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ANALYSIS OF THE DRIFT-DIFFUSION-POISSON–BOLTZMANN SYSTEM FOR NANOWIRE AND NANOPORE SENSORS IN THE ALTERNATING-CURRENT REGIME*

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Abstract. The basic analytical properties of the drift-diffusion-Poisson–Boltzmann system in the alternating-current (AC) regime are shown. The analysis of the AC case differs from the direct-current (DC) case and is based on extending the transport model to the frequency domain and writing the variables as periodic functions of the frequency in a small-signal approximation. We first present the DC and AC model equations to describe the three types of material in nanowire field-effect sensors: The drift-diffusion-Poisson system holds in the semiconductor, the Poisson–Boltzmann equation holds in the electrolyte, and the Poisson equation provides self-consistency. Then the AC model equations are derived. Finally, existence and local uniqueness of the solution of the AC model equations are shown. Real-world applications include nanowire field-effect bio- and gas sensors operating in the AC regime, which were only demonstrated experimentally recently. Furthermore, nanopore sensors are governed by the system of model equations and the analysis as well.

Keywords. Drift-diffusion-Poisson–Boltzmann system; existence, local uniqueness; charge transport; alternating current; field-effect sensor; nanowire sensor; nanocapacitor; nanopore sensor; nanotechnology.

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

1. Introduction

In this work, the mathematical modeling of affinity based field-effect sensors is considered in the alternating-current (AC) regime. While nanowire field-effect bio- and gas sensors operating in the direct-current (DC) regime have been established experimentally in the past decade, their use in the AC regime is more recent and has been shown to yield more physical insight and additional sensing information. Sensor based on nanopores and the principle of the Coulter counter are governed by the model equations in this work as well.

The working principle of nanowire field-effect sensors [22, 23, 27] is that the target molecules to be detected in a liquid change the charge concentration at the sensor surface after selectively binding to receptor molecules, which in turn modulates the conductance of the semiconducting nanowire. The currents through the nanowires are recorded and indicate the number of target molecules present. A schematic diagram 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 DNA and RNA oligomers as well as antigens with known antibodies can be detected. The functioning of nanowire gas sensors [7, 12, 13, 24, 25] is analogous.

The mathematical modeling of affinity based field-effect sensors and semiconductor devices in general has been addressed previously only in the DC regime [1, 9, 17, 26]. Furthermore, in [8], a multiscale problem inherent in nanowire sensors was solved and lead

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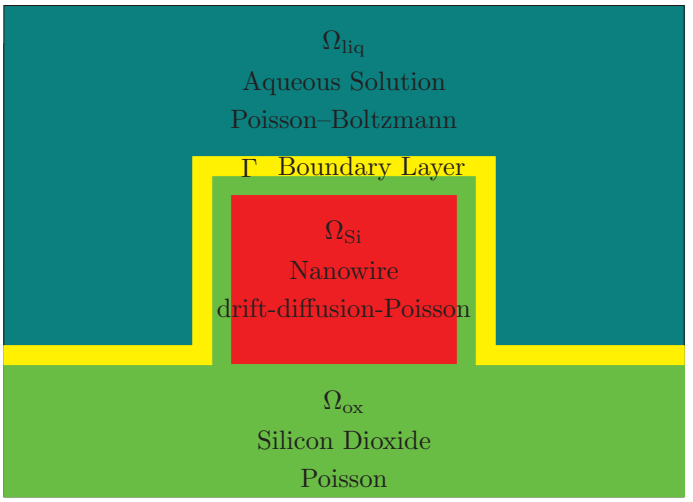

FIG. 1.1. *Schematic diagram of a cross section of a nanowire field-effect sensor.*

to the interface conditions used below. In [10], an effective equation for the covariance was derived after homogenization of a random charge distribution at a sensor surface. In [2], existence and uniqueness for the drift-diffusion-Poisson system with interface conditions were shown for the DC regime. A parallel numerical method was developed in [3]. These mathematical results have then been used to provide quantitative understanding and to optimize sensor design [4, 5].

More recently, such nanowire field-effect sensors have been fabricated for use in the AC regime and characterized [14, 18–21]. In the experiments, the electric potentials around the DC equilibrium are small and the frequencies are low enough to ensure that the free charge carriers in the liquid are equilibrated, avoiding spurious signals.

Nanopore sensors are also described by the same transport equations. Here the particles that move in a self-consistent manner are anions, cations, and target molecules. The principle of a nanopore sensor is similar to the Coulter counter. A schematic diagram is shown in Figure 1.2.

In this work, we derive the basic model equations for the AC small-signal regime for affinity-based field-effect sensors from the drift-diffusion-Poisson system. Whenever the frequency ω of the applied current is sufficiently small, the solution of the system of model equations can be written in terms of the real part of $\exp(\mathrm{i}\omega t)$. This makes it possible to derive the AC model equations, which are the drift-diffusion-Poisson system governing charge transport coupled to the Poisson–Boltzmann equation for the liquid. The unknowns are the electric potential and the concentrations of the positive and negative charge carriers. After the derivation of the system of model equations, the main results of this work are existence and local uniqueness shown for the AC model equations. As is known from the simpler DC drift-diffusion-Poisson system, only local uniqueness can be expected to hold so that the present results are strict.

The rest of the paper is organized as follows. The starting point, namely the DC model equations, is presented in Section 2 and, based on this discussion, the AC model equations are derived in Section 3. Then the main mathematical results, primarily existence and local uniqueness for the AC system, are shown in Section 3.3. Finally, the conclusions are drawn in Section 4.

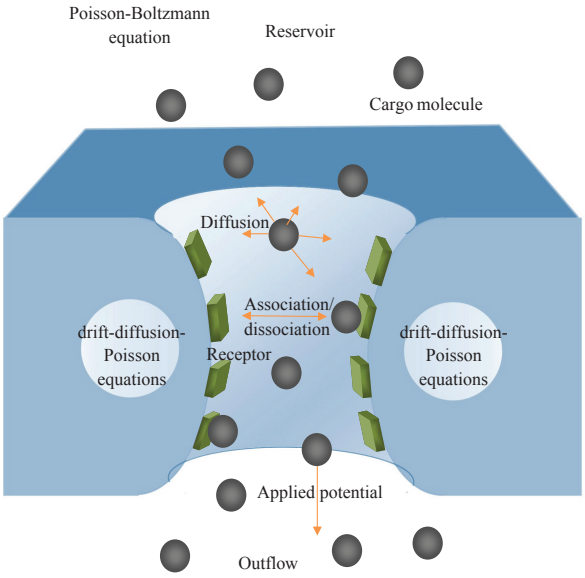

FIG. 1.2. *Schematic diagram of a nanopore sensor.*

2. The DC model equations

In this section, we start with a summary of the DC model equations, i.e., the drift-diffusion-Poisson system. In the next section, the AC model equations will be derived from these equations.

The domain $\Omega \subset \mathbb{R}^d$ $(d \leq 3)$ is assumed to be bounded and convex with smooth boundary $\partial\Omega$. In order to model an affinity based sensor, the domain is divided into three subdomains: the semiconductor Ω_{Si} (usually silicon), the dielectric Ω_{ox} (usually silicon oxide), and the electrolyte Ω_{liq} (a liquid containing free ions).

The Poisson equation for the electrostatic potential V is solved on the whole domain Ω and provides self-consistency. More precisely, in the subdomain Ω_{Si}, the drift-diffusion-Poisson system models charge transport. In the second subdomain Ω_{ox}, the Poisson equation holds with a vanishing right side, and in the third domain Ω_{liq}, the nonlinear Poisson–Boltzmann equation holds (see Figure 1.1).

The biofunctionalized layer at the manifold Γ between the subdomains Ω_{liq} and Ω_{ox} is responsible for the recognition of the target molecules. The charges there can be included as immobile charges in ρ_i and free charges in ρ_f, or—since they are many and small—they can be viewed as giving rise to a multiscale problem. Homogenization of a layer at a manifold in elliptic problems yields two interface conditions [8]. The rapidly oscillating charge concentration near Γ is replaced, as $\epsilon \to 0+$, by the two interface conditions

$$V(0+,y) - V(0-,y) = \alpha(y), \tag{2.1a}$$

$$A(0+)\partial_x V(0+,y) - A(0-)\partial_x V(0-,y) = \gamma(y), \tag{2.1b}$$

where α and γ are essentially given by the dipole-moment and the surface-charge densities of the boundary layer. The local (macroscopic) coordinates are chosen so that $x = 0$

corresponds to Γ and the y-coordinate is normal to Γ. The values of α and γ in the interface conditions result from microscopic models M_α and M_γ for the dipole-moment density and surface charge density of the boundary layer. They generally depend on the electrostatic potential and can be modeled by various means [6, 8].

In summary, the model equations for the DC case (see for example [2]) are the transient boundary-value problem

$$
\begin{aligned}
-\nabla\cdot(A\nabla V) &= q(C_{\mathrm{dop}} + Z_p p + Z_n n) && \text{in } \Omega_{\mathrm{Si}}, && \text{(2.2a)}\\
-\nabla\cdot(A\nabla V) &= 0 && \text{in } \Omega_{\mathrm{ox}}, && \text{(2.2b)}\\
-\nabla\cdot(A\nabla V) &= -2\eta\sinh(\beta(V-\Phi)) && \text{in } \Omega_{\mathrm{liq}}, && \text{(2.2c)}\\
\frac{\partial p}{\partial t} + R &= \frac{-1}{Z_p q}\nabla\cdot J_p && \text{in } \Omega_{\mathrm{Si}}, && \text{(2.2d)}\\
\frac{\partial n}{\partial t} + R &= \frac{-1}{Z_n q}\nabla\cdot J_n && \text{in } \Omega_{\mathrm{Si}}, && \text{(2.2e)}\\
J_p &= q(-D_p\nabla p - \mu_p p\nabla V) && && \text{(2.2f)}\\
J_n &= q(D_n\nabla n - \mu_n n\nabla V) && && \text{(2.2g)}\\
V(0+,y) - V(0-,y) &= \alpha(y) && \text{on } \Gamma, && \text{(2.2h)}\\
A(0+)\partial_x V(0+,y) - A(0-)\partial_x V(0-,y) &= \gamma(y) && \text{on } \Gamma, && \text{(2.2i)}\\
\alpha &= M_\alpha(V) && \text{on } \Gamma, && \text{(2.2j)}\\
\gamma &= M_\gamma(V) && \text{on } \Gamma, && \text{(2.2k)}\\
p(t=0) = p_I,\ n(t=0) &= n_I && \text{in } \Omega_{\mathrm{Si}} && \text{(2.2l)}\\
V &= V_D && \text{on } \partial\Omega_D, && \text{(2.2m)}\\
\nabla V\cdot\mathbf{n} &= 0 && \text{on } \partial\Omega_N, && \text{(2.2n)}\\
p = p_D, \quad n &= n_D && \text{on } \partial\Omega_{D,\mathrm{Si}}, && \text{(2.2o)}\\
J_p\cdot\mathbf{n} = 0, \quad J_n\cdot\mathbf{n} &= 0 && \text{on } \partial\Omega_{N,\mathrm{Si}} && \text{(2.2p)}
\end{aligned}
$$

for almost all $t\in[0,T_0]$, where V is the electrostatic potential, A is the electric permittivity, $q>0$ is the elementary charge, and C_{dop} is the doping concentration. D_p and D_n are the diffusion coefficients, and μ_p and μ_n are the mobilities of the charge carriers. In the case of a nanowire sensor, $p=p(t,x)$ and $n=n(t,x)$ are the concentrations of holes and electrons, respectively: $Z_p := 1$ for holes and $Z_n := -1$ for electrons. In the case of a nanopore sensor, the charge carriers are cations and anions and the constants Z_p and Z_n correspond to their valences. Furthermore, Φ is the Fermi potential, η is the bulk concentration and $\beta := q/(k_B T)$, where k_B is the Boltzmann constant and T is temperature. Finally, J_p and J_n are the current densities, and R is the recombination rate.

2.1. Existence and local uniqueness for the transient DC model equations. Existence and local uniqueness for the transient system (2.2) is an extension of the theory of the stationary drift-diffusion-Poisson system [15, 16], while extending to the additional subdomain Ω_{liq}, where the nonlinear Poisson–Boltzmann Equation (2.2c) holds, and including the interface conditions (2.2h)–(2.2i). The interface conditions necessitate an estimate for the electrostatic potential V so that the Schauder fixed-point theory can eventually be applied. The details of the stationary case can be found in [2]. Based on this result, the following result for the transient case, i.e., a system of parabolic and elliptic equations, can be shown. Note that in transient problems, the existence of a solution can only be established for a sufficiently small time interval by a fixed-point

argument.

We consider the general form of the elliptic part of the problem

$$-\nabla\cdot(A(x)\nabla V)+g(x,V)=f \qquad \forall x\in\Omega\setminus\Gamma, \tag{2.3a}$$

$$V=V_D \qquad \forall x\in\partial\Omega_D, \tag{2.3b}$$

$$\nabla V\cdot\mathbf{n}=0 \qquad \forall x\in\partial\Omega_N, \tag{2.3c}$$

$$V(0+,y)-V(0-,y)=\alpha(y) \qquad \forall x\in\Gamma, \tag{2.3d}$$

$$A(0+)\partial_x V(0+,y)-A(0-)\partial_x V(0-,y)=\gamma(y) \qquad \forall x\in\Gamma, \tag{2.3e}$$

and the coefficients and boundary conditions in system (2.2) must satisfy the following assumptions.

Assumptions 2.1.

(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 $\partial\Omega_N$ with $|\partial\Omega_N|>0$ consists of C^2 segments. The C^2 manifold $\Gamma\subset\Omega$ splits the domain Ω into two nonempty domains $\Omega^+=\Omega_{\mathrm{ox}}\cup\Omega_{\mathrm{Si}}$ and $\Omega^-=\Omega_{\mathrm{Si}}$ so that $\mathrm{meas}(\Gamma\cap\partial\Omega)=0$ and $\Gamma\cap\partial\Omega\subset\partial\Omega_N$ hold.*

(2) *The coefficient function $A(x)$ is uniformly elliptic, bounded function with*

$$0<A^-\le\operatorname{essinf}_{x\in\Omega}A(x)\le\|A(x)\|_{L^\infty(\Omega)}\le A^+<\infty \qquad \text{a.e. in } \Omega, \tag{2.4}$$

where $A(x)|_{\Omega^+}\in C^1(\Omega^+,\mathbb{R}^{3\times3})$ and $A(x)|_{\Omega^-}\in C^1(\Omega^-,\mathbb{R}^{3\times3})$. Furthermore, the inclusions $V_D(x)\in H^{1/2}(\partial\Omega)\cap L^\infty(\Gamma)$, $p_D(x,t),n_D(x,t)\in L^2((0,T_0);H^{1/2}(\partial\Omega_{\mathrm{Si}}))$, and $f(x)\in L^\infty(\Omega)$ hold.

(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) *The quasi Fermi-level $\Phi(x)$ is bounded above and below, and we define*

$$\underline{\Phi}:=\inf_{x\in\Omega}\Phi(x)\le\Phi(x)\le\sup_{x\in\Omega}\Phi(x)=:\overline{\Phi}.$$

(5) *There are constants $0\le R_0<\infty$ and $T_0>0$ such that*

$$\|(p_D,n_D)\|_X\le R_0 \qquad \forall(x,t)\in\partial\Omega_{\mathrm{Si}}\times[0,T_0],$$

where

$$X:=\left\{(p_D,n_D)\,\middle|\,p_D,n_D\in L^4((0,T_0);H^{1/2}(\partial\Omega_{\mathrm{Si}}))\right\}$$

with the norm

$$\|(p_D,n_D)\|_X:=\|p_D\|_{L^4((0,T_0);H^{1/2}(\partial\Omega_{\mathrm{Si}}))}+\|n_D\|_{L^4((0,T_0);H^{1/2}(\partial\Omega_{\mathrm{Si}}))}.$$

(6) *The microscopic models M_α and M_γ depend continuously in $H^1(\Omega)$ on the potential $V(x)$, and 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.*

Using the assumptions, we can formulate the existence of weak solutions of the system (2.2). Proof of this theorem is straightforward using the Schauder fixed-point theorem.

PROPOSITION 2.1 (Existence of weak solutions to the DC model). *Under Assumptions (2.1), there exist a time* $T_0 \in (0,\infty)$ *and a weak solution*

$$\begin{aligned}(V,p,n,\alpha,\gamma) \in &\left(H^1(\Omega)\cap L^\infty(\Omega)\right)\\ &\times \left(L^2\left((0,T_0);H^1(\Omega_{\mathrm{Si}})\right)\cap L^\infty(\Omega_{\mathrm{Si}}\times[0,T_0])\right)^2\\ &\times \left(L^\infty(\Gamma)\cap H^{1/2}(\Gamma)\right)\times L^2(\Gamma)\end{aligned}$$

of the system (2.2). The function V *satisfies the* L^∞*-estimate*

$$\underline{V} \le V(x) \le \overline{V} \qquad \text{in } \Omega, \tag{2.5}$$

where

$$\underline{V} := \min\left(\inf_{\partial\Omega_D} V_D, \underline{\Phi} - \sup_{\Omega} V_L, U_T \sinh^{-1}\left(\frac{\underline{C}}{2n_i}\right) + \underline{\Phi} - \sup_{\Omega} V_L\right), \tag{2.6a}$$

$$\overline{V} := \max\left(\sup_{\partial\Omega_D} V_D, \overline{\Phi} - \inf_{\Omega} V_L, U_T \sinh^{-1}\left(\frac{\overline{C}}{2n_i}\right) + \overline{\Phi} - \inf_{\Omega} V_L\right), \tag{2.6b}$$

$\underline{\Phi} \le \Phi(x) \le \overline{\Phi}$ *holds.* $U_T = 1/\beta$ *is the thermal voltage and* V_L *is the solution of the linear elliptic equation (equation (2.3) with* $g = 0$*), 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.

Furthermore, the estimate

$$\|(p,n)\|_X \le R_0$$

holds for every $x \in \Omega_{\mathrm{Si}}$ *and for almost all* $t \in [0,T_0]$*, where the constant* R_0 *is radius of the ball*

$$B_{R_0} := \{(p,n) \in X \mid \|(p,n)\|_X \le R_0\} \subset X$$

and $X := \left\{(p,n) \,\middle|\, p,n \in L^4\left((0,T_0);L^2(\Omega_{\mathrm{Si}})\right)\right\}$ *with the norm*

$$\|(p,n)\|_X := \|p\|_{L^4((0,T_0);L^2(\Omega_{\mathrm{Si}}))} + \|n\|_{L^4((0,T_0);L^2(\Omega_{\mathrm{Si}}))}.$$

Proposition 2.1 shows the existence of weak solutions of the DC model system (2.2). 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 one assumes that particle velocities or momenta are distributed according to a Maxwellian distribution, i.e., that they are in thermal equilibrium. However, large applied voltages result in fast particles which are modeled badly by a Maxwellian distribution.

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

Since the uniqueness is only local, the maximum principle is not helpful for proving uniqueness. The local uniqueness of solutions of the problem (2.2) is straightforward and can be shown using the implicit-function theorem around the equilibrium solution $(V_e,p_e,n_e,\alpha_e,\gamma_e)$. To apply the implicit-function theorem, one should show that the Fréchet derivative of the problem has a bounded inverse at the equilibrium solution. To this end, the norm estimation of the inverse of the linearization of the equations (2.2) at the equilibrium solution is needed. As mentioned before, the main assumption that we should make is that the applied voltages, i.e., the Dirichlet boundary conditions for the potential, are sufficiently small. We assume that the Dirichlet boundary conditions for the potential V are constants on each of r segments or contacts of the the Dirichlet boundary $\partial\Omega_D$ and denote the potentials there by the vector $(U_1,U_2,\dots,U_r)$.

In order to state local uniqueness for small applied voltages, we need the following assumptions:

Assumptions 2.2.

(1) The domain $\Omega\subset\mathbb{R}^3$ is open and bounded and the boundary $\partial\Omega$ is as smooth as necessary (see Assumptions (2.1)).

(2) The Dirichlet data (V_D,p_D,n_D) are a Lipschitz-continuously differentiable map of $U:=(U_1,U_2,\dots,U_r)$, $\mathbb{R}^r\to H^2(\Omega)\times L^2((0,T_0);H^2(\Omega_{\mathrm{Si}}))^2$.

(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

$$\|M'_\alpha(V)\|_{H^{1/2}(\Gamma)}+\|M'_\gamma(V)\|_{L^2(\Gamma)}\le C\|V\|_{H^2(\Omega)} \tag{2.7}$$

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

(4) The Shockley-Read-Hall recombination rate R has the form $R=(np-n_i^2)\kappa(t,x,n,p)$, where $\kappa(t,x,\cdot,\cdot)\in C^2(\mathbb{R}^2_+)$ holds for $x\in\Omega$ and for almost all $t\in[0,T_0]$, and where the derivatives $\partial^\nu_{(n,p)}\kappa(\cdot,\cdot,n,p)$ are bounded uniformly for all (n,p) in bounded subsets of $\mathbb{R}^2_+$ and for all multiindices ν with $|\nu|\le 2$. Furthermore, there are constants $\underline{\kappa}$ and $\overline{\kappa}$ such that either $0<\underline{\kappa}\le\kappa(t,x,n_e,p_e)\le\overline{\kappa}$ or $\kappa(t,x,n_e,p_e)=0$ for all $x\in\Omega_{\mathrm{Si}}$ and for almost all $t\in[0,T_0]$.

Proposition 2.2 (Local uniqueness of weak solutions to the DC model). *Under Assumptions (2.1) and (2.2), there exists a sufficiently small $\sigma\in\mathbb{R}$ with $|U|<\sigma$ such that the problem (2.2), has a locally unique solution*

$$\Big(V^*(U),p^*(U),n^*(U),\alpha^*(U)\gamma^*(U)\Big)\in H^2(\Omega)\times L^2((0,T_0);H^2(\Omega_{\mathrm{Si}}))^2 \times H^{1/2}(\Gamma)\times L^2(\Gamma).$$

The solution satisfies

$$\Big(V^*(0),p^*(0),n^*(0),\alpha^*(0),\gamma^*(0)\Big)=(V_e,p_e,n_e,\alpha_e,\gamma_e)$$

and it depends continuously differentiable on the Dirichlet boundary data U as a map from $\{U\in\mathbb{R}^r\,|\,|U|<\sigma\}$ into $H^2(\Omega)\times L^2((0,T_0);H^2(\Omega_{\mathrm{Si}}))^2\times H^{1/2}(\Gamma)\times L^2(\Gamma)$.

3. Main results: the AC model equations

The system (2.2) also models the specific physical situation when an alternating current is applied at the contacts, i.e., when the Dirichlet boundary conditions are transient linear combinations of sine and cosine functions. For these boundary conditions, we derive model equations in this section. These model equations will be stationary, albeit with double the number of unknowns. This means that in the case when the frequency is low enough to justify this model, no computationally expensive solutions of the full transient system (2.2) are necessary, but the stationary system derived here can be used instead.

To find the model equations in the frequency domain, we start by writing the AC solution (V,n,p) as what could be called a periodic perturbation of the DC solution (V_*,n_*,p_*) of system (2.2) as

$$V = V_* + \tilde{V}\exp(\mathrm{i}\omega t), \tag{3.1a}$$

$$n = n_* + \tilde{n}\exp(\mathrm{i}\omega t), \tag{3.1b}$$

$$p = p_* + \tilde{p}\exp(\mathrm{i}\omega t), \tag{3.1c}$$

where $\tilde{V}$, $\tilde{n}$, and $\tilde{p}$ are the complex amplitudes of the AC potential V, the AC electron concentration n, and the AC hole concentration p, respectively. The variables V_*, n_*, and p_* are the DC potential and charge concentrations.

The form (3.1) of the AC unknowns V, n, and p already contains physical assumptions. The main assumption is that the relaxation time of the charge carriers is small compared to the frequency of the sinusoidal applied potentials. The relaxation time here is in the order of the momentum relaxation time. If this were not the case, the solution (V,n,p) could not be written in this form and transport models more complicated than the drift-diffusion-Poisson system would have to be used. The small-frequency assumption is the first part of Assumptions 3.1, and it is satisfied in the experiments performed so far (e.g., [14, 20, 21]).

Assumptions 3.1.

(1) The frequency ω in equations (3.1) of the applied AC potentials (i.e., the Dirichlet boundary conditions) is sufficiently small such that the free charge carriers are essentially in equilibrium at each point in time.

(2) The amplitudes of the applied AC potentials are sufficiently small, and hence the amplitudes $\tilde{V}$, $\tilde{n}$, and $\tilde{p}$ in equations (3.1) are also small. More precisely, it is assumed that they are small compared to the thermal voltage k_BT/q, i.e.,

$$\|\tilde{n}\|_\infty \ll \frac{k_BT}{q}, \quad \|\tilde{p}\|_\infty \ll \frac{k_BT}{q}, \quad \text{and} \quad \|\tilde{V}\|_\infty \ll \frac{k_BT}{q}. \tag{3.2}$$

(3) $\|\tilde{V}\|_{H^1}$ is sufficiently small.

The second part of the assumptions means that the applied AC potentials are not too large. If they were too large, the validity of the drift-diffusion-Poisson model would be questionable to begin with, since only local uniqueness holds (see Section 2.1).

The third part of the assumptions is satisfied because of the regularity of solutions of elliptic problems. It is noted here since it plays an important role in the derivation of the model equations.

In order to find the model equations for the AC case, the next step is of course to substitute V, n, and p in equations (3.1) into the transient model equations (2.2).

3.1. The Poisson equation. We start with the Poisson equation (2.2a). Substituting equations (3.1), we get

$$\begin{aligned}\nabla\cdot(A\nabla V_*)+\nabla\cdot\big(A\nabla(\tilde{V}\exp(\mathrm{i}\omega t))\big)+qC_{\mathrm{dop}}\\ +q(Z_p p_*+Z_n n_*+Z_p\tilde{p}\exp(\mathrm{i}\omega t)+Z_n\tilde{n}\exp(\mathrm{i}\omega t))=0.\end{aligned}\tag{3.3}$$

Then, we subtract the DC Poisson equation for V_* and can cancel the exponential terms to obtain the AC Poisson equation

$$\nabla\cdot(A\nabla\tilde{V})+q(Z_p\tilde{p}+Z_n\tilde{n})=0\tag{3.4}$$

that holds in in Ω_{liq} and Ω_{Si}. In Ω_{ox}, the AC Poisson equation is simply

$$\nabla\cdot(A\nabla\tilde{V})=0.\tag{3.5}$$

3.2. The current equations. Regarding the transport part of the model, we consider the DC transport model (2.2d)–(2.2g) and substitute solutions of the form (3.1). The time derivative becomes

$$\frac{\partial p}{\partial t}=\frac{\partial p_*}{\partial t}+\mathrm{i}\omega\tilde{p}\exp(\mathrm{i}\omega t)\tag{3.6}$$

and the current is

$$J_p=-q\Big(D_p\nabla p+Z_p\mu_p p\nabla V\Big),\tag{3.7}$$

where $Z_p=1$. Then using equations (3.1), we have

$$\begin{aligned}J_p=-q\Big(&D_p\nabla p_*+D_p\exp(\mathrm{i}\omega t)\nabla\tilde{p}+\mu_p p_*\nabla V_*+\mu_p p_*\exp(\mathrm{i}\omega t)\nabla\tilde{V}\\ &+\mu_p\tilde{p}\exp(\mathrm{i}\omega t)\nabla V_*+\mu_p\tilde{p}\exp(2\mathrm{i}\omega t)\nabla\tilde{V}\Big).\end{aligned}\tag{3.8}$$

The last term is of second order in $\exp(\mathrm{i}\omega t)$. We will neglect it, because it is sufficiently small due to Assumption 3.1. Therefore, the transport equation becomes

$$\begin{aligned}\frac{\partial p_*}{\partial t}+\mathrm{i}\omega\tilde{p}\exp(\mathrm{i}\omega t)+R=\nabla\cdot\Big(&D_p\nabla p_*+D_p\exp(\mathrm{i}\omega t)\nabla\tilde{p}+\mu_p p_*\nabla V_*\\ &+\mu_p p_*\exp(\mathrm{i}\omega t)\nabla\tilde{V}+\mu_p\tilde{p}\exp(\mathrm{i}\omega t)\nabla V_*\Big).\end{aligned}\tag{3.9}$$

After subtracting the DC transport model (2.2d) and equation (3.7) and canceling the exponential terms, the first equation of the AC transport model is obtained as

$$\nabla\cdot(D_p\nabla\tilde{p})+\nabla\cdot\big(\mu_p\nabla V_*\tilde{p}\big)+\nabla\cdot\big(\mu_p p_*\nabla\tilde{V}\big)-\mathrm{i}\omega\tilde{p}=0.\tag{3.10}$$

Following the analogous calculation starting from the DC equations (2.2e) and (2.2g), we obtain the second equation of the AC transport model as

$$\nabla\cdot(D_n\nabla\tilde{n})+\nabla\cdot\big(\mu_n\nabla V_*\tilde{n}\big)+\nabla\cdot\big(\mu_n n_*\nabla\tilde{V}\big)-\mathrm{i}\omega\tilde{n}=0.\tag{3.11}$$

3.3. Existence and local uniqueness for the AC model equations. In this section, existence and uniqueness of the solution of the AC model equations (3.4), (3.10), and (3.11), which were derived in the previous section, will be shown. As the AC model is a system of complex valued equations, we consider the real and imaginary parts of the equations separately. To this end, we write the complex amplitudes as

$$\begin{aligned}\tilde{p} &= \Re(\tilde{p}) + \mathrm{i}\Im(\tilde{p}),\\ \tilde{n} &= \Re(\tilde{n}) + \mathrm{i}\Im(\tilde{n}),\\ \tilde{V} &= \Re(\tilde{V}) + \mathrm{i}\Im(\tilde{V}),\end{aligned}$$

where $\Re$ and $\Im$ denote the real and imaginary parts. Then the complex valued equations become the real valued equations

$$-\nabla\cdot(A\nabla\Re(\tilde{V})) = \begin{cases} q(\Re(\tilde{p}) - \Re(\tilde{n})) & \text{in } \Omega_{\mathrm{Si}}\cup\Omega_{\mathrm{liq}},\\ 0 & \text{in } \Omega_{\mathrm{ox}},\end{cases} \tag{3.12a}$$

$$-\nabla\cdot(A\nabla\Im(\tilde{V})) = \begin{cases} q(\Im(\tilde{p}) - \Im(\tilde{n})) & \text{in } \Omega_{\mathrm{Si}}\cup\Omega_{\mathrm{liq}},\\ 0 & \text{in } \Omega_{\mathrm{ox}},\end{cases} \tag{3.12b}$$

$$-\nabla\cdot(D_p\nabla\Re(\tilde{p})) - \nabla\cdot\big(\mu_p\nabla V_*\Re(\tilde{p})\big) = \nabla\cdot\big(\mu_p p_*\nabla\Re(\tilde{V})\big) + \omega\Im(\tilde{p}) \quad \text{in } \Omega_{\mathrm{Si}}, \tag{3.12c}$$

$$-\nabla\cdot(D_p\nabla\Im(\tilde{p})) - \nabla\cdot\big(\mu_p\nabla V_*\Im(\tilde{p})\big) = \nabla\cdot\big(\mu_p p_*\nabla\Im(\tilde{V})\big) - \omega\Re(\tilde{p}) \quad \text{in } \Omega_{\mathrm{Si}}, \tag{3.12d}$$

$$-\nabla\cdot(D_n\nabla\Re(\tilde{n})) + \nabla\cdot\big(\mu_n\nabla V_*\Re(\tilde{n})\big) = -\nabla\cdot\big(\mu_n n_*\nabla\Re(\tilde{V})\big) + \omega\Im(\tilde{n}) \quad \text{in } \Omega_{\mathrm{Si}}, \tag{3.12e}$$

$$-\nabla\cdot(D_n\nabla\Im(\tilde{n})) + \nabla\cdot\big(\mu_n\nabla V_*\Im(\tilde{n})\big) = -\nabla\cdot\big(\mu_n n_*\nabla\Im(\tilde{V})\big) - \omega\Re(\tilde{n}) \quad \text{in } \Omega_{\mathrm{Si}}. \tag{3.12f}$$

The interface between the liquid and the semiconductor in the AC model is described by the equations

$$\begin{aligned}\Re(\tilde{V})(0+,y) - \Re(\tilde{V})(0-,y) &= \alpha(y),\\ A(0+)\partial_x\Re(\tilde{V})(0+,y) - A(0-)\partial_x\Re(\tilde{V})(0-,y) &= \gamma(y),\\ \Im(\tilde{V})(0+,y) - \Im(\tilde{V})(0-,y) &= 0,\\ A(0+)\partial_x\Im(\tilde{V})(0+,y) - A(0-)\partial_x\Im(\tilde{V})(0-,y) &= 0\end{aligned} \tag{3.13}$$

on Γ. Moreover, the Dirichlet boundary conditions on $\partial\Omega_D$ in the AC model read as

$$\begin{aligned}\Re(\tilde{V}) &= \Re(\tilde{V}_D), & \Im(\tilde{V}) &= \Im(\tilde{V}_D),\\ \Re(\tilde{p}) &= \Re(\tilde{p}_D), & \Im(\tilde{p}) &= \Im(\tilde{p}_D),\\ \Re(\tilde{n}) &= \Re(\tilde{n}_D), & \Im(\tilde{n}) &= \Im(\tilde{n}_D),\end{aligned} \tag{3.14}$$

and the Neumann boundary conditions on $\partial\Omega_N$ as

$$\begin{aligned}\nabla\Re(\tilde{V})\cdot\mathbf{n} &= 0, & \nabla\Im(\tilde{V})\cdot\mathbf{n} &= 0,\\ \nabla\Re(\tilde{p})\cdot\mathbf{n} &= 0 & \nabla\Im(\tilde{p})\cdot\mathbf{n} &= 0,\\ \nabla\Re(\tilde{n})\cdot\mathbf{n} &= 0 & \nabla\Im(\tilde{n})\cdot\mathbf{n} &= 0.\end{aligned} \tag{3.15}$$

To discuss the system (3.12)–(3.15), we note that all the equations are special cases of the general form

$$-\nabla\cdot(A\nabla u) \mp \nabla\cdot(\mathbf{b}u) = f \qquad \forall x\in\Omega\setminus\Gamma, \tag{3.16a}$$

$$u = u_D \qquad \forall x \in \partial\Omega_D, \tag{3.16b}$$

$$\nabla u \cdot \mathbf{n} = 0 \qquad \forall x \in \partial\Omega_N, \tag{3.16c}$$

$$u(0+,y) - u(0-,y) = \alpha(y) \qquad \forall x \in \Gamma, \tag{3.16d}$$

$$A(0+)\partial_x u(0+,y) - A(0-)\partial_x u(0-,y) = \gamma(y) \qquad \forall x \in \Gamma, \tag{3.16e}$$

where u represents either $\Re(\tilde{V})$ and $\Im(\tilde{V})$. Because of Assumptions 2.1, A is uniformly bounded.

The second term on the left-hand side of equation (3.16a) is additional to fixed-point arguments for the usual drift-diffusion-Poisson system [11, 16], [2, Lemma 3.1]. The complications arising from this term are dealt with in the following lemma and the existence and uniqueness results below. The following lemma shows that under a certain condition, the above problem has a unique solution.

LEMMA 3.1 (Existence and uniqueness of solutions of equations (3.16)). *Under Assumptions 2.1, if*

$$BC_P \le A^-$$

holds, where $A^- \le \|A\|_{L^\infty} \le A^+$, $\|\mathbf{b}\|_{L^\infty} \le B$, *and* C_P *is a Poincaré constant, then the boundary-value problem with interface conditions* (3.16) *has a unique solution* $u \in H^1_{u_D}(\Omega)$. *Furthermore, the estimate*

$$\|u\|_{H^1(\Omega)} \le C(\|f\|_{L^2(\Omega)} + \|u_D\|_{H^{1/2}(\partial D_{\mathrm{Si},D})} + \|\alpha\|_{H^{1/2}(\Gamma)} + \|\gamma\|_{L^2(\Gamma)}) \tag{3.17}$$

holds true.

Proof. Multiplying the equations (3.16) by a test function $v \in H^1_0(\Omega)$ and integrating by parts, we obtain the weak formulation

$$\int_\Omega A\nabla w \cdot \nabla v \pm \int_\Omega \mathbf{b} w \cdot \nabla v = \int_\Omega fv - \int_\Omega A\nabla(\overline{u}_D + \overline{\alpha}) \cdot \nabla v \mp \int_\Omega \mathbf{b}(\overline{u}_D + \overline{\alpha}) \cdot \nabla v + \int_\Gamma \gamma v \qquad \forall v \in H^1_0(\Omega), \tag{3.18}$$

where $w := u - \overline{u}_D - \overline{\alpha}$ and $\overline{u}_D$ is the Dirichlet lift of u_D in Ω. Also, $\overline{\alpha} \in L^2(\overline{\Omega})$ is an extension of $\alpha \in H^{1/2}(\Gamma)$. Therefore, the weak solution of the boundary-value problem (3.16) is $u \in H^1_{u_D}(\Omega)$ which satisfies

$$a(u,v) = \ell(v) \qquad \forall v \in H^1_0(\Omega), \tag{3.19}$$

where

$$a(u,v) := \int_\Omega A\nabla u \cdot \nabla v \pm \int_\Omega \mathbf{b} u \cdot \nabla v \tag{3.20}$$

and

$$\ell(v) := \int_\Omega fv + \int_\Gamma \gamma v. \tag{3.21}$$

Equivalently, the weak solution of equations (3.16) is the $w \in H^1_0(\Omega)$ which satisfies

$$a(w,v) = \hat{\ell}(v) \quad \forall v \in H^1_0(\Omega), \tag{3.22}$$

where

$$a(w,v) := \int_\Omega A\nabla w\cdot\nabla v \pm \int_\Omega \mathbf{b}w\cdot\nabla v \tag{3.23}$$

and

$$\hat{\ell}(v) := \int_\Omega fv - \int_\Omega A\nabla(\overline{u}_D+\overline{\alpha})\cdot\nabla v \mp \int_\Omega \mathbf{b}(\overline{u}_D+\overline{\alpha})\cdot\nabla v + \int_\Gamma \gamma v. \tag{3.24}$$

In order to apply the Lax–Milgram Lemma, we first show that the bilinear form a is coercive. In other words, we show there exists a constant $C_A\in\mathbb{R}^+$ such that for every $w\in H^1(\Omega)$ the bilinear form a satisfies $|a(w,w)|\geq C_A\|w\|^2_{H^1(\Omega)}$.

Based on the Assumptions 2.1, we have

$$\begin{aligned} A^-\|\nabla w\|^2_{L^2(\Omega)} &\leq \int_\Omega A\nabla w\cdot\nabla w \\ &= a(w,w) \mp \int_\Omega \mathbf{b}w\cdot\nabla w \\ &\leq |a(w,w)| + \|\mathbf{b}\|_{L^\infty}\int_\Omega |w||\nabla w|, \end{aligned}$$

which is equivalent to

$$A^-\|\nabla w\|^2_{L^2(\Omega)} - \|\mathbf{b}\|_{L^\infty}\int_\Omega |w||\nabla w| \leq |a(w,w)| \qquad \forall w\in H^1(\Omega).$$

Thus, for coercivity, it is sufficient to show that there exists a positive constant C_A such that

$$C_A\|w\|^2_{H^1(\Omega)} \leq A^-\|\nabla w\|^2_{L^2(\Omega)} - \|\mathbf{b}\|_{L^\infty}\int_\Omega |w||\nabla w| \qquad \forall w\in H^1(\Omega).$$

Using the inequality

$$xy \leq \delta x^2 + \frac{1}{4\delta}y^2 \qquad \forall\delta\in\mathbb{R}^+ \quad \forall x\in\mathbb{R} \quad \forall x\in\mathbb{R}, \tag{3.25}$$

it is sufficient to find a positive constant C_A such that

$$\begin{aligned} &C_A(\|w\|^2_{L^2(\Omega)} + \|\nabla w\|^2_{L^2(\Omega)}) + \|\mathbf{b}\|_{L^\infty}\int_\Omega |w||\nabla w| \\ \leq &C_A(\|w\|^2_{L^2(\Omega)} + \|\nabla w\|^2_{L^2(\Omega)}) + \delta\|\mathbf{b}\|_{L^\infty}\|\nabla w\|^2_{L^2(\Omega)} + \frac{1}{4\delta}\|\mathbf{b}\|_{L^\infty}\|w\|^2_{L^2(\Omega)} \\ \leq &A^-\|\nabla w\|^2_{L^2(\Omega)}. \end{aligned} \tag{3.26}$$

We have to discern two cases. If $\|\nabla w\|_{L^2(\Omega)}=0$, then $\|w\|_{L^2(\Omega)}=0$ by the Poincaré inequality and the bilinear form a is coercive. If on the other hand $\|\nabla w\|_{L^2(\Omega)}\neq 0$, then dividing inequality (3.26) by $\|\nabla w\|^2_{L^2(\Omega)}$ and using the Poincaré inequality, we find

$$C_A(1+C_P^2) + B\delta + \frac{B}{4\delta}C_P^2 \leq A^-, \tag{3.27}$$

where $B := \|\mathbf{b}\|_{L_\infty}$ and C_P is the Poincaré constant. This inequality always holds for A^- large enough and C_P and B small enough. Maximizing the range of values when it holds leads to the minimization problem

$$\delta := \operatorname*{arg\,min}_{\delta\in\mathbb{R}^+} B\delta + \frac{B}{4\delta}C_P^2 \tag{3.28}$$

with the solution $\delta = C_P/2$. Substituting δ in inequality (3.27) results in the inequality

$$C_A \le \frac{A^- - BC_P}{1+C_P^2}. \tag{3.29}$$

Since C_A must be a positive constant, the nominator must be positive, i.e.,

$$BC_P \le A^-, \tag{3.30}$$

which is satisfied by assumption.

Next, the continuity of the bilinear form a is shown. Using the Cauchy-Schwarz inequality we have

$$\begin{aligned} |a(w,v)| &\le \|A\|_{L^\infty}\|\nabla w\|_{L^2(\Omega)}\|\nabla v\|_{L^2(\Omega)} + \|\mathbf{b}\|_{L^\infty}\|w\|_{L^2(\Omega)}\|\nabla v\|_{L^2(\Omega)} \\ &\le C_0\|w\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)}, \end{aligned} \tag{3.31}$$

where $C_0 := A^+ + B$. The continuity of the functional $\hat{\ell}$ is proved similarly by calculating

$$\begin{aligned} |\hat{\ell}(v)| &\le \|f\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} + \|\gamma\|_{L^2(\Gamma)}\|v\|_{L^2(\Omega)} \\ &\quad + \|A\|_{L^\infty}\|\nabla(\overline{u}_D + \overline{\alpha})\|_{L^2(\Omega)}\|\nabla v\|_{L^2(\Omega)} \\ &\quad + \|\mathbf{b}\|_{L^\infty}\|\overline{u}_D + \overline{\alpha}\|_{L^2(\Omega)}\|\nabla v\|_{L^2(\Omega)} \\ &\le \|f\|_{L^2(\Omega)}\|v\|_{H^1(\Omega)} + \|\gamma\|_{L^2(\Gamma)}\|v\|_{H^1(\Omega)} \\ &\quad + A^+\|\overline{u}_D + \overline{\alpha}\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} + B\|\overline{u}_D + \overline{\alpha}\|_{H^1(\Omega)}\|v\|_{H^1(\Omega)} \\ &\le C_1\|v\|_{H^1(\Omega)}, \end{aligned}$$

where

$$C_1 := \|f\|_{L^2(\Omega)} + \|\gamma\|_{L^2(\Gamma)} + C_T(A^+ + B)(\|u_D\|_{H^{1/2}(\partial\Omega)} + \|\alpha\|_{H^{1/2}(\Gamma)}).$$

Here, we used trace inequality (there exists a constant $C_T > 0$ such that $\|\overline{u}_D\|_{H^1(\Omega)} \le C_T\|u_D\|_{H^{1/2}(\partial\Omega)}$) to obtain the constant C_1.

Hence all the assumptions of the Lax–Milgram Lemma are satisfied. Therefore it proves the existence and uniqueness of the solution of equation (3.16).

Finally, we prove the estimate (3.17). We can write $H^1_{u_D}(\Omega) \ni u = w + \overline{u}_D + \overline{\alpha}$ with $w \in H^1_0(\Omega)$, and all $w \in H^1_0(\Omega)$ satisfy

$$\begin{aligned} a(w,w) &= a(u - \overline{u}_D - \overline{\alpha}, w) = a(u,w) - a(\overline{u}_D + \overline{\alpha}, w) \\ &= \ell(w) - a(\overline{u}_D + \overline{\alpha}, w) = \hat{\ell}(w). \end{aligned} \tag{3.32}$$

Here $\overline{u}_D \in H^1(\Omega)$ is the Dirichlet lift of u_D in Ω and thus satisfies $T\overline{u}_D = u_D$, where T is the trace operator. Due to coercivity and equation (3.32), we have

$$\|w\|^2_{H^1(\Omega)} \le \frac{1}{C_A}a(w,w) = \frac{1}{C_A}\hat{\ell}(w). \tag{3.33}$$

Using the bound for $\hat{\ell}$, we can write

$$\|w\|_{H^1(\Omega)} \le \frac{1}{C_A}|\hat{\ell}(w)| \le \frac{C_1}{C_A}. \tag{3.34}$$

Using the triangle and trace inequalities as well as inequality (3.34), we have

$$\begin{aligned}
&\|u\|_{H^1(\Omega)}\\
\le&\|w\|_{H^1(\Omega)} + \|\overline{u}_D\|_{H^1(\Omega)} + \|\overline{\alpha}\|_{H^1(\Omega)}\\
\le&\frac{1}{C_A}\big(\|f\|_{L^2(\Omega)} + \|\gamma\|_{L^2(\Gamma)} + C_T(A^+ + B)(\|u_D\|_{H^{1/2}(\partial\Omega)} + \|\alpha\|_{H^{1/2}(\Gamma)})\big)\\
&\quad + C_T\big(\|u_D\|_{H^{1/2}(\partial\Omega)} + \|\alpha\|_{H^{1/2}(\partial\Omega)}\big)\\
\le&\frac{1}{C_A}\left(\|f\|_{L^2(\Omega)} + \|\gamma\|_{L^2(\Gamma)}) + C_T\left(\frac{A^+ + B}{C_A} + 1\right)(\|u_D\|_{H^{1/2}(\partial\Omega)} + \|\alpha\|_{H^{1/2}(\partial\Omega)})\right)\\
\le&C\big(\|f\|_{L^2(\Omega)} + \|\gamma\|_{L^2(\Gamma)} + \|u_D\|_{H^{1/2}(\partial\Omega)} + \|\alpha\|_{H^{1/2}(\partial\Omega)}\big),
\end{aligned} \tag{3.35}$$

where $C := \max\{\frac{1}{C_A}, C_T(1 + \frac{A^+ + B}{C_A})\}$. ∎

Next, we prove the existence and local uniqueness of solutions of the AC model system (3.12)–(3.15). For the existence proof, we apply the Schauder fixed-point theorem to show the existence of a fixed point for a fixed-point map defined by the system of equations. Since a fixed point of this map is a solution of the equations, we thus prove the existence of a solution. To show local uniqueness, we apply the implicit-function theorem.

PROPOSITION 3.1 (Existence of weak solutions of the AC model). *Under Assumptions 2.1, the system of boundary-value problems* (3.12)–(3.15) *has a weak solution*

$$\begin{aligned}
&\big(\Re(\tilde{V}), \Im(\tilde{V}), \Re(\tilde{p}), \Im(\tilde{p}), \Re(\tilde{n}), \Im(\tilde{n}), \alpha, \gamma\big)\\
\in&\big(L^\infty(\Omega) \cap H^1(\Omega)\big)^2 \times \big(L^\infty(\Omega_{\mathrm{Si}}) \cap H^1(\Omega_{\mathrm{Si}})\big)^4 \times \big(L^\infty(\Gamma) \cap H^1(\Gamma)\big)^2.
\end{aligned}$$

Proof. We show the existence of solutions using the Schauder fixed-point theorem. To this end, we define a fixed-point map $G\colon M \to M$, where

$$\begin{aligned}
M := \Big\{ &\big(\Re(\tilde{V}), \Im(\tilde{V}), \Re(\tilde{p}), \Im(\tilde{p}), \Re(\tilde{n}), \Im(\tilde{n}), \alpha, \gamma\big)\\
&\in \big(L^2(\Omega)\big)^2 \times \big(L^2(\Omega_{\mathrm{Si}})\big)^4 \times \big(L^2(\Gamma)\big)^2 \,\big|\\
&\alpha, \gamma \text{ bounded a.e. on } \Gamma, \quad \Re(\tilde{V}), \Im(\tilde{V}) \text{ bounded a.e. on } \Omega,\\
&\Re(\tilde{p}), \Im(\tilde{p}), \Re(\tilde{n}), \Im(\tilde{n}) \text{ bounded a.e. on } \Omega_{\mathrm{Si}} \Big\}
\end{aligned}$$

is a closed and convex subset of $\big(L^2(\Omega)\big)^2 \times \big(L^2(\Omega_{\mathrm{Si}})\big)^4 \times \big(L^2(\Gamma)\big)^2$. For a given solution

$$\big(\Re(\tilde{V}_0), \Im(\tilde{V}_0), \Re(\tilde{p}_0), \Im(\tilde{p}_0), \Re(\tilde{n}_0), \Im(\tilde{n}_0), \alpha_0, \gamma_0\big), \tag{3.36}$$

the map G is defined by

$$G\big((\Re(\tilde{V}_0), \Im(\tilde{V}_0), \Re(\tilde{p}_0), \Im(\tilde{p}_0), \Re(\tilde{n}_0), \Im(\tilde{n}_0), \alpha_0, \gamma_0)\big)$$

$$:=\big(\Re(\tilde V_1),\Im(\tilde V_1),\Re(\tilde p_1),\Im(\tilde p_1),\Re(\tilde n_1),\Im(\tilde n_1),\alpha_1,\gamma_1\big).$$

The functions on the right-hand side are the solutions of the following boundary-value problems, which taken together are the given system of equations.

(1) Solve the boundary-value problem

$$-\nabla\cdot(A\nabla\Re(\tilde V))=\begin{cases} q\Big(\Re(\tilde p_0)-\Re(\tilde n_0)\Big) & \text{in } \Omega_{\mathrm{Si}}\cup\Omega_{\mathrm{liq}},\\ 0 & \text{in } \Omega_{\mathrm{ox}}\end{cases} \tag{3.37}$$

with the boundary conditions

$$\Re(\tilde V)=\Re(\tilde V_D)\quad\text{in } \partial\Omega_D\qquad\text{and}\qquad \nabla\Re(\tilde V)\cdot\mathbf{n}=0\quad\text{in } \partial\Omega_N$$

and the interface conditions

$$\begin{aligned}\Re(\tilde V)(0+,y)-\Re(\tilde V)(0-,y)&=\alpha_0(y) && \text{on } \Gamma,\\ A(0+)\partial_x\Re(\tilde V)(0+,y)-A(0-)\partial_x\Re(\tilde V)(0-,y)&=\gamma_0(y) && \text{on } \Gamma\end{aligned}$$

to obtain the solution $\Re(\tilde V)=\Re(\tilde V_1)$.

(2) Solve the boundary-value problem

$$-\nabla\cdot(A\nabla\Im(\tilde V))=\begin{cases} q\Big(\Im(\tilde p_0)-\Im(\tilde n_0)\Big) & \text{in } \Omega_{\mathrm{Si}}\cup\Omega_{\mathrm{liq}},\\ 0 & \text{in } \Omega_{\mathrm{ox}}\end{cases} \tag{3.38}$$

with the boundary conditions

$$\Im(\tilde V)=\Im(\tilde V_D)\quad\text{in } \partial\Omega_D\qquad\text{and}\qquad \nabla\Im(\tilde V)\cdot\mathbf{n}=0\quad\text{in } \partial\Omega_N$$

and the interface conditions

$$\begin{aligned}\Im(\tilde V)(0+,y)-\Im(\tilde V)(0-,y)&=0 && \text{on } \Gamma,\\ A(0+)\partial_x\Im(\tilde V)(0+,y)-A(0-)\partial_x\Im(\tilde V)(0-,y)&=0 && \text{on } \Gamma\end{aligned}$$

to obtain the solution $\Im(\tilde V)=\Im(\tilde V_1)$.

(3) Solve the boundary-value problem

$$-\nabla\cdot(D_p\nabla\Re(\tilde p))-\nabla\cdot\big(\mu_p\nabla V_*\Re(\tilde p)\big)=\nabla\cdot\big(\mu_p p_*\nabla\Re(\tilde V_1)\big)+\omega\Im(\tilde p_0) \tag{3.39}$$

in Ω_{Si} with the boundary conditions

$$\Re(\tilde p)=\Re(\tilde p_D)\quad\text{in } \partial\Omega_{D,\mathrm{Si}}\qquad\text{and}\qquad \nabla\Re(\tilde p)\cdot\mathbf{n}=0\quad\text{in } \partial\Omega_{N,\mathrm{Si}}$$

to obtain the solution $\Re(\tilde p)=\Re(\tilde p_1)$.

(4) Solve the boundary-value problem

$$-\nabla\cdot(D_p\nabla\Im(\tilde p))-\nabla\cdot\big(\mu_p\nabla V_*\Im(\tilde p)\big)=\nabla\cdot\big(\mu_p p_*\nabla\Im(\tilde V_1)\big)-\omega\Re(\tilde p_0) \tag{3.40}$$

in Ω_{Si} with the boundary conditions

$$\Im(\tilde p)=\Im(\tilde p_D)\quad\text{in } \partial\Omega_{D,\mathrm{Si}}\qquad\text{and}\qquad \nabla\Im(\tilde p)\cdot\mathbf{n}=0\quad\text{in } \partial\Omega_{N,\mathrm{Si}}$$

to obtain the solution $\Im(\tilde p)=\Im(\tilde p_1)$.

(5) Solve the boundary-value problem

$$-\nabla\cdot(D_n\nabla\Re(\tilde{n}))+\nabla\cdot\big(\mu_n\nabla V_*\Re(\tilde{n})\big)=-\nabla\cdot\big(\mu_n n_*\nabla\Re(\tilde{V}_1)\big)+\omega\Im(\tilde{n}_0) \tag{3.41}$$

in Ω_{Si} with the boundary conditions

$$\Re(\tilde{n})=\Re(\tilde{n}_D)\quad\text{in }\partial\Omega_{D,\mathrm{Si}}\qquad\text{and}\qquad\nabla\Re(\tilde{n})\cdot\mathbf{n}=0\quad\text{in }\partial\Omega_{N,\mathrm{Si}}$$

to obtain the solution $\Re(\tilde{n})=\Re(\tilde{n}_1)$.

(6) Solve the boundary-value problem

$$-\nabla\cdot(D_n\nabla\Im(\tilde{n}))+\nabla\cdot\big(\mu_n\nabla V_*\Im(\tilde{n})\big)=-\nabla\cdot\big(\mu_n n_*\nabla\Im(\tilde{V}_1)\big)-\omega\Re(\tilde{n}_0) \tag{3.42}$$

in Ω_{Si} with the boundary conditions

$$\Im(\tilde{n})=\Im(\tilde{n}_D)\quad\text{in }\partial\Omega_{D,\mathrm{Si}}\qquad\text{and}\qquad\nabla\Im(\tilde{n})\cdot\mathbf{n}=0\quad\text{in }\partial\Omega_{N,\mathrm{Si}}$$

to obtain the solution $\Im(\tilde{n})=\Im(\tilde{n}_1)$.

(7) Update the surface-charge density and dipole-moment density by the microscopic model

$$\begin{aligned}\alpha_1(y)&:=M_\alpha(\Re(\tilde{V}_1)+\mathrm{i}\Im(\tilde{V}_1)),\\ \gamma_1(y)&:=M_\gamma(\Re(\tilde{V}_1)+\mathrm{i}\Im(\tilde{V}_1)).\end{aligned} \tag{3.43}$$

Note that variables indexed with stars are the real valued DC model solutions which are known from Section 2.1.

All of these boundary-value problems are of the general form (3.16). Therefore existence and uniqueness of the solutions of all problems immediately follow from Lemma 3.1. Therefore, if we show that

$$\big(\Re(\tilde{V}_1),\Im(\tilde{V}_1),\Re(\tilde{p}_1),\Im(\tilde{p}_1),\Re(\tilde{n}_1),\Im(\tilde{n}_1),\alpha_1,\gamma_1\big)\in M,$$

then the fixed-point map G is well-defined. By Lemma 3.1, there exists a unique and bounded solution

$$\begin{aligned}&\big(\Re(\tilde{V}_1),\Im(\tilde{V}_1),\Re(\tilde{p}_1),\Im(\tilde{p}_1),\Re(\tilde{n}_1),\Im(\tilde{n}_1),\alpha_1,\gamma_1\big)\\ &\in\big(L^\infty(\Omega)\cap H^1(\Omega)\big)^2\times\big(L^\infty(\Omega_{\mathrm{Si}})\cap H^1(\Omega_{\mathrm{Si}})\big)^4\times\big(L^\infty(\Gamma)\cap H^1(\Gamma)\big)^2\end{aligned}$$

for a given $\big(\Re(\tilde{V}_0),\Im(\tilde{V}_0),\Re(\tilde{p}_0),\Im(\tilde{p}_0),\Re(\tilde{n}_0),\Im(\tilde{n}_0),\alpha_0,\gamma_0\big)$ in M. This implies

$$\big(\Re(\tilde{V}_1),\Im(\tilde{V}_1),\Re(\tilde{p}_1),\Im(\tilde{p}_1),\Re(\tilde{n}_1),\Im(\tilde{n}_1),\alpha_1,\gamma_1\big)\in M,$$

which shows the self-mapping property of G.

According to Lemma 3.1, continuous dependence of the solution

$$\big(\Re(\tilde{V}_1),\Im(\tilde{V}_1),\Re(\tilde{p}_1),\Im(\tilde{p}_1),\Re(\tilde{n}_1),\Im(\tilde{n}_1),\alpha_1,\gamma_1\big)$$

on the data of the problems (3.37)–(3.43) leads us to the estimate

$$\begin{aligned}&\|\Re(\tilde{V}_1)\|_{H^1(\Omega)}+\|\Im(\tilde{V}_1)\|_{H^1(\Omega)}+\|\Re(\tilde{p}_1)\|_{H^1(\Omega_{\mathrm{Si}})}+\|\Im(\tilde{p}_1)\|_{H^1(\Omega_{\mathrm{Si}})}\\ &\quad+\|\Re(\tilde{n}_1)\|_{H^1(\Omega_{\mathrm{Si}})}+\|\Im(\tilde{n}_1)\|_{H^1(\Omega_{\mathrm{Si}})}+\|\alpha_1\|_{H^1(\Gamma)}+\|\gamma_1\|_{L^2(\Gamma)}\\ &\le C\big(\|\Re(\tilde{V}_D)\|_{H^{1/2}(\partial\Omega)}+\|\Im(\tilde{V}_D)\|_{H^{1/2}(\partial\Omega)}+\|\Re(\tilde{p}_0)\|_{H^1(\Omega_{\mathrm{Si}})}+\|\Im(\tilde{p}_0)\|_{H^1(\Omega_{\mathrm{Si}})}\\ &\qquad+\|\Re(\tilde{n}_0)\|_{H^1(\Omega_{\mathrm{Si}})}+\|\Im(\tilde{n}_0)\|_{H^1(\Omega_{\mathrm{Si}})}+\|\Re(\tilde{p}_D)\|_{H^{1/2}(\partial\Omega_{\mathrm{Si}})}+\|\Im(\tilde{p}_D)\|_{H^{1/2}(\partial\Omega_{\mathrm{Si}})}\\ &\qquad+\|\Re(\tilde{n}_D)\|_{H^{1/2}(\partial\Omega_{\mathrm{Si}})}+\|\Im(\tilde{n}_D)\|_{H^{1/2}(\partial\Omega_{\mathrm{Si}})}\\ &\qquad+\|V_*\|_{H^1(\Omega)}+\|p_*\|_{H^1(\Omega_{\mathrm{Si}})}+\|n_*\|_{H^1(\Omega_{\mathrm{Si}})}+\|\alpha_0\|_{H^{1/2}(\Gamma)}+\|\gamma_0\|_{L^2(\Gamma)}\big)\end{aligned}$$

using inequality (3.35), where C is a constant. Furthermore, $\|\alpha_1\|_{H^1(\Gamma)}$ and $\|\gamma_1\|_{L^2(\Gamma)}$ are bounded due to the assumptions on M_α and M_γ. Thus, the image $G(M)$ is bounded as a subset of $H^1(\Omega)^2 \times H^1(\Omega_{\mathrm{Si}})^4 \times H^1(\Gamma)^2$, which is compactly embedded in $L^2(\Omega)^2 \times L^2(\Omega_{\mathrm{Si}})^4 \times L^2(\Gamma)^2$ according to the Rellich-Kondrachov theorem. This implies that the closure of $G(M)$ is compact and thus $G(M)$ is precompact. Therefore, G is compact. Compactness and continuity of G lead to the complete continuity of G. Finally, the Schauder fixed-point theorem implies the existence of a weak solution of the AC system of equations (3.12)–(3.15). ∎

Proposition 3.1 means that the AC model system (3.12)–(3.15) always has at least one weak solution. As mentioned before, the applied AC potentials are not too large. Otherwise, the validity of the drift-diffusion-Poisson model would be questionable to begin with, since only local uniqueness holds as discussed in Section 2.1. Therefore, similarly to the DC case, to show the local uniqueness, we use the implicit-function theorem. We denote the equilibrium solution using an index e.

The equilibrium solution is given by the solution

$$\big(\Re(\tilde{V}_e), \Im(\tilde{V}_e), \Re(\tilde{p}_e), \Im(\tilde{p}_e), \Re(\tilde{n}_e), \Im(\tilde{n}_e), \alpha_e, \gamma_e\big), \tag{3.44}$$

of the equilibrium boundary-value problem

$$\begin{aligned}
-\nabla\cdot(A\nabla\Re(\tilde{V}_e)) &= -2qn_i \sinh(\beta(\Re(\tilde{V}_e)-\Phi)) && \text{in } \Omega_{\mathrm{Si}},\\
-\nabla\cdot(A\nabla\Re(\tilde{V}_e)) &= 0 && \text{in } \Omega_{\mathrm{ox}},\\
-\nabla\cdot(A\nabla\Re(\tilde{V}_e)) &= -2q\eta \sinh(\beta(\Re(\tilde{V}_e)-\Phi)) && \text{in } \Omega_{\mathrm{liq}},\\
-\nabla\cdot(A\nabla\Im(\tilde{V}_e)) &= -2qn_i \sinh(\beta(\Im(\tilde{V}_e)-\Phi)) && \text{in } \Omega_{\mathrm{Si}},\\
-\nabla\cdot(A\nabla\Im(\tilde{V}_e)) &= 0 && \text{in } \Omega_{\mathrm{ox}},\\
-\nabla\cdot(A\nabla\Im(\tilde{V}_e)) &= -2q\eta \sinh(\beta(\Im(\tilde{V}_e)-\Phi)) && \text{in } \Omega_{\mathrm{liq}},\\
\Re(\tilde{V}_e)(0+,y) - \Re(\tilde{V}_e)(0-,y) &= \alpha_e(y) && \text{on } \Gamma,\\
A(0+)\partial_x\Re(\tilde{V}_e)(0+,y) - A(0-)\partial_x\Re(\tilde{V}_e)(0-,y) &= \gamma_e(y) && \text{on } \Gamma,\\
\Im(\tilde{V}_e)(0+,y) - \Im(\tilde{V}_e)(0-,y) &= 0 && \text{on } \Gamma,\\
A(0+)\partial_x\Im(\tilde{V}_e)(0+,y) - A(0-)\partial_x\Im(\tilde{V}_e)(0-,y) &= 0 && \text{on } \Gamma,\\
\Re(\tilde{V}_e) &= \Re(\tilde{V}_D)(0) && \text{on } \partial\Omega_D,\\
\Im(\tilde{V}_e) &= \Im(\tilde{V}_D)(0) && \text{on } \partial\Omega_D,\\
\nabla\Re(\tilde{V}_e)\cdot\mathbf{n} &= 0 && \text{on } \partial\Omega_N,\\
\nabla\Im(\tilde{V}_e)\cdot\mathbf{n} &= 0 && \text{on } \partial\Omega_N.
\end{aligned}$$

This solution exists uniquely due to [2, Lemma 3.2]. Furthermore, if all Fermi potentials are equal to Φ, the equilibrium concentrations of charge carriers in Ω_{Si}, i.e., $(\Re(\tilde{p}_e), \Im(\tilde{p}_e), \Re(\tilde{n}_e), \Im(\tilde{n}_e))$ are obtained by

$$\tilde{p}_e = n_i \exp\big(-\beta(\tilde{V}_e - \Phi)\big), \tag{3.46a}$$

$$\tilde{n}_e = n_i \exp\big(\beta(\tilde{V}_e - \Phi)\big). \tag{3.46b}$$

As mentioned, we apply the implicit-function theorem to show the local uniqueness of the solutions of the problem (3.12)–(3.15) around the equilibrium solution (3.44). To this end, similarly to the DC case we show that the Fréchet derivative of the problem

has a bounded inverse at the equilibrium solution. Again we assume that the Dirichlet boundary conditions for the potential, are sufficiently small and constant on each of r contacts that partition the whole Dirichlet boundary $\partial\Omega_D$ and denote the potentials there by the vector

$$\tilde{U} := (\tilde{U}_1,\dots,\tilde{U}_r) := \big((\Re(\tilde{U}_1),\Im(\tilde{U}_1)),\dots,(\Re(\tilde{U}_r),\Im(\tilde{U}_r))\big) \in \mathbb{C}^r.$$

In summary, the following assumptions are made to show local uniqueness for small applied voltages.

Assumptions 3.2.

(1) The Dirichlet data $(\Re(\tilde{V}_D),\Im(\tilde{V}_D),\Re(\tilde{p}_D),\Im(\tilde{p}_D),\Re(\tilde{n}_D),\Im(\tilde{n}_D))$ *are a Lipschitz-continuously differentiable map of* $\tilde{U} := (\tilde{U}_1,\dots,\tilde{U}_r)$ *from* $\mathbb{C}^r$ *into* $(H^2(\Omega))^2 \times (H^2(\Omega_{\mathrm{Si}}))^4$.

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

$$\|M'_\alpha(\tilde{V})\|_{H^{1/2}(\Gamma)} + \|M'_\gamma(\tilde{V})\|_{L^2(\Gamma)} \le C\|\tilde{V}\|_{H^2(\Omega)} \tag{3.47}$$

in a neighborhood of the equilibrium potential $\tilde{V}_e$ *with a sufficiently small constant* C.

Proposition 3.2 (Local uniqueness of weak solutions of the AC model). *Under Assumptions* (2.1) *and* (3.2), *there exists a sufficiently small* $\delta \in \mathbb{R}$ *with* $|\tilde{U}| < \delta$ *such that the AC system of equations* (3.12)–(3.15) *has a locally unique solution*

$$\begin{aligned}&\big(\Re(\tilde{V}^*)(\tilde{U}),\Im(\tilde{V}^*)(\tilde{U}),\Re(\tilde{p}^*)(\tilde{U}),\Im(\tilde{p}^*)(\tilde{U}),\Re(\tilde{n}^*)(\tilde{U}),\Re(\tilde{n}^*)(\tilde{U}),\alpha^*(\tilde{U}),\gamma^*(\tilde{U})\big)\\ &\in (H^2(\Omega))^2 \times (H^2(\Omega_{\mathrm{Si}}))^4 \times H^{1/2}(\Gamma) \times L^2(\Gamma).\end{aligned}$$

Furthermore, this solution satisfies

$$\begin{aligned}&\big(\Re(\tilde{V}^*)(0),\Im(\tilde{V}^*)(0),\Re(\tilde{p}^*)(0),\Im(\tilde{p}^*)(0),\Re(\tilde{n}^*)(0),\Re(\tilde{n}^*)(0),\alpha^*(0),\gamma^*(0)\big)\\ &= \big(\Re(\tilde{V}_e),\Im(\tilde{V}_e),\Re(\tilde{p}_e),\Im(\tilde{p}_e),\Re(\tilde{n}_e),\Im(\tilde{n}_e),\alpha_e,\gamma_e\big),\end{aligned}$$

and it depends continuously differentiably on $\tilde{U}$ *as a map from* $\big\{\tilde{U} \in \mathbb{C}^r \,\big|\, |\tilde{U}| < \delta, r \le 3\big\}$ *into* $(H^2(\Omega))^2 \times (H^2(\Omega_{\mathrm{Si}}))^4 \times H^{1/2}(\Gamma) \times L^2(\Gamma)$.

Proof. We rewrite the system of equations (3.12)–(3.15) using the substitutions

$$\begin{aligned}\Re(\hat{V}) &:= \Re(\tilde{V}) - \Re(\tilde{V}_D)(\tilde{U}), & \Im(\hat{V}) &:= \Im(\tilde{V}) - \Im(\tilde{V}_D)(\tilde{U}),\\ \Re(\hat{p}) &:= \Re(\tilde{p}) - \Re(\tilde{p}_D)(\tilde{U}), & \Im(\hat{p}) &:= \Im(\tilde{p}) - \Im(\tilde{p}_D)(\tilde{U}),\\ \Re(\hat{n}) &:= \Re(\tilde{n}) - \Re(\tilde{n}_D)(\tilde{U}), & \Im(\hat{n}) &:= \Im(\tilde{n}) - \Im(\tilde{n}_D)(\tilde{U}).\end{aligned}$$

Then, the system becomes

$$-\nabla\cdot(A\nabla\Re(\hat{V}+\tilde{V}_D)) = q\Big(\Re(\hat{p}+\tilde{p}_D) - \Re(\hat{n}+\tilde{n}_D)\Big) \qquad \text{in } \Omega_{\mathrm{Si}}, \tag{3.48a}$$

$$-\nabla\cdot(A\nabla\Re(\hat{V}+\tilde{V}_D)) = 0 \qquad \text{in } \Omega_{\mathrm{ox}}, \tag{3.48b}$$

$$-\nabla\cdot(A\nabla\Re(\hat{V}+\tilde{V}_D)) = -2\eta\sinh(\beta(\Re(\hat{V}+\tilde{V}_D) - \Phi)) \qquad \text{in } \Omega_{\mathrm{liq}}, \tag{3.48c}$$

$$-\nabla\cdot(A\nabla\Im(\hat V+\tilde V_D))=q\Big(\Im(\hat p+\tilde p_D)-\Im(\hat n+\tilde n_D)\Big) \quad \text{in } \Omega_{\mathrm{Si}}, \tag{3.48d}$$

$$-\nabla\cdot(A\nabla\Im(\hat V+\tilde V_D))=0 \quad \text{in } \Omega_{\mathrm{ox}}, \tag{3.48e}$$

$$-\nabla\cdot(A\nabla\Im(\hat V+\tilde V_D))=-2\eta\sinh(\beta(\Im(\hat V+\tilde V_D)-\Phi)) \quad \text{in } \Omega_{\mathrm{liq}}, \tag{3.48f}$$

$$\begin{aligned}&-\nabla\cdot(D_p\nabla\Re(\hat p+\tilde p_D))-\nabla\cdot\big(\mu_p\nabla V_*\Re(\hat p+\tilde p_D)\big)\\ &=\nabla\cdot\big(\mu_p p_*\nabla\Re(\hat V+\tilde V_D)\big)+\omega\Im(\hat p+\tilde p_D) \quad \text{in } \Omega_{\mathrm{Si}},\end{aligned} \tag{3.48g}$$

$$\begin{aligned}&-\nabla\cdot(D_p\nabla\Im(\hat p+\tilde p_D))-\nabla\cdot\big(\mu_p\nabla V_*\Im(\hat p+\tilde p_D)\big)\\ &=\nabla\cdot\big(\mu_p p_*\nabla\Im(\hat V+\tilde V_D)\big)-\omega\Re(\hat p+\tilde p_D) \quad \text{in } \Omega_{\mathrm{Si}},\end{aligned} \tag{3.48h}$$

$$\begin{aligned}&-\nabla\cdot(D_n\nabla\Re(\hat n+\tilde n_D))+\nabla\cdot\big(\mu_n\nabla V_*\Re(\hat n+\tilde n_D)\big)\\ &=-\nabla\cdot\big(\mu_n n_*\nabla\Re(\hat V+\tilde V_D)\big)+\omega\Im(\hat n+\tilde n_D) \quad \text{in } \Omega_{\mathrm{Si}},\end{aligned} \tag{3.48i}$$

$$\begin{aligned}&-\nabla\cdot(D_n\nabla\Im(\hat n+\tilde n_D))+\nabla\cdot\big(\mu_n\nabla V_*\Im(\hat n+\tilde n_D)\big)\\ &=-\nabla\cdot\big(\mu_n n_*\nabla\Im(\hat V+\tilde V_D)\big)-\omega\Re(\hat n+\tilde n_D) \quad \text{in } \Omega_{\mathrm{Si}},\end{aligned} \tag{3.48j}$$

$$\Re(\hat V)(0+,y)-\Re(\hat V)(0-,y)=\alpha(y) \quad \text{on } \Gamma, \tag{3.48k}$$

$$A(0+)\partial_x\Re(\hat V)(0+,y)-A(0-)\partial_x\Re(\hat V)(0-,y)=\gamma(y) \quad \text{on } \Gamma, \tag{3.48l}$$

$$\Im(\hat V)(0+,y)-\Im(\hat V)(0-,y)=0 \quad \text{on } \Gamma, \tag{3.48m}$$

$$A(0+)\partial_x\Im(\hat V)(0+,y)-A(0-)\partial_x\Im(\hat V)(0-,y)=0 \quad \text{on } \Gamma, \tag{3.48n}$$

$$\alpha=M_\alpha(\Re(\hat V+\tilde V_D)+\Im(\hat V+\tilde V_D)) \quad \text{on } \Gamma, \tag{3.48o}$$

$$\gamma=M_\gamma(\Re(\hat V+\tilde V_D)+\Im(\hat V+\tilde V_D)) \quad \text{on } \Gamma, \tag{3.48p}$$

$$\Re(\hat V)=\Im(\hat V)=0 \quad \text{on } \partial\Omega_D, \tag{3.48q}$$

$$\Re(\hat p)=\Im(\hat p)=0 \quad \text{on } \partial\Omega_{D,\mathrm{Si}}, \tag{3.48r}$$

$$\Re(\hat n)=\Im(\hat n)=0 \quad \text{on } \partial\Omega_{D,\mathrm{Si}}, \tag{3.48s}$$

$$\nabla\Re(\hat V)\cdot\mathbf{n}=\nabla\Im(\hat V)\cdot\mathbf{n}=0 \quad \text{on } \partial\Omega_N, \tag{3.48t}$$

$$\nabla\Re(\hat p)\cdot\mathbf{n}=\nabla\Im(\hat p)\cdot\mathbf{n}=0 \quad \text{on } \partial\Omega_{N,\mathrm{Si}}, \tag{3.48u}$$

$$\nabla\Re(\hat n)\cdot\mathbf{n}=\nabla\Im(\hat n)\cdot\mathbf{n}=0 \quad \text{on } \partial\Omega_{N,\mathrm{Si}}. \tag{3.48v}$$

The above system can be written as the operator equation

$$Q\big((\Re(\hat V),\Im(\hat V),\Re(\hat p),\Im(\hat p),\Re(\hat n),\Im(\hat n),\alpha,\gamma),\tilde U\big)=0,$$

where the operator

$$Q\colon D\times S_{\delta_1}(0)\to(L^2(\Omega))^2\times(L^2(\Omega_{\mathrm{Si}}))^4\times H^{1/2}(\Gamma)\times L^2(\Gamma)$$

is given by solving the above system. D is an open subset of $H^2_\partial(\Omega\setminus\Gamma)\times H^2_\partial(\Omega_{\mathrm{Si}})^2\times H^{1/2}(\Gamma)\times L^2(\Gamma)$, where H^2_∂ is defined by

$$H^2_\partial(\Omega):=\{\phi\in H^2(\Omega)\,|\,\nabla\phi\cdot\mathbf{n}=0\text{ on }\partial\Omega_{\mathrm{N}},\ \phi=0\text{ on }\partial\Omega_{\mathrm{D}}\}, \tag{3.49}$$

and $S_{\delta_1}(0)\subset\mathbb{C}^r$, $r\le 3$, is a sphere with radius δ_1 and center 0.

Since

$$\begin{aligned}&Q\big((\Re(\hat{V}),\Im(\hat{V}),\Re(\hat{p}),\Im(\hat{p}),\Re(\hat{n}),\Im(\hat{n}),\alpha,\gamma),\tilde{U}\big)\\&\in(L^2(\Omega))^2\times(L^2(\Omega_{\mathrm{Si}}))^4\times H^{1/2}(\Gamma)\times L^2(\Gamma)\end{aligned}$$

results in $(\Re(\hat{V}),\Im(\hat{V}),\Re(\hat{p}),\Im(\hat{p}),\Re(\hat{n}),\Im(\hat{n}),\alpha,\gamma)\in D$ and $\tilde{U}\in S_{\delta_1}(\tilde{U})$ and since any product of functions in D is in $L^2(\Omega)$ because of the inequality $\|uv\|_{L^2(\tilde{U})}\le C\|u\|_{H^1(\tilde{U})}\|v\|_{H^1(\tilde{U})}$ for all u and $v\in H^1(\tilde{U})$, the operator Q is well-defined.

To apply the implicit-function theorem, the Fréchet derivative

$$D_{(\Re(\hat{V}),\Im(\hat{V}),\Re(\hat{p}),\Im(\hat{p}),\Re(\hat{n}),\Im(\hat{n}),\alpha,\gamma)}Q$$

must have a bounded inverse at the equilibrium solution

$$\begin{aligned}\big(\Re(\tilde{V}_e)-\Re(\tilde{V}_D)(0),\Im(\tilde{V}_e)-\Im(\tilde{V}_D)(0),\Re(\tilde{p}_e)-\Re(\tilde{p}_D)(0),\Im(\tilde{p}_e)-\Im(\tilde{p}_D)(0),\\ \Re(\tilde{n}_e)-\Re(\tilde{n}_D)(0),\Im(\tilde{n}_e)-\Im(\tilde{n}_D)(0),\alpha_e,\gamma_e,0\big),\end{aligned}$$

which is by definition also a solution of the equation $Q=0$.

Suppose $(g_1,g_2,g_3,g_4,g_5,g_6,g_7,g_8)\in L^2(\Omega)\times L^2(\Omega_{\mathrm{Si}})^4\times H^{1/2}(\Gamma)\times L^2(\Gamma)$. To find the inverse of the Fréchet derivative, we have to solve the equation

$$\begin{aligned}&D_{(\Re(\hat{V}),\Im(\hat{V}),\Re(\hat{p}),\Im(\hat{p}),\Re(\hat{n}),\Im(\hat{n}),\alpha,\gamma)}Q(a_1,a_2,a_3,a_4,a_5,a_6,a_7,a_8)\\&=(g_1,g_2,g_3,g_4,g_5,g_6,g_7,g_8)\end{aligned}\tag{3.50}$$

for a_i, $i\in\{1,\dots,8\}$, where $(g_1,g_2,g_3,g_4,g_5,g_6,g_7,g_8)\in L^2(\Omega)\times L^2(\Omega_{\mathrm{Si}})^4\times H^{1/2}(\Gamma)\times L^2(\Gamma)$ and Q are calculated at the equilibrium solution. To write this equation as a boundary-value problem, we have to linearize the original equation (3.48) around the equilibrium solution first. The derivative $D_{(\Re(\hat{V}),\Im(\hat{V}),\Re(\hat{p}),\Im(\hat{p}),\Re(\hat{n}),\Im(\hat{n}),\alpha,\gamma)}Q$ at the equilibrium solution is

$$\begin{pmatrix}
-\nabla\cdot(A\nabla) & 0 & -q & 0 & q & 0 & 0 & 0\\
0 & -\nabla\cdot(A\nabla) & 0 & -q & 0 & q & 0 & 0\\
0 & 0 & L_1 & -\omega & 0 & 0 & 0 & 0\\
0 & 0 & \omega & L_2 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & L_3 & -\omega & 0 & 0\\
0 & 0 & 0 & 0 & \omega & L_4 & 0 & 0\\
-M'_\alpha(\Re(\tilde{V}_e)) & -M'_\alpha(\Im(\tilde{V}_e)) & 0 & 0 & 0 & 0 & 1 & 0\\
-M'_\gamma(\Re(\tilde{V}_e)) & -M'_\gamma(\Im(\tilde{V}_e)) & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}$$

in Ω_{Si}, where

$$\begin{aligned}L_1&:=-\nabla\cdot(D_p\nabla)-\nabla\cdot(\mu_p\nabla V_*),\\L_2&:=-\nabla\cdot(D_p\nabla)-\nabla\cdot(\mu_p\nabla V_*),\\L_3&:=-\nabla\cdot(D_n\nabla)+\nabla\cdot(\mu_n\nabla V_*),\\L_4&:=-\nabla\cdot(D_n\nabla)+\nabla\cdot(\mu_n\nabla V_*).\end{aligned}$$

In the matrix above, the first and second rows pertain to the linearizations of the Poisson equation with respect to $\Re(\tilde{V})$ and $\Im(\tilde{V})$, respectively, and hence they depend

on the subdomain. In the three subdomains Ω_{Si}, Ω_{ox}, and Ω_{liq}, the linearizations with respect to $\Re(\tilde{V})$ are given by the rows of the matrix

$$\begin{pmatrix} -\nabla\cdot(A\nabla) & 0 & -q & 0 & q & 0 & 0 & 0 \\ -\nabla\cdot(A\nabla) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\nabla\cdot(A\nabla)+2\eta\beta\cosh(\beta(\Re(\tilde{V}_e)-\Phi)) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

and the linearizations with respect to $\Im(\tilde{V})$ are given by

$$\begin{pmatrix} 0 & -\nabla\cdot(A\nabla) & 0 & -q & 0 & q & 0 & 0 \\ 0 & -\nabla\cdot(A\nabla) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\nabla\cdot(A\nabla)+2\eta\beta\cosh(\beta(\Im(\tilde{V}_e)-\Phi)) & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Therefore, equation (3.50) is equivalent to the boundary-value problem

$$\begin{aligned}
&-\nabla\cdot(A\nabla a_1) = q(a_3-a_5)+g_1 && \text{in } \Omega_{\mathrm{Si}}, && (3.51a)\\
&-\nabla\cdot(A\nabla a_1) = g_2 && \text{in } \Omega_{\mathrm{ox}}, && (3.51b)\\
&-\nabla\cdot(A\nabla a_1) = -2\eta\cosh(\beta(\Re(\tilde{V}_e)-\Phi))a_1+g_1 && \text{in } \Omega_{\mathrm{liq}}, && (3.51c)\\
&-\nabla\cdot(A\nabla a_2) = q(a_4-a_6)+g_2 && \text{in } \Omega_{\mathrm{Si}}, && (3.51d)\\
&-\nabla\cdot(A\nabla a_2) = g_2 && \text{in } \Omega_{\mathrm{ox}}, && (3.51e)\\
&-\nabla\cdot(A\nabla a_2) = -2\eta\cosh(\beta(\Im(\tilde{V}_e)-\Phi))a_2+g_2 && \text{in } \Omega_{\mathrm{liq}}, && (3.51f)\\
&-\nabla\cdot(D_p\nabla a_3)-\nabla\cdot\left(\mu_p\nabla V_* a_3\right) = \omega a_4+g_3 && \text{in } \Omega_{\mathrm{Si}}, && (3.51g)\\
&-\nabla\cdot(D_p\nabla a_4)-\nabla\cdot\left(\mu_p\nabla V_* a_4\right) = -\omega a_3+g_4 && \text{in } \Omega_{\mathrm{Si}}, && (3.51h)\\
&-\nabla\cdot(D_n\nabla a_5)+\nabla\cdot\left(\mu_n\nabla V_* a_5\right) = \omega a_6+g_5 && \text{in } \Omega_{\mathrm{Si}}, && (3.51i)\\
&-\nabla\cdot(D_n\nabla a_6)+\nabla\cdot\left(\mu_n\nabla V_* a_6\right) = -\omega a_5+g_6 && \text{in } \Omega_{\mathrm{Si}}, && (3.51j)\\
&a_1(0+,y)-a_1(0-,y) = a_7 && \text{on } \Gamma, && (3.51k)\\
&A(0+)\partial_x a_1(0+,y)-A(0-)\partial_x a_1(0-,y) = a_8 && \text{on } \Gamma, && (3.51l)\\
&a_2(0+,y)-a_2(0-,y) = 0 && \text{on } \Gamma, && (3.51m)\\
&A(0+)\partial_x a_2(0+,y)-A(0-)\partial_x a_2(0-,y) = 0 && \text{on } \Gamma, && (3.51n)\\
&a_7 = M_\alpha'(\Re(\tilde{V}_e))a_1+M_\alpha'(\Im(\tilde{V}_e))a_2+g_7 && \text{on } \Gamma, && (3.51o)\\
&a_8 = M_\gamma'(\Re(\tilde{V}_e))a_1+M_\gamma'(\Im(\tilde{V}_e))a_2+g_8 && \text{on } \Gamma, && (3.51p)\\
&a_1 = a_2 = 0 && \text{on } \partial\Omega_D, && (3.51q)\\
&a_3 = a_4 = a_5 = a_6 = 0 && \text{on } \partial\Omega_{D,\mathrm{Si}}, && (3.51r)\\
&\nabla a_1\cdot\mathbf{n} = \nabla a_2\cdot\mathbf{n} = 0 && \text{on } \partial\Omega_N, && (3.51s)\\
&\nabla a_3\cdot\mathbf{n} = \nabla a_4\cdot\mathbf{n} = \nabla a_5\cdot\mathbf{n} = \nabla a_6\cdot\mathbf{n} = 0 && \text{on } \partial\Omega_{N,\mathrm{Si}}. && (3.51t)
\end{aligned}$$

There exist unique solutions a_3, a_4, a_5, and a_6 of the semilinear elliptic equations (3.51g)–(3.51j) due to [2, Lemma 3.2], and the estimates

$$\begin{aligned}
&\|a_3\|_{H^2(\Omega_{\mathrm{Si}})}+\|a_4\|_{H^2(\Omega_{\mathrm{Si}})}+\|a_5\|_{H^2(\Omega_{\mathrm{Si}})}+\|a_6\|_{H^2(\Omega_{\mathrm{Si}})}\\
&\le C(\|g_3\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_4\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_5\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_6\|_{L^2(\Omega_{\mathrm{Si}})})
\end{aligned}$$

holds in Ω_{Si}. Substituting a_3, a_4, a_5, and a_6 in equations (3.51a)–(3.51f) and then summing the estimates, we find

$$\|a_1\|_{H^2(\Omega)}+\|a_2\|_{H^2(\Omega)} \le C_1(\|g_1\|_{L^2(\Omega)}+\|g_2\|_{L^2(\Omega)}+\|g_3\|_{L^2(\Omega_{\mathrm{Si}})}$$

$$+\|g_4\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_5\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_6\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_7\|_{H^{1/2}(\Gamma)}$$
$$+\|g_8\|_{L^2(\Gamma)}+\|a_7\|_{H^{1/2}(\Gamma)}+\|a_8\|_{L^2(\Gamma)}).$$

Using equations (3.51o)–(3.51p) and Assumption 3.2 on M_α and M_γ, there exists a sufficiently small constant C_2 such that the estimate

$$\|a_7\|_{H^{1/2}(\Gamma)}+\|a_8\|_{L^2(\Gamma)}\le C_2(\|a_1\|_{H^2(\Omega)}+\|a_2\|_{H^2(\Omega)})+\|g_7\|_{H^{1/2}(\Gamma)}+\|g_8\|_{L^2(\Gamma)}$$

holds. For sufficiently small C_2, i.e., if $C_1C_2<1$, we obtain from the last two inequalities

$$\begin{aligned}&(1-C_1C_2)\big(\|a_1\|_{H^2(\Omega)}+\|a_2\|_{H^2(\Omega)}\big)\\ \le& C_1\big(\|g_1\|_{L^2(\Omega)}+\|g_2\|_{L^2(\Omega)}+\|g_3\|_{L^2(\Omega_{\mathrm{Si}})}\\ &+\|g_4\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_5\|_{L^2(\Omega_{\mathrm{Si}})}+\|g_6\|_{L^2(\Omega_{\mathrm{Si}})}+2\|g_7\|_{H^{1/2}(\Gamma)}+2\|g_8\|_{L^2(\Gamma)}\big).\end{aligned}$$

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

$$\|(D_{(\Re(\hat V),\Im(\hat V),\Re(\hat p),\Im(\hat p),\Re(\hat n),\Im(\hat n),\alpha,\gamma)}Q)^{-1}\|\le C, \tag{3.52}$$

where the norm is the operator norm of

$$H^2(\Omega)\times H^2(\Omega_{\mathrm{Si}})^4\times H^{1/2}(\Gamma)\times L^2(\Gamma)\to L^2(\Omega)\times L^2(\Omega_{\mathrm{Si}})^4\times H^{1/2}(\Gamma)\times L^2(\Gamma). \tag{3.53}$$

Finally, the implicit-function theorem proves the local uniqueness of the solution. ∎

4. Conclusions

Many devices, especially sensors, can be used in the AC regime. Still, these model equations have barely been analyzed mathematically. We started from a general model for affinity based field-effect sensors, namely the transient drift-diffusion-Poisson system coupled with the Poisson–Boltzmann equation. Assuming sufficiently low frequencies and sufficiently small signals, the model equations for the AC regime were derived based on the DC regime. The main results are existence and uniqueness for the AC model equations.

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