

Some results on the Euler-Poisson system for plasmas and semiconductors

Ingrid Lacroix-Violet

‡ Laboratoire Paul Painlevé UMR 8524 CNRS-USTLille

E-mails: ingrid.violet@math.univ-lille1.fr

Abstract

This paper is a review of different results already published concerning the steady state Euler-Poisson system for a potential flow. In a first part we present results on the zero electron mass limit and the quasineutral limit of the system using an asymptotic expansion method. For the quasineutral limit, we consider the case where boundary layers can appear. In a second part, we present some numerical schemes of finite volume type to compute approximate solutions of the system for semiconductors in the unipolar case. In particular, some numerical simulations are given to illustrate some smallness conditions on given data and parameters in the proof of existence of solutions to the system.

Keywords : Steady-state Euler-Poisson system, potential and subsonic flow, quasineutral limit, asymptotic expansion, semiconductors and plasmas, numerical simulation, finite volume method.

1 Introduction

In this paper we consider the Euler-Poisson system which is a hydrodynamic model widely used in the mathematical modeling and numerical simulation for plasmas [9] and semiconductors [32]. It consists in two

nonlinear equations given by the conservation laws of momentum and density, called the Euler equations, plus a Poisson equation for the electrostatic potential. Due to the hyperbolicity of the transient nonlinear Euler equations, the weak solution is only studied in one space dimension. In such a situation, the existence of global weak solution is shown in the set of bounded functions [31].

Here we only consider the unipolar steady-state case for a potential flow. In the scaled variables, the Euler-Poisson system reads then as follows (see [13, 34, 35]):

$$-\operatorname{div}(n\nabla\psi) = 0, \quad (1.1)$$

$$\frac{\varepsilon}{2}|\nabla\psi|^2 + h(n) = V + \frac{\varepsilon\psi}{\tau}, \quad (1.2)$$

$$-\lambda^2\Delta V = n - C. \quad (1.3)$$

This system will be studied in an open and bounded domain Ω in \mathbb{R}^d ($d = 2$ or $d = 3$ in practice) with sufficiently smooth boundary Γ . The unknowns of the system are $n = n(x)$, $\psi = \psi(x)$ and $V = V(x)$ which represent respectively the electron density, the velocity potential and the electrostatic potential. The function $h = h(n)$ corresponds to the enthalpy of the system and is defined by:

$$h'(n) = \frac{p'(n)}{n}, \quad n > 0, \quad \text{and } h(1) = 0,$$

where $p = p(n)$ is the pressure function, supposed to be sufficiently smooth and strictly increasing for $n > 0$. In practice, the pressure function is typically governed by the γ -law, $p(n) = cn^\gamma$ where $c > 0$ and $\gamma \geq 1$ are constants. The case $\gamma = 1$ corresponds to the isothermal flow, since in this case the temperature is constant. The function $C = C(x)$ stands for the doping profile for a semiconductor and for the ion density for a plasma. The physical scaled parameters λ , ε , τ represent respectively the Debye length, the electron mass and the relaxation time of the system. They are dimensionless and small compared to the characteristic length of physical interest.

In all the following, system (1.1)-(1.3) will be completed with Dirichlet type boundary conditions. We will see later which ones exactly.

First of all let us say that this system was already studied a lot. In particular let us mention [13] where the authors have shown existence and uniqueness of solutions (with all the physical parameters equal to one) under a smallness condition on the data, which implies that the

problem is in the subsonic region. In [34], it is shown that the smallness condition on the data can be replaced by a smallness condition on the parameter ε . Then the existence and uniqueness hold for large data provided that ε is small enough. In the same article, the author was also interested in the asymptotic limit of the system when the physical parameters tend, independently, to zero. There are then three limits called respectively the zero electron mass limit (case ε tends to zero), the zero relaxation time limit (case τ tends to zero) and the quasineutral limit (case λ tends to zero). In particular, in [34], the author obtained the convergence, for the electron mass limit, in $O(\varepsilon)$ for an asymptotic expansion of order zero, and, a convergence in $O(\lambda^2)$ for the quasineutral limit in case of an asymptotic expansion of order zero under a compatibility condition. In [35], the asymptotic expansions are justified up to any order for the zero electron mass limit and the zero relaxation time limit. In [40], the same result is obtained for the quasineutral limit without compatibility condition.

Let us note that the asymptotic limits for the Euler-Poisson system have been studied by a lot of authors. In one-dimensional steady state Euler-Poisson system, the quasineutral limit was performed in [39] for well-prepared boundary data and in [33] for general boundary data. In [12], by using pseudo-differential techniques, the quasineutral limit was studied for local smooth solutions of a one-dimensional and isothermal model for plasmas in which the electron density is described by the Maxwell-Boltzmann relation. This relation can be obtained in the zero electron mass limit of the Euler-Poisson equations which we will discuss below. See also [4] for the study of the quasineutral limit in a semi-linear Poisson equation in which the Maxwell-Boltzmann relation is also used.

The zero relaxation time limit in one dimensional transient Euler-Poisson system has been investigated in [31] and [26, 27] by the compensated compactness arguments for global weak solutions. The limit system is governed by the classical drift-diffusion model. In multi-dimensional case and for local smooth solutions this limit has been studied in [1].

From a numerical point of view, the hydrodynamic model has essentially been studied in its complete form (with the energy balance equation). In [3] the authors provide numerical simulations and show that the model exhibits velocity overshoot. In [19] the authors propose numerical methods for the hydrodynamic model and give numerical results for the ballistic diode. In [18], the author extend the simulations to the case of transonic flow. There exists also a wide litterature on the analysis and simulation of the drift-diffusion equations (see

[2, 5, 6, 7, 10, 11, 25, 29, 38] for instance). The steady-state drift-diffusion system, as the steady state Euler-Poisson model, is a fully nonlinear system which is frequently solved with a Gummel map method [24]. In [8] the authors propose iterative schemes to solve a system of linear partial differential equations for the electrostatic and velocity potentials and nonlinear algebraic equation for the density instead of solving a fully nonlinear system of partial differential equations. They consider in their article also the case of the bi-polar system (which means that they consider the two species : electrons and ions). In particular they can see numerically the smallness condition on the parameter ε for the existence of solutions. They can also obtain some current-voltage characteristics and the case of a ballistic diode.

In this paper we make a review of results for the steady state Euler-Poisson system for a potential flow obtained by the author and co-authors. In particular we will present the construction and justification of an asymptotic expansion up to any order, and in the multidimensional case, for the zero electron mass limit and the quasineutral limit. Let us note that for the quasineutral limit, we will consider a case without compatibility condition, which means that boundary layers can appear. These two results were the objects of two previous papers [35, 40] and will be here presented in section 2. Moreover we will be interested in numerical simulation for system (1.1)-(1.3). As mention above, in [8] the authors propose two numerical schemes of finite volume type with reconstruction of the gradient appearing in (1.2). We will present them in section 3.

2 Asymptotic limits

In this section we are interested in two asymptotic limits: the zero electron mass limit and the quasineutral limit. We will just give the main ideas of the results and we refer to [35] and [40] for more details. In all this section we take $\tau = 1$.

First of all, as mention in the introduction, we complete the system (1.1)-(1.3) with Dirichlet type boundary conditions on the density and the velocity potential:

$$n = n_D, \quad \psi = \psi_D, \quad \text{on } \Gamma. \quad (2.1)$$

By eliminating V of (1.2) and (1.3) and using (1.1) we have:

$$\begin{aligned} -\Delta h(n) + \frac{\varepsilon}{n} \sum_{i,j=1}^d \frac{\partial \psi}{\partial x_i} \frac{\partial \psi}{\partial x_j} \frac{\partial^2 n}{\partial x_i \partial x_j} - \frac{\varepsilon}{\tau n} \nabla \psi \cdot \nabla n - \frac{\varepsilon}{n^2} (\nabla \psi \cdot \nabla n)^2 \\ + \frac{\varepsilon}{n} \sum_{i,j=1}^d \frac{\partial \psi}{\partial x_i} \frac{\partial^2 \psi}{\partial x_i \partial x_j} \frac{\partial n}{\partial x_j} + n - C(x) = Q(\psi), \end{aligned} \quad (2.2)$$

where Q is given by

$$Q(\psi) = \sum_{i,j=1}^d \left(\frac{\partial^2 \psi}{\partial x_i \partial x_j} \right)^2. \quad (2.3)$$

For $n > 0$ it is easy to see that (n, ψ, V) is a smooth solution to the system (1.1)-(1.3) if and only if (n, ψ) is a smooth solution to (1.1) and (2.2). Moreover, for ψ given, equation (2.2) is elliptic if and only if the flow is subsonic, i.e., the condition $|\nabla \psi| < \sqrt{p'(n)}/\varepsilon$ holds.

The first goal of this part is to construct asymptotic expansions in the case of the zero electron mass limit and the quasineutral limit. The second one is to justify them, which means that we can obtain the existence and uniqueness of each profile, and estimates of the difference between the exact solution and the asymptotic expansions.

2.1 Zero electron mass limit

Here we are interested in the construction and justification of an asymptotic expansion for the zero electron mass limit i.e. for ε tends to zero. Then we assume in all this part $\lambda = 1$ and we note $(n_\varepsilon, \psi_\varepsilon, V_\varepsilon)$ the solution of (1.1)-(1.3) supplemented with the boundary conditions:

$$n_\varepsilon = \sum_{k=0}^m \varepsilon^k \bar{n}_k + n_{D,\varepsilon}^{m+1}, \quad \psi_\varepsilon = \sum_{k=0}^m \varepsilon^k \bar{\psi}_k + \psi_{D,\varepsilon}^{m+1} \quad \text{sur } \Gamma, \quad (2.4)$$

where $n_{D,\varepsilon}^{m+1}$ and $\psi_{D,\varepsilon}^{m+1}$ are smooth enough and defined in $\bar{\Omega}$ such that $n_{D,\varepsilon}^{m+1} = O(\varepsilon^{m+1})$ and $\psi_{D,\varepsilon}^{m+1} = O(\varepsilon^{m+1})$ uniformly in ε .

Let us recall that for fixed ε , the existence and uniqueness of solutions to the system have been already shown in the space

$$B \stackrel{\text{def}}{=} \mathcal{W}^{2,q}(\Omega) \times \mathcal{C}^{2,\delta}(\bar{\Omega}) \times \mathcal{C}^{1,\delta}(\bar{\Omega})$$

for small boundary data [13] or on a smallness condition on ε [34] which guarantee that the problem is located in the subsonic region.

2.1.1 Construction of the asymptotic expansion

Let us first explain how to derive the profile equations. We assume that:

- (A1) Ω is a bounded and convex domain of \mathbb{R}^d with $\Gamma \in \mathcal{C}^{2,\delta}$, $\delta \in]0, 1[$,
- (A2) $p \in \mathcal{C}^{m+4}(\mathbb{R}^+)$, $m \in \mathbb{N}$, $p'(n) > 0 \forall n > 0$,
- (A3) $C \in L^\infty(\Omega)$, $0 < \underline{C} \leq C(x)$,
- (A4) $\bar{n}_k \in \mathcal{W}^{2,q}(\Omega)$ for $q > \frac{d}{1-\delta}$ and $\forall 0 \leq k \leq m$, $0 < \underline{n} \leq \bar{n}_0(x) \forall x \in \Gamma$,
- (A5) $\bar{\psi}_k \in \mathcal{C}^{2,\delta}(\bar{\Omega})$, $\forall 0 \leq k \leq m$,
- (A6) the sequence $(\varepsilon^{-(m+1)} n_{D,\varepsilon}^{m+1})_{\varepsilon>0}$ is bounded in $\mathcal{W}^{2,q}(\Omega)$,
- (A7) the sequence $(\varepsilon^{-(m+1)} \psi_{D,\varepsilon}^{m+1})_{\varepsilon>0}$ is bounded in $\mathcal{C}^{2,\delta}(\bar{\Omega})$.

Let $(n_{a,\varepsilon}, \psi_{a,\varepsilon}, V_{a,\varepsilon})$ be defined by the following ansatz :

$$n_{a,\varepsilon} = \sum_{k \geq 0} \varepsilon^k n_k, \quad \psi_{a,\varepsilon} = \sum_{k \geq 0} \varepsilon^k \psi_k, \quad V_{a,\varepsilon} = \sum_{k \geq 0} \varepsilon^k \phi_k \quad \text{in } \Omega, \quad (2.5)$$

with the boundary conditions :

$$n_{a,\varepsilon} = \sum_{k \geq 0} \varepsilon^k \bar{n}_k, \quad \psi_{a,\varepsilon} = \sum_{k \geq 0} \varepsilon^k \bar{\psi}_k \quad \text{on } \Gamma. \quad (2.6)$$

Plugging expression (2.5) into the system (1.1)-(1.3), using the Taylor's formula to developp

$$h\left(\sum_{k \geq 0} \varepsilon^k n_k\right),$$

and by identification of the power of ε , we obtain the system for each (n_k, ψ_k, V_k) , $k \geq 0$. More precisely, the first order (n_0, ψ_0, V_0) satisfies the nonlinear problem in Ω :

$$-\operatorname{div}(n_0 \nabla \psi_0) = 0, \quad (2.7)$$

$$h(n_0) = V_0, \quad (2.8)$$

$$-\Delta V_0 = C(x) - n_0, \quad (2.9)$$

with the following boundary conditions :

$$n_0 = \bar{n}_0, \quad \psi_0 = \bar{\psi}_0 \quad \text{on } \Gamma. \quad (2.10)$$

For all $k \geq 1$, (n_k, ψ_k, V_k) is obtained by induction on k in the following linear problem in Ω :

$$-\operatorname{div}(n_0 \nabla \psi_k) = \sum_{i=1}^k \operatorname{div}(n_i \nabla \psi_{k-i}), \quad (2.11)$$

$$h'(n_0)n_k - V_k = f_k, \quad (2.12)$$

$$-\Delta V_k = -n_k, \quad (2.13)$$

with the boundary conditions :

$$n_k = \bar{n}_k, \quad \psi_k = \bar{\psi}_k \quad \text{on } \Gamma, \quad (2.14)$$

where

$$f_k = \psi_{k-1} - \frac{1}{2} \sum_{i=0}^{k-1} \nabla \psi_{k-1-i} \cdot \nabla \psi_i - \bar{h}_k((n_i)_{0 \leq i \leq k-1}). \quad (2.15)$$

Remark 2.1. Equation (2.8) expresses a Maxwell-Boltzmann type relation. Indeed for the isothermal plasma, the pressure is a linear function. Then $p(n) = a^2 n$ with $a > 0$. This implies from the definition of h that $h(n) = a^2 \log n$ and hence, from (2.8) $n_0 = \exp(V_0/a^2)$. This is the classical Maxwell-Boltzmann relation which has been used in [4, 12, 37] for the study of the quasineutral limit.

2.1.2 Justification of the asymptotic expansion

To justify the asymptotic expansion there are two necessary steps. First, we have to show that each profile exists and is unique. Then we have to obtain estimates for the difference between the exact solution and the asymptotic expansion in the good spaces.

Using classical results we can prove

Theorem 2.2. *Let assumptions (A1)-(A5) hold. The problem (2.7)-(2.10) has a unique solution (n_0, ψ_0, V_0) in $\mathcal{W}^{2,q}(\Omega) \times \mathcal{C}^{2,\delta}(\bar{\Omega}) \times \mathcal{C}^{1,\delta}(\bar{\Omega})$ which satisfies*

$$n_0(x) \geq \min(\underline{C}, \underline{n}) > 0, \quad \forall x \in \bar{\Omega}.$$

We refer to [35] for the details of proof. Considering now the problem (2.11)-(2.14), we can prove by induction on k that it has also a unique solution

Theorem 2.3. *Let assumptions (A1)-(A5) hold and $1 \leq k \leq m$. The problem (2.11)-(2.14) has a unique solution (n_k, ψ_k, V_k) in $\mathcal{W}^{2,q}(\Omega) \times \mathcal{C}^{2,\delta}(\bar{\Omega}) \times \mathcal{C}^{1,\delta}(\bar{\Omega})$.*

We refer again to [35] for more details on proof. The two theorems 2.2 and 2.3 give immediately

Theorem 2.4. *Let $m \in \mathbb{N}$ and assumptions (A1)-(A5) hold. Then there exists a unique asymptotic expansion (2.5) up to order m , i.e., for all $0 \leq k \leq m$, there exists a unique profile $(n_k, \psi_k, V_k) \in B$, solution to the problem (2.7)-(2.10) of $k = 0$ or (2.11)-(2.14) if $1 \leq k \leq m$.*

It remains now to obtain estimates for the difference between a sequence of exact solution and the asymptotic expansion. Let $(n_\varepsilon, \psi_\varepsilon, V_\varepsilon)$ be a smooth solution of (1.1)-(1.3) and (2.4) and $(n_{a,\varepsilon}^m, \psi_{a,\varepsilon}^m, V_{a,\varepsilon}^m)$ be approximate solution of order m defined by

$$n_{a,\varepsilon}^m = \sum_{k=0}^m \varepsilon^k n_k, \quad \psi_{a,\varepsilon}^m = \sum_{k=0}^m \varepsilon^k \psi_k, \quad V_{a,\varepsilon}^m = \sum_{k=0}^m \varepsilon^k V_k, \quad (2.16)$$

where $(n_k, \psi_k, V_k)_{0 \leq k \leq m}$ is the unique solution of (2.7)-(2.10) for $k = 0$ and (2.11)-(2.14) for $1 \leq k \leq m$. In [35] it is shown

Theorem 2.5. *Let $(n_\varepsilon, \psi_\varepsilon, V_\varepsilon)$ be the solution of the system (1.1)-(1.3) and (2.4) and $(n_{a,\varepsilon}^m, \psi_{a,\varepsilon}^m, V_{a,\varepsilon}^m)$ be the approximate solution given by the asymptotic expansion (2.16). Let assumptions (A1)-(A7) hold. Then there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0]$, we have the following estimates*

$$\begin{aligned} \|n_\varepsilon - n_{a,\varepsilon}^m\|_{\mathcal{W}^{2,q}(\Omega)} &\leq A_1 \varepsilon^{m+1}, \quad \|\psi_\varepsilon - \psi_{a,\varepsilon}^m\|_{\mathcal{C}^{2,\delta}(\bar{\Omega})} \leq A_1 \varepsilon^{m+1}, \\ \|V_\varepsilon - V_{a,\varepsilon}^m\|_{\mathcal{C}^{1,\delta}(\bar{\Omega})} &\leq A_1 \varepsilon^{m+1}, \end{aligned} \quad (2.17)$$

where $A_1 > 0$ is a constant independent of ε .

Here we give only the main steps of the proof of theorem 2.4 and we refer one more times to [35] for more details.

The first step consists in obtaining the system satisfied by the approximate solution $(n_{a,\varepsilon}^m, \psi_{a,\varepsilon}^m, V_{a,\varepsilon}^m)$. To this end we use the problems satisfied by each profile of the asymptotic expansion. Then we subtract the systems verified by the exact solution and the approximate solution to obtain

$$-\operatorname{div}(n_\varepsilon \nabla \psi_\varepsilon) + \operatorname{div}(n_{a,\varepsilon}^m \nabla \psi_{a,\varepsilon}^m) = \varepsilon^{m+1} D_1^\varepsilon, \quad (2.18)$$

$$\frac{\varepsilon}{2}(|\nabla\psi_\varepsilon|^2 - |\nabla\psi_{a,\varepsilon}^m|^2) + h(n_\varepsilon) - h(n_{a,\varepsilon}^m) = V_\varepsilon - V_{a,\varepsilon}^m + \varepsilon(\psi_\varepsilon - \psi_{a,\varepsilon}^m) + \varepsilon^{m+1}D_2^\varepsilon, \quad (2.19)$$

$$-\Delta(V_\varepsilon - V_{a,\varepsilon}^m) = -(n_\varepsilon - n_{a,\varepsilon}^m), \quad (2.20)$$

and

$$n_\varepsilon - n_{a,\varepsilon}^m = n_{D,\varepsilon}^{m+1}, \quad \psi_\varepsilon - \psi_{a,\varepsilon}^m = \psi_{D,\varepsilon}^{m+1} \quad \text{on } \Gamma. \quad (2.21)$$

where

$$D_1^\varepsilon = \sum_{k=m+1}^{2m} \left(\varepsilon^{k-m-1} \sum_{i=k-m}^m \operatorname{div}(n_i \nabla \psi_{k-i}) \right),$$

$$D_2^\varepsilon = -\frac{1}{2} \sum_{k=m}^{2m} \left(\varepsilon^{k-m} \sum_{i=k-m}^m \nabla \psi_i \cdot \nabla \psi_{k-i} \right) - r_\varepsilon(n) + \psi_m,$$

and

$$r_\varepsilon(n) = \frac{1}{(m+1)!} \frac{d^{m+1}h(n_{a,\xi}^m)}{d\varepsilon^{m+1}} \quad \text{with } \xi \in [0, \varepsilon].$$

We eliminate first $V_\varepsilon - V_{a,\varepsilon}^m$ to obtain an elliptic nonlinear system satisfied by $(n_\varepsilon - n_{a,\varepsilon}^m, \psi_\varepsilon - \psi_{a,\varepsilon}^m)$. Using different lemmas and uniform boundedness of the sequence of solution $(n_\varepsilon, \psi_\varepsilon, V_\varepsilon)$, we can show the estimates (2.17) for $(n_\varepsilon - n_{a,\varepsilon}^m, \psi_\varepsilon - \psi_{a,\varepsilon}^m)$. Then, using (2.19), we obtain easily the last estimate of (2.17) for $V_\varepsilon - V_{a,\varepsilon}^m$.

Remark 2.6. Here, this kind of proof is possible only due to the fact that we have already existence, uniqueness and uniform boundedness of a sequence of solution to the problem (1.1)-(1.3) and (2.1) thanks to [34]. In the following section for the quasineutral limit, the situation will be very different, since without compatibility condition, we don't have anymore existence of solutions for the problem (1.1)-(1.3) and (2.1).

Remark 2.7. In a same way, it is shown in [35] an analogous result for the zero relaxation time limit. Moreover, as an application of theorem 2.4 here and theorem 4.2 in [35], when the boundary data are compatible with the function C , it is possible to obtain the convergence to the incompressible Euler equations via the zero electron mass limit and the zero relaxation time limit.

2.2 Quasineutral limit

Here we are interested in the construction and justification of an asymptotic expansion for the quasineutral limit, i.e. λ tends to zero, without compatibility condition which means that boundary layers can appear. Indeed, if we formally take $\lambda = 0$ in (1.3) and (2.1) we obtain

$$C(x) = n(x), \quad \text{in } \Omega \quad \text{and} \quad n = n_D \quad \text{on } \Gamma.$$

Then, if $n_D \neq C$ on Γ some boundary layers appear.

In all the section we keep $\varepsilon > 0$ as a small parameter independent of λ in the equations and we note $(n_\lambda, \psi_\lambda, V_\lambda)$ a solution of (1.1)-(1.3) supplemented with the boundary conditions

$$n_\lambda = \sum_{j=0}^m \lambda^j n_D^j + n_{D,\lambda}^m, \quad \psi_\lambda = \sum_{j=0}^m \lambda^j \psi_D^j + \psi_{D,\lambda}^m, \quad \text{on } \Gamma, \quad (2.22)$$

where $n_{D,\lambda}^m$ and $\psi_{D,\lambda}^m$ are smooth enough and defined on $\bar{\Omega}$. Let us note that here since we consider the case without compatibility condition, we don't have existence and uniqueness of solution to (1.1)-(1.3) and (2.22) contrary to previously. We will see later, that it is important to keep ε in the equations since the ellipticity of the system would be equivalent to a smallness condition on ε as before.

2.2.1 Construction of the asymptotic expansion

Let us first explain how to construct the asymptotic expansions. The method used here is the one presented in [36]. We assume that:

- (H1) $C \in C^\infty(\bar{\Omega})$, $0 < \underline{n} \leq C(x) \leq \bar{n}$, $x \in \bar{\Omega}$, $\underline{n}, \bar{n} \in \mathbb{R}$,
- (H2) $n_D^j \in C^\infty(\bar{\Omega})$ for $0 \leq j \leq m$,
- (H3) $\psi_D^j \in C^{2,\delta}(\bar{\Omega})$ for $0 \leq j \leq m$,
- (H4) $n_D^0(x) = C(x)$, $n_D^1(x) = 0$, $x \in \bar{\Omega}$,
- (H5) $(\lambda^{-m-1} n_{D,\lambda}^m)_{\lambda>0}$ is bounded in $W^{2,q}(\Omega)$, $q > \frac{d}{1-\delta}$, $\delta \in (0, 1)$,
- (H6) $(\lambda^{-m+1} \psi_{D,\lambda}^m)_{\lambda>0}$ is bounded in $C^{2,\delta}(\bar{\Omega})$.

Remark 2.8. The assumption (H4) is a compatibility condition for the first and second order terms. It assures that there will not appear any boundary layers in these two terms. The case without compatibility conditions presents some difficulties in which we didn't succeed in the study [40]. We will give more details on it below.

Here due to the boundary layers, to construct the asymptotic expansion, we have to consider to type of ansatz : an internal ansatz and an external ansatz.

Internal expansion Let

$$n(x) = \sum_{k \geq 0} \lambda^k n_k(x); \quad \psi(x) = \sum_{k \geq 0} \lambda^k \psi_k(x); \quad V(x) = \sum_{k \geq 0} \lambda^k V_k(x).$$

Plugging this into (1.1)-(1.3), using the same method as in the previous section, and by identification of the power of λ , we obtain the problems satisfy by (n_k, ψ_k, V_k) for all k . More precisely

$$V_0 = -\frac{\varepsilon}{2} |\nabla \psi_0|^2 - h(n_0) + \varepsilon \psi_0, \quad (2.23)$$

$$\operatorname{div}(n_0 \nabla \psi_0) = 0, \quad (2.24)$$

$$n_0 = C(x), \quad (2.25)$$

$$V_1 = -\varepsilon \nabla \psi_0 \cdot \nabla \psi_1 - h'(n_0) n_1 + \varepsilon \psi_1, \quad (2.26)$$

$$-\operatorname{div}(n_0 \nabla \psi_1) = \operatorname{div}(n_1 \nabla \psi_0), \quad (2.27)$$

$$n_1 = 0, \quad (2.28)$$

and for all $k \geq 2$

$$V_k = -\frac{\varepsilon}{2} \sum_{i=0}^k \nabla \psi_i \cdot \nabla \psi_{k-i} - h'(n_0) n_k - \bar{h}_k((n_i)_{0 \leq i \leq k-1}) + \varepsilon \psi_k \quad (2.29)$$

$$-\operatorname{div}(n_0 \nabla \psi_k) = \sum_{i=1}^k \operatorname{div}(n_i \nabla \psi_{k-i}), \quad (2.30)$$

$$n_k = \Delta V_{k-2}, \quad (2.31)$$

where \bar{h}_k is smooth and $\bar{h}_1 \equiv 0$ (see [35]).

All the profiles (n_k, ψ_k, V_k) can be determined uniquely and sufficiently smooth by induction on k with boundary conditions given later. Then the internal expansion is constructed. For $m \geq 2$ let us denote

$$n_{I,m}^\lambda = \sum_{k=0}^m \lambda^k n_k; \quad \psi_{I,m}^\lambda = \sum_{k=0}^m \lambda^k \psi_k; \quad V_{I,m}^\lambda = \sum_{k=0}^m \lambda^k V_k.$$

By construction, it is easy to see that if (n_k, ψ_k, V_k) are smooth enough, then the error equations are of order $O(\lambda^{m+1})$. Since $n_k = \Delta V_{k-2}$, for $k \geq 2$, and is not necessarily equal to n_D^k on Γ , a boundary layer can appear.

External expansion We follow the notations in [40]. For $x \in \Omega$, we note $t(x)$ the distance from Γ to x and $s(x)$ the point of Γ nearest from x . For $\theta > 0$, let Ω_θ be the boundary layer of size θ :

$$\Omega_\theta = \{x \in \Omega; |x - y| < \theta, y \in \Gamma\}.$$

If θ is small enough, $s(x)$ is defined uniquely for all $x \in \Omega_\theta$. In Ω_θ , we define the fast variable by $\xi(x, \lambda) = t(x)/\lambda$. For $x \in \Omega_\theta$, let $\nu(x) =$

(ν_1, \dots, ν_d) the unit interior-directional normal vector of Γ passing from x . Then from :

$$t(x) = \|x - s(x)\|, \quad x - s(x) = t(x)\nu(x),$$

and due to the fact that for all $i = 1, \dots, d$, $\partial s(x)/\partial x_i$ is orthogonal to $\nu(x)$, it is easy to see that $\nabla_x t = \nu(x)$. Hence the partial derivative of a function $w(s(x), \xi(x, \lambda))$ may be decomposed as :

$$\frac{\partial w(s(x), \xi(x, \lambda))}{\partial x_i} = \lambda^{-1} \nu_i \frac{\partial w}{\partial \xi} + D_i w, \quad (2.32)$$

where D_i is a first order differential operator in s defined by : $D_i w = \nabla_s w \cdot \frac{\partial s}{\partial x_i}$. Similarly :

$$\frac{\partial^2 w(s(x), \xi(x, \lambda))}{\partial x_i \partial x_j} = \lambda^{-2} \nu_i \frac{\partial^2 w}{\partial \xi^2} + \lambda^{-1} D_{ji} \frac{\partial w}{\partial \xi} + D_j D_i w + \nabla_s w \cdot \frac{\partial^2 s}{\partial x_i \partial x_j}, \quad (2.33)$$

where $D_{ji} = \nu_i D_j + \nu_j D_i + \partial \nu_i / \partial x_j$. Note that for all i, j we have : $D_{ji} = D_{ij}$.

For each function $w(x)$ defined in Ω_θ the equivalent function of (s, t) is denoted by \tilde{w} i.e. $w(x) = \tilde{w}(s(x), t(x)) = \tilde{w}(s(x), \lambda \xi(x, \lambda))$. We develop $\tilde{w}(s(x), \lambda \xi(x, \lambda))$ formally to obtain

$$\tilde{w}(s(x), \lambda \xi(x, \lambda)) = \tilde{w}(s(x), 0) + O(\lambda).$$

Let $\bar{w}(s) = \tilde{w}(s, 0)$. Then the ansatz of an approximate solution up to order m of (1.1)-(1.3) in Ω_θ are given by

$$\begin{aligned} \tilde{n}_{a,m}^\lambda(x) &= n_{I,m}^\lambda(x) + \tilde{n}_{B,m}^\lambda(s(x), \xi(x, \lambda)), \\ \tilde{\psi}_{a,m}^\lambda(x) &= \psi_{I,m}^\lambda(x) + \tilde{\psi}_{B,m}^\lambda(s(x), \xi(x, \lambda)), \\ \tilde{V}_{a,m}^\lambda(x) &= V_{I,m}^\lambda(x) + \tilde{V}_{B,m}^\lambda(s(x), \xi(x, \lambda)); \end{aligned}$$

where the boundary layers $(\tilde{n}_{B,m}^\lambda, \tilde{\psi}_{B,m}^\lambda, \tilde{V}_{B,m}^\lambda)$ have the expansions :

$$\tilde{n}_{B,m}^\lambda = \sum_{k=0}^m \lambda^k n_k^b, \quad \tilde{\psi}_{B,m}^\lambda = \sum_{k=0}^{m+1} \lambda^k \psi_k^b, \quad \tilde{V}_{B,m}^\lambda = \sum_{k=0}^m \lambda^k V_k^b,$$

in which each term $(n_k^b(s, \xi), \psi_k^b(s, \xi), V_k^b(s, \xi))$ will be chosen to decay exponentially when ξ tends to $+\infty$. They are determined by setting $(\tilde{n}_{a,m}^\lambda, \tilde{\psi}_{a,m}^\lambda, \tilde{V}_{a,m}^\lambda)$ in (1.1)-(1.3) and identification of the power of λ . Let $\partial/\partial \nu = \sum_{i=1}^d \nu_i \partial/\partial x_i$. After computation we obtain

$$\psi_0^b \equiv 0,$$

$$(S_0) \quad \begin{cases} (\bar{n}_0 + n_0^b) \frac{\partial^2 \psi_1^b}{\partial \xi^2} + \left(\frac{\partial \bar{\psi}_0}{\partial \nu} + \frac{\partial \psi_1^b}{\partial \xi} \right) \frac{\partial n_0^b}{\partial \xi} = 0, \\ \frac{\varepsilon}{2} \left(\frac{\partial \psi_1^b}{\partial \xi} \right)^2 + \varepsilon \frac{\partial \psi_1^b}{\partial \xi} \frac{\partial \bar{\psi}_0}{\partial \nu} + h(\bar{n}_0 + n_0^b) - V_0^b = \bar{V}_0 + \varepsilon \bar{\psi}_0, \\ \frac{\partial^2 V_0^b}{\partial \xi^2} = n_0^b, \end{cases}$$

and for $k \geq 1$:

$$(S_k) \quad \begin{cases} \varepsilon \frac{\partial \psi_{k+1}^b}{\partial \xi} \left(\frac{\partial \psi_1^b}{\partial \xi} + \frac{\partial \bar{\psi}_0}{\partial \nu} \right) + h'(\bar{n}_0 + n_0^b) n_k^b - V_k^b \\ \quad \quad \quad = F_{1,k}(n_l^b, \psi_{l+1}^b, 0 \leq l \leq k-1), \\ (\bar{n}_0 + n_0^b) \frac{\partial^2 \psi_{k+1}^b}{\partial \xi^2} + \left(\frac{\partial \bar{\psi}_0}{\partial \nu} + \frac{\partial \psi_1^b}{\partial \xi} \right) \frac{\partial n_k^b}{\partial \xi} + n_k^b \frac{\partial^2 \psi_1^b}{\partial \xi^2} \\ \quad \quad \quad + \frac{\partial n_0^b}{\partial \xi} \frac{\partial \psi_{k+1}^b}{\partial \xi} = F_{2,k}(n_l^b, \psi_{l+1}^b, 0 \leq l \leq k-1), \\ -\frac{\partial^2 V_k^b}{\partial \xi^2} + n_k^b = F_{3,k}(V_l^b, k-1 \leq l \leq k-2), \end{cases}$$

where $F_{i,k}$, $i = 1, 2, 3$, are given functions of $(n_l^b, \psi_{l+1}^b)_{0 \leq l \leq k-1}$ for $F_{1,k}$, $F_{2,k}$, and of $(V_l^b)_{k-1 \leq l \leq k-2}$ for $F_{3,k}$.

Hence the approximate solution is constructed in Ω_θ . To complete the definition of the approximate solution in $\bar{\Omega}$, let $\sigma \in C^\infty(0, \infty)$ be a smooth function such that $\sigma(t) = 1$ for $0 \leq t \leq \theta/2$ and $\sigma \equiv 0$ for $t \geq \theta$ and $(n_{B,m}^\lambda(x), \psi_{B,m}^\lambda(x), V_{B,m}^\lambda(x))$ defined by

$$\begin{cases} (\tilde{n}_{B,m}^\lambda(s(x), t(x)/\lambda), \tilde{\psi}_{B,m}^\lambda(s(x)t(x)/\lambda), \tilde{V}_{B,m}^\lambda(s(x)t(x)/\lambda))\sigma(t(x)), \\ \quad \quad \quad \text{for } x \in \Omega_\theta, \\ 0, \quad \text{for } x \in \Omega - \Omega_\theta. \end{cases}$$

Then, $(n_{B,m}^\lambda, \psi_{B,m}^\lambda, V_{B,m}^\lambda)$ has the same regularity as $(\tilde{n}_{B,m}^\lambda, \tilde{\psi}_{B,m}^\lambda, \tilde{V}_{B,m}^\lambda)$. For $(n_k^b(s, \xi), \psi_k^b(s, \xi), V_k^b(s, \xi))$ decreasing exponentially when ξ tends to $+\infty$, it is easy to see that the difference between $(n_{B,m}^\lambda, \psi_{B,m}^\lambda, V_{B,m}^\lambda)$ and $(\tilde{n}_{B,m}^\lambda, \tilde{\psi}_{B,m}^\lambda, \tilde{V}_{B,m}^\lambda)$ is uniform of order of $e^{-\mu/\lambda}$ for a constant $\mu > 0$.

Finally, the boundary conditions (2.22) give for $s \in \Gamma$:

$$n_0 = n_D^0, n_1 = n_D^1, n_0^b(s, 0) = n_1^b(s, 0) = 0, \bar{n}_k(s) + n_k^b(s, 0) = n_D^k, k \geq 2, \quad (2.34)$$

$$\begin{aligned} \psi_0 &= \psi_D^0, \psi_1 = \psi_D^1, \psi_2 = \psi_D^2, \\ \psi_1^b(s, 0) &= \psi_2^b(s, 0) = 0, \bar{\psi}_k(s) + \psi_k^b(s, 0) = \psi_D^k, k \geq 3. \end{aligned} \quad (2.35)$$

We refer to [36] for the scheme of determination of $(n_k, \psi_k, V_k, n_k^b, \psi_{k+1}^b, V_k^b)$.

Remark 2.9. Due to the assumption (H4) :

$$n_0^b = n_1^b = \psi_1^b = \psi_2^b = 0.$$

This means that there is no boundary layers terms of order zero and one for the density and zero, one and two for the velocity potential.

The approximate solution up to order m is now constructed in the form :

$$(n_\lambda^a, \psi_\lambda^a, V_\lambda^a) = (n_{I,m}^\lambda + n_{B,m}^\lambda, \psi_{I,m}^\lambda + \psi_{B,m}^\lambda, V_{I,m}^\lambda + V_{B,m}^\lambda), \text{ in } \bar{\Omega}. \quad (2.36)$$

Moreover : $n_\lambda^a = \sum_{k=0}^m \lambda^k n_D^k$, $\psi_\lambda^a = \sum_{k=0}^m \lambda^k \psi_D^k$ on Γ and :

$$n_\lambda^a = n_0 + \sum_{j=2}^m \lambda^j (n_j + n_j^b), \quad (2.37)$$

$$\psi_\lambda^a = \psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \sum_{j=3}^m \lambda^j (\psi_j + \psi_j^b) + \lambda^{m+1} \psi_{m+1}^b. \quad (2.38)$$

2.2.2 Justification of the asymptotic expansion

One more times to justify the asymptotic expansions, we have to prove the existence and uniqueness of each profile and to obtain some estimates for the difference between the exact solution and the approximate solution. Moreover, here, since we consider the case where boundary layers can appear, we have also to prove existence of solutions to the problem (1.1)-(1.3) and (2.22). We will give here only the results and we refer to [40] for more details.

Theorem 2.10. *Under the assumptions (H1)-(H6), there exists a unique asymptotic expansion (2.36) up to order m , sufficiently smooth satisfying (2.37)-(2.38).*

We have already seen that (1.1)-(1.3) and (2.22) is equivalent to (1.1), (2.2) and (2.22). Then

Theorem 2.11. *Let the assumptions (H1)-(H6) hold. For λ small enough there is an $\varepsilon_0 > 0$ independent of λ such that for all $\varepsilon \in [0, \varepsilon_0]$, the*

problem (1.1), (2.2), (2.22) has a unique solution $(n_\lambda, \psi_\lambda)$ in $\mathcal{W}^{2,q}(\Omega) \times \mathcal{C}^{2,\delta}(\bar{\Omega})$ which satisfy

$$\|n_\lambda - n_\lambda^a\|_{W^{2,q}(\Omega)} \leq A\lambda^{m-1}, \quad \|\psi_\lambda - \psi_\lambda^a\|_{C^{2,\delta}(\bar{\Omega})} \leq A\lambda^{m-1}, \quad (2.39)$$

where A is a constant independent of λ .

Remark 2.12. Using equation (1.2), the continuity of h and estimates (2.39), we can easily obtain, for λ small enough

$$\|V_\lambda - V_\lambda^a\|_{C^{1,\delta}(\bar{\Omega})} \leq A\lambda^{m-1},$$

where A is a constant independent of λ .

The proof of theorem 2.11 is long and complicate and we refer to [40] for details. Let us just mention that the main idea is to search a solution under the form

$$n_\lambda = n_\lambda^a + \lambda^{m-1}r_\lambda, \quad \psi_\lambda = \psi_\lambda^a + \lambda^{m-1}p_\lambda.$$

Then we consider the problem verified by r_λ and p_λ . It is clear that if we obtain the existence and the boundedness of r_λ and p_λ we immediately have the result of theorem 2.11. The problem for r_λ and p_λ is a nonlinear elliptic problem. To solve it, we use the Schauder fixed point theorem, in which, to obtain the existence, uniqueness and boundedness of solution for the linearized problem, we use an another fixed point theorem: the Leray-Schauder fixed point theorem.

3 Numerical simulations

In this section we construct numerical schemes to the system (1.1)-(1.3). As seen before, from a theoretical point of view, to study this system ones uses (1.1) and (1.3) to eliminate V in (1.2) to obtain a system of two equations of unknowns (n, ψ) , supplemented with Dirichlet boundary conditions. Recall that the resulting equation for n , equation (2.2), is elliptic if and only if the flow is subsonic which corresponds to a smallness condition on the data or on the parameter ε . When (n, ψ) are solved ones obtains easily V from (1.2). However, equation (2.2) is fully nonlinear and coupled to ψ till its second derivatives, so that the numerical discretization is not an easy task. Let us now recall the system (1.1)-(1.3):

$$-\operatorname{div}(n\nabla\psi) = 0, \quad (3.1)$$

$$\frac{\varepsilon}{2}|\nabla\psi|^2 + h(n) = V + \frac{\varepsilon\psi}{\tau}, \quad (3.2)$$

$$-\lambda^2\Delta V = n - C, \quad \in \Omega. \quad (3.3)$$

The first and last equations are linear for (ψ, V) and the second one is nonlinear only algebraically for n . This motivates us to make the following iterative scheme: for a given n^m ($m \geq 0$), we first solve (ψ^m, V^m) by:

$$-\operatorname{div}(n^m \nabla \psi^m) = 0, \quad (3.4)$$

$$-\Delta V^m = C - n^m, \quad \text{in } \Omega, \quad (3.5)$$

subject to mixed Dirichlet-Neumann boundary conditions:

$$V^m = \bar{V}, \quad \psi^m = \bar{\psi}, \quad \text{on } \Gamma_D, \quad (3.6)$$

$$\nabla V^m \cdot \nu = \nabla \psi^m \cdot \nu = 0, \quad \text{on } \Gamma_N, \quad (3.7)$$

where ν is the unit outward normal to $\Gamma = \Gamma_D \cup \Gamma_N$.

Remark 3.1. Let us note that these boundary conditions are physically motivated in the case of a semiconductor. However, usually, for a semiconductor the boundary conditions are given for the electrostatic potential and the electron density. But, since here we need some boundary conditions on ψ and not on n , we choose

$$\bar{\psi} \stackrel{\text{def}}{=} (h(n_D) - \bar{V})/\varepsilon. \quad (3.8)$$

With such boundary conditions we are able to obtain Dirichlet type boundary conditions for n on Γ_D (see Remark 2.1 in [8] for more details).

Then, n^{m+1} is computed with the algebraic equation

$$h(n^{m+1}) + \frac{\varepsilon}{2} |\nabla \psi^m|^2 = V^m + \varepsilon \psi^m. \quad (3.9)$$

Equations (3.4) and (3.5) are of elliptic type (provided that n remains positive). There are several numerical methods to solve them. In [8], we choose to use two finite volume schemes. The first scheme is "classical" with a two point discretization of the fluxes through the edges, see [15]. It leads to piecewise constant approximate solutions and needs to be completed by a reconstruction of the gradients $\nabla \psi^m$, necessary for the computation of n^{m+1} in (3.9). The second scheme is of mixed finite volume type as introduced in [14], in which the construction of the gradients is intrinsic. Here we will only present the first scheme and we refer to [8] for details on the second scheme. Let us just mention that the results obtained with each scheme are really similar. Our first goal in this study was to see numerically the necessary smallness condition on ε for the existence of solutions. But our schemes can also be used to obtain the current-voltage characteristics or to simulate a ballistic diode.

3.1 Mesh and notations

Let us first of all introduce some notations usefull in the presentation of the schemes. It concerns the mesh, the initial and boundary data.

A mesh of Ω is given by a family \mathcal{T} of control volumes (open polygonal convex disjoint subsets of Ω), a family \mathcal{E} of edges in 2-d (faces in 3-d) and a set \mathcal{P} of points of Ω indexed by \mathcal{T} : $\mathcal{P} = (\mathbf{x}_K)_{K \in \mathcal{T}}$. For a control volume $K \in \mathcal{T}$ we denote by $m(K)$ the measure of K and \mathcal{E}_K the set of edges of K . The (d-1)-dimensional measure of an edge σ is denoted $m(\sigma)$. In the case where $\sigma \in \mathcal{E}$ such that $\bar{\sigma} = \bar{K} \cap \bar{L}$ with K and L being two neighboring cells, we note $\sigma = K|L$.

The set of interior (resp. boundary) edges is denoted by \mathcal{E}^{int} (resp. \mathcal{E}^{ext}), that is $\mathcal{E}^{int} = \{\sigma \in \mathcal{E}; \sigma \not\subset \partial\Omega\}$ (resp. $\mathcal{E}^{ext} = \{\sigma \in \mathcal{E}; \sigma \subset \partial\Omega\}$). We note \mathcal{E}_D^{ext} (resp. \mathcal{E}_N^{ext}) the set of $\sigma \subset \Gamma_D$ (resp. $\sigma \subset \Gamma_N$). For all $K \in \mathcal{T}$, we note $\mathcal{E}_K^{ext} = \mathcal{E}_K \cap \mathcal{E}^{ext}$, $\mathcal{E}_{D,K}^{ext}$ (resp. $\mathcal{E}_{N,K}^{ext}$) the edges of K included in Γ_D (resp. Γ_N), and $\mathcal{E}_K^{int} = \mathcal{E}_K \cap \mathcal{E}^{int}$. Finally, for $\sigma \in \mathcal{E}_K$, we denote by \mathbf{x}_σ its barycenter and by $\nu_{K,\sigma}$ the exterior unit normal vector to σ .

Given an initial datum n^0 and boundary data \bar{V} , $\bar{\psi}$, their approximations on each control volume or on each boundary edge are denoted by

$$\begin{aligned} n_K^0 &= \frac{1}{m(K)} \int_K n^0, \\ \bar{V}_\sigma &= \frac{1}{m(\sigma)} \int_\sigma \bar{V}, \\ \bar{\psi}_\sigma &= \frac{1}{m(\sigma)} \int_\sigma \bar{\psi}, \end{aligned}$$

We also set

$$f_K^m = C_K - n_K^m, \quad \text{with} \quad C_K = \frac{1}{m(K)} \int_K C.$$

3.2 Classical finite volume scheme (VF4-scheme)

Now we are able to present the classical finite volume scheme used in [8] to solve the problem (3.1)-(3.3).

Let us consider an admissible mesh of Ω given by \mathcal{T} , \mathcal{E} and \mathcal{P} which satisfy Definition 3.8 in [15]. We recall that the admissibility of \mathcal{T} implies that the straight line between two neighboring centers of cells $(\mathbf{x}_K, \mathbf{x}_L)$ is orthogonal to the edge $\sigma = K|L$. Finally, let us define the transmissibility coefficients :

$$\tau_\sigma = \frac{m(\sigma)}{d(\mathbf{x}_K, \mathbf{x}_L)} \quad \text{if } \sigma = K|L \in \mathcal{E}_K^{int} \quad \text{and} \quad \tau_\sigma = \frac{m(\sigma)}{d(\mathbf{x}_K, \Gamma)} \quad \text{if } \sigma \in \mathcal{E}_K^{ext}, \quad (3.10)$$

and the size of the mesh :

$$H = \max_{K \in \mathcal{T}} \text{diam}(K). \quad (3.11)$$

In all the sequel, we assume that the points \mathbf{x}_K are located inside each control volume. Let $(V_K^m)_{K \in \mathcal{T}}$ and $(\psi_K^m)_{K \in \mathcal{T}}$ be the discrete unknowns. A finite volume scheme to the mixed Dirichlet-Neumann problem (3.4)-(3.7) is defined by the following set of equations (see [15]) :

$$- \sum_{\sigma \in \mathcal{E}_K} dV_{K,\sigma}^m = m(K)f_K^m, \quad (3.12)$$

$$- \sum_{\sigma \in \mathcal{E}_K} n_\sigma^m d\psi_{K,\sigma}^m = 0, \quad (3.13)$$

where

$$dV_{K,\sigma}^m = \begin{cases} \tau_\sigma (V_L^m - V_K^m), & \sigma = K|L, \\ \tau_\sigma (\bar{V}_\sigma - V_K^m), & \sigma \in \mathcal{E}_{D,K}^{ext}, \\ 0, & \sigma \in \mathcal{E}_{N,K}^{ext}, \end{cases}$$

$$d\psi_{K,\sigma}^m = \begin{cases} \tau_\sigma (\psi_L^m - \psi_K^m), & \sigma = K|L, \\ \tau_\sigma (\bar{\psi}_\sigma - \psi_K^m), & \sigma \in \mathcal{E}_{D,K}^{ext}, \\ 0, & \sigma \in \mathcal{E}_{N,K}^{ext}, \end{cases}$$

$$n_\sigma^m = \begin{cases} \frac{n_K^m + n_L^m}{2}, & \sigma = K|L, \\ n_K^m, & \sigma \in \mathcal{E}_K^{ext}. \end{cases}$$

The quantities $dV_{K,\sigma}^m$ and $d\psi_{K,\sigma}^m$ are the approximations of the fluxes through each edge for each function i.e.

$$dV_{K,\sigma}^m \approx \int_\sigma \nabla V^m \cdot \nu_{K,\sigma} \quad \text{and} \quad d\psi_{K,\sigma}^m \approx \int_\sigma \nabla \psi^m \cdot \nu_{K,\sigma}.$$

For given n^m , since the equations (3.4)-(3.5) are linear, we obtain the piecewise constant functions ψ^m and V^m , unique solution of (3.12)-(3.13). Then we need to define the gradient of ψ^m . Therefore, we use the reconstruction proposed in [16]; the approximate gradient is a piecewise constant function, defined on each control volume by

$$\mathbf{w}_K^m = \frac{1}{m(K)} \sum_{\sigma \in \mathcal{E}_K} d\psi_{K,\sigma}^m(\mathbf{x}_\sigma - \mathbf{x}_K), \quad \forall K \in \mathcal{T}.$$

Finally, from (3.2) we obtain the piecewise constant function n^{m+1} by:

$$n_K^{m+1} = h^{-1}\left(V_K^m + \varepsilon\psi_K^m - \frac{\varepsilon}{2}|\mathbf{w}_K^m|^2\right), \quad (3.14)$$

with h^{-1} being the inverse function of h (see [8] for a discussion on the invertibility of h).

3.3 Numerical results

In [8] the numerical simulations are performed in two space dimensions by taking the domain $\Omega = [0, 1] \times [0, 1]$. A point \mathbf{x} of Ω is denoted by its coordinates $\mathbf{x} = (x_1, x_2)$ and then the boundary $\Gamma = \Gamma_N \cup \Gamma_D$ is defined by $\Gamma_N = \{(x_1, x_2), x_1 \in [0, 1], x_2 \in \{0, 1\}\}$ and $\Gamma_D = \Gamma_{D,l} \cup \Gamma_{D,r}$ with

$$\begin{aligned} \Gamma_{D,l} &= \{(x_1, x_2), x_1 = 0, x_2 \in [0, 1]\}, \\ \Gamma_{D,r} &= \{(x_1, x_2), x_1 = 1, x_2 \in [0, 1]\}. \end{aligned}$$

The considered pressure functions are $p(s) = s^\gamma$ with $\gamma = 1$ or $5/3$, which implies for the enthalpy :

$$h(s) = \begin{cases} \ln(s), & \text{if } \gamma = 1, \\ \frac{5}{2}(s^{2/3} - 1), & \text{if } \gamma = 5/3. \end{cases}$$

For the case $\gamma = 5/3$, the inverse function of h is defined on all \mathbb{R} by setting

$$h^{-1}(t) = \begin{cases} \left(\frac{2}{5}t + 1\right)^{3/2}, & \text{if } t > -5/2, \\ 0, & \text{else.} \end{cases}$$

We refer again to [8] for more details. In all the simulations, the used mesh is a triangular mesh of size 5×10^{-2} and the accuracy of the

numerical results is defined as the difference between n^m and n^{m+1} in $L^2(\Omega)$ or $L^\infty(\Omega)$ norm. For results on the validity of the schemes, on the bipolar case, we refer one more times to [8]. Here we present the obtained results for a ballistic diode using either the VF4-scheme or the mixed finite volume scheme (DE-scheme) since they are always very similar.

A ballistic diode is a semiconductor which consists of a weakly doped n -region S between two highly doped n^+ -regions $\Omega \setminus S$. It corresponds to the unipolar case since in such devices the charge transport is only due to electrons. In [8] the numerical solution of the system (3.1)-(3.3) is computed with the doping profile

$$C(\mathbf{x}) = \begin{cases} 10^{-3}, & \text{if } (x_1, x_2) \in S = [1/6, 5/6] \times [0, 1], \\ 1, & \text{else.} \end{cases}$$

The considered boundary conditions for the electrostatic potential are the following

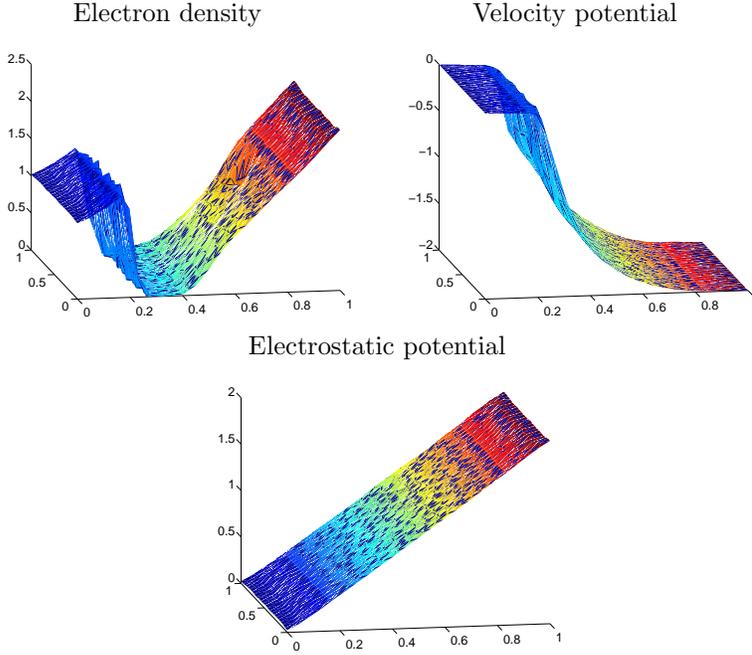
$$V^m = 0, \quad \text{on } \Gamma_{D,l} \quad \text{and} \quad V^m = U, \quad \text{on } \Gamma_{D,r}, \quad m \geq 0, \quad (3.15)$$

where U is a given applied voltage. Two kind of boundary conditions are considered for the velocity potential. First the authors consider the following one:

$$\psi^m = 0, \quad \text{on } \Gamma_{D,l} \quad \text{and} \quad \psi^m = -U, \quad \text{on } \Gamma_{D,r}, \quad m \geq 0. \quad (3.16)$$

For different values of γ , U and ε , the numerical solutions of the electron density, velocity potential and electrostatic potential are calculated. Note that the smallness condition on ε , for boundary conditions independent of ε (see [34]), which ensures the strict ellipticity of the system, appears clearly in the numerical simulations. Indeed, when ε is not small enough, the gradient of the velocity potential becomes more and more large in the iteration. Moreover, due to the negative sign before $|\nabla \psi_K^m|^2$ in the formula (3.14), the condition $n > 0$ is not numerically satisfied and the matrix involved in the computation of ψ^m becomes singular. A numerical example in this case is given in Figure 3.1 (the computation is stopped after 4 iterations).

In the case $\gamma = 5/3$, due to the definition of the inverse function of h , U should satisfy $U > -5/2$. Indeed, for ε small enough, n_K^{m+1} is nearly given by $h^{-1}(V_K^m)$ according to (3.14). If $\phi_K^m \leq -5/2$, then $h^{-1}(V_K^m) = 0$ and $n_K^{m+1} \approx 0$, so that the matrix involved in the computation of ψ^{m+1} becomes singular.

Figure 3.1: Case $\gamma = 1$, $U = 2$, $\varepsilon = 0.6$.

Note that the usual boundary conditions used for a ballistic diode are on V and n instead of ψ and in general we choose $n = n_D = C(x) = 1$ on Γ_D (see Remark 2.6). Since $h(1) = 0$ by definition, from (3.8) we deduce the following boundary conditions on ψ :

$$\psi^m = 0, \quad \text{on } \Gamma_{D,l} \text{ and } \psi^m = -U/\varepsilon, \quad \text{on } \Gamma_{D,r}, \quad m \geq 0. \quad (3.17)$$

For such boundary conditions, the ellipticity condition depends on the ratio of U and $\sqrt{\varepsilon}$ and not only on ε . This ratio has to be small enough to ensure the ellipticity condition (which remains to ensure that we are in the subsonic region). In Figure 3.2 we show the obtained solution for $\varepsilon = 0.6$ and $U = 0.1$ with the DE-scheme. The required accuracy is of order 10^{-7} in $L^\infty(\Omega)$ norm for stopping the iterations (the iteration number is 8).

Let us now present the current-voltage characteristics for the boundary conditions (3.15) and (3.17). By definition of Γ_N , the second coordinate of the electron current density is vanishing. Then, the problem is

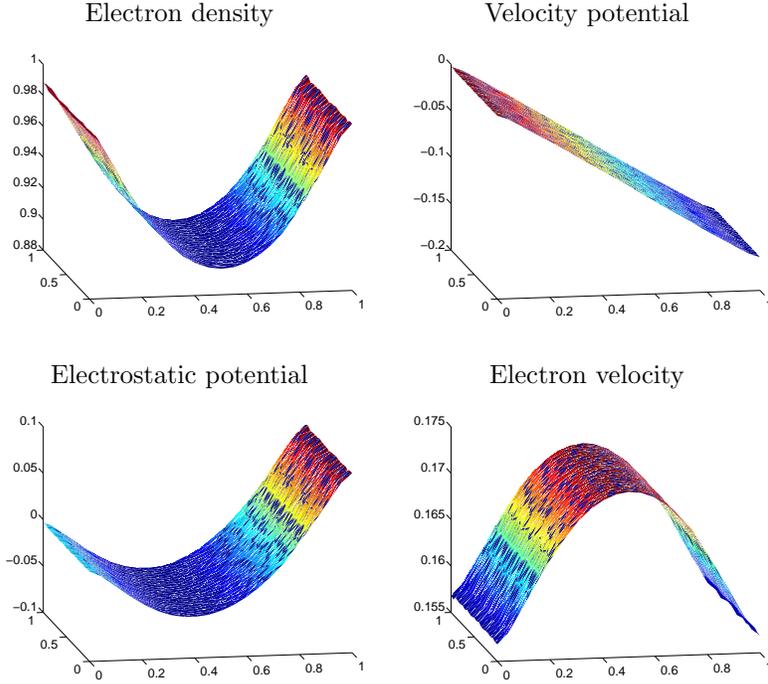


Figure 3.2: Case $\gamma = 1$, $U = 0.1$, $\varepsilon = 0.6$ for a ballistic diode.

reduced to a one-dimensional case and the first coordinate of the electron current density is constant in the device. To obtain the current-voltage characteristics, we compute the electron current density on each control volume and we take the average of these values. Here by definition of the boundary conditions on ψ , the ellipticity condition is satisfied when $|U|/\sqrt{\varepsilon}$ is strictly less than 1. Then for $\varepsilon = 1$ we choose $-0.83 \leq U \leq 0.83$ and for $\varepsilon = 0.6$, $-0.66 \leq U \leq 0.66$. We show the results in Figure 3.3. The required accuracy in $L^\infty(\Omega)$ norm for stopping the iterations is 10^{-7} and we still present the results for the DE-scheme.

In conclusion, in [8], two kinds of finite volume schemes for the numerical approximation of the steady state Euler-Poisson system for potential flows are proposed. Both schemes give similar results for different test cases with similar times computation. They permit to show the importance of the smallness of ε and the boundary data for the ellipticity of the system.

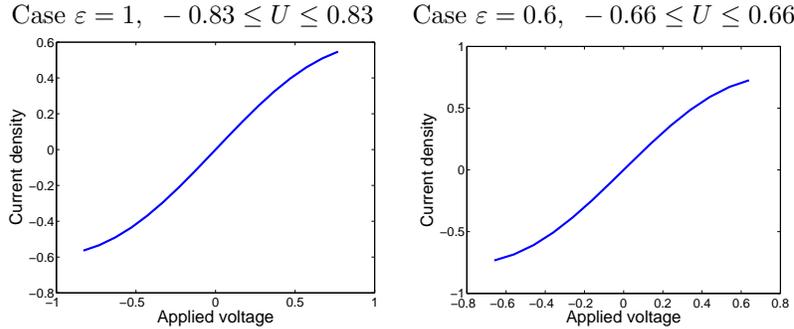


Figure 3.3: Current-voltage characteristics for different values of ε when the considered boundary conditions on ψ depend on ε .

The VF4-scheme is a bit simpler to implement but it only works on admissible meshes, whereas the DE-scheme enables to treat very general meshes.

References

- [1] G.Ali and A.Jüngel, Global smooth solutions to the multi-dimensional hydrodynamic model for two-carrier plasmas, *J. Diff. Eqn.*, 190 (2003).
- [2] F. Arimburgo, C.Baiocchi and L.D.Marini, Numerical approximation of the 1-D nonlinear drift-diffusion model in semiconductors, *Nonlinear Kinetic Theory and Mathematical Aspects of Hyperbolic Systems* (Rappallo, 1992) (World Scientific, 1992).
- [3] G. Baccarani and M.R. Wordeman, An investigation of steady-state velocity overshoot effects in Si and GaAs devices, *Solid State Electronics*, 28 (1985).
- [4] H.Brézis, F.Golse and R.Sentis, Analyse asymptotique de l'équation de Poisson couplée à la relation de Boltzmann. Quasi-neutralité des plasmas, *C. R. Acad. Sci. Paris*, 321 (1995).
- [5] F.Brezzi, L.D.Marini and P.Pietra, Numerical simulation of semiconductor devices, *Comput. Meth. Appl. Mech. Engrg.* 75 (1989).
- [6] C.Chainais-Hillairet, J.G.Liu and Y.J.Peng, Finite volume scheme for multi-dimensional drift-diffusion equations and convergence analysis, *Math. Mod. Anal. Numer.*, 37 (2003).

- [7] C.Chainais-Hillairet and Y.J.Peng, Finite volume approximation for degenerate drift-diffusion system in several space dimensions, *Math. Mod. Meth. Appl. Sci.*, 14 (3) (2004).
- [8] C.Chainais, Y.J.Peng, I.Violet, Numerical solutions of the Euler-Poisson system for a potential flow, *Applied Numerical Mathematics*, 59 (2009).
- [9] F.Chen, Introduction to plasma physics and controlled fusion, *Vol1, Plenum Press, New-York*, (1984).
- [10] Z.X.Chen and B.Cockburn, Analysis of a finite element method for the drift-diffusion semiconductor device equations : The multidimensional case, *Numer. Math.*, 71 (1995).
- [11] B.Cockburn and I.Triandaf, Error estimates for a finite element method for the drift-diffusion semiconductor device equations : The zero diffusion case, *Math. Comput.*, 63 (1994).
- [12] S.Cordier and E.Grenier, Quasi-neutral limit of an Euler-Poisson system arising from plasma physics, *Comm. Part. Diff. Eqs*, 25 (2000).
- [13] P.Degond and P.A.Markowich, A steady state potential flow model for semiconductors, *Annali di matematica pura ed applicata*, (IV), Vol CLXV, (1993).
- [14] J.Droniou and R.Eymard, A mixed finite volume scheme for anisotropic diffusion problems on any grid, *Num. Math.*, 105 (2006).
- [15] R.Eymard, T.Gallouët and R.Herbin, Finite volume methods, *Handbook of numerical analysis, North-Holland, Amsterdam*, Vol. VII, (2000).
- [16] R.Eymard, T.Gallouët and R.Herbin, A cell-centred finite-volume approximation for anisotropic diffusion operators on unstructured meshes in any space dimension, *IMA Journal of Numerical Analysis*, 26 (2) (2006).
- [17] P.C.Fife, Semilinear elliptic boundary value problems with small parameters, *Arch. Ration. Mech. Anal*, 52 (1973).
- [18] C.L. Gardner, Numerical simulation of a steady-state electron shock wave in a submicrometer semiconductor device, *IEEE Trans. Electron Devices*, 28 (1991).
- [19] C.L. Gardner, J.W. Jerome and D.J. Rose, Numerical methods for the hydrodynamic device model: subsonic flow, *IEEE Trans. Computer-Aided Design.*, 8 (1989).
- [20] I.Gasser, The initial time layer problem and the quasineutral limit in a nonlinear drift-diffusion model for semiconductors, *Nonlinear Differential Equations and Applications*, 8 (2001).

- [21] I.Gasser, D.Levermore, P.A.Markowich and C.Schmeiser, The initial time layer problem and the quasineutral limit in the semiconductor drift-diffusion model, *European J. Appl. Math.*, 12 (2001).
- [22] I.Gasser and P.Marcati, The combined relaxation and vanishing Debye length limit in the hydrodynamic model for semiconductors, *Math. Mech. Appl. Sci.*, 24 (2001).
- [23] D.Gilbarg and N.S.Trudinger, Elliptic partial differential equations of second order, *Springer, Berlin, New-York*, (1984).
- [24] H.K. Gummel, A self-consistent iterative scheme for one-dimensional steady-state transistor calculations, *IEEE Trans. Electron Devices*, 11 (1964).
- [25] A.Jüngel, Numerical approximation of a drift-diffusion model for semiconductors with nonlinear diffusion, *Z. Angew. Math. Mech.*, 75 (1995).
- [26] A.Jüngel and Y.J.Peng, A hierarchy of hydrodynamic models for plasmas. Zero-relaxation-time limit, *Comm. Part. Diff. Eqs*, 24 (1999).
- [27] A.Jüngel and Y.J.Peng, Zero-relaxation-time limits in hydrodynamic models for plasmas revisited, *Z. Angew. Math. Phys.*, 51 (2000).
- [28] A.Jüngel and Y.J.Peng, A hierarchy of hydrodynamic models for plasmas. Quasineutral limits in the drift-diffusion equations, *Asymptotic Analysis*, 28 (2001).
- [29] A.Jüngel and P.Pietra, A discretization scheme for a quasi-hydrodynamic semiconductor model, *Math. Mod. Meth. Appl. Sci*, 7 (1997).
- [30] C.Lattanzio and P.Marcati, The relaxation to the drift-diffusion system for the 3-D isentropic Euler-Poisson model for semiconductors, *Discr. contin. dyn. syst.*, 5 (1999).
- [31] P.Marcati and R.Natalini, Weak solutions to a hydrodynamic model for semiconductors and relaxation to the drift-diffusion equation, *Arch. Rat. Mech. Anal.*, 129 (1995).
- [32] P.A.Markowich, The stationary semiconductor device equations, *Springer, New-York*, (1986).
- [33] Y.J.Peng, Asymptotic limits of one-dimensional hydrodynamic models for plasmas and semiconductors, *Chinese Ann. Math.*, 23B (2002).
- [34] Y.J.Peng, Some asymptotic analysis in steady state Euler-Poisson equations for potential flow, *Asymptotic analysis*, 36 (2003).

- [35] Y.J.Peng and I.Violet, Asymptotic expansions in a steady state Euler-Poisson system and convergence to incompressible Euler equations, *M3AS*, 15 (2005).
- [36] Y.J.Peng and Y.G.Wang, Boundary layers and quasi-neutral limit in steady state Euler-Poisson equations for potential flows, *Nonlinearity*, 17 (2004).
- [37] P.Raviart, On singular perturbation problems for the nonlinear Poisson equation : A mathematical approach to electrostatic sheaths and plasma erosion, *Lecture Notes of the Summer school in Ile d'Oléron, France*, (1997).
- [38] R.Sacco and F.Saleri, Mixed finite volume methods for semiconductor device simulation, *Numer. Meth. Part. Diff. Equations*, 13 (1997).
- [39] M.Slemrod and N.Sternberg, Quasi-neutral limit for the Euler-Poisson system, *J.Nonlinear Sciences*, 11 (2001).
- [40] I.Violet, High order expansions in quasi-neutral limit of the Euler-Poisson system for a potential flow, *Proceedings of the Royal Society of Edinburgh*, 137A, (2007).