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Mathematical Advances and Horizons for Classical and Quantum-Perturbed Drift-Diffusion Systems: Solid State Devices and Beyond [1]

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Abstract. The classical drift-diffusion model employed in semi-conductor simulation is now seen as part of a hierarchy of mathematical models designed to capture the intricate patterns of current flow in solid-state devices. These models include those incorporating quantum mechanical effects. Scientific computation has vastly outpaced our mathematical understanding of these models. This article is restricted in its focus, and describes mathematical understanding achieved during the last few decades primarily in terms of Gummel decomposition, as applied to drift-diffusion models and the closely related family of quantum corrected drift-diffusion models. Drift-diffusion models are being employed once again in *organic* devices, and in bio-chip devices, and a re-examination is now seen as timely, as such studies proceed beyond solid state devices.

Keywords: Gummel decomposition, drift-diffusion, quantum-perturbed drift-diffusion, solar cells, bio-chips

1. Historical Introduction

As organic devices emerge with a variety of applications (see [17] for a detailed solar cell model), it seems appropriate to take stock of drift-diffusion models and quantum-perturbed drift-diffusion models, in terms of the understanding achieved via Gummel decomposition for the analysis of these systems. We shall restrict our detailed attention to the steady case. Since evolution models are often employed to reach steady-state, some discussion of these models is appropriate. The plan for this article is as follows. In the introduction, we sketch out briefly the progression of macroscopic models for device simulation, including macroscopic models more involved than drift-diffusion, such as hydrodynamic and energy transport models. This treatment is not intended to be exhaustive. We mention, only in passing, kinetic and strictly quantum mechanical models. The goal is to describe mathematical advances which provide the underpinning for scientific computation: Gummel decomposition and invariant regions. The quantum-perturbed drift-diffusion model has proven to be quite challenging. It occupies a significant portion of the following sections.

1..1 Relevant Literature

In this section, citations for both the steady and unsteady models are given. The papers of Gummel [46] and Scharfetter-Gummel [97] were the milestone papers in introducing Gummel decomposition (Gummel iteration) and the advection-diffusion flux approximation, sometimes called exponential fitting, to resolve disparate diffusion rates. These studies were based on the classical Van Roosbroeck model [93] (see also [100]). The paper of Mock [86] appears to be the first mathematical study of the model; this was followed by Seidman's article [98]. The article [8] described computational and well-posedness approaches, later detailed in [11] and [55]. The former study involved a finite volume approach in two dimensions, representing a generalization of the Scharfetter-Gummel discretization (see [7, 43, 44, 104] for more recent presentations). The study [55] introduced the fixed point approach based upon Gummel decomposition; the invariant domains were defined by maximum principles, and convex analysis; [35] was exploited for this model for the first time. Although it is sometimes inferred that Gummel iteration implies the convergence of suc-

cessive approximations, this is only selectively true; a rigorous study was carried out in [56] and in the Yale dissertation of Kerkhoven [71]. This thesis blended the analytical and convergence properties associated with the semiconductor model (see also [72]). Well-posedness for the unsteady problem was studied in [57]. A significant paper which described the numerical linear algebra involved in an approximate Newton iteration was [74].

Noteworthy during this period were the books [9, 10, 48, 49, 81–83, 87, 99, 103]. At about this time, more attention was devoted to sophisticated models which incorporated energy tracking and/or quantum mechanical effects. The study [75] addressed the resonant tunneling diode. The hydrodynamic model, introduced earlier by Blotekjaer [13], was re-introduced with systematic analysis and discretization, by Rudan and Odeh [96]. Ancona and Tiersten [4] and Ancona and Iafrate [3] introduced and studied the quantum-corrected drift-diffusion model (QCDD; see also [5]). Mathematical progress on the QCDD model has lagged. A survey of this progress is one of the goals of this article, and will be discussed in subsequent sections. This paper does not discuss the quantum hydrodynamic model. A comprehensive recent study is given in [34] (for earlier studies, including numerical simulations, cf. [23, 41, 69, 106]). Reference [106] was the first well-posedness result based upon [41].

The remainder of the introduction will round out the above discussion. The derivation of the hydrodynamic model is typically based on phase space moments of the Boltzmann equation (for an in depth presentation of the Boltzmann equation, see [19, 20]; for an early analysis of particle simulations, see [32, 33, 88]; for a ballistic study, see [102]; for an outline of the hydrodynamic methodology, see [58, 60]). The version of this model utilized in the device community makes use of the so-called inertial approximation, effectively suppressing the convective term in the momentum equation. The study [67] examines the effect of this approximation. The approximation induces a type of energy transport system, although this term is usually reserved for a special structure of the type examined in [21] (see also [66, 68]). A relatively recent presentation, based upon entropy principles, can be found in [69, Chapter 4]; numerical simulation is carried out in [40]. When the inertial approximation is not employed, the unsteady system is hyperbolic. This presents challenges to both the mathematical analysis and the numerical approximations, which in the general setting are required to be shock capturing in the time-dependent case. In the steady case, it is possible to identify subsonic regimes [42] and to compute directly, but, in general, the computational literature in this area has emphasized convergence to steady state (see[36]) via time-stepping. A substantial mathematical literature has developed around this; see [47] for a recent rigorous analysis (also, cf. the bibliography of [47] for parallel mathematical studies of convergence to scaled drift-diffusion models). Various mathematical papers have appeared on the topic of the hydrodynamic model, and tend to fall into two classes. The Cauchy problem for the unsteady system (pure initial value problem) is known to be well-posed for short time or small initial data if the latter are smooth. The general underlying theory is due to Kato (see [61] for the coupled Poisson/hydrodynamic system). Kato's theory is very powerful, and has been used to study the equations of gravitation (see [51]; see also the final two chapters of [53] for a presentation of Kato's theory). However, the situation is quite different for global (in time) solutions. The most general analytical studies in this regard are given by [37] and [22]; the former is strictly analytical, while the latter also contains simulations of the Gunn oscillator and the MESFET. Finally, the closely related field of electrodiffusion of ions can lead to models similar to drift-diffusion. Early contributions were due to Rubinstein [94, 95]. We close the paper with a brief summary of the general case, which couples fluid transport to ion diffusion.

1..2 Finite Element Approximation

Two elegant theories of approximation appeared concurrently in the early 1970s. One was termed the inf-sup theory (see [6, 15]; a comprehensive theory can be found in [14]). This theory is valid, however, only for linear formulations.and applications. A second theory for nonlinear formulations required a functional analytic framework, which had been discovered at approximately the same time as the inf-sup theory, by a group of authors working in the former Soviet Union [76]. It was later shown in [59] that this *nonlinear* theory logically generalizes the inf-sup theory of [6]. In a series of two papers [64, 73], Kerkhoven and the writer made use of the results of [76] to position the steady Van Roosbroeck system within this framework, and thereby obtain convergence results for the classical drift-diffusion system. They are consistent with the convergence order expected from linear equations, though with greater anticipated computational complexity. The convergence order is that of best ap-

proximation in the Hilbert space energy metric. A significant aspect of the theory is the use of discrete maximum principles; this was first outlined in [27, 73] (see also [70] for a more recent study). The notions of maximum and discrete maximum principles have been generalized via invariant region theory. These regions are seen as indispensable for the Gummel decomposition theory (see [63] for a very recent and general study). Since this theory is well understood only for 'de facto' diffusion-reaction' systems, the quasi-Fermi levels are employed in the application to the semi-conductor model. Early studies for the unsteady problem are due to Smoller and others [101], who introduced the concepts of outward and inward pointing vector fields on the boundary of the invariant region. This has been retained, or generalized, in subsequent studies, including those of trapping regions. Finite elements (discontinuous Galerkin method) have also been used for the hydrodynamic model [24].

2. The Quantum-Corrected Drift-Diffusion Model

. There are two principal reasons to seek an enhanced drift-diffusion model. First, as noted in [30], quantization of energy states for electrons confined in the channel produces a shift of the charge peak, increasing the equivalent oxide thickness in such a way that the coupling of the gate and channel voltages is reduced. Second, the penetration of electrons under the channel barrier effectively smooths and lowers this barrier, increasing the off–state leakage current. New device structures and geometries have been investigated to limit quantization effects (see [105]). The quantum models proposed in the literature (Wigner transport equation [52], non-equilibrium Green's functions [29]) do not appear to be uniformly incorporated into industrial applications. Quantum Corrected Drift–Diffusion (QCDD) models are based on the introduction of a correction potential in the DD equation to account for quantum effects on the spatial distribution of charge carriers within the devices (see [3, 4, 90]). This approximation neglects quantum effects on transport which can be considered of higher order [77].

We follow the original idea contained in [55] to characterize the solution of the QCDD transport model as a fixed point of the the Gummel decomposition mapping. This close link between the theoretical existence analysis and the numerical algorithms was lacking in previous nonconstructive proofs (cf. [2, 89]). The article [2] formed the basis of the study [30]. The authors of [2] employed a truncation operator, to prevent the occurrence of singularities in the quantum corrections, and then proved convergence to the solution of the original system. This was retained in [30], whose notable mathematical features included a new theory of gradient equations for the Poisson equation, and a theory of invariant regions for the quantum correction equations, for which uniqueness is not guaranteed due to the lack of monotonicity of the semi-linear terms. We present, in summary form, the constructive aspects of [30].

2..1 Equations of the Quantum Drift–Diffusion Model

Under isothermal and steady–state regimes, the Quantum Corrected Drift–Diffusion (QCDD) model can be written in the following dimensionless form [3, 69]:

$$\begin{cases} -\operatorname{div}\left(\lambda^2\,\boldsymbol{\nabla}\varphi\right) = p - n + D, \\ -\delta_n^2 \triangle\sqrt{n} + \sqrt{n}\,\left(\varphi_n - \varphi + \ln\left(n\right)\right) = 0, \\ \quad G_n = \varphi_n - \varphi + \ln\left(n\right), \\ -\delta_p^2 \triangle\sqrt{p} + \sqrt{p}\,\left(-\varphi_p + \varphi + \ln\left(p\right)\right) = 0, \\ \quad G_p = \varphi_p - \varphi - \ln\left(p\right), \\ -\operatorname{div}\left(\mu_n\left(\boldsymbol{\nabla} n - n\boldsymbol{\nabla}\left(\varphi + G_n\right)\right)\right) = -U, \\ -\operatorname{div}\left(\mu_p\left(\boldsymbol{\nabla} p + p\boldsymbol{\nabla}\left(\varphi + G_p\right)\right)\right) = -U. \end{cases} \tag{1}$$

$(1)_1$ is the Poisson equation for the electrostatic potential φ, $(1)_6$–$(1)_7$ are the carrier continuity equations for the electron and hole carrier concentrations n and p, while $(1)_2$–$(1)_3$ and $(1)_4$–$(1)_5$ provide a self-consistent definition of the quantum corrections G_n and G_p as functions of φ, n, p and the quantum quasi–Fermi potentials φ_n and φ_p. Generalized Maxwell–Boltzmann statistics are given by:

$$n = \exp\left(\left(\varphi + G_n\right) - \varphi_n\right), \quad p = \exp\left(\varphi_p - \left(\varphi + G_p\right)\right). \tag{2}$$

System (1) is solved in a domain $\Omega \subset \mathbf{R}^d$, with boundary $\Gamma = \Gamma_D \cup \Gamma_N$ and outward unit normal vector $\mathbf{n}$, with $\Gamma_D = \Gamma_+ \cup \Gamma_0$. The pairwise disjoint partitions of Γ_+ and Γ_0 physically represent the ohmic contacts and material interfaces, while Γ_N physically represents the portions of the boundary separating the device domain from the exterior region. Boundary conditions for system (1) are:

$$\begin{cases} \varphi = \varphi_D, \qquad n = n_D, \qquad p = p_D & \text{on } \Gamma_+, \\ \varphi = \varphi_D, \qquad n = p = 0 & \text{on } \Gamma_0, \\ \boldsymbol{\nabla}\varphi \cdot \mathbf{n} = \mathbf{J}_n \cdot \mathbf{n} = \mathbf{J}_p \cdot \mathbf{n} = 0 & \text{on } \Gamma_N, \end{cases} \tag{3}$$

with the current densities $\mathbf{J}_n = \mu_n\left(\boldsymbol{\nabla} n - n\boldsymbol{\nabla}\left(\varphi + G_n\right)\right)$ and $\mathbf{J}_p = -\mu_p\left(\boldsymbol{\nabla} p + p\boldsymbol{\nabla}\left(\varphi + G_p\right)\right)$. The boundary data φ_D, n_D and p_D are computed assuming charge neutrality and thermal equilibrium on Γ_+, while on Γ_0 the prescribed value of φ_D is the external voltage applied at the gate contact up to the voltage drop across the gate oxide layer. The quantities λ, δ_n and δ_p in (1) are positive singular perturbation parameters resulting from the application of a scaling procedure [31]. Setting $\delta_n = \delta_p = 0$, which corresponds to formally performing the classical limit $\hbar \to 0$, allows the recovery of the standard DD model. We refer to [31, Sect. 2.4], for the explicit expressions of the parameters and of their numerical values. The quantity D is a given function and represents the doping profile of the device. We assume that D is a bounded function. The quantities μ_n and μ_p are the carrier mobilities. These are discussed in [99, Chapt. 4]. We assume that $\mu_\nu, \nu = n, p$, are strictly positive bounded functions. The quantity U is the net recombination rate, and accounts for recombination (R) and generation (G) effects in the semiconductor material. Several models for U are proposed in the literature to describe R/G effects in a quantum–modified setting (see [2] and [5]). The impact of R/G phenomena is not relevant for the present discussion; its effects are not included.

2..2 Preliminaries

Proceeding as in the case of the DD model (cf. [60], Sect.4.3), we define the following constants:

$$\alpha = \min\left(\inf_{\Gamma_+}\varphi_n,\, \inf_{\Gamma_+}\varphi_p\right) = \inf_{\Gamma_+}\varphi_a + \ln\left(\theta\right),$$
$$\beta = \max\left(\sup_{\Gamma_+}\varphi_n,\, \sup_{\Gamma_+}\varphi_p\right) = \sup_{\Gamma_+}\varphi_a - \ln\left(\theta\right),$$

where φ_a is the externally applied bias and $\theta := n_{int}/\overline{n}$, n_{int} and $\overline{n}$ denoting the intrinsic concentration in the semiconductor material and the scaling factor for carrier concentrations, respectively. For the purpose of the analysis of the existence of a fixed point of the Gummel Decomposition Map (GDM), defined in the following section, the above quantities should provide the upper and lower bounds for the invariant region to which the fixed point belongs. With this aim, it is useful to *symmetrize* the bounding interval $[\alpha,\, \beta]$ by introducing, as in Ref. [2], the following constants:

$$m = -\|\varphi_a\|_{L^\infty(\Gamma_+)} + \ln\left(\theta\right) - 1 \le \alpha,$$
$$M = -m = \|\varphi_a\|_{L^\infty(\Gamma_+)} - \ln\left(\theta\right) + 1 \ge \beta,$$

with $m \le 0$ and $M \ge 0$. For any nonnegative carrier concentrations n and p, we set $w := n^{1/2}$ and $z := p^{1/2}$, and for any bounded potential φ, we define the auxiliary variables,

$$\sigma_n(w, \varphi) := w^2 e^{-\varphi}, \qquad \sigma_p(z, \varphi) := z^2 e^{\varphi}. \tag{4}$$

For any bounded quantum quasi–Fermi potentials φ_n and φ_p, we introduce the quantum Slotboom variables

$$\rho := \exp\left(-\varphi_n\right), \qquad \omega := \exp\left(\varphi_p\right), \tag{5}$$

in such a way that the generalized Maxwell-Boltzmann statistics (2) can be written in the equivalent form

$$n = \rho\, \exp\left(\varphi + G_n\right), \qquad p = \omega\, \exp\left(-\left(\varphi + G_p\right)\right). \tag{6}$$

Then, we define the closed convex set

$$K = \{[v,\, w] \in \left(L^2(\Omega) \times L^2(\Omega)\right) : \\ m \le [v(x),\, w(x)] \le M,\ \text{a.e. in } \Omega\}, \tag{7}$$

and for any function g and any fixed $\delta \in (0, 1]$, we introduce the *truncation operator*

$$[g]_\delta := \max\left(g,\, \delta\right).$$

We also let $\mathcal{V} := H^1(\Omega) \cap L^\infty(\Omega)$.

2..3 The Gummel Decomposition Map

Given a pair $[\widetilde{\varphi}_n,\, \widetilde{\varphi}_p] \in K$, and $\delta \in (0, 1]$, the GDM for the iterative solution of the QCDD system (1) consists of the following steps (*Outer Loop*):

(1): solve in the domain Ω the nonlinear system:

$$\begin{cases} -\operatorname{div}\left(\lambda^2\, \boldsymbol{\nabla}\varphi_\delta\right) + w_\delta^2 - z_\delta^2 - D = 0, \\ -\delta_n^2 \triangle w_\delta + w_\delta\, \left(\widetilde{\varphi}_n - \varphi_\delta + 2\ln\left([w_\delta]_\delta\right)\right) = 0, \\ -\delta_p^2 \triangle z_\delta - z_\delta\, \left(\widetilde{\varphi}_p - \varphi_\delta - 2\ln\left([z_\delta]_\delta\right)\right) = 0, \end{cases} \tag{8}$$

subject to the boundary conditions:

$$\begin{cases} \varphi_\delta = \varphi_D \quad \text{on } \Gamma_D, & \boldsymbol{\nabla}\varphi_\delta \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N, \\ w_\delta = n_D^{1/2} \quad \text{on } \Gamma_+, & w_\delta = 0 \quad \text{on } \Gamma_0, \\ & \boldsymbol{\nabla} w_\delta \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N, \\ z_\delta = p_D^{1/2} \quad \text{on } \Gamma_+, & z_\delta = 0 \quad \text{on } \Gamma_0, \\ & \boldsymbol{\nabla} z_\delta \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_N. \end{cases} \tag{9}$$

(2): Define the regularized quantum corrections:

$$G_{n_\delta} = \widetilde{\varphi}_n - \varphi_\delta + 2\ln\left([w_\delta]_\delta\right), \\ G_{p_\delta} = \widetilde{\varphi}_p - \varphi_\delta - 2\ln\left([z_\delta]_\delta\right), \tag{10}$$

and the quantum–corrected potentials

$$V_{n_\delta} := \varphi_\delta + G_{n_\delta}, \qquad V_{p_\delta} := \varphi_\delta + G_{p_\delta}. \tag{11}$$

(3): Solve in the domain Ω the linear, uncoupled continuity equations:

$$-\operatorname{div}\left(\mu_n e^{V_{n\delta}}\,\boldsymbol{\nabla}\rho_\delta\right)=0, \tag{12}$$

$$-\operatorname{div}\left(\mu_p e^{-V_{p\delta}}\,\boldsymbol{\nabla}\omega_\delta\right)=0, \tag{13}$$

subject to the boundary conditions:

$$\begin{cases} \rho_\delta=\rho_D \quad \text{on } \Gamma_+, & \boldsymbol{\nabla}\rho_\delta\cdot\mathbf{n}=0 \text{ on } \Gamma_0\cup\Gamma_N,\\ \omega_\delta=\omega_D \quad \text{on } \Gamma_+, & \boldsymbol{\nabla}\omega_\delta\cdot\mathbf{n}=0 \text{ on } \Gamma_0\cup\Gamma_N. \end{cases} \tag{14}$$

(4): Update the quantum quasi–Fermi potentials by inverting (5):

$$\varphi_n=-\ln\left(\rho_\delta\right), \qquad \varphi_p=\ln\left(\omega_\delta\right). \tag{15}$$

The GDM T is now defined. We summarize: Given a pair $[\widetilde{\varphi}_n,\,\widetilde{\varphi}_p]\in K$, carry out Steps (1–4) to determine the image of this pair under the action of T.

3. Analysis of the Gummel Decomposition

In [30], the Gummel decomposition is described as the outer iteration, which it is in a computing procedure. Two major results are derived in [2]: (i) a derivation of the bounds m, M, followed by a proof of existence of a fixed point for each pair of regularization parameters (the methods are nonconstructive, and differ from the Gummel decomposition approach); (ii) a proof of convergence as the regularization parameters tend to zero. In this paper, we explain the original contribution of [30] in analyzing the well-posedness of the individual components of the Gummel decomposition. The 'a priori' bounds m, M of [2] translate immediately into bounds (see eq. (23) of [30] and (4) above) given by:

$$0\le\sigma_{n,\delta}\le\beta_n,\ 0\le\sigma_{p,\delta}\le\beta_p. \tag{16}$$

3..1 The Inner Iteration Loop

Given $[\widehat{\varphi}_\delta,\,\widehat{w}_\delta,\,\widehat{z}_\delta]$, satisfying the essential boundary conditions in (9), the inner loop for the solution of the nonlinear system (8) consists of the following steps:

(A): Solve the nonlinear Poisson equation for the updated potential φ_δ:

$$\begin{cases} -\operatorname{div}\left(\lambda^2\,\boldsymbol{\nabla}\varphi_\delta\right)+\sigma_{n,\delta}(\widehat{w}_\delta,\widehat{\varphi}_\delta)\\ \quad e^{\varphi_\delta}-\sigma_{p,\delta}(\widehat{z}_\delta,\widehat{\varphi}_\delta)\,e^{-\varphi_\delta}-D=0, & \text{in } \Omega\\ \varphi_\delta=\varphi_D & \text{on } \Gamma_D,\\ \boldsymbol{\nabla}\varphi_\delta\cdot\mathbf{n}=0 & \text{on } \Gamma_N. \end{cases} \tag{17}$$

(B): Solve the nonlinear Bohm equation for the updated square root of the electron concentration w_δ:

$$\begin{cases} -\delta_n^2\triangle w_\delta+\\ w_\delta\,\left(\widetilde{\varphi}_n-\varphi_\delta+2\ln\left([w_\delta]_\delta\right)\right)=0, & \text{in } \Omega,\\ w_\delta=n_D^{1/2} & \text{on } \Gamma_+,\\ w_\delta=0 & \text{on } \Gamma_0,\\ \boldsymbol{\nabla}w_\delta\cdot\mathbf{n}=0 & \text{on } \Gamma_N. \end{cases} \tag{18}$$

(C): Solve the nonlinear Bohm equation for the updated square root of the hole concentration z_δ:

$$\begin{cases} -\delta_p^2\triangle z_\delta-\\ z_\delta\,\left(\widetilde{\varphi}_p-\varphi_\delta-2\ln\left([z_\delta]_\delta\right)\right)=0, & \text{in } \Omega,\\ z_\delta=p_D^{1/2} & \text{on } \Gamma_+,\\ z_\delta=0 & \text{on } \Gamma_0,\\ \boldsymbol{\nabla}z_\delta\cdot\mathbf{n}=0 & \text{on } \Gamma_N. \end{cases} \tag{19}$$

3..1.1 Gradient Equation

The following result is quoted from [30]. Full details of the proof are given in this reference.

Lemma 3..1 *Let $\sigma_{n,\delta}$ and $\sigma_{p,\delta}$ be given functions satisfying* (16). *Then, problem* (17) *has a uniquely defined solution φ_δ within the order interval $[\varphi_{min},\varphi_{max}]$, where the quantities $\varphi_{min}\equiv\inf_\Omega\,(\underline{\varphi})$ and $\varphi_{max}\equiv\sup_\Omega\,(\overline{\varphi})$ are independent of δ and the functions $\underline{\varphi}$ and $\overline{\varphi}$ are the solutions of the gradient equations*

$$-\lambda^2\Delta\underline{\varphi}+\beta_n\exp(\underline{\varphi})=D_{\min} \tag{20}$$

and

$$-\lambda^2\Delta\bar{\varphi}-\beta_p\exp(-\bar{\varphi})=D_{\max}, \tag{21}$$

to which the boundary conditions $(17)_{2-3}$ *must be adjoined.*

It is surprising that the maximum principles, originally derived in [55], and also found in [82], are not adequate to derive the bounds for the potential equation analyzed here. The explanation lies in the core definition of the closed convex set introduced above in (7), and in the corresponding generality of inequalities (16).

3..1.2 The Density System

Lemma 3..2 *Let $\widetilde{\varphi}_n$ and $\widetilde{\varphi}_p$ be given functions in K and let φ_δ be the unique solution of* (17) *as in Lemma 3..1. Then, problems* (18) *and* (19) *have uniquely defined solutions w_δ and z_δ within the order intervals $Q_w = [0, w_{\max}]$ and $Q_z = [0, z_{\max}]$, resp. $w_{\max}$ and $z_{\max}$ are the following positive quantities, independent of δ:*

$$w_{\max} = \max\{\sup_{\Gamma_+} w,\, \exp[(M + \varphi_{\max})/2]\},$$
$$z_{\max} = \max\{\sup_{\Gamma_+} z,\, \exp[(M - \varphi_{\min})/2]\}.$$

Since neither of the nonlinear equations in Steps B and C of the inner iteration loop is a gradient equation, a new theory is required to examine the corresponding boundary value problems. This is outlined in detail in the appendices of [30], based on invariant regions. The bounds of the lemma define the respective invariant regions for the principal variables. A key connection between the vector field and the boundary of the invariant region is that it is outward pointing on the region's boundary. Since solutions are not unique, in general, a continuous selection principle, based upon a homotopy argument, insures that the mapping is well-defined. The selection principle is based upon the functional-analytic arguments of [54], where an Euler predictor/Newton corrector method is introduced. The method is designed so that, along the homotopy path, the approximations remain in the domain of convergence of Newton's method. This construction overcomes the lack of demonstrated uniqueness in the system. The hypothesis, justified in [30], is stated as follows.

Assumption 3..1 (*Continuous Selection Hypothesis) Let (N, P) denote the components of the mapping introduced in Steps B,C above, via w, z. The homotopy mappings for N, P, starting with Laplace's equation, and terminating in a specified solution, are continuous in the L^2 sense with respect to the functions $\tilde{\varphi}_n, \tilde{\varphi}_p, \varphi_\delta$.*

3..2 Existence of a Fixed Point for The Generalized Gummel Map

In section 2..3, we have defined a consolidated mapping $\mathbf{T} : K \to K$, with the properties:

(*i*) Components act *invariantly* on the closed convex subsets of L^2, defined pointwise by the bounds given in Lemma 3..1 and Lemma 3..2.

(*ii*) Composition mapping $\mathbf{T}$ acts *invariantly on* K.

The following is quoted from [30].

Theorem 3..1 *Under the hypotheses expressed in the bounds of inequalities* (16) *and the Continuous Selection hypothesis 3..1, the fixed point map defined as the result of steps A,B,C above has a fixed point in K. Moreover, a solution triple φ, n and p to the BVP* (1) *exists in $H^1(\Omega) \cap L^\infty(\Omega)$.*

Remark 3..1 *This strategy of a generalized Gummel method was extensively device-tested via the simulations of [30], where one, two, and three dimensional examples were studied. The numerical experiments include a careful study of $\delta \to 0$, which was verified analytically in [2].*

4. Model for a Solar Cell

We cite the following drift-diffusion model as a template [17]. It is the most advanced macroscopic model we have identified in the literature. The densities of electrons n, holes p and excitons x, and the electrostatic potential ϕ evolve according to:

$$\begin{aligned}
\frac{\partial n}{\partial t} &= D(\nabla\phi, x) - R(n,p) \\
&\quad -\frac{1}{q}\nabla\cdot[qn\mu_n\nabla\phi - kT\mu_n\nabla n], \\
\frac{\partial p}{\partial t} &= D(\nabla\phi, x) - R(n,p) \\
&\quad -\frac{1}{q}\nabla\cdot[-qp\mu_p\nabla\phi - kT\mu_p\nabla p], \\
\frac{\partial x}{\partial t} &= G - D(\nabla\phi, x) + \frac{1}{4}R(n,p) - R'(x) \\
&\quad +\frac{1}{q}\nabla\cdot[kT\mu_x\nabla x], \\
\nabla\cdot(\varepsilon\nabla\phi) &= -q(p-n). \qquad (22)
\end{aligned}$$

The quantities D and G are exciton dissociation and generation rates, resp. The former is expressed by Onsager's theory [45], whereas photo-generation is tracked by experimentally measured flux expansions [38]. Recombination is expressed via the Langevin form of $R(n,p)$ [12] and $R'(x)$ expresses relaxation of excitons. The first three equations are standard continuity equations for the carriers, whereas the Gauss law for the electric force is expressed in the final equation. The constants q, k, T, ε denote charge modulus, the Boltzmann constant, the ambient temperature, and the permittivity. For the ith carrier, μ_i is the mobility.

The model must be able to predict concentrations and fluxes of carriers, and their response to changes of morphology. The cell as designed currently has a significant number of donor/acceptor interfaces, and the particular phenomena at these interfaces represent a critical factor in the device performance. Thus far, no definitive mathematical results exist for this model.

5. Electrodiffusion: Influence of Electrolytes

We consider the nonlinearly coupled Poisson-Nernst-Planck/Navier-Stokes (PNP/NS) system of PDEs, suitably coupled with generation/reaction zero-order terms. The basic system was introduced by Rubinstein in [95]. This discussion is based upon the recent article [65]. In the consolidated model, self-consistent charge transport is represented by the Poisson-Nernst-Planck system, and the fluid motion by a Navier-Stokes system with forcing terms. This model is capable of describing electro-chemical and fluid-mechanical transport throughout the fluid environment. This already engages a range of spatial and temporal scales. Chemical reactions in cellular metabolism can be studied by coupling this system to generation/reaction zero order terms, denoted by R_n, R_p below. We formulate the initial/mixed-boundary value problem in $\Omega \subset \mathbf{R}^m$. Existence of weak solutions, based upon Rothe's method, was demonstrated in [65]. A local smooth theory based upon these equations was derived earlier for the Cauchy problem in [62]. For fluid-structure systems which are modeled *linearly*, there are results; see [1] for a fluid/elasticity model analyzed via semigroup methods. In addition, the results of [84] extend semigroup methods to the Navier-Stokes system.

5..1 The Fluid/Transport System

We begin by formulating the constitutive relations for the ionic current densities. They extend the usual relations, given in PNP theory, by the inclusion of velocity convection terms. If $\vec{v}$ is the velocity of the electrolyte, and the ionic concentrations are denoted by n, p, respectively, the current densities are:

$$\vec{J_n} = eD_n\nabla n - e\mu_n n\nabla\phi - e\vec{v}n, \quad (23)$$

$$\vec{J_p} = -eD_p\nabla p - e\mu_p p\nabla\phi + e\vec{v}p. \quad (24)$$

Here, $\vec{J_n}, \vec{J_p}$ are the anion and cation current densities, with corresponding (constant) diffusion and mobility coefficients, D_n, D_p, μ_n, μ_p, respectively. The charge modulus is given by e, and ϕ is the electric potential. The Poisson equation, given shortly, describes the coupling. The enhanced PNP system is then given by, with ε the dielectric constant of the medium:

$$\begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{e}\nabla\cdot\vec{J_n} &= -R_n, \\ \frac{\partial p}{\partial t} + \frac{1}{e}\nabla\cdot\vec{J_p} &= -R_p, \\ \vec{E} &= -\nabla\phi, \\ \nabla\cdot(\varepsilon\nabla\phi) &= e(n-p-d). \end{aligned} \quad (25)$$

In the above, the 'fixed' charge concentration is denoted by d; though not mobile, it is an input which may change in time. The Einstein relations are employed as usual. For convenience, R_n, R_p are assumed bounded and continuous in their arguments $\vec{v}, n, p$.

The velocity of the electrolyte is determined by the Navier-Stokes equations:

$$\begin{aligned} &\rho(\vec{v}_t + \vec{v}\cdot\nabla\vec{v}) - \eta\Delta\vec{v} = -\nabla P_f - e(p-n)\nabla\phi, \\ &\nabla\cdot\vec{v} = 0, \end{aligned} \quad (26)$$

where ρ is the constant (mass) density of the electrolyte, P_f denotes fluid pressure, and η is the constant dynamic viscosity. Note that d has been neglected in the electric 'volume force' term. We shall make use of the kinematic viscosity, $\nu_* = \eta/\rho$, in the statement of the mathematical model. Note that the signs of R_n, R_p are those adopted in semiconductor physics, but the explicit forms are not essential for this discussion.

5..2 Algorithm and Modeling Summary

In this concluding section, we briefly discuss the main relevant issues concerning the numerical treatment of the PNP/NS system, and its application in the modeling of several realistic problems arising in Bio-Engineering.

5..2.1 Numerical Approximation

A staggered algorithm is adopted for the successive solution of the PNP and NS subsystems, in the same fashion as in the treatment of fluid-structure interaction problems. For each time level t_k, a PNP system with a given velocity field $\mathbf{v}^{(k)}$ is solved using the Gummel Map discussed earlier. This provides in output the updated concentrations $n^{(k+1)}$, $p^{(k+1)}$ and electric field $\mathbf{E}^{(k+1)}$. Then, the NS system is solved using a fixed point iteration based on Oseen sub-problems [91]. This provides in output the updated velocity $\mathbf{v}^{(k+1)}$ and pressure $P_f^{(k+1)}$. The process is repeated until

self-consistency is achieved for the solution at the considered time level. The numerical discretization of the linearized sub-problems is carried out using (stabilized) dual–mixed hybridized finite element formulations [16, 18]. This ensures the same computational accuracy for scalar and vector/tensor–valued unknowns, local conservation and self–equilibrium, and nonnegativity of concentrations. In the case of the continuity equations in the linearized PNP system, exponential fitting is included in the scheme to deal with the presence of highly dominating advective terms. In the case of the momentum balance equation in the linearized NS system, a Discontinuous Galerkin upwind treatment is introduced for stabilization.

5..2.2 Applications

Contemporary applications in Bio-Engineering are characterized by sophisticated interacting systems, as in Lab-On-Chip technology, where electrochemical and fluid–mechanical transport of substances, chemical reactions and electrical transduction of biological signals simultaneously occur, at strongly varying spatial and temporal scales. Significant examples of such systems, for which the PNP/NS model provides an appropriate description in most relevant situations, are:

- Bio-chips for neuronal cell monitoring. The basic configuration of such bio-hybrid devices consists of a cell in an electrolyte solution, that is grown onto the surface of an electronic substrate with the aim of transducing an ionic current signal into an electric output current. Bio-chips encompass significant spatial and temporal scales. For example, the ion channels in the cell membrane are nanometers in length, and the current is gauged on the nanosecond scale. The channel gating is on the millisecond scale. The cell is of micron dimensions, and the communication between cell and transistor is affected by gating. We refer to [39] for a thorough description of the system and to [85] for further details on the characterization of the neuronal/transistor interface. For simulations related to such models, we refer to [78–80].

- Bio-reactors for cell growth in tissue engineering. The basic configuration of such devices is a three–layer structure including two fluid layers and, in between, a porous scaffolded biocompatible matrix where cells are grown upon hydrodynamical perfusion of a nutrient culture medium. Again, the device encompasses significant spatial and temporal scales, the scaffold being of centimeter dimensions, and the single pore being of micron dimensions, while a typical culture period is of the order of weeks. We refer to [28, 92] for a detailed description of the bioreactor architecture and of the analysis of the role of shear stress and perfusion rate on the effectiveness of the culture procedure. A recent example of mathematical modeling and numerical simulation of bio-reactors can also be found in [26].

- Microfluidic chambers in Lab-On-Chip technology. These devices are frequently used in micro-electro-mechanical systems (MEMS) in the chemical and bio-medical industry, or in electro-kinetic transport processes such as electro-osmosis and electro-phoresis. A mathematical model similar to the one discussed in this article, together with extensive numerical investigation, is presented in [25, 50].

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