0(\Omega)=\{w\in H^1(\Omega)\,|\,Tw=0\}. \tag{3.3}$$

We additionally define

$$H^1_{\mathrm{div},0}(\Omega;\mathbb{R}^3):=\left\{w\in L^2(\Omega;\mathbb{R}^3)\,|\,\nabla\cdot w\in L^2(\Omega)\wedge u\cdot\mathbf{n}=0 \text{ on } \partial\Omega\right\}$$

as the solution space of admissible velocity, and

$$L^2_0(\Omega):=\{w\in L^2(\Omega)\,|\,\textstyle\int_\Omega w=0\}$$

as the test spaces of admissible pressures. Vanishing averages are enforced in order to make the solution unique. Multiplying the Equations (3.1) by a test function $\phi_1\in H^1_0(\Omega)$ and integrating by parts, we obtain the weak formulation

$$a_1(w,\phi_1)=\ell_1(\phi_1) \qquad \forall\phi_1\in H^1_0(\Omega), \tag{3.4}$$

where the bilinear form $a_1(\cdot,\cdot)\colon H^1_g(\Omega)\times H^1_0(\Omega)\to\mathbb{R}$ and the functional $\ell_1(\cdot)\colon H^1_0(\Omega)\to\mathbb{R}$ are defined by

$$a_1(w,\phi_1):=\int_\Omega A^*\nabla w\cdot\nabla\phi_1+\int_\Omega g(w)\phi_1$$

and

$$\ell_1(\phi_1) := \int_\Omega f\phi_1 + \int_\Gamma \gamma\phi_1.$$

For $w := V \in H^1_{V_D}(\Omega)$ we recover the Poisson equation and for $w := u \in H^1_{u_D}(\Omega_{\mathrm{Si}})$ or $w := v \in H^1_{v_D}(\Omega_{\mathrm{Si}})$ with $\gamma = 0$, we recover the transport equations.

To find the weak formulation of the Stokes equations

$$-\rho\Delta\mathbf{u} + \nabla P = -q(c^+ - c^-)\nabla V \qquad \forall x \in \Omega_{\mathrm{liq}}, \tag{3.5a}$$
$$\nabla\cdot\mathbf{u} = 0 \qquad \forall x \in \Omega_{\mathrm{liq}}, \tag{3.5b}$$
$$\mathbf{u} = 0 \qquad \forall x \in \partial\Omega_{D,\mathrm{liq}} \tag{3.5c}$$

and the Nernst-Planck equations

$$-\nabla\cdot(D^\pm\nabla c^\pm) \mp \mu^\pm\nabla\cdot(c^\pm\nabla V) + (\mathbf{u}\cdot\nabla)c^\pm = 0 \qquad \forall x \in \Omega_{\mathrm{liq}}, \tag{3.6a}$$
$$c^\pm = c^\pm_D \qquad \forall x \in \partial\Omega_{D,\mathrm{liq}}, \tag{3.6b}$$
$$J^\pm\cdot\mathbf{n} = 0 \qquad \forall x \in \partial\Omega_{N,\mathrm{liq}}, \tag{3.6c}$$

we multiply the Equations (3.5a) and (3.5b) by test functions $\mathbf{v} \in H^1_{\mathrm{div},0}(\Omega;\mathbb{R}^3) =: X$ and $Q \in L^2_0(\Omega) =: Z$, respectively to obtain

$$a(\mathbf{u},\mathbf{v}) + b(P,\mathbf{v}) = \ell(\mathbf{v}) \qquad \forall \mathbf{v} \in X, \tag{3.7a}$$
$$b(Q,\mathbf{u}) = 0 \qquad \forall Q \in Z, \tag{3.7b}$$

which is a mixed problem. The two bilinear forms $a\colon X\times X\to\mathbb{R}$ and $b\colon Z\times X\to\mathbb{R}$ and the functional $\ell(\cdot)\colon X\to\mathbb{R}$ are defined by

$$a(\mathbf{u},\mathbf{v}) := \int_\Omega \rho\nabla\mathbf{u} : \nabla\mathbf{v},$$
$$b(z,\mathbf{w}) := -\int_\Omega \mathrm{div}\mathbf{w}\, z,$$

and

$$\ell(\mathbf{v}) := \int_\Omega \mathbf{f}_s\mathbf{v}$$

with $\mathbf{f}_s := -q(c^+ - c^-)\nabla V$ for $\mathbf{u} \in X$ and $P \in Z$.

Furthermore, multiplying (3.6a) by a test function $\phi_2 \in H^1_0(\Omega)$, we introduce the bilinear form $a_2\colon H^1_{c^\pm_D}(\Omega)\times H^1_0(\Omega)\to\mathbb{R}$ and the functional $\ell_2\colon H^1_0(\Omega)\to\mathbb{R}$ and to find the weak formulation

$$a_2(c^\pm,\phi_2) = \ell_2(\phi_2) \qquad \forall \phi_2 \in H^1_0(\Omega), \tag{3.8}$$

where

$$a_2(c^\pm,\phi_2) := \int_\Omega D^\pm\nabla c^\pm\cdot\nabla\phi_2 \pm \int_\Omega \mu^\pm c^\pm\nabla V\cdot\nabla\phi_2,$$
$$\ell_2(\phi_2) := 0$$

for $c^\pm \in H^1_{c^\pm_D}(\Omega)$.

We can now define the notion of a weak solution of system (2.14).

DEFINITION 3.1 (Weak solution of system (2.14)). *The vector* $(V,u,v,\mathbf{u},P,c^+,c^-,\alpha,\gamma)$ *is a weak solution of the drift-diffusion-Nernst-Planck-Stokes-Poisson system* (2.14) *if it satisfies the following conditions.*

(i) $V(x)\in L^\infty(\Omega)\cap H^1_{V_D}(\Omega)$ *and* $u(x),v(x)\in L^\infty(\Omega)\cap H^1_{u_D,v_D}(\Omega)$ *solve* (3.4) *for all* $\phi_1\in H^1_0(\Omega)$.
$\mathbf{u}(x)\in H^1_{\mathrm{div},0}(\Omega;\mathbb{R}^d)\cap L^\infty(\Omega;\mathbb{R}^d)$ *and* $P\in L^2_0(\Omega)$ *solve* (3.7a) *and* (3.7b) *for all* $\mathbf{v}\in H^1_{\mathrm{div},0}(\Omega;\mathbb{R}^d)$ *and* $Q\in L^2_0(\Omega)$, *respectively.*
$c^\pm(x)\in L^\infty(\Omega)\cap H^1_{c_D^\pm}(\Omega)$ *solves* (3.8) *for all* $\phi_2\in H^1_0(\Omega)$.
Moreover, $\alpha(x)\in L^\infty(\Gamma)\cap H^{1/2}(\Gamma)$ *and* $\gamma(x)\in L^2(\Gamma)$ *satisfy* (3.4).

(ii) The boundary conditions

$$\begin{aligned}
&V=V_D && \forall x\in\partial\Omega_D,\\
&u=u_D && \forall x\in\partial\Omega_{D,\mathrm{Si}},\\
&v=v_D && \forall x\in\partial\Omega_{D,\mathrm{Si}},\\
&\mathbf{u}=0 && \forall x\in\partial\Omega_{D,\mathrm{liq}},\\
&c^\pm=c_D^\pm && \forall x\in\partial\Omega_{D,\mathrm{liq}},\\
&J^\pm\cdot\mathbf{n}=0 && \forall x\in\partial\Omega_{N,\mathrm{liq}},\\
&\mathbf{n}\cdot\nabla V=0 && \forall x\in\partial\Omega_N,\\
&\mathbf{n}\cdot\nabla u=0=\mathbf{n}\cdot\nabla v && \forall x\in\partial\Omega_{N,\mathrm{Si}}
\end{aligned}$$

hold, where $\mathbf{n}$ *is the unit outward facing normal vector of the boundary* $\partial\Omega$. *The interface conditions*

$$\begin{aligned}
&V(0+,y)-V(0-,y)=\alpha(y) && \forall x\in\Gamma,\\
&A(0+)\partial_x V(0+,y)-A(0-)\partial_x V(0-,y)=\gamma(y) && \forall x\in\Gamma
\end{aligned}$$

hold as well.

4. Main results

In this section, we state the main results and prove the existence and local uniqueness of a solution by applying the Schauder fixed-point theorem and the implicit-function theorem, respectively. The main issue of the model equations is how to treat the different equations on a single domain and how the interface conditions (2.8) influence the estimates of the solution. The interface conditions result in jumps in the potential V and in the field $-\partial_x V$. The size of the jumps depends on the values of α and γ so that large values of α or γ yield large absolute values of the potential.

Using the assumptions above, we state and prove the main results in the following subsections.

4.1. Existence of weak solutions.

The main result which states the existence of a solution of system (2.14) is the following theorem.

THEOREM 4.1 (Existence of a weak solution of system (2.14)). *Under Assumptions 3.1, there exists a weak solution*

$$\begin{aligned}
&(V,u,v,\mathbf{u},P,c^+,c^-,\alpha,\gamma)\in\left(H^1(\Omega)\cap L^\infty(\Omega)\right)\times\left(H^1(\Omega_{\mathrm{Si}})\cap L^\infty(\Omega_{\mathrm{Si}})\right)^2\\
&\quad\times\left(H^1_{\mathrm{div},0}(\Omega_{\mathrm{liq}};\mathbb{R}^d)\cap L^\infty\left(\Omega_{\mathrm{liq}};\mathbb{R}^d\right)\right)\times\left(L^2_0(\Omega_{\mathrm{liq}})\cap L^\infty\left(\Omega_{\mathrm{liq}}\right)\right)
\end{aligned}$$

$$\times \left(H^1(\Omega_{\mathrm{liq}}) \cap L^\infty(\Omega_{\mathrm{liq}})\right)^2 \times \left(L^\infty(\Gamma) \cap H^{1/2}(\Gamma)\right) \times L^2(\Gamma)$$

of system (2.14). *The solution furthermore satisfies the* L^∞*-estimates*

$$\begin{aligned} V^- \le V(x) \le V^+ \qquad & \text{in } \Omega, \\ \frac{1}{K} \le u(x) \le K \qquad & \text{in } \Omega_{\mathrm{Si}}, \\ \frac{1}{K} \le v(x) \le K \qquad & \text{in } \Omega_{\mathrm{Si}}, \\ \underline{C}^\pm \le c^\pm(x) \le \overline{C}^\pm \qquad & \text{in } \Omega_{\mathrm{liq}}, \end{aligned}$$

where $C^+ \in \mathbb{R}^+$, $C^- \in \mathbb{R}^+$, $K \in \mathbb{R}^+$, *and*

$$V^- := \min\left(\inf_{\partial\Omega_D} V_D, U_T \ln\left(\frac{1}{2Kn_i}\left(\underline{C} + \sqrt{\underline{C}^2 + 4n_i^2}\right)\right) - \sup_{\Omega} V_L\right), \tag{4.1a}$$

$$V^+ := \max\left(\sup_{\partial\Omega_D} V_D, U_T \ln\left(\frac{K}{2n_i}\left(\overline{C} + \sqrt{\overline{C}^2 + 4n_i^2}\right)\right) - \inf_{\Omega} V_L\right). \tag{4.1b}$$

Here $\underline{C} \le C(x) \le \overline{C}$ *holds and* V_L *is the solution of the linear equation [2, Lemma 3.1], for which the estimate*

$$\|V_L\|_{H^1(\Omega)} \le C\left(\|f\|_{L^2(\Omega)} + \|V_D\|_{H^{1/2}(\partial\Omega)} + \|\alpha\|_{H^{1/2}(\Gamma)} + \|\gamma\|_{L^2(\Gamma)}\right)$$

holds for a positive constant C.

Proof. The proof is based on the Schauder fixed-point theorem and the estimates are obtained from a maximum principle. The main idea of the proof follows [2, 31, 37], while the emphasis is on the different fixed-point map and the different estimates.

(1) We start by defining the fixed-point function. First we choose a suitable space N to define the function $F\colon N \to N$, which will be shown to satisfy the assumptions of the Schauder fixed-point theorem. We define

$$N := \Big\{(u,v,c^+,c^-,\alpha,\gamma) \mid \frac{1}{K} \le u(x), v(x) \le K \text{ a.e. in } \Omega_{\mathrm{Si}}, \underline{C}^\pm \le c^\pm(x) \le \overline{C}^\pm \text{ a.e. in } \Omega_{\mathrm{liq}}, \\ \alpha,\gamma \text{ bounded a.e. on } \Gamma,\ K, \overline{C}^\pm, \underline{C}^\pm \in \mathbb{R}^+\Big\}.$$

The function F is defined as

$$F(u_1,v_1,c_1^+,c_1^-,\alpha_1,\gamma_1) := (u_0,v_0,c_0^+,c_0^-,\alpha_0,\gamma_0),$$

where $(u_0,v_0,c_0^+,c_0^-,\alpha_0,\gamma_0)$ is given (from the previous iteration) and $(u_1,v_1,c_1^+,c_1^-,\alpha_1,\gamma_1)$ is computed from the given solution as follows.

1) Solve the elliptic boundary-value problem with interface conditions

$$\begin{aligned} -\nabla\cdot(A\nabla V_1) &= C_{\mathrm{dop}} - n_i\left(e^{V_1/U_T}u_0 - e^{-V_1/U_T}v_0\right) && \forall x \in \Omega_{\mathrm{Si}}, && (4.2a)\\ -\nabla\cdot(A\nabla V_1) &= 0 && \forall x \in \Omega_{\mathrm{ox}}, && (4.2b)\\ -\nabla\cdot(A\nabla V_1) &= c_0^+ - c_0^- && \forall x \in \Omega_{\mathrm{liq}}, && (4.2c)\\ V_1(0+,y) - V_1(0-,y) &= \alpha_0(y) && \forall x \in \Gamma, && (4.2d)\\ A(0+)\partial_x V_1(0+,y) - A(0-)\partial_x V_1(0-,y) &= \gamma_0(y) && \forall x \in \Gamma, && (4.2e)\\ V_1 &= V_D && \forall x \in \partial\Omega_D, && (4.2f)\\ \mathbf{n}\cdot\nabla V_1 &= 0 && \forall x \in \partial\Omega_N && (4.2g) \end{aligned}$$

for V_1.

2) Solve the elliptic problem

$$U_T\nabla\cdot(\mu_n e^{V_1/U_T}\nabla u_1)=\frac{u_1v_0-1}{\tau_p(e^{V_1/U_T}u_0+1)+\tau_n(e^{-V_1/U_T}v_0+1)} \quad \forall x\in\Omega_{\mathrm{Si}}, \tag{4.3a}$$

$$u_1=u_D \qquad \forall x\in\partial\Omega_{D,\mathrm{Si}}, \tag{4.3b}$$

$$\mathbf{n}\cdot\nabla u_1=0 \qquad \forall x\in\partial\Omega_{N,\mathrm{Si}}, \tag{4.3c}$$

for u_1.

3) Solve the elliptic problem

$$U_T\nabla\cdot(\mu_p e^{-V_1/U_T}\nabla v_1)=\frac{u_0v_1-1}{\tau_p(e^{V_1/U_T}u_0+1)+\tau_n(e^{-V_1/U_T}v_0+1)} \quad \forall x\in\Omega_{\mathrm{Si}}, \tag{4.4a}$$

$$v_1=v_D \qquad \forall x\in\partial\Omega_{D,\mathrm{Si}}, \tag{4.4b}$$

$$\mathbf{n}\cdot\nabla v_1=0 \qquad \forall x\in\partial\Omega_{N,\mathrm{Si}}, \tag{4.4c}$$

for v_1.

4) Solve the elliptic problem

$$-\rho\Delta\mathbf{u}_1+\nabla P_1=-(c_0^+-c_0^-)\nabla V_1 \qquad \forall x\in\Omega_{\mathrm{liq}}, \tag{4.5a}$$

$$\nabla\cdot\mathbf{u}_1=0 \qquad \forall x\in\Omega_{\mathrm{liq}}, \tag{4.5b}$$

$$\mathbf{u}_1=0 \qquad \forall x\in\partial\Omega_{\mathrm{liq}}, \tag{4.5c}$$

for $\mathbf{u}_1$ and P_1.

5) Solve the elliptic problem

$$-\nabla\cdot(D^\pm\nabla c_1^\pm)\mp\mu^\pm\nabla\cdot(c_1^\pm\nabla V_1)+(\mathbf{u}_1\cdot\nabla)c_0^\pm=0 \qquad \forall x\in\Omega_{\mathrm{liq}}, \tag{4.6a}$$

$$c_1^\pm=c_D^\pm \qquad \forall x\in\partial\Omega_{D,\mathrm{liq}}, \tag{4.6b}$$

$$J^\pm\cdot\mathbf{n}=0 \qquad \forall x\in\partial\Omega_{N,\mathrm{liq}}. \tag{4.6c}$$

for $c_1^\pm$.

6) Update the surface-charge density and dipole-moment density according to the microscopic models by

$$\alpha_1(y):=M_\alpha(V_1) \qquad x\in\Gamma, \tag{4.7a}$$

$$\gamma_1(y):=M_\gamma(V_1) \qquad x\in\Gamma. \tag{4.7b}$$

For simplicity, from now on we will denote the solution of iterations by $(V,u,v,\mathbf{u},P,c^+,c^-,\alpha,\gamma)$ instead of using the index 1.

(2) All boundary-value and initial-boundary-value problems are understood in the weak sense. Hence, a fixed point of the nonlinear operator F is a weak solution of our coupled problem (2.14). We show the existence of a fixed point for the function F by showing that it is well-defined and completely continuous. Finally, we apply the Schauder fixed-point theorem after verifying its assumptions in (i)–(v).

(i) First, we check that F is well-defined. One can apply standard elliptic existence results to the aforementioned problems, see e.g. [32, 36], in general. Poisson and drift-diffusion Equations (4.2)–(4.4) have unique weak solutions $(V,u,v,\alpha,\gamma)\in\big(H^1(\Omega)\cap L^\infty(\Omega)\big)\times\big(H^1(\Omega_{\mathrm{Si}})\cap L^\infty(\Omega_{\mathrm{Si}})\big)^2\times\big(L^\infty(\Gamma)\cap H^{1/2}(\Gamma)\big)$ due to [2, Theorem 2.2]. The Stokes problem (4.5) is also uniquely solvable (see e.g. [9, Theorem 2.1] and [36, Theorem 7.4.1]), i.e., there exists a unique weak solution

$(\mathbf{u},P)\in H^1_{\mathrm{div},0}(\Omega_{\mathrm{liq}};\mathbb{R}^3)\times L^2_0(\Omega_{\mathrm{liq}})$, while the pressure P is only determined up to a constant. Imposing a zero mean value, i.e., imposing $\int_\Omega P=0$, leads to uniqueness of P in $L^2_0(\Omega_{\mathrm{liq}})$. Furthermore, a unique weak solution $(c^+,c^-)\in H^1(\Omega_{\mathrm{liq}})\cap L^\infty(\Omega)$ of the Nernst-Planck Equations (4.6) exists due to [32, Theorem 3.3.16]. We note that the fixed-point operator F is solely a function of concentrations the $(\overline{c}^+,\overline{c}^-,\overline{u},\overline{v})$. Therefore a fixed-point (c^+,c^+,u,v) of F only solves the respective transport equations for $c^\pm$, u, and v. However, two suboperators which solve the Poisson and Stokes equations contain the necessary information about the electrostatic potential V, the velocity field $\mathbf{u}$, and the pressure P.
Therefore, all boundary-value problems involved in the definition of fixed-point map F are uniquely solvable. Hence, F is well-defined.

(ii) N is closed and convex due to its definition.

(iii) We show that F maps N into itself. To obtain the estimates, we apply Lemma 3.3.14 in [32] to the first problem (4.2) to find a unique solution V. To this end, we define

$$\underset{\sim}{g}(V):=qn_i\big(\frac{1}{K}e^{V/U_T}-Ke^{-V/U_T}\big)-q\overline{C},$$
$$\widetilde{g}(V):=qn_i\big(Ke^{V/U_T}-\frac{1}{K}e^{-V/U_T}\big)-q\overline{C},$$

where $\underset{\sim}{g}$ and $\widetilde{g}$ are monotonically increasing for all $x\in\Omega$.
Solving the algebraic equations

$$\underset{\sim}{g}(\widetilde{V}+\inf_\Omega V_L)=0,$$
$$\widetilde{g}(\underset{\sim}{V}+\sup_\Omega V_L)=0,$$

where V_L is the solution of the linear elliptic boundary-value problem in the existence lemma [2, Lemma 3.1] yields

$$\widetilde{V}+\inf_\Omega V_L=U_T\ln\big(\frac{K}{2n_i}(\overline{C}+\sqrt{\overline{C}^2+4n_i^2})\big),$$
$$\underset{\sim}{V}+\sup_\Omega V_L=U_T\ln\big(\frac{1}{2Kn_i}(\underline{C}+\sqrt{\underline{C}^2+4n_i^2})\big).$$

Hence, using Lemma 3.3.14 in [32], we find the estimates

$$V(x)\geq\min\Big(\inf_{\partial\Omega_D}V_D,U_T\ln\big(\frac{1}{2Kn_i}(\underline{C}+\sqrt{\underline{C}^2+4n_i^2})\big)-\sup_\Omega V_L\Big)=:V^-,$$
$$V(x)\leq\max\Big(\sup_{\partial\Omega_D}V_D,U_T\ln\big(\frac{K}{2n_i}(\overline{C}+\sqrt{\overline{C}^2+4n_i^2})\big)-\inf_\Omega V_L\Big)=:V^+$$

for all $x\in\Omega$. Therefore, we obtain a unique solution V_1, and it satisfies the estimate

$$V^-\leq V(x)\leq V^+\qquad\text{in }\Omega.$$

Additionally, we define

$$\underset{\sim}{g}(u):=\frac{\frac{1}{K}u-1}{\tau_p\big(Ke^{V^+/U_T}+1\big)+\tau_n\big(Ke^{-V^+/U_T}+1\big)},$$

$$\widetilde{g}(u) := \frac{Ku-1}{\tau_p\left(\frac{1}{K}e^{V^-/U_T}+1\right)+\tau_n\left(\frac{1}{K}e^{-V^-/U_T}+1\right)}.$$

Then the equation $g(\widetilde{u})=0$ yields $\widetilde{u}=K$ and the equation $\widetilde{g}(\underset{\sim}{u})=0$ yields $\underset{\sim}{u}=1/K$. Similarly, we find $\widetilde{v}=K$ and $\underset{\sim}{v}=1/K$. Thus, we have $1/K\le u(x),v(x)\le K$ in Ω_{Si}. Regarding $c^{\pm}(x)$, we use the same lemma as for u and v and consider

$$\underset{\sim}{g}(c^{\pm}) := \mp\mu^{\pm}\nabla\cdot(c^{\pm}\nabla V^{\pm}),$$
$$\widetilde{g}(c^{\pm}) := \mp\mu^{\pm}\nabla\cdot(c^{\pm}\nabla V^{\mp}).$$

Solving the equations $\underset{\sim}{g}(\widetilde{c^{\pm}})=0$ and $\widetilde{g}(\underset{\sim}{c^{\pm}})=0$ yields

$$\widetilde{c^{\pm}} := \frac{c_1}{\nabla V^{\pm}},$$
$$\underset{\sim}{c^{\pm}} := \frac{c_2}{\nabla V^{\mp}},$$

where c_1 and c_2 are constants. Then using Lemma 3.3.14 in [32], we obtain the estimates

$$\underline{C}^{\pm} := \max\Big(\sup_{\partial\Omega_{D,\mathrm{liq}}} c_D^{\pm}, \frac{c_1}{\nabla V^{\pm}}\Big),$$
$$\overline{C}^{\pm} := \min\Big(\inf_{\partial\Omega_{D,\mathrm{liq}}} c_D^{\pm}, \frac{c_2}{\nabla V^{\mp}}\Big)$$

for all $x\in\Omega_{\mathrm{liq}}$. Therefore, we obtain unique solutions $c^{\pm}$ which satisfy the estimate

$$\underline{C}^{\pm} \le c^{\pm}(x) \le \overline{C}^{\pm} \qquad \text{in } \Omega_{\mathrm{liq}}.$$

Therefore, F maps N into itself.

(iv) We now show that F is continuous. The continuity of F is a consequence of its well-posedness, meaning that a unique solution exists for each problem and it depends continuously on the data. The continuous dependence of the H^1-norm of the solution on the data follows from the estimate in [2, Lemma 3.2] for the semilinear elliptic problems and continuity of the right-hand sides of the corresponding problems. Also, α and γ depend continuously on α_0 and γ_0 due to the continuous dependence of V and the continuity of the microscopic models M_α and M_γ. Therefore, F is continuous.

The continuous dependence of $(V,u,v,\mathbf{u},P,c^+,c^-,\alpha,\gamma)$ on the data of the problems in (4.2)–(4.7) implies that there is a positive and continuous function H such that

$$\begin{aligned}&\|V\|_{H^1(\Omega)}+\|\mathbf{u}\|_{H^1(\Omega_{\mathrm{liq}};\mathbb{R}^d)}+\|c^{\pm}\|_{H^1(\Omega_{\mathrm{liq}})}+\|P\|_{H^1(\Omega_{\mathrm{liq}})}+\|u\|_{H^1(\Omega_{\mathrm{Si}})}+\|v\|_{H^1(\Omega_{\mathrm{Si}})}\\ &\le H\big(\|C_{\mathrm{dop}}\|_{L^2(\Omega)},\|c_D^{\pm}\|_{L^2(\Omega_{\mathrm{liq}})},\|V_D\|_{H^{1/2}(\partial\Omega)},\|u_D\|_{H^{1/2}(\partial\Omega_{\mathrm{Si}})},\\ &\qquad\qquad \|v_D\|_{H^{1/2}(\partial\Omega_{\mathrm{Si}})},\|\alpha_0\|_{H^{1/2}(\Gamma)},\|\gamma_0\|_{L^2(\Gamma)}\big)\end{aligned}$$

holds. Hence the inequality

$$\|V\|_{H^1(\Omega)}+\|\mathbf{u}\|_{H^1(\Omega_{\mathrm{liq}};\mathbb{R}^d)}+\|P\|_{H^1(\Omega_{\mathrm{liq}})}+\|c^+\|_{H^1(\Omega_{\mathrm{liq}})}+\|c^-\|_{H^1(\Omega_{\mathrm{liq}})}$$

$$+\|u\|_{H^1(\Omega_{\mathrm{Si}})}+\|v\|_{H^1(\Omega_{\mathrm{Si}})}\le C$$

holds for a positive constant C. Furthermore, $\|\alpha\|_{H^1(\Gamma)}$ and $\|\gamma\|_{H^1(\Gamma)}$ are bounded due to the assumptions on M_α and M_γ.

(v) We show that the image $F(N)$ is precompact, i.e., the closure of $F(N)$ is compact. The image $F(N)$ is bounded as a subset of $H^1(\Omega)\times H^1(\Omega_{\mathrm{liq}};\mathbb{R}^d)\times H^1(\Omega_{\mathrm{liq}})^2\times H^1(\Omega_{\mathrm{Si}})^2\times H^1(\Gamma)^2$ which – based on the Rellich-Kondrachov theorem – is compactly embedded in $L^2(\Omega)\times L^2(\Omega_{\mathrm{liq}};\mathbb{R}^d)\times L^2(\Omega_{\mathrm{liq}})^2\times L^2(\Omega_{\mathrm{Si}})^2\times L^2(\Gamma)^2$. This means that the closure of $F(N)$ is compact, which implies that $F(N)$ is precompact.

(3) According to (i)–(v), the Schauder fixed-point theorem can be applied to the function F, which proves existence of a fixed-point of this function, and thus the existence of a weak solution of the original problem is shown.

∎

4.2. Uniqueness of weak solutions. Theorem 4.1 shows the existence of weak solutions of the system (2.14). Then the question arises whether the solutions are unique. Based on numerical evidence, the solution starts to oscillate between two functions when large voltages are applied as Dirichlet boundary conditions.

Furthermore, it is well-known that in the derivation of the drift-diffusion equations from the Boltzmann equation one essentially assumes that the particle momenta are distributed according to a Boltzmann-Maxwell distribution. However, large applied voltages result in fast particles which are not taken into account by this distribution.

These two reasons, namely the shortcomings of the drift-diffusion equations as a transport model as well as the numerical evidence, suggest that the solutions are not unique in the case of large applied voltages. Indeed, we will show next that the solution is unique in a neighborhood around thermal equilibrium and hence uniqueness is only a local property for sufficiently small Dirichlet boundary conditions.

Since uniqueness is only local, the maximum principle is not helpful for proving uniqueness. To prove local uniqueness, we will use the implicit-function theorem.

Before we can state and prove local uniqueness, we must specify thermal equilibrium more precisely. The situation where the current densities of ions and molecules, i.e., $J^\pm$, J_n, and J_p vanish is called thermal equilibrium. Then the applied potentials at all r contacts that constitute the Dirichlet boundary $\partial\Omega_D$ are equal to the Fermi level. If the equilibrium dipole-moment and surface-charge densities are called α_e and γ_e, respectively, and the equilibrium potential V_e, the liquid velocity $\mathbf{u}_e$, and liquid pressure P_e, then V_e, $\mathbf{u}_e$, and P_e are solutions of the equilibrium boundary-value problems

$$\begin{aligned}
&-\nabla\cdot(A\nabla V_e)=qC_{\mathrm{dop}}-qn_i(e^{V_e/U_T}-e^{-V_e/U_T}) && \forall x\in\Omega_{\mathrm{Si}},\\
&-\nabla\cdot(A\nabla V_e)=0 && \forall x\in\Omega_{\mathrm{ox}},\\
&-\nabla\cdot(A\nabla V_e)=q(c_e^+-c_e^-) && \forall x\in\Omega_{\mathrm{liq}},\\
&V_e(0+,y)-V_e(0-,y)=\alpha_e(y) && \forall x\in\Gamma,\\
&A(0+)\partial_x V_e(0+,y)-A(0-)\partial_x V_e(0-,y)=\gamma_e(y) && \forall x\in\Gamma,\\
&V_e=V_D(0) && \forall x\in\partial\Omega_D,\\
&\nabla V_e\cdot\mathbf{n}=0 && \forall x\in\partial\Omega_N,
\end{aligned}$$

whose solution V_e exists uniquely due to [2, Lemma 3.2], and the solution $(\mathbf{u}_e,P_e)$ of

$$\begin{aligned}
&-\rho\Delta\mathbf{u}_e+\nabla P_e=-q(c_e^+-c_e^-)\nabla V_e && \forall x\in\Omega_{\mathrm{liq}},\\
&\nabla\cdot\mathbf{u}_e=0 && \forall x\in\Omega_{\mathrm{liq}},
\end{aligned}$$

$$\mathbf{u}_e = 0 \qquad \forall x \in \partial\Omega_{D,\mathrm{liq}},$$

exists because of [9, Theorem 2.1]. In the first equation above, α_e and γ_e are the equilibrium values and at the second problem, V_e is obtained from the first problem.

The above system is solved by introducing an initial equilibrium solution and a fixed-point map which is defined by the above BVPs similar to what we did in (4.2)–(4.7).

We will be able to show local uniqueness of solutions of the problem (2.14) around the equilibrium solution $(V_e, u_e, v_e, c_e^{\pm}, \mathbf{u}_e, P_e)$. To apply the implicit-function theorem, we have to show that the Fréchet derivative of the problem has a bounded inverse at the equilibrium solution. To this end, we estimate the norm of the inverse of the linearization of the system (2.14) at the equilibrium solution. As mentioned before, the main assumption is that the Dirichlet boundary conditions for the potential are sufficiently small. More precisely, we assume that the Dirichlet boundary conditions for the potential V are constants on each of the r segments of the the Dirichlet boundary $\partial\Omega_{D,\mathrm{Si}}$ and denote the potentials there by the vector $U := (U_1, U_2, \cdots, U_r)$.

In order to prove local uniqueness for small applied voltages, the following assumptions are used.

Assumptions 4.1.

(1) *The domain $\Omega \subset \mathbb{R}^3$ is open and bounded, and the boundary $\partial\Omega$ is as smooth as necessary (see Assumptions 3.1).*

(2) *The Dirichlet data $(V_D, u_D, v_D, \mathbf{u}_D, c_D^+, c_D^-)$ are a Lipschitz-continuously differentiable function of $U := (U_1, U_2, \cdots, U_r)$, $\mathbb{R}^r \to H^2(\Omega) \times H^2(\Omega_{\mathrm{Si}})^2 \times H^2(\Omega_{\mathrm{liq}})^3$.*

(3) *The Fréchet derivatives M_α' and M_γ' of the interface models M_α and M_γ with respect to V exist, they are in $H^{1/2}(\Gamma)$ and $L^2(\Gamma)$, respectively, and they satisfy the inequality*

$$\|M_\alpha'(V)\|_{H^{1/2}(\Gamma)} + \|M_\gamma'(V)\|_{L^2(\Gamma)} \le C\|V\|_{H^2(\Omega)} \tag{4.8}$$

in a neighborhood of the equilibrium potential V_e with a sufficiently small constant C.

(4) *The recombination rate R has the form $R = (uv-1)K(x,V,u,v)$, where $K(x,\cdot,\cdot,\cdot) \in C^2(\mathbb{R} \times \mathbb{R}^2_+)$ holds for $x \in \Omega$ where the derivatives $\partial^\nu_{(V,u,v)} K(\cdot, V, u, v)$ are bounded uniformly for all (V,u,v) in bounded subsets of $\mathbb{R} \times \mathbb{R}^2_+$ and for all multiindices ν with $|\nu| \le 2$. Furthermore, there are constants $\underline{\kappa}$ and $\overline{\kappa}$ such that either $0 < \underline{\kappa} \le K(x, V_e(x), 1, 1) \le \overline{\kappa}$ or $K(x, V_e(x), 1, 1) = 0$ for all $x \in \Omega$.*

Theorem 4.2 (Local uniqueness of weak solutions of (2.14)). *Under Assumptions 3.1 and 4.1, there exists a sufficiently small $\sigma \in \mathbb{R}$ with $|U| < \sigma$ such that the system (2.14) has a locally unique solution*

$$\begin{aligned}&\big(V^*(U), u^*(U), v^*(U), \mathbf{u}^*(U), P^*(U), c^{\pm *}(U), \alpha^*(U), \gamma^*(U)\big)\\ &\qquad \in H^2(\Omega) \times H^2(\Omega_{\mathrm{Si}})^2 H^2_{\mathrm{div},0}(\Omega_{\mathrm{liq}}; \mathbb{R}^3) \times H^2(\Omega_{\mathrm{liq}})^3 \times H^{1/2}(\Gamma) \times L^2(\Gamma).\end{aligned}$$

It depends continuously differentiably on the Dirichlet boundary data U as a function

$$\begin{aligned}\{U \in \mathbb{R}^r \mid |U| < \sigma\} \to\ & H^2(\Omega) \times H^2(\Omega_{\mathrm{Si}})^2 \times H^2_{\mathrm{div},0}(\Omega_{\mathrm{liq}}; \mathbb{R}^3) \times H^2(\Omega_{\mathrm{liq}})^3\\ & \times H^{1/2}(\Gamma) \times L^2(\Gamma).\end{aligned}$$

Proof. Uniqueness is proved using the implicit-function theorem. We define the function

$$G\colon B\times S_{\sigma_1}(0)\to\chi,$$
$$G\big((\hat V,\hat u,\hat v,\mathbf{u},P,\hat{c^+},\hat{c^-},\alpha,\gamma),U\big)=0,$$

where

$$\chi:=L^2(\Omega)\times L^2(\Omega_{\mathrm{Si}})^2\times H^1_{\mathrm{div},0}\big(\Omega_{\mathrm{liq}};\mathbb{R}^3\big)\times L^2(\Omega_{\mathrm{liq}})^3\times H^{1/2}(\Gamma)\times L^2(\Gamma),$$

and G is defined by the left-hand sides of the boundary-value problems

$$-\nabla\cdot\big(A\nabla(\hat V+V_D)\big)-qC_{\mathrm{dop}}$$
$$+qn_i\big(e^{(\hat V+V_D)/U_T}(\hat u+u_D)-e^{-(\hat V+V_D)/U_T}(\hat v+v_D)\big)=0 \qquad \forall x\in\Omega_{\mathrm{Si}}, \quad (4.9a)$$
$$-\nabla\cdot\big(A\nabla(\hat V+V_D)\big)=0 \qquad \forall x\in\Omega_{\mathrm{ox}}, \quad (4.9b)$$
$$-\nabla\cdot\big(A\nabla(\hat V+V_D)\big)-q\big((\hat{c^+}+c_D^+)-(\hat{c^-}+c_D^-)\big)=0 \qquad \forall x\in\Omega_{\mathrm{liq}}, \quad (4.9c)$$
$$-\rho\Delta\mathbf{u}+q\big((\hat{c^+}+c_D^+)-(\hat{c^-}+c_D^-)\big)\nabla(\hat V+V_D)+\nabla P=0 \qquad \forall x\in\Omega_{\mathrm{liq}}, \quad (4.9d)$$
$$\nabla\cdot\mathbf{u}=0 \qquad \forall x\in\Omega_{\mathrm{liq}}, \quad (4.9e)$$
$$-D^\pm\Delta(\hat{c^\pm}+c_D^\pm)\mp\mu^\pm\nabla\cdot\big((\hat{c^\pm}+c_D^\pm)\nabla(\hat V+V_D)\big)+(\mathbf{u}\cdot\nabla)(\hat{c^\pm}+c_D^\pm)=0 \quad \forall x\in\Omega_{\mathrm{liq}}, \quad (4.9f)$$
$$U_T n_i\nabla\cdot(\mu_n e^{(\hat V+V_D)/U_T}\nabla(\hat u+u_D))$$
$$-((\hat u+u_D)(\hat v+v_D)-1)K(x,\hat V+V_D,\hat u+u_D,\hat v+v_D)=0 \qquad \forall x\in\Omega_{\mathrm{Si}}, \quad (4.9g)$$
$$U_T n_i\nabla\cdot(\mu_p e^{-(\hat V+V_D)/U_T}\nabla(\hat v+v_D))$$
$$-((\hat u+u_D)(\hat v+v_D)-1)K(x,\hat V+V_D,\hat u+u_D,\hat v+v_D)=0 \qquad \forall x\in\Omega_{\mathrm{Si}}, \quad (4.9h)$$
$$\hat V(0+,y)-\hat V(0-,y)=\alpha(y) \qquad \forall x\in\Gamma, \quad (4.9i)$$
$$A(0+)\partial_x\hat V(0+,y)-A(0-)\partial_x\hat V(0-,y)=\gamma(y) \qquad \forall x\in\Gamma, \quad (4.9j)$$
$$\alpha=M_\alpha(\hat V+V_D) \qquad \forall x\in\Gamma, \quad (4.9k)$$
$$\gamma=M_\gamma(\hat V+V_D) \qquad \forall x\in\Gamma, \quad (4.9l)$$
$$\hat V=0 \qquad \forall x\in\partial\Omega_D, \quad (4.9m)$$
$$\hat u=0=\hat v \qquad \forall x\in\partial\Omega_{D,\mathrm{Si}}, \quad (4.9n)$$
$$\mathbf{n}\cdot\nabla\hat V=0 \qquad \forall x\in\partial\Omega_N, \quad (4.9o)$$
$$\mathbf{n}\cdot\nabla\hat u=0=\mathbf{n}\cdot\nabla\hat v \qquad \forall x\in\partial\Omega_{N,\mathrm{Si}}, \quad (4.9p)$$
$$\mathbf{u}=0 \qquad \forall x\in\partial\Omega_{D,\mathrm{liq}}, \quad (4.9q)$$
$$\hat{c^\pm}=0 \qquad \forall x\in\partial\Omega_{D,\mathrm{liq}}, \quad (4.9r)$$
$$J^\pm\cdot\mathbf{n}=0 \qquad \forall x\in\partial\Omega_{N,\mathrm{liq}}, \quad (4.9s)$$

which are obtained by substituting $\hat V:=V-V_D(U)$, $\hat u:=u-u_D(U)$, $\hat v:=v-v_D(U)$, and $\hat{c^\pm}:=c^\pm-c_D^\pm(U)$ into the system (2.14). B is an open subset of $H^2_\partial(\Omega\setminus\Gamma)\times H^2_\partial(\Omega_{\mathrm{Si}})^2\times H^2_{\partial,\mathrm{div}}(\Omega_{\mathrm{liq}};\mathbb{R}^3)\times H^2_\partial(\Omega_{\mathrm{liq}})^3\times H^{1/2}(\Gamma)\times L^2(\Gamma)$ with

$$H^2_\partial(\Omega):=\{\phi\in H^2(\Omega)\,|\,\nabla\phi\cdot\mathbf{n}=0\text{ on }\partial\Omega_{\mathrm{N}},\ \phi=0\text{ on }\partial\Omega_{\mathrm{D}}\}, \quad (4.10a)$$
$$H^2_{\partial,\mathrm{div}}(\Omega):=\{\phi\in H^2(\Omega)\,|\,\nabla\cdot\phi=0\text{ in }\Omega_{\mathrm{liq}},\ \phi=0\text{ on }\partial\Omega_{\mathrm{D}}\}. \quad (4.10b)$$

The sphere S_{σ_1} with radius σ_1 and center 0 is a subset of $\mathbb{R}^r$.

We claim that the set B and the radius σ_1 can be chosen such that

$$u=\hat{u}+u_D(U)>0, \quad v=\hat{v}+v_D(U)>0, \quad \text{and} \quad c^{\pm}=\hat{c}^{\pm}+c_D^{\pm}(U)>0.$$

holds for all $U\in S_{\sigma_1}(0)$ and for all $(\hat{V},\hat{u},\hat{v},\mathbf{u},P,\hat{c}^+,\hat{c}^-,\alpha,\gamma)\in B$. Since the recombination rate R is only defined for positive concentrations u and v and the concentrations $c^{\pm}$ are nonnegative [37], the above conditions are satisfied. To this end, it is sufficient to choose B bounded and small enough, i.e., $\|\hat{u}\|_{H^2(\Omega_{\mathrm{Si}})}$ is sufficiently small. This results in a small $\|\hat{u}\|_{L^\infty(\Omega_{\mathrm{Si}})}$, since $\|\hat{u}\|_{L^\infty(U)}\le C\|\hat{u}\|_{H^2(U)}$ holds for all $u\in H^2(U)$. Therefore, we can conclude that $u>0$. The same argument ensures that v and $c^{\pm}$ are positive if B is bounded and small enough.

On the other hand, since $G\big((\hat{V},\hat{u},\hat{v},\mathbf{u},P,\hat{c}^+,\hat{c}^-,\alpha,\gamma),U\big)\in\chi$ implies that $(\hat{V},\hat{u},\hat{v},\mathbf{u},P,\hat{c}^+,\hat{c}^-,\alpha,\gamma)\in B$ and $U\in S_{\sigma_1(U)}$, and products of functions in B (a subset of H^2) are in L^2, it follows that the function G is well-defined.

The equilibrium solution $\big((V_e-V_D(0),0,0,\mathbf{u}_e,P_e,0,0,\alpha_e,\gamma_e),0\big)$ is a solution of the equation $G\big((\hat{V},\hat{u},\hat{v},\mathbf{u},P,\hat{c^+},\hat{c^-},\alpha,\gamma),U\big)=0$. To apply the implicit-function theorem, the Fréchet derivative

$$DG:=D_{(\hat{V},\hat{u},\hat{v},\mathbf{u},P,\hat{c^+},\hat{c^-},\alpha,\gamma)}G\big((V_e-V_D(0),0,0,\mathbf{u}_e,P_e,0,0,\alpha_e,\gamma_e),0\big)$$

must have a bounded inverse. Suppose $(g_1,g_2,g_3,g_4,g_5,g_6,g_7,g_8,g_9)\in\chi$. To find the inverse of the Fréchet derivative, we have to solve the equation

$$DG(a_1,a_2,a_3,a_4,a_5,a_6,a_7,a_8,a_9)=(g_1,g_2,g_3,g_4,g_5,g_6,g_7,g_8,g_9) \tag{4.11}$$

for a_i, $i\in\{1,2,\dots,9\}$. To write this equation as a boundary-value problem, we have to linearize the original equation (4.9) first. Thus, DG takes the form

$$\begin{pmatrix}
-\nabla\cdot(A\nabla)+L_1 & qn_ie^{V_e/U_T} & -qn_ie^{-V_e/U_T} & 0 & 0 & 0 & 0 & 0\ 0\\
0 & L_2 & -K & 0 & 0 & 0 & 0 & 0\ 0\\
0 & -K & L_3 & 0 & 0 & 0 & 0 & 0\ 0\\
0 & 0 & 0 & -\rho\Delta & \nabla & q\nabla V_e & -q\nabla V_e & 0\ 0\\
0 & 0 & 0 & \nabla\cdot & 0 & 0 & 0 & 0\ 0\\
0 & 0 & 0 & \nabla c_e^+ & 0 & L_4 & 0 & 0\ 0\\
0 & 0 & 0 & \nabla c_e^- & 0 & 0 & L_5 & 0\ 0\\
-M_\alpha'(V_e) & 0 & 0 & 0 & 0 & 0 & 0 & 1\ 0\\
-M_\gamma'(V_e) & 0 & 0 & 0 & 0 & 0 & 0 & 0\ 1
\end{pmatrix},$$

where

$$\begin{aligned}
L_1&:=qn_i\Big(\frac{e^{V_e/U_T}+e^{-V_e/U_T}}{U_T}\Big),\\
L_2&:=U_Tn_i\nabla\cdot\big(\mu_ne^{V_e/U_T}\nabla\big)-K,\\
L_3&:=U_Tn_i\nabla\cdot\big(\mu_pe^{-V_e/U_T}\nabla\big)-K,\\
L_4&:=-D^+\Delta+\mathbf{u}_e\cdot\nabla,\\
L_5&:=-D^-\Delta+\mathbf{u}_e\cdot\nabla.
\end{aligned}$$

The first row corresponds to the linearized Poisson equation in Ω_{Si}. The three rows in

$$\begin{pmatrix}
-\nabla\cdot(A\nabla)+L_1 & qn_ie^{V_e/U_T} & -qn_ie^{-V_e/U_T} & 0\ 0 & 0 & 0\ 0\ 0\\
-\nabla\cdot(A\nabla) & 0 & 0 & 0\ 0 & 0 & 0\ 0\ 0\\
-\nabla\cdot(A\nabla) & 0 & 0 & 0\ 0 & -q & q\ 0\ 0
\end{pmatrix}.$$

correspond to the linearized Poisson equation in Ω_{Si}, Ω_{ox}, and Ω_{liq}, respectively.

Therefore, Equation (4.11) is equivalent to the boundary-value problem

$$
\begin{aligned}
&-\nabla\cdot(A\nabla a_1) = -qn_i\Big(\Big(\frac{e^{V_e/U_T}+e^{-V_e/U_T}}{U_T}\Big)a_1 && && \text{(4.12a)}\\
&\quad + e^{V_e/U_T}a_2 - e^{-V_e/U_T}a_3\Big) + g_1 && \forall x\in\Omega_{\mathrm{Si}}, && \text{(4.12b)}\\
&-\nabla\cdot(A\nabla a_1) = g_1 && \forall x\in\Omega_{\mathrm{ox}}, && \text{(4.12c)}\\
&-\nabla\cdot(A\nabla a_1) = q(a_6-a_7)+g_1 && \forall x\in\Omega_{\mathrm{liq}}, && \text{(4.12d)}\\
&U_T n_i\nabla\cdot\big(\mu_n e^{V_e/U_T}\nabla a_2\big) = Ka_2+Ka_3+g_2 && \forall x\in\Omega_{\mathrm{Si}}, && \text{(4.12e)}\\
&U_T n_i\nabla\cdot\big(\mu_p e^{-V_e/U_T}\nabla a_3\big) = Ka_3+Ka_2+g_3 && \forall x\in\Omega_{\mathrm{Si}}, && \text{(4.12f)}\\
&-\rho\Delta a_4+\nabla a_5 = -q\nabla V_e(a_6-a_7)+g_4 && \forall x\in\Omega_{\mathrm{liq}}, && \text{(4.12g)}\\
&\nabla\cdot a_4 = g_5 && \forall x\in\Omega_{\mathrm{liq}}, && \text{(4.12h)}\\
&-D^+\Delta a_6+\mathbf{u}_e\cdot\nabla a_6 = -\nabla c_e^+ a_4+g_6 && \forall x\in\Omega_{\mathrm{liq}}, && \text{(4.12i)}\\
&-D^-\Delta a_7-\mathbf{u}_e\cdot\nabla a_7 = -\nabla c_e^- a_4+g_7 && \forall x\in\Omega_{\mathrm{liq}}, && \text{(4.12j)}\\
&a_1(0^+,y)-a_1(0^-,y) = a_8 && \forall x\in\Gamma, && \text{(4.12k)}\\
&A(0^+)\partial_x a_1(0^+,y)-A(0^+)\partial_x a_1(0^-,y) = a_9 && \forall x\in\Gamma, && \text{(4.12l)}\\
&a_8 = M_\alpha'(V_e)a_1+g_8 && \forall x\in\Gamma, && \text{(4.12m)}\\
&a_9 = M_\gamma'(V_e)a_1+g_9 && \forall x\in\Gamma, && \text{(4.12n)}\\
&a_1 = 0 && \forall x\in\partial\Omega_D, && \text{(4.12o)}\\
&a_2 = 0 = a_3 && \forall x\in\partial\Omega_{D,\mathrm{Si}}, && \text{(4.12p)}\\
&\mathbf{n}\cdot\nabla a_1 = 0 && \forall x\in\partial\Omega_N, && \text{(4.12q)}\\
&\mathbf{n}\cdot\nabla a_2 = 0 = \mathbf{n}\cdot\nabla a_3 && \forall x\in\partial\Omega_{N,\mathrm{Si}}, && \text{(4.12r)}\\
&a_4 = 0 && \forall x\in\partial\Omega_{D,\mathrm{liq}}, && \text{(4.12s)}\\
&\mathbf{n}\cdot\nabla a_6 = 0 = \mathbf{n}\cdot\nabla a_7 && \forall x\in\partial\Omega_{N,\mathrm{liq}}. && \text{(4.12t)}
\end{aligned}
$$

As stated in Assumptions 4.1, either $0<\underline{\kappa}\le K\le\overline{\kappa}$ or $K=0$ holds in Ω_{Si}. In both cases, there exist unique solutions a_2 and a_3 of the Equations (4.12e)–(4.12f) due to [2, Lemma 3.2]. Therefore, there exists a positive constant C such that the estimate

$$
\|a_2\|_{H^2(\Omega_{\mathrm{Si}})}+\|a_3\|_{H^2(\Omega_{\mathrm{Si}})}\le C\big(\|g_2\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_3\|_{L^2(\Omega_{\mathrm{Si}})}\big) \tag{4.13}
$$

in Ω_{Si} holds. Furthermore, there exist solutions a_6 and a_7 for equations (4.12i)–(4.12j) and a sufficiently small constant C_2 such that the estimate

$$
\|a_6\|_{H^2(\Omega_{\mathrm{liq}})}+\|a_7\|_{H^2(\Omega_{\mathrm{liq}})}\le\|g_6\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_7\|_{L^2(\Omega_{\mathrm{liq}})}+C_1\|a_4\|_{H^2(\Omega_{\mathrm{liq}})} \tag{4.14}
$$

holds. The Stokes Equations (4.12g)–(4.12h) also have unique solutions a_4 and a_5 with the estimate

$$
\begin{aligned}
&\|a_4\|_{H^2(\Omega_{\mathrm{liq}})}+\|a_5\|_{H^2(\Omega_{\mathrm{liq}})}\\
&\le C_2\big(\|g_4\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_5\|_{L^2(\Omega_{\mathrm{liq}})}+\|a_6\|_{H^2(\Omega_{\mathrm{liq}})}+\|a_7\|_{H^2(\Omega_{\mathrm{liq}})}\big)\\
&\le C_2\big(\|g_4\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_5\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_6\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_7\|_{L^2(\Omega_{\mathrm{liq}})}+C_1\|a_4\|_{H^2(\Omega_{\mathrm{liq}})}\big).
\end{aligned}
$$

Hence, we have

$$
(1-C_1C_2)\|a_4\|_{H^2(\Omega_{\mathrm{liq}})}\le C_2\big(\|g_4\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_5\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_6\|_{L^2(\Omega_{\mathrm{liq}})}+\|g_7\|_{L^2(\Omega_{\mathrm{liq}})}\big)
$$

for sufficiently small C_2, i.e., if $C_1C_2<1$. We conclude that

$$\|a_6\|_{H^2(\Omega_{\rm liq})}+\|a_7\|_{H^2(\Omega_{\rm liq})}\le 2\|g_6\|_{L^2(\Omega_{\rm liq})}+2\|g_7\|_{L^2(\Omega_{\rm liq})}+\|g_4\|_{L^2(\Omega_{\rm liq})}+\|g_5\|_{L^2(\Omega_{\rm liq})}. \tag{4.15}$$

After substituting a_2, a_3, a_5 and a_6 into (4.12a), the estimate

$$\begin{aligned}\|a_1\|_{H^2(\Omega)}\le C_3(&\|g_1\|_{L^2(\Omega)}+\|g_2\|_{L^2(\Omega_{\rm Si})}+\|g_3\|_{L^2(\Omega_{\rm Si})}+2\|g_6\|_{L^2(\Omega_{\rm liq})}\\&+2\|g_7\|_{L^2(\Omega_{\rm liq})}+\|g_4\|_{H^2(\Omega_{\rm liq})}+\|g_5\|_{H^2(\Omega_{\rm liq})}+\|a_8\|_{H^{1/2}(\Gamma)}+\|a_9\|_{L^2(\Gamma)})\end{aligned}$$

follows. By Equations (4.12m)–(4.12n) and Assumption 4.1, there exists a sufficiently small constant C_4 such that the inequality

$$\|a_8\|_{H^{1/2}(\Gamma)}+\|a_9\|_{L^2(\Gamma)}\le C_4\|a_1\|_{H^2(\Omega)}+\|g_7\|_{H^{1/2}(\Gamma)}+\|g_8\|_{L^2(\Gamma)}$$

holds. For sufficiently small C_4, i.e., if $C_3C_4<1$, we find

$$\begin{aligned}(1-C_3C_4)\|a_1\|_{H^2(\Omega)}\le C_3(&\|g_1\|_{L^2(\Omega)}+\|g_2\|_{L^2(\Omega_{\rm liq})}+\|g_3\|_{L^2(\Omega_{\rm liq})}+\|g_4\|_{L^2(\Omega_{\rm liq})}\\&+\|g_5\|_{L^2(\Omega_{\rm liq})}+2\|g_6\|_{L^2(\Omega_{\rm liq})}+2\|g_7\|_{L^2(\Omega_{\rm liq})}+2\|g_8\|_{H^{1/2}(\Gamma)}+2\|g_9\|_{L^2(\Gamma)}).\end{aligned}$$

Therefore, the Fréchet derivative of G at the equilibrium solution has a bounded inverse, i.e., there is a constant C such that

$$\|D_{(\hat V,\hat u,\hat v,\mathbf{u},P,\hat{c^+},\hat{c^-},\alpha,\gamma)}G\big((V_e-V_D(0),0,0,\mathbf{u}_e,P_e,0,0,\alpha_e,\gamma_e),0\big)^{-1}\|\le C,$$

where the norm is the operator norm of

$$\chi\to H^2(\Omega)\times H^2(\Omega_{\rm Si})^2\times H^2_{{\rm div},0}(\Omega_{\rm liq};\mathbb{R}^3)\times H^2(\Omega_{\rm liq})^3\times H^{1/2}(\Gamma)\times L^2(\Gamma).$$

Finally, the implicit-function theorem yields the assertion. ∎

5. Conclusions

This work presents a fully coupled stationary system of partial differential equations as the basic mathematical model for nanowire sensors as well as for nanopore sensors. It also presents existence and uniqueness results for this system of equations. The new model considers all three subdomains with different transport properties in nanoscale devices of these kinds and includes the Stokes equations for describing the background medium. This model completes the predominant model which does not take into account the flow of the background medium and only uses the drift-diffusion-Poisson system.

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