NUMERICAL SOLUTIONS OF EULER-POISSON SYSTEMS FOR POTENTIAL FLOWS

CLAIREE CHAINAIS-HILLAIRET, YUE-JUE PENG AND INGRID VIOLET

Laboratoire de Mathématiques, CNRS UMR 6620
Université Blaise Pascal (Clermont-Ferrand 2), 63177 Aubière cedex, France
chainais@math.univ-bpclermont.fr, peng@math.univ-bpclermont.fr,
violet@math.univ-bpclermont.fr

Abstract : Steady-state Euler-Poisson systems for potential flows are studied here from a numerical point of view. The main idea is to use iterative schemes to solve a system of linear partial differential equations together with nonlinear algebraic equations instead of solving a fully nonlinear system of partial differential equations. We present two numerical schemes of finite volume type to compute approximate solutions of the systems for semiconductors in unipolar and bipolar cases. The numerical simulations are carried out in two space dimensions, in which some smallness conditions on given data and parameters in the proof of existence of solutions to the systems are clearly illustrated.

Keywords. Euler-Poisson system, numerical simulation, finite volume method, potential flow, steady-state.

1. Introduction

The hydrodynamic model introduced by Blotkjaer in [5] plays an important role in the mathematical modeling and in the numerical simulation of semiconductor devices [28, 29] and plasmas [9]. In this paper, we consider a classical simplified hydrodynamic model in which the energy equation is replaced by a pressure-density relationship. It means that the electrons behave like a gas and that the flow is either isentropic or isothermal. This simplified hydrodynamic model leads to the Euler-Poisson system. It consists of two nonlinear equations given by the conservation of mass and momentum for each species (Euler equations), coupled to a Poisson equation for the electrostatic potential. Here we neglect the collision terms in the mass conservation equations. Then, the hydrodynamic system introduced by Blotkjaer in [5], extended to the bipolar case, reads in the scaled variables:
\[
\begin{align*}
\frac{\partial}{\partial t} p + \text{div}(pu_p) &= 0, \quad \text{in } \Omega \times \mathbb{R}_+, \\
\frac{\partial}{\partial t} (pu_p) + \text{div}(pu_p \otimes u_p) + \nabla P_p(p) &= -p\nabla \phi - \frac{pu_p}{\tau}, \quad \text{in } \Omega \times \mathbb{R}_+, \\
\frac{\partial}{\partial t} n + \text{div}(nu_n) &= 0, \quad \text{in } \Omega \times \mathbb{R}_+, \\
\varepsilon \frac{\partial}{\partial t} (nu_n) + \varepsilon \text{div}(nu_n \otimes u_n) + \nabla P_n(n) &= n\nabla \phi - \varepsilon \frac{nu_n}{\tau}, \quad \text{in } \Omega \times \mathbb{R}_+, \\
\lambda^2 \Delta \phi &= n - p - C, \quad \text{in } \Omega \times \mathbb{R}_+,
\end{align*}
\]

where \( \Omega \) is an open and bounded domain of \( \mathbb{R}^d \) (\( d = 2 \) or \( d = 3 \) in practice) representing the geometry of the semiconductor device or the plasma. The unknowns of the system are the electron and hole (ions in the case of a plasma) densities \( n = n(x,t) \), \( p = p(x,t) \), the electron and hole velocities \( u_n = u_n(x,t), \ u_p = u_p(x,t) \), and the electrostatic potential \( \phi = \phi(x,t) \). The function \( C = C(x) \) stands for the doping profile of the device in the case of a semiconductor. For a plasma, this function is equal to zero. The pressure functions are in general the same for electrons and holes, \( P_n(s) = P_p(s) = P(s) \), and in all the applications we have \( P(s) = s^\gamma \) with \( \gamma = 1 \) (isothermal flow) or \( \gamma = 5/3 \) (isentropic flow).

The physical parameters \( \lambda, \varepsilon \) and \( \tau \) are respectively the Debye length, the ratio of the effective masses of electrons and holes, and the relaxation time. They are small compared to the characteristic lengths of physical interest. In the sequel, \( \lambda \) and \( \tau \) are supposed to be equal to 1.

In this paper we only consider the steady-state case of potential flows. Then, \( \text{rot}(u_n) = \text{rot}(u_p) = 0 \) and there exist \( \psi_n \) and \( \psi_p \) such that \( u_n = -\nabla \psi_n, \ u_p = -\nabla \psi_p \), where \( \psi_n \) and \( \psi_p \) are the electron and hole velocity potentials. Under these assumptions and with \( \lambda = \tau = 1 \), the Euler-Poisson system (1.1)-(1.5) can be rewritten as (see [16]) :

\[
\begin{align*}
-\text{div}(p\nabla \psi_p) &= 0, \quad \text{in } \Omega, \\
H(p) + \frac{1}{2}|\nabla \psi_p|^2 &= -\phi + \psi_p, \quad \text{in } \Omega, \\
-\text{div}(n\nabla \psi_n) &= 0, \quad \text{in } \Omega, \\
H(n) + \frac{\varepsilon}{2}|\nabla \psi_n|^2 &= \phi + \varepsilon \psi_n, \quad \text{in } \Omega, \\
\Delta \phi &= n - p - C, \quad \text{in } \Omega,
\end{align*}
\]

where \( H = H(s) \) is the enthalpy function of the system defined by:

\[
H'(s) = \frac{P'(s)}{s} \quad \text{and} \quad H(1) = 0.
\]

In the unipolar case, the system is reduced to three equations (1.8)-(1.10) in which \( p = p(x) \) can be neglected and \( \varepsilon \) is the effective mass of electrons. The system (1.6)-(1.10) or (1.8)-(1.10) is in general supplemented with Dirichlet-Neumann boundary conditions on the densities and velocity potentials.

There are many works dealing with the hydrodynamic model. This model treats the propagation of charges in the device as a compressible charged fluid. Therefore, as it is well known in gas dynamics, the particle flow can be either fully subsonic, or fully supersonic or transonic.

The transient hydrodynamic model has been studied by Marcati and Natalini [27] (global existence of entropy solutions in one-dimension), Ali and Jüngel [1] (local existence
of smooth solutions and asymptotic limits in multi-dimension) and Jüngel and Peng [25] (asymptotic limits of entropy solutions in one dimension). Numerical schemes in the quasineutral limit have been developed by Crispel, Degond and Vignal [13, 14]. The zero relaxation time limit of the hydrodynamic model leads to the classical drift-diffusion systems (see [25]) for which finite volume methods have been developed and analyzed in [7, 8].

A mathematical analysis for the one-dimensional steady-state hydrodynamic model, in the unipolar case, has been introduced by Degond and Markowich in [15]. For the isentropic case, these authors give an existence and a uniqueness result in the subsonic case, which is characterized by a smallness assumption on the current flowing through the device. For the same problem, Ascher, Markowich, Pietra and Schmeiser [3] present an analysis of transonic solutions and Gamba [20] establishes the existence of transonic solution without any smallness condition. The behaviour of the solution near the boundary is also studied in [20].

In the multidimensional case, the steady-state hydrodynamic model, in the unipolar case, has been first studied by Degond and Markowich. In [16], these authors prove the existence and local uniqueness of solutions for the model with potential flows. This result holds under a smallness condition on the boundary data, which implies that the problem is in the subsonic region. It has been proved by Peng in [30] that this smallness condition on the boundary data can be replaced by a smallness condition on $\varepsilon$. The results can be extended to the bipolar case provided that $\varepsilon$ and the boundary data for $\psi_p$ are small enough. In [31, 33], the asymptotic limits are performed by using a method of asymptotic expansions.

From a numerical point of view, the hydrodynamic model has essentially been studied in its complete form (with the energy-balance equation). Baccarini and Wordeman in [4] provide numerical simulations and show that the model exhibits velocity overshoot. Gardner, Jerome and Rose in [22] propose numerical methods for the hydrodynamic model and give numerical results for the ballistic diode in the case of subsonic flow. They obtain the hot electron effect in the channel of the diode. In [21], Gardner extend the simulations to the case of transonic flow.

There exists also a wide literature on the analysis and simulation of the drift-diffusion equations (see [2, 6, 7, 8, 10, 11, 24, 26, 32] and references therein). 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 [23].

The goal of this paper is to develop numerical schemes to compute solutions of the bidimensional steady-state Euler-Poisson system for potential flows. In particular, we want to illustrate the smallness condition on $\varepsilon$, [30], or on the boundary data, [16], for the existence of solutions to the problem (1.1)-(1.5). The main idea is to use iterative schemes to solve a system of linear partial differential equations for $(\phi, \psi_n, \psi_p)$ and nonlinear algebraic equations for $(n, p)$ instead of solving a fully nonlinear system of partial differential equations. We present two numerical schemes of finite volume type with reconstruction of the gradients appearing in (1.7) or (1.9). They are based on the previous work by Eymard, Gallouët and Herbin in [18, 19] and by Eymard and Droniou [17].

In Section 2, we present our numerical schemes in the unipolar case. The numerical results in two space dimensions in the unipolar and bipolar cases are given in Section 3.
2. Presentation of the numerical schemes

In this section we construct numerical schemes to the system in the unipolar case. The corresponding schemes in the bipolar case are similar. Omitting the subscript \( n \) for simplicity, the set of equations (1.8)-(1.10) for the unipolar model can be rewritten as:

\[
\begin{align*}
-\text{div}(n\nabla \psi) &= 0, \\
H(n) + \frac{\varepsilon}{2} |\nabla \psi|^2 &= \phi + \varepsilon \psi, \\
\Delta \phi &= n - C(x), \quad \text{in } \Omega.
\end{align*}
\]

From a theoretical point of view, to study this system one uses equation (2.1) and (2.3) to eliminate \( \phi \) in (2.2) to obtain a system of two equations of unknowns \((n, \psi)\), supplemented with Dirichlet boundary conditions. The resulting equation for \( n \) is

\[
-\Delta H(n) + \frac{\varepsilon}{n} \sum_{i,j=1}^{d} \frac{\partial \psi}{\partial x_i} \frac{\partial \psi}{\partial x_j} \frac{\partial^2 n}{\partial x_i \partial x_j} - \frac{\varepsilon}{n} \nabla \psi \cdot \nabla n - \frac{\varepsilon}{n^2} (\nabla \psi \cdot \nabla n)^2 \\
+ \frac{\varepsilon}{n} \sum_{i,j=1}^{d} \frac{\partial \psi}{\partial x_i} \frac{\partial^2 \psi}{\partial x_i \partial x_j} \frac{\partial n}{\partial x_j} + n - C(x) = \varepsilon Q(\psi),
\]

where \( Q \) is given by

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

When \( \psi \) is given, equation (2.4) on \( n \) is elliptic if and only if the flow is subsonic (see [16, 30]), i.e.

\[
|\nabla \psi| < \sqrt{\frac{P'(n)}{\varepsilon}},
\]

where \(| \cdot |\) stands for the Euclidean norm.

The existence and uniqueness of solutions to the system (2.1) and (2.4) can be proved under a smallness condition on the boundary data [16] or on \( \varepsilon \) [30] which ensures the strict ellipticity of the equation (2.4) for \( n \). When \((n, \psi)\) are solved one obtains easily \( \phi \) from (2.2). However, the equation (2.4) is fully nonlinear and coupled to \( \psi \) till its second derivatives, so that its numerical discretization is not an easy task. Note that the first and last equations in the system (2.1)-(2.3) are linear for \((\psi, \phi)\) 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 \((\psi^m, \phi^m)\) by:

\[
\begin{align*}
-\text{div}(n^m \nabla \psi^m) &= 0, \\
-\Delta \phi^m &= C - n^m, \quad \text{in } \Omega,
\end{align*}
\]

subject to mixed Dirichlet-Neumann boundary conditions:

\[
\begin{align*}
\phi^m &= \bar{\phi}, \quad \psi^m = \bar{\psi}, \quad \text{on } \Gamma_D, \\
\nabla \phi^m \cdot \nu = \nabla \psi^m \cdot \nu &= 0, \quad \text{on } \Gamma_N,
\end{align*}
\]

where \( \nu \) is the unit outward normal to \( \Gamma = \partial \Omega = \Gamma_D \cup \Gamma_N \).
Remark 2.1. These boundary conditions are physically motivated in the case of a semiconductor (see [16]). For such a device, $\Gamma_D$ stands for the ohmic contacts and $\Gamma_N$ for the insulating boundary segments. In particular, condition (2.9) means that there is no current flow throughout $\Gamma_N$. However, usually, for a semiconductor, the boundary conditions are given for the electrostatic potential $\phi$ and the electron density $n$ with homogeneous Neumann conditions on the insulating segments and Dirichlet type conditions on the ohmic contacts. This means in particular that one imposes $n = n_D$ on $\Gamma_D$. Since here we need some boundary conditions on $\psi$ and not on $n$, we choose:

\[(2.10) \quad \bar{\psi} \overset{\text{def}}{=} \left( H(n_D) - \bar{\phi} \right)/\varepsilon.\]

With such boundary conditions, we are able to then obtain $n = n_D$ on $\Gamma_D$.

Then we compute $n^{m+1}$ by the algebraic equation

\[(2.11) \quad H(n^{m+1}) + \frac{\varepsilon}{2} |\nabla \psi^m|^2 = \phi^m + \varepsilon \psi^m.\]

Equations (2.6) and (2.7) are of elliptic type (provided $n^m$ remains positive). There are several numerical methods to solve this kind of equations (e.g. finite element method, mixed finite element method, finite volume methods...). Here, some finite volume schemes are used. The first scheme is "classical" with a two point discretization of the fluxes through the edges, see [18]. 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 (2.11). The second scheme is of mixed finite volume type as introduced by J. Droniou and R. Eymard in [17], in which the construction of the gradients is intrinsic.

2.1. Mesh and notations. First, we introduce some notations that are useful for both schemes. It concerns the mesh, the initial and boundary data.

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

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

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

\[
n^0_K = \frac{1}{m(K)} \int_K n^0,
\]
\[
\bar{\phi}_\sigma = \frac{1}{m(\sigma)} \int_\sigma \bar{\phi},
\]
\[
\bar{\psi}_\sigma = \frac{1}{m(\sigma)} \int_\sigma \bar{\psi},
\]
We also set
\[ f_K^m = C_K - n_K^m, \quad \text{with} \quad C_K = \frac{1}{m(K)} \int_K C. \]

2.2. Classical finite volume scheme. Let us consider an admissible mesh of \( \Omega \) given by \( T, E \) and \( P \) which satisfy Definition 3.8 in [18]. We recall that the admissibility of \( T \) implies that the straight line between two neighboring centers of cells \((x_K, x_L)\) is orthogonal to the edge \( \sigma = K|L \). Finally, let us define the transmissibility coefficients:

\[ \tau_\sigma = \frac{m(\sigma)}{d(x_K, x_L)} \quad \text{if} \quad \sigma = K|L \in E^\text{int}_K \quad \text{and} \quad \tau_\sigma = \frac{m(\sigma)}{d(x_K, \Gamma)} \quad \text{if} \quad \sigma \in E^\text{ext}_K, \]

and the size of the mesh:

\[ h = \max_{K \in T} \text{diam}(K). \]

In all the sequel, we assume that the points \( x_K \) are located inside each control volume. Let \((\phi_K^m)_{K \in T}\) and \((\psi_K^m)_{K \in T}\) be the discrete unknowns. A finite volume scheme to the mixed Dirichlet-Neumann problem (2.6)-(2.9) is defined by the following set of equations (see [18]):

\[ \begin{aligned}
- \sum_{\sigma \in E_K} d\phi_{K,\sigma}^m &= m(K)f_K^m, \\
- \sum_{\sigma \in E_K} n_\sigma^m d\psi_{K,\sigma}^m &= 0,
\end{aligned} \]

where

\[ d\phi_{K,\sigma}^m = \begin{cases} 
\tau_\sigma (\phi_L^m - \phi_K^m), & \sigma = K|L, \\
\tau_\sigma (\bar{\phi}_\sigma - \phi_K^m), & \sigma \in E^\text{ext}_{D,K}, \\
0, & \sigma \in E^\text{ext}_{N,K}, 
\end{cases} \]

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

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

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

\[ d\phi_{K,\sigma}^m \approx \int_\sigma \nabla \phi_{K,\sigma}^m \cdot \nu_{K,\sigma} \quad \text{and} \quad d\psi_{K,\sigma}^m \approx \int_\sigma \nabla \psi_{K,\sigma}^m \cdot \nu_{K,\sigma}. \]

For given \( n^m \), since the equations (2.6)-(2.7) are linear, we obtain the piecewise constant functions \( \psi^m \) and \( \phi^m \), unique solution of (2.14)-(2.15). Then we need to define the gradient
of $\psi_m$. Therefore, we use the reconstruction proposed in [19]; 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 (2.2) we obtain the piecewise constant function $n^{m+1}$ by:
\[
n_K^{m+1} = H^{-1} \left( \phi_K^m + \varepsilon \psi_K^m - \frac{\varepsilon}{2} |\mathbf{w}_K^m|^2 \right),
\]
with $H^{-1}$ being the inverse function of $H$ (the invertibility of $H$ will be discussed later).

2.3. Mixed finite volume scheme. As seen previously, the definition of $n^{m+1}$ through the algebraic equation (2.11) needs construction of an approximate gradient, which is not usual in classical finite volume schemes. However, the penalized mixed finite volume scheme introduced by J.Droniou and R.Eymard in [17] for an elliptic equation is a scheme whose unknowns are the function, its gradient on each control volume and the fluxes through each edge. Then the definition of the piecewise constant gradient of the solution is intrinsic. Furthermore this scheme can be used on very general meshes.

Let us consider a mesh of $\Omega$ given by $\mathcal{T}$, $\mathcal{E}$ and $\mathcal{P}$ which satisfy definition 2.1 in [17]. We denote by $(\phi_K^m)_{K \in \mathcal{T}}$ and $(\psi_K^m)_{K \in \mathcal{T}}$ the approximate values of $\phi$ and $\psi$, by $(\mathbf{v}_K^m)_{K \in \mathcal{T}}$ and $(\mathbf{w}_K^m)_{K \in \mathcal{T}}$ the approximate gradients of $\phi^m$ and $\psi^m$, respectively. Let $\xi = (\xi_K)_{K \in \mathcal{T}}$ be a family of small positive numbers and
\[
F_{K,\sigma}^m \approx \frac{1}{m(\sigma)} \int_{\sigma} \nabla \phi^m \cdot \mathbf{n}_{K,\sigma} \quad \text{and} \quad G_{K,\sigma}^m \approx \frac{1}{m(\sigma)} \int_{\sigma} \nabla \psi^m \cdot \mathbf{n}_{K,\sigma}.
\]
The penalized mixed finite volume scheme to the problems (2.6)-(2.7) and (2.8)-(2.9) can be written as (see [17]):
\[
\mathbf{v}_K^m \cdot (\mathbf{x}_\sigma - \mathbf{x}_K) + \mathbf{v}_L^m \cdot (\mathbf{x}_\sigma - \mathbf{x}_L) + \xi_K m(K) F_{K,\sigma} - \xi_L m(L) F_{L,\sigma} = \phi_L^m - \phi_K^m, \quad \forall K \in \mathcal{M}, \forall L \in \mathcal{N}_K \text{ with } \sigma = K|L,
\]
\[
\mathbf{v}_K^m \cdot (\mathbf{x}_\sigma - \mathbf{x}_K) + \xi_K m(K) F_{K,\sigma} = \phi^m_K - \phi^m_K, \quad \forall K \in \mathcal{M}, \forall \sigma \in \mathcal{E}^{ext}_{D,K},
\]
\[
F_{K,\sigma} + F_{L,\sigma} = 0, \quad \forall \sigma = K|L \in \mathcal{E}^{int}, \quad F_{K,\sigma} = 0, \quad \forall \sigma \in \mathcal{E}^{ext}_{N,K},
\]
\[
m(K) \mathbf{w}_K^m = \sum_{\sigma \in \mathcal{E}_K} F_{K,\sigma} (\mathbf{x}_\sigma - \mathbf{x}_K), \quad \forall K \in \mathcal{M},
\]
\[
- \sum_{\sigma \in \mathcal{E}_K} F_{K,\sigma} = m(K) f_K^m, \quad \forall K \in \mathcal{M},
\]
\[
\mathbf{w}_K^m \cdot (\mathbf{x}_\sigma - \mathbf{x}_K) + \mathbf{w}_L^m \cdot (\mathbf{x}_\sigma - \mathbf{x}_L) + \xi_K m(K) G_{K,\sigma} - \xi_L m(L) G_{L,\sigma} = \psi_L^m - \psi_K^m, \quad \forall K \in \mathcal{M}, \forall L \in \mathcal{N}_K \text{ with } \sigma = K|L,
\]
\[
\mathbf{w}_K^m \cdot (\mathbf{x}_\sigma - \mathbf{x}_K) + \xi_K m(K) G_{K,\sigma} = \psi^m_K - \psi^m_K, \quad \forall K \in \mathcal{M}, \forall \sigma \in \mathcal{E}^{ext}_{D,K},
\]
\[
G_{K,\sigma} + G_{L,\sigma} = 0, \quad \forall \sigma = K|L \in \mathcal{E}^{int}, \quad G_{K,\sigma} = 0, \quad \forall \sigma \in \mathcal{E}^{ext}_{N,K},
\]
\[
m(K) n_K^m \mathbf{w}_K^m = \sum_{\sigma \in \mathcal{E}_K} G_{K,\sigma} (\mathbf{x}_\sigma - \mathbf{x}_K), \quad \forall K \in \mathcal{M},
\]
\[
- \sum_{\sigma \in \mathcal{E}_K} G_{K,\sigma} = 0, \quad \forall K \in \mathcal{M}.
\]
Then $n_{K}^{m+1}$ is given by (2.16).

In both schemes, the iterations on $m$ are stopped when the difference between $n^{m}$ and $n^{m+1}$ is sufficiently small in $L^2(\Omega)$ or $L^\infty(\Omega)$ norm. Notice that for the penalized mixed finite volume scheme we have to solve two systems whose size is $3\text{Card}(M) + \text{Card}(E)$. However it is possible to proceed to an algebraic elimination which leads for each one to a system of size $\text{Card}(E^{int})$, following the same principles as in the hybrid resolution presented in [17].

Let us denote by $n_{K}$ and $w_{K}$ the values of the electron density and the gradient of the electron potential velocity on each control volume when the iterations are stopped. Then we calculate, for each scheme, the electron current density $J_{K}$ on each control volume by:

\begin{equation}
J_{K} = -n_{K}w_{K}.
\end{equation}

In all the sequel, the classical finite volume scheme is referred to as the VF4-scheme and the penalized mixed finite volume scheme as the DE-scheme. The schemes for the bipolar case are almost the same. The only difference is that there are three linear equations (instead of two) and two nonlinear algebraic equations (instead of one), which can be solved exactly with the same methods.

3. Numerical results

We perform the numerical simulations in two space dimensions by taking the domain $\Omega = [0,1] \times [0,1]$. A point $x$ of $\Omega$ is denoted by its coordinates $x = (x_1, x_2)$. Let us define $\Gamma_N = \{(x_1, x_2), x_1 \in [0,1], x_2 \in \{0,1\}\}$ and $\Gamma_D = \Gamma_{D,l} \cup \Gamma_{D,r}$ with

\begin{align*}
\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{align*}

The pressure function is taken to be $P(s) = s^\gamma$ with $\gamma = 1$ or $5/3$, which implies for the enthalpy :

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

In the case $\gamma = 1$, $H$ is defined from $]0, +\infty[$ to $\mathbb{R}$ and admits an inverse function on all $\mathbb{R}$ defined by $H^{-1}(t) = \exp(t)$. In the case $\gamma = 5/3$, $H$ is only defined from $]0, +\infty[$ to $]-5/2, +\infty[$. In order to define its inverse function on all $\mathbb{R}$ we extend the function by continuity by setting :

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

In the numerical simulations below, we use a triangular mesh of size $5 \times 10^{-2}$. 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.
3.1. **Validity of the schemes.** To our knowledge, in the literature there do not exist numerical results to the steady-state Euler-Poisson system in the isentropic and subsonic case. Therefore it is impossible to compare our results with those obtained by other numerical methods. To ensure that our schemes provide a good approximation of the solution, we compare the numerical solutions obtained with each scheme to exact solutions. To this end we consider two different test cases for the unipolar system (2.1)-(2.3).

3.1.1. **First test case.** This test case is only academic. For it, we are able to obtain the exact solution to the Euler-Poisson system (2.1)-(2.3) for appropriate boundary conditions. In particular, we use it to obtain the errors between the numerical and the exact solutions as functions of the mesh size. Here, the doping profile is defined as follows:

\[ C(x_1, x_2) = 1 - 2\varepsilon A^2 \pi^4 \exp(2\pi x_1), \ (x_1, x_2) \text{ in } \Omega, \]

where \( A \) is a given constant. This doping profile is strictly positive on \( \bar{\Omega} \) provided that \( A^2 \varepsilon \) is small (for instance, \( \varepsilon = 9.5 \times 10^{-6} \) and \( A = 1 \)). We supplement the system (2.1)-(2.3) with the following mixed Dirichlet-Neumann boundary conditions

\[ \nabla \psi \cdot \nu = \nabla \phi \cdot \nu = 0, \text{ on } \Gamma_N, \]
\[ \psi = A \cos(\pi x_2), \ \phi = \frac{1}{2} A^2 \varepsilon \pi^2 - A \varepsilon \cos(\pi x_2), \text{ on } \Gamma_{D,t}, \]
\[ \psi = A \exp(\pi) \cos(\pi x_2), \ \phi = \frac{1}{2} A^2 \varepsilon \pi^2 \exp(2\pi) - A \varepsilon \exp(\pi) \cos(\pi x_2), \text{ on } \Gamma_{D,r}. \]

Then it is easy to check that the exact solution of (2.1)-(2.3) and (3.1)-(3.2) is given by

\[ n(x_1, x_2) = 1, \]
\[ \psi(x_1, x_2) = A \exp(\pi x_1) \cos(\pi x_2), \]
\[ \phi(x_1, x_2) = \frac{1}{2} A^2 \varepsilon \pi^2 \exp(2\pi x_1) - A \varepsilon \exp(\pi x_1) \cos(\pi x_2), \text{ in } \bar{\Omega}. \]

We choose \( \varepsilon = 9.5 \times 10^{-6} \) and \( A = 1 \). We start the computation with \( n^0_1(x_1, x_2) = 1/2 \) on \( \Omega \). The computations are stopped when the relative \( L^2 \)-error between two following iterations is smaller than \( 10^{-3} \).

We compute the errors between the numerical and exact solutions for different mesh size for each scheme and for each value of \( \gamma \). The results are shown in Figure 1. We can see that for both schemes and for each unknown, the errors are decreasing with the mesh size. The DE-scheme seems to be more efficient in particular for the velocity and electrostatic potentials. Moreover, the errors are smaller in the case \( \gamma = 5/3 \) than in the case \( \gamma = 1 \). They are of order of \( h \) for each quantity.

We now consider the initial density \( n^0_1(x_1, x_2) = 1 \) and the same values for \( \varepsilon \) and \( A \) as above. The required accuracy is of order \( O(h) \) in \( L^2(\Omega) \) norm for stopping the iterations. The results are shown in Figure 2, from which we see that again the errors are increasing functions of \( h \). They are of the same order as previously. Again, they are smaller in the case \( \gamma = 5/3 \) than in the case \( \gamma = 1 \).
3.1.2. Second test case. For this test case we are also able to obtain the exact solution for appropriate boundary conditions. It remains in fact to a one-dimensional test case. Here, the doping profile is defined as a constant being equal to 1 and we consider the following boundary conditions:

\begin{align}
\phi(0, x_2) &= 0, \quad \phi(1, x_2) = U, \\
\psi(0, x_2) &= \frac{U^2}{2\varepsilon}, \quad \psi(1, x_2) = \frac{U}{\varepsilon} \left( \frac{U}{2\varepsilon} - 1 \right).
\end{align}

It is easy to check that the exact solution is then given by:

\begin{align}
\phi(x_1, x_2) &= Ux_1, \\
\psi(x_1, x_2) &= -\frac{U}{\varepsilon}x_1 + \frac{U^2}{2\varepsilon^2}, \\
n(x_1, x_2) &= 1, \quad \text{in } \bar{\Omega}.
\end{align}

Let us note that here the errors between the exact and the numerical solutions are of the order of the computer precision even if the mesh size is not small. Then, we are here more interested with the ellipticity condition (which remains to the subsonic condition)
Numerical solution of Euler-Poisson system

Case $\gamma = 1$

a) Electron density
b) Velocity potential
c) Electrostatic potential

Case $\gamma = 5/3$

c) Electron density
d) Velocity potential
c) Electrostatic potential

Figure 2. Errors of the electron density, the velocity potential and the electrostatic potential as a function of the mesh size for $n_0^1 \equiv 1$.

and the current-voltage characteristics. Since the electron current density $J$ is given by $J = -n\nabla \psi$, using (3.7)-(3.8), we have:

$$J = \left( \frac{U}{\varepsilon}, 0 \right),$$

which is in agreement with the result obtain by Degond and Markowich for the one-dimensional case in [15].

Moreover, since $|\nabla \psi| = |U|/\varepsilon$, by (2.5) the ellipticity condition for the system is given by:

$$|U| < \sqrt{\varepsilon P'(n)}.$$

This gives respectively in the case $\gamma = 1$ and $\gamma = 5/3$:

$$|U| < \sqrt{\varepsilon} \quad \text{and} \quad |U| < \sqrt{(5\varepsilon)/3}.$$
values of $U$ for which we are able to obtain the current density is more or less large in function of the value of $\varepsilon$.

Let us choose as initialization $n^0(x_1, x_2) = 1/2$. The iterations are stopped when the relative $L^2$-error between two following iterations is smaller than $10^{-3}$. In Figure 3 we show the obtained current-voltage characteristics for different values of $\varepsilon$: $\varepsilon = 1$ and $\varepsilon = 0.1$ (which give respectively $\sqrt{\varepsilon} = 1$ and $\sqrt{\varepsilon} \approx 0.31$). We only show results obtained by the VF4-scheme since they are exactly the same for the DE-scheme. It is clear that (3.9) is verified.

**Case $\gamma = 1$**

a) Case $\varepsilon = 1$, $-0.9 \leq U \leq 0.9$

b) Case $\varepsilon = 0.1$, $-0.3 \leq U \leq 0.3$

**Case $\gamma = 5/3$**

c) Case $\varepsilon = 1$, $-1.2 \leq U \leq 1.2$

d) Case $\varepsilon = 0.1$, $-0.39 \leq U \leq 0.39$

**Figure 3.** Current-voltage characteristics for the second test case for $\varepsilon = 1$ and $\varepsilon = 0, 1$.

### 3.2. Case of a ballistic diode.

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. Here we want to compute the numerical solution of the system (2.1)-(2.3) with the doping profile

$$C(x) = \begin{cases} 
10^{-3}, & \text{if } (x_1, x_2) \in S = [1/6, 5/6] \times [0, 1], \\
1, & \text{else}.
\end{cases}$$
We consider the following boundary conditions for the electrostatic potential:

\begin{equation}
\phi^m = 0, \quad \text{on } \Gamma_{D,l} \quad \text{and} \quad \phi^m = U, \quad \text{on } \Gamma_{D,r}, \quad m \geq 0.
\end{equation}

Here U is a given applied voltage. Let us first consider the following boundary conditions on the velocity potential:

\begin{equation}
\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.
\end{equation}

For different values of \( \gamma \), \( U \) and \( \varepsilon \), the numerical solutions of the electron density, velocity potential and electrostatic potential are calculated. Note that the smallness condition on \( \varepsilon \), for boundary conditions independent of \( \varepsilon \) (see [30]), which ensures the strict ellipticity of the system, appears clearly in the numerical simulation. Indeed, when \( \varepsilon \) 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 \( |\nabla \psi_K|^2 \) in the formula (2.16), the condition \( n > 0 \) is not numerically satisfied and the matrix involved in the computation of \( \psi^m \) becomes singular. A numerical example in this case is given in Figure 4 (the computation is stopped after 4 iterations). We use the VF4-scheme to obtain a), b) and c), and the DE-scheme for d), e) and f).

In the case \( \gamma = 5/3 \), due to the definition of the inverse function of \( H \), \( U \) should satisfy \( U > -5/2 \). Indeed, for \( \varepsilon \) small enough, \( n_K^{m+1} \) is nearly given by \( H^{-1}(\phi_K^m) \) according to (2.16). If \( \phi_K^m \leq -5/2 \), then \( H^{-1}(\phi_K^m) = 0 \) and \( n_K^{m+1} \approx 0 \), so that the matrix involved in the computation of \( \psi^{m+1} \) becomes singular.

Note that the usual boundary conditions used for a ballistic diode are on \( \phi \) and \( n \) instead of \( \psi \) and in general we choose \( n = n_D = C(x) = 1 \) on \( \Gamma_D \) (see Remark 2.1). Since
$H(1) = 0$ by definition, from (2.10) we deduce the following boundary conditions on $\psi$:

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

(3.12)

For such boundary conditions, the ellipticity condition depends on the ratio of $U$ and $\sqrt{\varepsilon}$ and not only on $\varepsilon$. 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 5 we show the obtained solution for $\varepsilon = 0.6$ and $U = 0.1$. We require an accuracy of order $10^{-7}$ in $L^\infty(\Omega)$ norm for stopping the iterations (the iteration number is 8). We only show the results for the DE-scheme since they are similar to the ones obtained with the VF4-scheme.

Let us now consider the current-voltage characteristics for the boundary conditions (3.10) and (3.12). By definition of $\Gamma_N$, the second coordinate of the electron current density is vanishing. Then, the problem is 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 $\psi$, the ellipticity condition is satisfied when $|U|/\sqrt{\varepsilon}$ is stricly 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 6. The required accuracy in $L^\infty(\Omega)$ norm for stopping the iterations is $10^{-7}$. Here we still only present the results for the DE-scheme.
a) Case $\varepsilon = 1$, $-0.83 \leq U \leq 0.83$  b) Case $\varepsilon = 0.6$, $-0.66 \leq U \leq 0.66$

**Figure 6.** Current-voltage characteristics for different values of $\varepsilon$ when we consider boundary conditions on $\psi$ which depend on $\varepsilon$.

### 3.3. Bipolar case

Recall that in this case the system reads as follows

\begin{align}
-\text{div}(p\nabla \psi_p) &= 0, \\
H(p) + \frac{1}{2}|\nabla \psi_p|^2 &= -\phi + \psi_p, \\
-\text{div}(n\nabla \psi_n) &= 0, \\
H(n) + \frac{\varepsilon}{2}|\nabla \psi_n|^2 &= \phi + \varepsilon \psi_n, \\
\Delta \phi &= n - p - C, \quad \text{on } \Omega.
\end{align}

Let us define the initial hole density $p^0 = p^0(x)$ and the initial electron density $n^0 = n^0(x)$ by:

\begin{align*}
p^0(x) &= \begin{cases} 1/2, & \text{if } (x_1, x_2) \in [1/3, 2/3] \times [0, 1], \\ 1, & \text{else,} \end{cases} \\
n^0(x) &= \begin{cases} 1/4, & \text{if } (x_1, x_2) \in [1/3, 2/3] \times [0, 1], \\ 1, & \text{else.} \end{cases}
\end{align*}

For simplicity we take a vanishing doping profile $C \equiv 0$ and supplement the system (3.13)-(3.17) with the boundary conditions (3.10) for $\phi^m$, $m \geq 0$ and the following Dirichlet boundary conditions for $\psi_p^m$ and $\psi_n^m$, $m \geq 0$:

\begin{equation}
\psi_p^m = \psi_n^m = 0, \quad \text{on } \Gamma_{D,l} \quad \text{and} \quad \psi_p^m = U, \quad \psi_n^m = -U, \quad \text{on } \Gamma_{D,r}.
\end{equation}

Remark that the formula for computing the hole density $p^{m+1}$ is

\begin{equation}
p_K^{m+1} = H^{-1}\left(-\phi_K^m + \psi_p^m + \frac{1}{2}|\nabla \psi_p^m|^2\right), \quad K \in T \text{ or } M, \quad m \geq 0.
\end{equation}

In this subsection the smallness condition on $\varepsilon$ is still needed because of the same reason as in the unipolar case. The common value of $\varepsilon$ is $\varepsilon = 10^{-2}$. In Fig 7 and Fig. 9 the iteration is stopped when the maximum of $p^{m+1} - p^m$ and $n^{m+1} - n^m$ is of order $10^{-8}$ in $L^\infty(\Omega)$ norm (respectively after 5 and 9 iterations). For $\gamma = 1$, the numerical solutions of the electron density, hole density and hole velocity potential are given in Fig. 7 and Fig. 8, in which the sub-figures a), b) and c) are obtained with the VF4-scheme and d), e)
and f) with the DE-scheme. In the computation, we need also that the value of $|U|$ to be small. An example for large $|U|$ ($U = 1$) is given in Fig. 8 (for 5 iterations), from which we see that the hole density is near zero, so that the matrix involved in the computation of $\psi_p$ is almost singular. However, the computation of the electron density and electron velocity potential can still be carried out, due to the smallness value of $\varepsilon$. Finally, for $\gamma = 5/3$, the numerical solutions of the hole density and electron density are shown in Fig. 9, in which the subFigures a) and b) are obtained with the VF4-scheme and c) and d) with the DE-scheme (here the iteration number equals 9).

**Figure 7.** Case $\gamma = 1$, $U = 10^{-1}$, $\varepsilon = 10^{-2}$.

### 4. Conclusion

In this paper, we propose two kinds of finite volume schemes for the numerical approximation of the steady-state Euler-Poisson system for potential flows. Both schemes give similar results for different test cases with similar times of computation. They permit us to show the importance of the smallness of $\varepsilon$ and the boundary data for the ellipticity of the system.

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.
Figure 8. Case $\gamma = 1$, $U = 1$, $\varepsilon = 10^{-2}$.

References


Figure 9. Case $\gamma = 5/3$, $U = 10^{-1}$, $\varepsilon = 10^{-2}$. 


