CHARGE TRANSPORT IN AN INCOMPRESSIBLE FLUID: NEW DEVICES IN COMPUTATIONAL ELECTRONICS

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Abstract. A model for electro-diffusion is discussed, characterized by the Navier-Stokes/Poisson-Nernst-Planck system. In particular, we emphasize: (i) significant applications; (ii) existence for the initial/boundary-value problem; (iii) aspects of the steady problem.

Key words. Navier-Stokes/Poisson-Nernst-Planck, charge transport, ionic channels, slip condition, initial/boundary-value problem, steady problem, EOSFET

AMS(MOS) subject classifications. Primary 35Q30, 76D03, 76C05.

1. Introduction.

Comprehensive conservation law models began to be used in computational electronics for simulation in the latter 1980s, when the charged carriers were characterized as a compressible (energetic) fluid in a solid state semiconductor device. Earlier, Blotekjaer [1] had characterized energy valleys as a basis for carrier distinction in a hydrodynamic model, derived from the Boltzmann equation. However, the timely paper [37] serves as a marker for the confluence of emerging technology and numerical algorithms. It was shortly after this time that the International Workshops on Computational Electronics [16] began to be held, permitting the systematic presentation and publication of hydrodynamic model simulations and analysis for charge transport [14, 11, 7, 25, 4, 5, 19, 21] and those of the closely related energy transport model [24, 26, 27]. In addition, devices such as the resonant tunneling diode motivated the study of quantum hydrodynamic models, based upon Madelung's transformation [13, 6, 41, 27, 10]. The use of charge conservation as a legitimate, physics-based, modeling tool for electrons and holes dates to the period shortly after the invention of the transistor (see [39]). A recent survey [22] fills in this discussion.

1.1. New devices.

By the term, 'new devices', is meant those electronic devices that do not function exclusively via solid-state physics technology. Among these, organic devices and hybrid devices have recently emerged. Bio-chips (discussed below) and solar cells [2] are included, for example. As an illustration, we consider the study of charge transport in Voltage Operated ionic Channels (VOCs) for application in Bio–Electronics and biophysics more generally. VOCs are present on cellular membranes, where they regulate and maintain the dynamical electro-chemical equilibrium between the cell-surrounding environment and the intracellular en-

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vironment. Single channel current recordings have been made possible by the development of the patch clamp by E. Neher and B. Sakmann. VOCs can be included in a more comprehensive model: Nanoscale Biological Chips (NBC). An example of such a device is the Electrolyte Oxide Silicon Field Effect Transistor (EOSFET) in which a transistor is gated by cell-generated ionic current via an electrolyte (see [40, 12] for studies and [32] for illuminating graphics and discussion). This cited work also includes a characterization of the electrolyte as an equivalent circuit model. In this paper we rely on biophysical conservation laws to define the appropriate system of partial differential equations. In particular, we discuss: (i) a Navier-Stokes/Poisson-Nernst-Planck model; (ii) the existence theory for the initial/boundary-value problem; (iii) the steady problem. These issues are characterized by electro-diffusion.

1.2. Related literature. The mathematical model presented in the next section is due to Rubinstein [36]. Analytical studies include local smooth solutions of the Cauchy problem [20], and global weak solutions of the initial/boundary-value problem [23, 38]. For simulations of the model presented here, see [30, 28, 29]. Since the determination of the current density was a prime goal of these studies, a critical byproduct was the conclusion that the fluid fluctuations in the ion channels decisively impacted the current. This conclusion mandates, in some sense, the analysis of the extended model. Another application is that of tissue engineering in bioreactors [9, 35]. A culture medium creates hydrodynamic stress within a scaffolded micro-architecture. Future models may permit charge flow. Growth of neuronal cells [33] and electro-hydrodynamics [15] provide additional applications. Finally, a mathematical model similar to the one employed here is employed for electro-osmotic flow [8].

2. The mathematical model. The equations are discussed in the first subsection, and a weak solution is defined following this.

2.1. The Fluid/Transport System. If $\vec{v}$ is the velocity of the electrolyte, and the ionic concentrations are denoted by n, p, the current densities are:

$$\vec{J}_n = eD_n \nabla n + e\mu_n n\vec{E} - e\vec{v}n,$$
$$\vec{J}_p = -eD_p \nabla p + e\mu_p p\vec{E} + e\vec{v}p.$$

$\vec{J}_n, \vec{J}_p$ are the anion and cation current densities, with corresponding diffusion and mobility coefficients, D_n, D_p, μ_n, μ_p. The charge modulus is given by e, and ϕ is the electric potential, with electric field $\vec{E} = -\nabla\phi$. The enhanced PNP system is, with ϵ the dielectric constant:

$$\frac{\partial n}{\partial t} - \frac{1}{e}\nabla\cdot \vec{J}_n = 0, \quad D_n = (kT_0/e)\mu_n,$$
$$\frac{\partial p}{\partial t} + \frac{1}{e}\nabla\cdot \vec{J}_p = 0, \quad D_p = (kT_0/e)\mu_p,$$

$$\nabla\cdot(\epsilon\nabla\phi) = e(n-p-d) \quad \text{(Poisson equation).}$$

The Einstein relations have been used: T_0 is the ambient temperature; k denotes Boltzmann's constant; d is the non-mobile charge. The velocity of the electrolyte is determined by the Navier-Stokes system:

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

where ρ is the (mass) density of the electrolyte, P_f denotes fluid pressure, and η is the dynamic viscosity. We shall make use of the kinematic viscosity, $\nu_* = \eta/\rho$, which has a nominal value of $1\text{nm}^2/\text{ps}$ at room temperature.

2.2. Weak solution in the sense of Leray. We first introduce the required function spaces. Note that Σ_D denotes the Dirichlet boundary for the variables n, p, ϕ. For $\vec{v}$, the entire boundary of Ω is used for the specification of (possibly) slip boundary conditions. Let m denote the Euclidean space dimension, and let $s \geq m/2$ be prescribed ($H^{s-1} \subset L_m$). Denote by $\mathcal{H}$ the divergence free functions in the m-fold Cartesian product of $H^1(\Omega)$, by $\mathcal{H}^s$ the intersection of $\mathcal{H}$ with the m-fold Cartesian product of $H^s(\Omega)$; by $\mathcal{H}^s_0$ the zero trace (on $\partial\Omega$) subspace of $\mathcal{H}^s$. $(\mathcal{H}^s_0)^*$ is the corresponding dual. Analogously, H^s_{0,Σ_D} denotes those H^s functions with zero trace on Σ_D. The space-time domain is: $\mathcal{D} = \Omega \times [0,T]$. Define

$$\begin{aligned}\mathcal{C} = \{\vec{u} = (\vec{v},\phi,n,p) : \vec{v} \in L_2((0,T);\mathcal{H}); n,p \in L_2((0,T);H^1);\\ \phi \in L_2((0,T);H^2);\ (\vec{v}_t, n_t, p_t) \in L_2((0,T);(\mathcal{H}^s_0)^* \times (H^s_{0,\Sigma_D})^* \times (H^s_{0,\Sigma_D})^*)\}.\end{aligned}$$

A weak solution of the Navier-Stokes/PNP system is a vector $\vec{u} \in \mathcal{C}$ such that boundary conditions are satisfied, such that ϕ is related to n, p via the Poisson equation, and, for $a(\vec{v},\vec{v},\vec{\psi}) = \int_\Omega \vec{v}\cdot\nabla\vec{v}\vec{\psi}\, d\xi$, and for test functions $\vec{\psi}, \omega_n, \omega_p$, continuous from $[0,T]$ into the space $\mathcal{H}^s_0 \times H^s_{0,\Sigma_D} \times H^s_{0,\Sigma_D}$, with time derivatives in $L^2(\mathcal{D})$, we have (the highlighted term is the NS-term):

$\vec{v}$ equation

$$\begin{aligned}&\int_{\mathcal{D}} [\rho\vec{v}\frac{\partial\vec{\psi}}{\partial t} - \eta\nabla\vec{v}\cdot\nabla\vec{\psi}]d\xi dt \boxed{-\textstyle\int_0^T \rho a(\vec{v},\vec{v},\vec{\psi})dt}\\ &-e\int_{\mathcal{D}} (p-n)\nabla\phi\cdot\vec{\psi}\, d\xi dt = \int_{\Omega\times\{T\}} \vec{v}\cdot\vec{\psi}\, d\xi - \int_{\Omega\times\{0\}} \vec{v}_0\cdot\vec{\psi}\, d\xi\end{aligned}$$

n equation

$$\begin{aligned}&\int_{\mathcal{D}} [n\frac{\partial\omega_n}{\partial t} - D_n\nabla n\cdot\nabla\omega_n + \left(\frac{neD_n}{kT_0}\right)\nabla\phi\cdot\nabla\omega_n + \vec{v}n\cdot\nabla\omega_n]d\xi dt\\ &= \int_{\Omega\times\{T\}} n\omega_n\, d\xi - \int_{\Omega\times\{0\}} n_0\omega_n\, d\xi\end{aligned}$$

p equation

$$\int_{\mathcal{D}} [p\frac{\partial \omega_p}{\partial t} - D_p \nabla p \cdot \nabla \omega_p - \left(\frac{peD_p}{kT_0}\right) \nabla \phi \cdot \nabla \omega_p + \vec{v} p \cdot \nabla \omega_p] d\xi dt$$
$$= \int_{\Omega \times \{T\}} p\omega_p \, d\xi - \int_{\Omega \times \{0\}} p_0 \omega_p \, d\xi$$

2.3. Multiscales in the EOSFET.

2.3.1. Brief description of the EOSFET. The EOSFET consists of a single cell immersed in a surrounding bath, connected to an electronic substrate: oxide/transistor. Gating of the transistor is achieved via electrolyte current. Vertical cross-sections can be used to define two-dimensional computational domains. The role of the boundary conditions becomes important here in the separation of the domain components. For example, Dirichlet boundary conditions are imposed on a portion of the top of the cell, to specify cell-reference ionic concentrations. Dirichlet conditions are again specified on a reference portion of the lower cell, near the cleft separating the cell from the electronic substrate. These conditions also contain information regarding potential differences in the device. The EOSFET has extraordinary long-term implications for use: (i) transduction of chemical signals generated by the biological component into an electronically identifiable signal; (ii) activation of the biological component by an applied electronic signal.

2.3.2. Disparity of scales. This model encompasses significant spatial and temporal scales. 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. Moreover, experience in the case of the PNP model and also the hydrodynamic model has shown that the dynamic problem reaches a steady state much more rapidly than the gating time scale. This indicates the importance of the steady problem in the open channel. An early simulation of this case, via the full conservation law model, can be found in [3].

2.4. Assumptions. In this section, we summarize the assumptions.

2.4.1. Boundary conditions. Dirichlet boundary values for $\vec{v}$ are imposed on all of $\partial\Omega$ with the stipulation that a nonnegative normal fluid velocity component condition is imposed on $\partial\Omega$. For the remaining variables, Σ_D serves as the Dirichlet boundary, with homogeneous Neumann boundary conditions on the boundary complement. Thus, we assume the existence of functions $\vec{v}_B, \phi_B, n_B, p_B$, defined continuously from $[0, T]$ into appropriately smooth spaces, such that the following requirements hold for the solution vector: $\vec{v}_{|\partial\Omega} = \vec{v}_{B|\partial\Omega}$, $\phi_{|\Sigma_D} = \phi_{B|\Sigma_D}$, $n_{|\Sigma_D} = n_{B|\Sigma_D}$, $p_{|\Sigma_D} = p_{B|\Sigma_D}$. Moreover, it is assumed that $\vec{v}_B$ is divergence free on Ω.

2.4.2. Boundary regularity. We assume the boundary of Ω is sufficiently regular that the classical trace formulas and Green's integration by parts formulas are valid, and we assume that the Poisson solver is H^2 regularizing for L_2 data. Note that this implies that the mixed boundary conditions imposed by ϕ_B are not completely arbitrary.

2.4.3. Technical assumptions on given data. $\vec{v}_B(\cdot\,,t)$ has components in $\mathcal{H}^s \cap L^\infty\ \forall t \in [0,T]$; $\phi_B(\cdot\,,t) \in H^{\max(s,2)}$; and $n_B(\cdot\,,t), p_B(\cdot\,,t) \in H^s$. The functions $\vec{v}_B, n_B, p_B$ have time derivatives in $L^2(\mathcal{D})$ and (trace time derivatives) in $L^2(\mathcal{D}_b)$. The initial data functions, $\vec{v}_0, n_0, p_0$, are of finite energy, with $\vec{v}_0$ divergence free. The non-mobile charge d is continuous from $[0,T]$ into L^2.

3. The existence theory. The essential approach of [23] is summarized; Rothe's method forms the basis for the existence proof. Because of this, we begin with the stationary case.

3.1. Abstract stationary result. The analysis is based upon finite-dimensional approximations, combined with an appropriate passage to the limit. Let X, Y be separable, reflexive Banach spaces, with Y a subspace, densely and continuously embedded in X; X is compactly embedded in the reflexive Banach space W. Consider $A : X \mapsto Y^*$,

$$A(u) = Lu + a(u,u,\cdot\,) + F(u,\cdot\,),$$

where $L : X \mapsto X^*$ is an isomorphism. The structure of L is induced by a continuous, coercive bilinear form $B(\cdot\,,\cdot\,)$ on $X \times X$:

$$\langle Lu, v\rangle = B(u,v),\ B(u,u) \geq c\|u\|^2.$$

We outline the general assumptions now.

- a is continuous on $X \times X \times Y$ and F is continuous on $X \times Y$.
- For each $u \in X$, $a(u,u,\cdot\,), F(u,\cdot\,)$ are continuous *linear* functionals on Y.
- The coerciveness property,

  $$\langle A(u), u\rangle / \|u\|_X \to \infty,\ \text{as } \|u\|_X \to \infty, u \in Y,$$

  holds in the norm on X for elements in Y.
- If $u_k \rightharpoonup u$ (weakly) in X and $u_k \to u$ in W, then

  $$a(u_k, u_k, v) \to a(u,u,v),\ \forall v \in Y,$$

  $$F(u_k, v) \to F(u,v),\ \forall v \in Y.$$

The following theorem is proved in [23].

THEOREM 3.1. *Under the stated hypotheses, there is an element $u \in X$ satisfying $A(u) = f_{|Y}$ for any given $f \in X^*$.*

3.2. Rothe's method. Given a partition $\{t_k = k\Delta t : 0 \le k \le K\}$ of $[0,T]$, we define the following semidiscrete system:

$$\frac{\vec{v}_k - \vec{v}_{k-1}}{\Delta t} + V(\vec{v}_k, \vec{v}_k, n_k, p_k, \cdot\,) = 0,$$
$$\frac{n_k - n_{k-1}}{\Delta t} + N(\vec{v}_k, \vec{v}_k, n_k, p_k, \cdot\,) = 0,$$
$$\frac{p_k - p_{k-1}}{\Delta t} - P(\vec{v}_k, \vec{v}_k, n_k, p_k, \cdot\,) = 0,$$
$$\nabla\cdot(\epsilon\nabla\phi_k) = e(n_k - p_k - d_k).$$

Here, d_k is the obvious trace of d on $t_k = k\Delta t$. Adjoined to these semidiscrete equations are the traces of the prescribed boundary data functions. An explanation of the mappings is as follows. A typical domain element is written $(\vec{v}, \vec{w}, n, p)$. V has range in the dual of divergence free functions in $\prod_1^m \mathcal{H}_0^s$. Thus, for $\vec{\psi}$ in $\mathcal{H}_0^s$, this can be written as follows.

$$V(\vec{v}, \vec{w}, n, p, \vec{\psi}) = \nu_*(\nabla\vec{v}, \nabla\vec{\psi})_{L_2} + (\vec{v}\cdot\nabla\vec{w}, \vec{\psi})_{L_2} + (e/\rho)((p-n)\nabla\phi, \vec{\psi})_{L_2}.$$

The mappings N, P are each defined into the dual of H^s_{0,Σ_D} as follows. For ω_n, ω_p in H^s_{0,Σ_D},

$$N(\vec{v}, \vec{w}, n, p, \omega_n) = \frac{1}{e}(\vec{J}_n, \nabla\omega_n)_{L_2},$$

$$P(\vec{v}, \vec{w}, n, p, \omega_p) = -\frac{1}{e}(\vec{J}_p, \nabla\omega_p)_{L_2}.$$

3.3. Analysis of the hypotheses for the semidiscrete system. We begin with the identifications of the spaces in the abstract theorem.

3.3.1. Identifications. The space X is a product of finite energy spaces, with appropriate zero boundary trace and divergence free first component. The spaces Y, W are now defined: $Y = \mathcal{H}_0^s \times H^s_{0,\Sigma_D} \times H^s_{0,\Sigma_D}$, and $W = W_0 \times L_2 \times L_2$, where $W_0 = \prod_1^m L_2$. We now make the identifications with mappings of the previous subsection. Because of the definition of X used here, where the homogeneous boundary conditions are employed, we necessarily carry this over to B, a, and F. We write: $\vec{u} = (\vec{v}, n, p) = (\vec{v}_B + \vec{\sigma}, n_B + \nu, p_B + \pi)$, and formulate the definitions in terms of $\vec{\zeta} = (\vec{\sigma}, \nu, \pi)$ in order to accommodate the choice of X. Thus,

$$B(\vec{\zeta}, \vec{\zeta}) = \nu_*(\nabla\vec{\sigma}, \nabla\vec{\sigma})_{L_2} + \Delta t^{-1}(\vec{\sigma}, \vec{\sigma})_{L_2}$$
$$+D_n(\nabla\nu, \nabla\nu)_{L_2} + \Delta t^{-1}(\nu, \nu)_{L_2} + D_p(\nabla\pi, \nabla\pi)_{L_2} + \Delta t^{-1}(\pi, \pi)_{L_2},$$
$$a(\vec{\sigma}, \vec{\tau}, \cdot\,) = ((\vec{v}_B + \vec{\sigma})\cdot\nabla(\vec{v}_B + \vec{\tau}), \cdot\,)_{L_2} = (\vec{v}\cdot\nabla\vec{w}, \cdot\,)_{L_2}.$$

For later reference, we write: $b(\vec{v}, \vec{w}, \cdot\,) := a(\vec{\sigma}, \vec{\tau}, \cdot\,)$. A technical issue in verifying (stationary) convergence is the requirement of employing truncation to modify F (and later passing to the limit). Truncation outside the interval $[-M, M]$ for each component in the case of $\vec{v}$, and for a scalar function otherwise, is indicated by τ_M. Set: $c_n = \frac{eD_n}{kT_0}$, $c_p = \frac{eD_p}{kT_0}$, and

$$\begin{aligned} F_M(\vec{v}, n, p; \vec{\psi}, \omega_n, \omega_p) &= (e/\rho)((\tau_M(p) - \tau_M(n))\nabla\phi, \vec{\psi})_{L^2} - c_n(\tau_M(n)\nabla\phi, \nabla\omega_n)_{L^2} \\ &\quad -(n\tau_M(\vec{v}), \nabla\omega_n)_{L^2} + c_p(\tau_M(p)\nabla\phi, \nabla\omega_p)_{L^2} - (p\tau_M(\vec{v}), \nabla\omega_p)_{L^2} \\ f(\vec{\psi}, \omega_n, \omega_p) &= -\nu_*(\nabla\vec{v}_B, \nabla\vec{\psi})_{L^2} - D_n(\nabla n_B, \nabla\omega_n)_{L^2} - D_p(\nabla p_B, \nabla\omega_p)_{L^2} \\ &\quad +\Delta t^{-1}(\vec{u}_{k-1}, \vec{\psi})_{L^2} + \Delta t^{-1}(n_{k-1}, \omega_n)_{L^2} + \Delta t^{-1}(p_{k-1}, \omega_p)_{L^2} \\ &\quad -\Delta t^{-1}(\vec{u}_B(t_k), \vec{\psi})_{L^2} - \Delta t^{-1}(n_B(t_k), \omega_n)_{L^2} - \Delta t^{-1}(p_B(t_k), \omega_p)_{L^2}. \end{aligned}$$

It is understood that ϕ is implicitly defined via the Poisson equation.

3.3.2. Continuity. It is not possible in this review to do more than indicate general techniques of proof. The analysis of the bilinear form B is standard. For a, continuity in the argument $(\vec{\sigma}, \vec{\tau}, \vec{\psi})$, (i. e. , on $X \times X \times Y$) is equivalent to continuity of b in the argument $(\vec{v}, \vec{w}, \vec{\psi})$; for $s \geq m/2$:

$$|a(\vec{\sigma}, \vec{\tau}, \vec{\psi})| = |b(\vec{v}, \vec{w}, \vec{\psi})| \leq C\|\vec{v}\|_{L^2}\|\vec{w}\|_{H^1}\|\vec{\psi}\|_{H^s}.$$

This estimate uses $b(\vec{v}, \vec{w}, \vec{\psi}) = -b(\vec{v}, \vec{\psi}, \vec{w})$, followed by the Hölder inequality with reciprocal indices $1/2, 1/m, (m-2)/(2m)$, and the Sobolev inequality. Estimation of the other terms is similar.

3.3.3. Coerciveness. The bilinear form B is coercive by hypothesis. For a, we observe: $a(\vec{\sigma}, \vec{\sigma}, \vec{\sigma}) = b(\vec{v}, \vec{v}, \vec{v} - \vec{v}_B)$, and we estimate:

$$b(\vec{v}, \vec{v}, \vec{v} - \vec{v}_B) = b(\vec{v}, \vec{v}, \vec{v}) - b(\vec{v}, \vec{v}, \vec{v}_B) \geq -C\|\vec{v}\|_{L^2}\|\vec{v}\|_{\mathcal{H}}\|\vec{v}_B\|_{L^\infty}.$$

Notice that the inequality $b(\vec{v}, \vec{v}, \vec{v}) \geq 0$, has been used. The homogeneous trace terms may be absorbed into B for Δt sufficiently small; the remaining terms are controlled by problem dependent constants.

$b(\vec{v}, \vec{v}, \vec{v}) \geq 0$ follows from:

$$b(\vec{v}, \vec{v}, \vec{v}) = \frac{1}{2}\int_\Omega \vec{v}\cdot\nabla|\vec{v}|^2\, dx = \frac{1}{2}\int_\Omega \nabla\cdot(\vec{v}|\vec{v}|^2)\, dx,$$

which is then integrated by parts, and observed to have a nonnegative boundary integral by the assumption on the sign of the normal boundary component of $\vec{v}_B$. Notice that, prior to integration by parts, we have used the divergence free property of $\vec{v}$. Estimation of the other terms follows a similar line of argument. The truncation is used here in a fundamental way. The sequential hypothesis is routine.

One concludes: For each fixed M, solutions of the stationary problem $(F \mapsto F_M)$ exist for Δt sufficiently small.

4. Existence of weak solutions for the dynamic problem. We make use of the stationary solutions previously constructed.

4.1. Step function and piecewise linear sequences. We now define the sequences which permit weak compactness estimates. Indeed, $\vec{u}_{S,\Delta t}$ is the step function and $\vec{u}_{PL,\Delta t}$ the piecewise linear interpolant, both given explicitly: for $(k-1)\Delta t \leq t < k\Delta t$,

$$\vec{u}_{S,\Delta t}(\cdot\,,t) = \vec{u}_{k,\Delta t},\ \vec{u}_{PL,\Delta t}(\cdot\,,t) = \vec{u}_{k,\Delta t} + \frac{(t-k\Delta t)(\vec{u}_{k,\Delta t} - \vec{u}_{k-1,\Delta t})}{\Delta t}.$$

We have the following fundamental estimates.

LEMMA 4.1. *The sequences, $\vec{u}_{S,\Delta t}(x,t), \vec{u}_{PL,\Delta t}(x,t)$, are bounded in the topology of $L^2((0,T);X)$, and $\vec{u}_{PL,\Delta t}(x,t)$ is bounded in $H^1((0,T);Y^*)$. The bounds do not depend on the truncation parameter M.*

4.2. Weak solutions of the reduced system. The technique of proof is to extract weakly convergent subsequences of $\vec{u}_{S,\Delta t}$ and $\vec{u}_{PL,\Delta t}$ in $L^2((0,T);X)$; the Aubin lemma [18, Lemma 5.4.2], based upon Lemma 4.1, allows one to obtain a further $L^2(\mathcal{D})$-convergent subsequence of the piecewise linear sequence. Any limit can be identified with a weak solution, in the sense of Leray, of the modified (via truncation) evolution system.

4.3. Conclusion of the proof. It remains to conclude the proof. The same arguments used to obtain a solution of the reduced problem may be repeated, as applied to the sequence with $M \to \infty$. Similar weak limits, together with the Aubin lemma, are valid. We have the following theorem.

THEOREM 4.1. *Under the hypotheses stated earlier, there is a weak solution of the Navier-Stokes/PNP system. The requirement that the normal component of the velocity boundary data be nonnegative can be relaxed in the case of the Stokes system.*

REMARK 4.1. *The question arises as to whether n, p can be chosen to be nonnegative. One can implement this argument at the level of the semidiscrete equations, via a discrete Gronwall inequality, as derived in [18]. Initial and boundary values are required to be nonnegative in this case, for the validity of the argument via the discrete Gronwall inequality. Altogether, one obtains nonnegativity for the modified system, and, finally, for the system of the definition.*

5. Computational Aspects and Open Problems.

5.1. 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 typically employed in semiconductor device simulation [18]. This provides 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 subproblems [34]. This provides 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. Note here that the pressure is employed explicitly, indicating the gap between the theoretical Leray framework, and the implicit strong solution framework used for computation.

5.2. Open problems and promising research directions. The regularity presently demonstrated for the NS/PNP model, i.e. , that associated with Leray solutions, is not appropriately aligned with the regularity of the assumptions, particularly regarding boundary data. Also, a more explicit treatment of the pressure, as is done in the numerical algorithm, is desirable. In brief, a strong solution theory would be desirable. It would be helpful if the role of the non-slip boundary condition could be clarified. A *challenging* open problem is the existence theory for the steady-state NS/PNP model.

In terms of scientific significance, a clearer understanding of the impact of the fluid fluctuations on the current density is highly desirable. Moreover, even if it is determined that these are significant, what is the physical role of the convective term in the NS/PNP system? Is this system actually required for modeling, or is the Stokes/PNP system adequate? Computationally, what are the precise time scale observations as the dynamic model approaches steady-state? Finally, this model is no longer out of reach of skilled computational science. Can the three-dimensional problem now be solved for a meaningful application?

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