Asymptotic behavior of a finite volume scheme for the transient drift-diffusion model

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In this paper, we propose a finite volume discretization for multidimensional nonlinear drift-diffusion system. Such a system arises in semi-conductors modeling and is composed of two parabolic equations and an elliptic one. We prove that the numerical solution converges to a steady state when time goes to infinity. Several numerical tests show the efficiency of the method.

Keywords: Drift-diffusion system, thermal equilibrium, boundary problem, finite volume scheme.
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1. Introduction

In the modeling of semi-conductor devices, there exists a hierarchy of models ranging from the kinetic transport equations to the drift-diffusion equations, see (23). In semi-conductor simulations, the drift-diffusion system is the most widely used because it displays both computational efficiency and physical consistency. This system consists of two continuity equations for the electron density $N := N(t,x)$ and the hole density $P := P(t,x)$ and a Poisson equation for the electrostatic potential $V := V(t,x)$ for $t \in \mathbb{R}^+$ and $x \in \mathbb{R}^d$.

More precisely, let $\Omega \subset \mathbb{R}^d$ ($d \geqslant 1$) be an open and bounded domain such that Ω is polygonal or polyhedral and we set $\Gamma = \partial\Omega$. For $T > 0$, we denote by $\Omega_T = (0,T) \times \Omega$ and $\Gamma_T = (0,T) \times \Gamma$. Then, setting all physical parameters equal to 1, the drift-diffusion system for a bipolar semiconductor reads

$$\begin{cases} \dfrac{\partial N}{\partial t} - \operatorname{div}(\nabla r(N) - N\nabla V) = 0, \quad (t,x) \in \Omega_T, \\ \\ \dfrac{\partial P}{\partial t} - \operatorname{div}(\nabla r(P) + P\nabla V) = 0, \quad (t,x) \in \Omega_T, \\ \\ \Delta V = N - P - C, \quad (t,x) \in \Omega_T, \end{cases} \tag{1.1}$$

where $C \in L^\infty(\Omega)$ is the prescribed doping profile characterizing the device under consideration

$$|C(x)| \leqslant \overline{C}, \qquad x \in \Omega. \tag{1.2}$$

The usual considerations on which the isentropic hydrodynamic model are based suggest a pressure of the form

$$r(s) = s^\alpha, \quad \alpha > 1.$$

The linear case, where $\alpha = 1$, corresponds to the isothermal model. In the general case, we will assume that $r \in \mathscr{C}^1(\mathbb{R}), \quad r(0) = r'(0) = 0$, with $r'(s) \geqslant c_0 s^{\alpha-1}$.

Equations (1.1) are supplemented with initial data at time $t = 0$

$$N(0,x) = N^0(x), \quad P(0,x) = P^0(x), \quad x \in \Omega, \tag{1.3}$$

such that there exist two constants $0 \leqslant m \leqslant M$ satisfying

$$m \leqslant N^0(x), P^0(x) \leqslant M, \quad x \in \Omega. \tag{1.4}$$

Moreover, we will consider Dirichlet-Neumann boundary conditions. Indeed, the physically motivated boundary conditions are either Dirichlet boundary conditions on N, P, V or homogeneous Neumann boundary conditions on N, P and V. This means that the boundary Γ is split into two parts $\Gamma = \Gamma_D \cup \Gamma_N$ and, if we denote by ν the outward normal to Γ, that the boundary conditions read on the boundary Γ_D

$$\begin{cases} N(t,x) = N^D(x), \quad (t,x) \in (0,T) \times \Gamma_D, \\ P(t,x) = P^D(x), \quad (t,x) \in (0,T) \times \Gamma_D, \\ V(t,x) = V^D(x), \quad (t,x) \in (0,T) \times \Gamma_D \end{cases} \tag{1.5}$$

and homogeneous Neumann boundary conditions on Γ_N:

$$\nabla r(N) \cdot \nu = \nabla r(P) \cdot \nu = \nabla V \cdot \nu = 0 \text{ on } \Gamma_N. \tag{1.6}$$

We assume that the Dirichlet boundary conditions satisfy

$$m \leqslant N^D(x), P^D(x) \leqslant M, \quad x \in \Gamma_D. \tag{1.7}$$

On the one hand, the existence of solutions to the system (1.1)-(1.6) has been proven under natural assumptions. In some situations, the uniqueness of solutions is also obtained, see (3; 13; 15; 17; 20). On the other hand, a lot of numerical algorithms for solving the drift-diffusion system, in the stationary case as well as in the transient case, have already been proposed. It started with 1-D finite difference methods and the so-called Scharfetter-Gummel scheme (26). In the linear pressure case ($r(s) = s$), finite element methods (1; 8; 7; 9; 10; 16; 25), mixed exponential fitting finite element methods (4) have also been successfully developed. The extension of the mixed exponential fitting finite element methods to the case of nonlinear pressures ($r(s) = s^\alpha$) has been considered in (2; 18) and (21) where numerical results are given in 1-D and 2-D respectively. The convergence of finite volume schemes in the nonlinear case has been established in (6).

The large time behavior of the solutions to the nonlinear drift-diffusion model (1.1)-(1.6) has been studied in(19). It is proven that the solution to the transient system converges to a solution to the thermal equilibrium state as $t \to \infty$ if the boundary conditions (1.5) are in thermal equilibrium. The stationary drift-diffusion system reads

$$\begin{cases} -\operatorname{div}(\nabla r(N) - N\nabla V) = 0, \quad x \in \Omega, \\ -\operatorname{div}(\nabla r(P) + P\nabla V) = 0, \quad x \in \Omega, \\ \Delta V = N - P - C, \quad x \in \Omega, \end{cases} \tag{1.8}$$

with the boundary conditions (1.5)-(1.6). The thermal equilibrium is a steady-state for which electron and hole currents ($\nabla r(N) - N\nabla V$ and $\nabla r(P) + P\nabla V$) vanish. The existence of a thermal equilibrium has been proven in (24). Let us introduce the enthalpy function h defined by

$$h(s) = \int_1^s \frac{r'(\tau)}{\tau}\, d\tau \tag{1.9}$$

and the generalized inverse g of h, defined by

$$g(s) = \begin{cases} h^{-1}(s) & \text{if } h(0^+) < s < \infty, \\ 0 & \text{if } s \leqslant h(0^+), \end{cases}$$

where we have implicitly assumed that $h(+\infty) = \infty$. If the boundary conditions satisfy $N^D, P^D > 0$ and

$$h(N^D) - V^D = \alpha_N \text{ and } h(P^D) + V^D = \alpha_P \text{ on } \Gamma_D,$$

the thermal equilibrium is defined by

$$N(x) = g(\alpha_N + V(x)), \quad P(x) = g(\alpha_P - V(x)), \quad x \in \Omega, \tag{1.10}$$

whereas V satisfies the following semi-linear elliptic problem

$$\begin{aligned} &\Delta V = g(\alpha_N + V) - g(\alpha_P - V) - C, \quad \text{in } \Omega, \\ &V(x) = V^D(x) \text{ on } \Gamma_D, \quad \nabla V \cdot \nu = 0 \text{ on } \Gamma_N. \end{aligned} \tag{1.11}$$

In this paper we are concerned by the theoretical study of the large time behavior of the numerical solution given by a finite volume scheme for the transient drift-diffusion model (1.1)-(1.6) . This work is motivated by a very practical question. Indeed, in numerical analysis the numerical solution is classically proven to converge to the exact solution of the continuous model on a fixed time interval when the mesh size goes to zero. However, in engineering the numerical solution is often computed on a fixed mesh where the final time is increasing and goes to infinity. Thus, in such a situation, it becomes crucial to study the stability and consistency of the numerical solution in the long time asymptotic limit. Moreover in engineering numerical solutions are often performed to find stationary solution, then the question of consistency of the computed solution with respect to the exact one is usually not known.

This article is the first step of a research program in numerical analysis on the long time asymptotic behavior of discrete solutions (spectral methods for Boltzmann's equation, finite volume for 2-D Navier-Stokes equations, etc). Here, we focus on a drift-diffusion model for semi-conductors when the thermal equilibrium holds at the boundary.

We first study the stationary case and propose a finite volume scheme for the steady state problem. On the one hand, we prove existence and uniqueness of a numerical solution. On the other hand, we establish *a priori* estimates which will lead to the convergence of the numerical solution to the exact solution of the steady state problem. The second part is devoted to the evolution problem (1.1)-(1.6). We construct a new finite volume scheme and rigorously prove that the numerical solution converges to the solution of the discrete steady state problem given in the first part. The proof is based on the control of the discrete energy dissipation.

2. Numerical scheme and main results

In this section, we present the finite volume schemes for the thermal equilibrium (1.11), with (1.10), and for the time evolution drift-diffusion system (1.1)-(1.6). Then we give the main results of the paper.

We first define the space discretization of Ω. An admissible mesh of Ω is given by a family $\mathcal{T}$ of control volumes (open and convex polygons in 2-D, polyhedra in 3-D), a family $\mathcal{E}$ of edges in 2-D (faces in 3-D) and a family of points $(x_K)_{K\in\mathcal{T}}$ which satisfy Definition 5.1 in (12). It implies that the straight line between two neighboring centers of cells (x_K, x_L) is orthogonal to the edge $\sigma = K|L$. In the set of edges $\mathcal{E}$, we distinguish the interior edges $\sigma \in \mathcal{E}_{int}$ and the boundary edges $\sigma \in \mathcal{E}_{ext}$. Because of the Dirichlet-Neumann boundary conditions, we split $\mathcal{E}_{ext}$ into $\mathcal{E}_{ext} = \mathcal{E}_{ext}^D \cup \mathcal{E}_{ext}^N$ where $\mathcal{E}_{ext}^D$ is the set of Dirichlet boundary edges and $\mathcal{E}_{ext}^N$ is the set of Neumann boundary edges. For a control volume $K \in \mathcal{T}$, we denote by $\mathcal{E}_K$ the set of its edges, $\mathcal{E}_{int,K}$ the set of its interior edges, $\mathcal{E}_{ext,K}^D$ the set of edges of K included in Γ_D and $\mathcal{E}_{ext,K}^N$ the set of edges of K included in Γ_N.

In the sequel, we denote by d the distance in $\mathbb{R}^d$, m the measure in $\mathbb{R}^d$ or $\mathbb{R}^{d-1}$. We assume that the family of mesh considered satisfies the following regularity constraint there exists $\xi > 0$ such that

$$\mathrm{d}(x_K, \sigma) \geqslant \xi\, \mathrm{d}(x_K, x_L), \quad \text{for } K \in \mathcal{T}, \text{ for } \sigma \in \mathcal{E}_{int,K}, \ \sigma = K|L. \tag{2.1}$$

The size of the mesh is defined by

$$\delta = \max_{K\in\mathcal{T}} (\mathrm{diam(K)})\,. \tag{2.2}$$

For all $\sigma \in \mathcal{E}$, we define the transmissibility coefficient:

$$\tau_\sigma = \begin{cases} \dfrac{\mathrm{m}(\sigma)}{\mathrm{d}(x_K, x_L)}, & \text{for } \sigma \in \mathcal{E}_{int},\ \sigma = K|L, \\[2mm] \dfrac{\mathrm{m}(\sigma)}{\mathrm{d}(x_K, \sigma)}, & \text{for } \sigma \in \mathcal{E}_{ext,K}. \end{cases}$$

Then, we set

$$G(x, V) = g(\alpha_N + V) - g(\alpha_P - V) - C(x).$$

The scheme corresponding to the equation (1.11) on the potential V reads

$$\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, DV_{K,\sigma} = \mathrm{m}(K)\, G_K(V_K), \quad K \in \mathcal{T}, \tag{2.3}$$

where the $(DV_{K,\sigma})_{\sigma\in\mathscr{E}}$ are defined by

$$DV_{K,\sigma} = \begin{cases} V_L - V_K, & \text{if } \sigma \in \mathscr{E}_{int},\ \sigma = K|L, \\ V_\sigma - V_K & \text{if } \sigma \in \mathscr{E}^D_{ext,K}, \\ 0 & \text{if } \sigma \in \mathscr{E}^N_{ext,K}. \end{cases} \tag{2.4}$$

with

$$V_\sigma = \frac{1}{\mathrm{m}(\sigma)} \int_\sigma V^D(x)\, dx, \quad \sigma \in \mathscr{E}^D_{ext} \tag{2.5}$$

and

$$G_K(V) = \frac{1}{\mathrm{m}(K)} \int_K G(x,V)\, dx, \quad K \in \mathscr{T}. \tag{2.6}$$

Then, we define an approximate solution V_δ associated to the discretization $\mathscr{T}$ (we recall that δ is the size of the discretization), which is a piecewise constant function :

$$V_\delta(x) = V_K \quad x \in K. \tag{2.7}$$

The scheme leads to a system of nonlinear algebraic equations. In the next section, we will establish existence and uniqueness of a solution to the scheme (2.3)-(2.7) and a priori estimates giving some compactness and allowing to pass to the limit on the sequence of approximate solutions $(V_\delta)_{\delta>0}$ towards the solution $V \in H^1(\Omega)\cap L^\infty(\Omega)$ of (1.11) coupled with boundary conditions (1.5)-(1.6). The result is the following:

THEOREM 2.1 Assume that the boundary conditions satisfy (1.7) with $m > 0$ and the thermal equilibrium on Γ_D

$$h(N^D) - V^D = \alpha_N, \text{ and } h(P^D) + V^D = \alpha_P,$$

where the enthalpy h is given by (1.9).

The scheme (2.3)-(2.6) admits an unique solution, which satisfies the following L^∞ estimate and discrete H^1 estimate : there exists a constant $\mathscr{C} > 0$, only depending on V^D and g, such that for all $K \in \mathscr{T}$

$$|V_K| \leqslant \mathscr{C} \qquad \forall K \in \mathscr{T}$$

$$\sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_K} \tau_\sigma |DV_{K,\sigma}|^2 \leqslant \mathscr{C}.$$

We may now define the finite volume approximation of the drift-diffusion system (1.1)-(1.6) in the case of mixed Dirichlet-Neumann boundary conditions. The scheme is almost the same as the one proposed in (5) except that the diffusion is approximated in a different way.

Let $(\mathscr{T},\mathscr{E},(x_K)_{K\in\mathscr{T}})$ be an admissible space discretization of Ω and let us define the time step Δt and $M_T = E(T/\Delta t)$ in order to get a space-time discretization of Ω_T. First of all, the initial and boundary conditions and the doping profile are approximated by their L^2 projections on control volumes or on edges:

$$N_K^0 = \frac{1}{\mathrm{m}(K)} \int_K N^0, \quad P_K^0 = \frac{1}{\mathrm{m}(K)} \int_K P^0, \quad C_K = \frac{1}{\mathrm{m}(K)} \int_K C, \quad K \in \mathscr{T}, \tag{2.8}$$

$$N_\sigma = \frac{1}{\mathrm{m}(\sigma)} \int_\sigma N^D, \quad P_\sigma = \frac{1}{\mathrm{m}(\sigma)} \int_\sigma P^D, \quad V_\sigma = \frac{1}{\mathrm{m}(\sigma)} \int_\sigma V^D, \quad \sigma \in \mathscr{E}^D_{ext} \tag{2.9}$$

For $n \in \mathbb{N}$, we construct the approximate potential V^n from the density (N^n, P^n) and then we update the density (N^{n+1}, P^{n+1}) at iteration $n+1$. On the one hand, for the potential V^n we use a classical finite volume scheme

$$\sum_{\sigma \in \mathscr{E}_K} \tau_\sigma \, DV^n_{K,\sigma} = \mathrm{m}(K)\,(N^n_K - P^n_K - C_K), \quad K \in \mathscr{T}, \tag{2.10}$$

where $DV^n_{K,\sigma}$ are defined analogously to (2.4). On the other hand, for the scheme on N^{n+1} and P^{n+1}, we choose a fully implicit discretization, with a standard upwinding for the convective fluxes and a new nonlinear approximation for the diffusive fluxes. Then the scheme for N^{n+1} and P^{n+1} is given for $K \in \mathscr{T}$ by

$$\begin{aligned} &\mathrm{m}(K)\,\frac{N^{n+1}_K - N^n_K}{\Delta t} \\ &- \sum_{\substack{\sigma \in \mathscr{E}_K,\\ \sigma = K|L}} \tau_\sigma \left[\min(N^{n+1}_K, N^{n+1}_L)\, Dh(N^{n+1})_{K,\sigma} - (DV^n_{K,\sigma})^+ N^{n+1}_K - (DV^n_{K,\sigma})^- N^{n+1}_L\right] \\ &- \sum_{\sigma \in \mathscr{E}^D_{ext,K}} \tau_\sigma \left[\min(N^{n+1}_K, N_\sigma)\, Dh(N^{n+1})_{K,\sigma} - (DV^n_{K,\sigma})^+ N^{n+1}_K - (DV^n_{K,\sigma})^- N_\sigma\right] = 0, \end{aligned} \tag{2.11}$$

$$\begin{aligned} &\mathrm{m}(K)\,\frac{P^{n+1}_K - P^n_K}{\Delta t} \\ &- \sum_{\substack{\sigma \in \mathscr{E}_K,\\ \sigma = K|L}} \tau_\sigma \left[\min(P^{n+1}_K, P^{n+1}_L)\, Dh(P^{n+1})_{K,\sigma} + (DV^n_{K,\sigma})^+ P^{n+1}_L + (DV^n_{K,\sigma})^- P^{n+1}_K\right] \\ &- \sum_{\sigma \in \mathscr{E}^D_{ext,K}} \tau_\sigma \left[\min(P^{n+1}_K, P_\sigma)\, Dh(P^{n+1})_{K,\sigma} + (DV^n_{K,\sigma})^+ P_\sigma + (DV^n_{K,\sigma})^- P^{n+1}_K\right] = 0, \end{aligned} \tag{2.12}$$

where $Dh(P)_{K,\sigma}$ is defined by

$$Dh(P)_{K,\sigma} = \begin{cases} h(P_L) - h(P_K), & \text{if } \sigma \in \mathscr{E}_{int},\ \sigma = K|L, \\ h(P_\sigma) - h(P_K) & \text{if } \sigma \in \mathscr{E}^D_{ext,K}, \\ 0 & \text{if } \sigma \in \mathscr{E}^N_{ext,K}. \end{cases} \tag{2.13}$$

and $u^+ = \max\{u, 0\}$ and $u^- = \min\{u, 0\}$.

Then, the approximate solution $(N_\delta, P_\delta, V_\delta)$ to the problem (1.1)-(1.6) associated to the discretization $\mathscr{D}$ is defined as piecewise constant function by

$$N_\delta(t,x) = N^{n+1}_K, \quad P_\delta(t,x) = P^{n+1}_K, \quad V_\delta(t,x) = V^{n+1}_K \quad (t,x) \in [T^n, t^{n+1}) \times K,$$

where $\{(N^n_K, P^n_K, V^n_K),\ K \in \mathscr{T},\ 0 \leqslant n \leqslant M_T + 1\}$ is the solution to the scheme (2.10)-(2.12). We may now state our main result.

THEOREM 2.2 We assume that there is no doping profile ($C = 0$), that the initial and boundary conditions satisfy (1.4) and (1.7) with $0 < m \leqslant M$ and that the following condition on the time step is fulfilled

$$\Delta t\, D < 1, \quad \text{where } D := \frac{M^2}{m}. \tag{2.14}$$

Then, the solution $(N_\delta, P_\delta, V_\delta)$ given by the finite volume scheme (2.8)-(2.12) satisfies for each $K \in \mathscr{T}$

$$\begin{array}{rcl} (N_K^n, P_K^n) & \to & (N_K, P_K) \text{ when } n \to \infty, \\ V_K^n & \to & V_K \text{ when } n \to \infty, \end{array}$$

where (N_K, P_K, V_K) is an approximation to the solution of the steady state equation (1.10)-(1.11) given by (2.3)-(2.4).

3. Drift diffusion system at thermal equilibrium

In this section, we study the numerical solution corresponding to the steady state (1.8) with boundary conditions (1.5), (1.6) in the thermal equilibrium case where the steady state rewrites (1.10)-(1.11).

3.1 *A semi-linear elliptic problem*

The aim of this section is to prove the convergence of a finite volume scheme for a semi-linear elliptic problem like (1.11). More precisely, we are interested in problems of the form:

$$\begin{cases} \Delta V = G(x,V), \quad x \in \Omega, \\ V = V^D \text{ on } \Gamma_D, \quad \nabla V \cdot \nu = 0 \text{ on } \Gamma_N. \end{cases} \tag{3.1}$$

The assumptions are the following:

$$G(x,V) \text{ is monotonically increasing with respect to } V \text{ for all } x \in \Omega. \tag{3.2}$$

There exist functions $G_1(V)$ and $G_2(V)$ monotically increasing such that

$$G_1(V) \leqslant G(x,V) \leqslant G_2(V) \text{ for all } x \in \Omega. \tag{3.3}$$

Moreover,

$$\text{there exist } V_1 \text{ and } V_2 \text{ satisfying } G_1(V_1) = 0 \text{ and } G_2(V_2) = 0. \tag{3.4}$$

Finally, the function V^D can be extended in the whole domain Ω and satisfies

$$V^D \in H^1(\Omega). \tag{3.5}$$

Under such assumptions, the problem (3.1) admits a unique solution $V \in H^1(\Omega) \cap L^\infty(\Omega)$. The proof of this result can be found in (22). For the thermal equilibrium (1.11), the assumptions (3.2), (3.3) are clearly satisfied. Indeed,

$$G(x,V) = g(\alpha_N + V) - g(\alpha_P - V) - C(x)$$

is monotonically increasing with respect to V. The functions G_1 and G_2 are the following

$$G_1(V) = g(\alpha_N + V) - g(\alpha_P - V) - \overline{C}, \quad G_2(V) = g(\alpha_N + V) - g(\alpha_P - V) - \underline{C},$$

where $\underline{C} = \inf_{x \in \Omega} C(x)$, $\overline{C} = \sup_{x \in \Omega} C(x)$ and since $\lim_{V \to -\infty} g(V) = 0$ and $\lim_{V \to +\infty} g(V) = +\infty$, we have

$$\lim_{V \to \pm\infty} G_1(V) = \pm\infty, \quad \lim_{V \to \pm\infty} G_2(V) = \pm\infty$$

therefore from the continuity of G we show that there exist V_1 and V_2 such that $G_1(V_1) = G_2(V_2) = 0$ and (3.4) is satisfied.

3.2 *Existence and uniqueness*

First we prove that if (V_K,V_σ) is solution to the scheme (2.3)-(2.6) exists, it satisfies an L^∞-estimate.

LEMMA 3.1 We assume that (3.2), (3.3) , (3.4) and (3.5) are satisfied. Let us set

$$\widetilde{\mathrm{V}} = \max\{V_1, \sup_{\Gamma_D} V^D\}, \quad \underset{\sim}{\mathrm{V}} = \min\{V_2, \inf_{\Gamma_D} V^D\}. \tag{3.6}$$

If the scheme (2.3)-(2.6) admits a solution, then it satisfies the following L^∞ estimate :

$$\underset{\sim}{\mathrm{V}} \leqslant V_K \leqslant \widetilde{\mathrm{V}}, \quad \forall K \in \mathscr{T}. \tag{3.7}$$

Proof. The definition (3.6), combined with the monotonicity of G_1 and G_2 and with (3.3) lead to

$$G_1(\widetilde{\mathrm{V}}) \geqslant G_1(V_1) = 0 \quad \text{and} \quad G_2(\underset{\sim}{\mathrm{V}}) \leqslant G_2(V_2) = 0.$$

Then, we define $\widetilde{\mathrm{V}}_K = \widetilde{\mathrm{V}}$ for $K \in \mathscr{T}$ and $\widetilde{\mathrm{V}}_\sigma = \widetilde{\mathrm{V}}$ for $\sigma \in \mathscr{E}^D_{ext}$, and $\widetilde{\mathrm{W}}$ by

$$\widetilde{\mathrm{W}} = \begin{cases} \widetilde{\mathrm{W}}_K = V_K - \widetilde{\mathrm{V}}_K, & \text{for } K \in \mathscr{T}, \\ \widetilde{\mathrm{W}}_\sigma = V_\sigma - \widetilde{\mathrm{V}}_\sigma, & \text{for } \sigma \in \mathscr{E}^D_{ext}. \end{cases}$$

From the definitions of G_1, (3.3) and $\widetilde{\mathrm{V}}$, it follows that for $K \in \mathscr{T}$

$$\sum_{\sigma\in\mathscr{E}_K} \tau_\sigma \, d\widetilde{\mathrm{V}}_{K,\sigma} - \mathrm{m}(K)\, G_K(\widetilde{\mathrm{V}}_K) \leqslant 0 - \mathrm{m}(K)\, G_1(\widetilde{\mathrm{V}}_K) \leqslant -\mathrm{m}(K)\, G_1(V_1) = 0$$

and using that V is a solution to (2.3)-(2.6), it yields for all $K \in \mathscr{T}$

$$\sum_{\sigma\in\mathscr{E}_K} \tau_\sigma \, d\widetilde{\mathrm{W}}_{K,\sigma} \geqslant \mathrm{m}(K) \Big(G_K(V_K) - G_K(\widetilde{\mathrm{V}}_K) \Big). \tag{3.8}$$

On the one hand, using the definition of $\widetilde{\mathrm{V}}$ (3.6), we know that $\widetilde{\mathrm{W}}_\sigma \leqslant 0$ for all $\sigma \in \mathscr{E}^D_{ext}$.

On the other hand, we denote by $\widetilde{\mathrm{W}}_{K_0} = \max_{K\in\mathscr{T}} \widetilde{\mathrm{W}}_K$ and assume that

$$\widetilde{\mathrm{W}}_{K_0} = V_{K_0} - \widetilde{\mathrm{V}}_{K_0} > 0.$$

Then, writing (3.8) for $K = K_0$ and using that $G_K(V)$ is nondecreasing with respect to V, the right hand side is positive whereas the left hand side is negative. Therefore, we have shown that for all $K \in \mathscr{T}$, $\widetilde{\mathrm{W}}_K \leqslant 0$, hence the upper bound

$$V_K \leqslant \widetilde{\mathrm{V}}, \quad \forall K \in \mathscr{T}.$$

The lower bound is obtained by the same way. □

The result of existence and uniqueness of a solution to the numerical scheme (2.3)-(2.6) is a consequence of the L^∞-estimate (3.7) and comes from an application of Leray-Schauder fixed point theorem.

PROPOSITION 3.1 We assume that (3.2), (3.3), (3.4) and (3.5) are satisfied. Then, the numerical scheme (2.3)-(2.6) admits a unique solution $V = (V_K)_{K\in\mathscr{T}}$ which satisfies the L^∞-estimate (3.7).

Proof. We start by uniqueness and consider two solutions U^1 and U^2 to (2.3)-(2.6). Multiplying by $U^1_K - U^2_K$ and summing over $K \in \mathscr{T}$, it follows

$$\sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_K} \tau_\sigma \left[D(U^1 - U^2)_{K,\sigma} \right]^2 + \sum_{K\in\mathscr{T}} \mathrm{m}(K) \left[G_K(U^1_K) - G_K(U^2_K) \right] \left[U^1_K - U^2_K \right] = 0.$$

Since $G(x,V)$ is increasing with respect to V

$$\left[G_K(U_K^1)-G_K(U_K^2)\right]\,\left[U_K^1-U_K^2\right]\geqslant 0,\quad \forall K\in\mathscr{T};$$

we conclude that

$$\sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma\,\left[D(U^1-U^2)_{K,\sigma}\right]^2\leqslant 0$$

and since $(U^1-U^2)_\sigma=0$, for $\sigma\in\mathscr{E}_{ext}^D$, then $U^1=U^2$.

For the existence proof, we introduce the application $T\ :\ (V,\lambda)\to W$ where W is the solution to the linear system

$$\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma\,DW_{K,\sigma}\ =\ \lambda\,\mathrm{m}(K)\,G_K(V_K),\quad\forall\,K\in\mathscr{T},$$

with

$$W_\sigma=\frac{1}{\mathrm{m}(\sigma)}\int_\sigma\lambda\,V^D(x)\,d\gamma.$$

The operator T is a linear mapping from $\mathbb{R}^\theta\times[0,1]\to\mathbb{R}^\theta$, where θ is the number of control volumes, continuous and compact. Furthermore, it satisfies :

- $T(V,0)=0,$
- for all $(V,\lambda)\in\mathbb{R}^\theta\times[0,1]$ such that $T(V,\lambda)=V$, we have $\underset{\sim}{\mathrm{V}}\leqslant V_K\leqslant\widetilde{\mathrm{V}}$.

Thanks to the Leray-Schauder fixed point theorem, it follows that $T_1:V\mapsto T(V,1)$ admits a unique fixed point, which concludes the proof of Proposition 3.1. □

From the L^∞ bound, we can now establish a discrete H^1 estimate giving strong compactness on the approximation. Assume that $(u_\sigma)_{\sigma\in\mathscr{E}_{ext}^D}$ is given on the boundary Γ^D. For $u=(u_K)_{K\in\mathscr{T}}$, we define the L^2-norm and the H^1-seminorm as follows:

$$\begin{aligned}\|u\|_{0,\Omega}^2&=\sum_{K\in\mathscr{T}}\mathrm{m}(K)\,|u_K|^2\\ |u|_{1,\Omega}^2&=\sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}}\tau_\sigma\,|u_K-u_L|^2+\sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}_{ext,K}^D}\tau_\sigma\,|u_K-u_\sigma|^2.\end{aligned}$$

We recall the discrete Poincaré inequality:

LEMMA 3.2 Let Ω be an open convex bounded polygonal or polyhedral subset of $\mathbb{R}^d$ ($d=2$ or 3). Then, there exists $C_\Omega\in\mathbb{R}_+$ only depending on Ω such that, for all admissible mesh of Ω satisfying the regularity assumption (2.1), for all $(u_K)_{K\in\mathscr{T}}$ and $(u_\sigma)_{\sigma\in\mathscr{E}_{ext}^D}$ satisfying $u_\sigma=0$ for all $\sigma\in\mathscr{E}_{ext}^D$, we have

$$\|u\|_{0,\Omega}\ \leqslant\ \frac{C_\Omega\sqrt{d}}{\sqrt{\xi}}\,|u|_{1,\Omega}\tag{3.9}$$

Proof. We perform a similar proof as in (14). Let $\mathscr{T}$ be an admissible mesh and denote by $X(\mathscr{T})$ the set of functions from Ω to $\mathbb{R}$ which are constant over each control volume $K\in\mathscr{T}$ and which are zero on the set of edges $\sigma\subset\Gamma_D$. We consider $v\in X(\mathscr{T})$ and since the function v is piecewise constant and has a finite number of jumps (which corresponds to the number of edges), we get that $v\in BV(\Omega)$. Moreover in dimension d, the space of BV functions which are zero on the boundary Γ_D is continuously embedded in $L^{\frac{d}{d-1}}(\Omega)$ (11, Theorem 3.5). Then, there exists a constant $C_\Omega > 0$, depending only on Ω, such that

$$\int_\Omega |v(x)|^{\frac{d}{d-1}} dx \leqslant C_\Omega \left[BV_\Omega(v)\right]^{\frac{d}{d-1}},$$

where

$$BV_\Omega(v) = \sup\left\{\int_\Omega v(x)\,\mathrm{div}\varphi(x)dx, \quad \varphi \in C_o^\infty(\Omega), \quad |\varphi(x)| \leqslant 1, \quad \forall x \in \Omega\right\}.$$

Applying this latter result to our function $v \in X(\mathscr{T})$, we get

$$\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|v_K|^{\frac{d}{d-1}}\right)^{\frac{d-1}{d}} \leqslant C_\Omega\, BV_\Omega(v)$$

and since v is piecewise constant, for all $\varphi \in C_o^\infty(\Omega)$

$$\int_\Omega v(x)\,\mathrm{div}\varphi(x)dx = \sum_{K\in\mathscr{T}} v_K \int_K \mathrm{div}\varphi(x)dx.$$

Thus, applying the Green formula to the smooth and compactly supported function φ

$$\int_\Omega v(x)\,\mathrm{div}\varphi(x)dx = \sum_{K\in\mathscr{T}} v_K \sum_{\sigma\in\mathscr{E}_{int,K}} \int_\sigma \varphi(\gamma)\cdot \nu_{K,\sigma}\, d\gamma,$$

where $\nu_{K,\sigma}$ is the unit normal to the edge σ, oriented outwards K. Next, we perform a discrete integration by part

$$\begin{aligned}
\int_\Omega v(x)\mathrm{div}\varphi(x)dx &= \sum_{\substack{\sigma\in\mathscr{E}_{int},\\ \sigma=K|L}} (v_K - v_L) \int_\sigma \varphi(\gamma)\cdot\nu_{K,\sigma}\, d\gamma,\\
&\leqslant \sum_{\substack{\sigma\in\mathscr{E}_{int},\\ \sigma=K|L}} \mathrm{m}(\sigma)\,|v_K - v_L|\,||\varphi||_\infty,\\
&\leqslant \sum_{\substack{\sigma\in\mathscr{E}_{int},\\ \sigma=K|L}} \mathrm{m}(\sigma)\,|v_K - v_L|.
\end{aligned}$$

Hence, we get

$$\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|v_K|^{\frac{d}{d-1}}\right)^{\frac{d-1}{d}} \leqslant C_\Omega \sum_{\substack{\sigma\in\mathscr{E}_{int},\\ \sigma=K|L}} \mathrm{m}(\sigma)|v_K - v_L|.$$

Now, we take $v = |u|^{\frac{2(d-1)}{d}}$ and use that

$$\left| |u_K|^{\frac{2(d-1)}{d}} - |u_L|^{\frac{2(d-1)}{d}} \right| \leqslant \frac{2(d-1)}{d} \left(|u_K|^{\frac{d-2}{d}} + |u_L|^{\frac{d-2}{d}}\right) |u_K - u_L|.$$

Integrating by parts and applying the Cauchy-Schwarz inequality, it yields, thanks to (2.1),

$$\begin{aligned}
\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|u_K|^2\right)^{\frac{d-1}{d}} &\leqslant C_\Omega \sum_{K\in\mathscr{T}} \sum_{\substack{\sigma\in\mathscr{E}_{int,K}\\ \sigma=K|L}} \mathrm{m}(\sigma)|u_K|^{\frac{d-2}{d}}|u_K - u_L|\\
&\leqslant \frac{C_\Omega}{\sqrt{\xi}}\, |u|_{1,\Omega} \left(\sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_K} \mathrm{m}(\sigma)\mathrm{d}(x_K,\sigma)|u_K|^{\frac{2(d-2)}{d}}\right)^{1/2}.
\end{aligned}$$

Since $\sum_{\sigma\in\mathscr{E}_K} \mathrm{m}(\sigma)\,\mathrm{d}(x_K,\sigma) = d\,\mathrm{m}(K)$, this gives

$$\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|u_K|^2\right)^{\frac{d-1}{d}} \leqslant \frac{C_\Omega\sqrt{d}}{\sqrt{\xi}}\,|u|_{1,\Omega}\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|u_K|^{\frac{2(d-2)}{d}}\right)^{1/2}.$$

Finally using the Hölder inequality, we get

$$\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|u_K|^2\right)^{\frac{d-1}{d}} \leqslant \frac{C_\Omega\sqrt{d}}{\sqrt{\xi}}\,|u|_{1,\Omega}\left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)|u_K|^2\right)^{\frac{d-2}{2d}}$$

and then (3.9). □

The next lemma provides an L^2 estimate and an H^1 estimate on the numerical solution to the scheme (2.3)-(2.6).

LEMMA 3.3 We assume that (3.2), (3.3) , (3.4) and (3.5) are satisfied. Then, there exists $\mathscr{C} > 0$ such that the solution $(V_K)_{K\in\mathscr{T}}$, $(V_\sigma)_{\sigma\in\mathscr{E}^D_{ext}}$ to the scheme (2.3)-(2.6) satisfies

$$\sum_{K\in\mathscr{T}} \mathrm{m}(K)\,|V_K|^2 + \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma\,|V_K-V_L|^2 + \sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma\,|V_K-V_\sigma|^2 \leqslant \mathscr{C}. \tag{3.10}$$

Proof. As $V^D\in H^1(\Omega)$, we can define $(V^D_K)_{K\in\mathscr{T}}$ and $(V^D_\sigma)_{\sigma\in\mathscr{E}^D_{ext}}$ by

$$\begin{aligned} V^D_K &= \frac{1}{\mathrm{m}(K)}\int_K V^D(x)\,dx, \quad \text{for } K\in\mathscr{T},\\ V^D_\sigma &= \frac{1}{\mathrm{m}(\sigma)}\int_\sigma V^D(x)\,dx, \quad \text{for } \sigma\in\mathscr{E}^D_{ext}. \end{aligned}$$

Multiplying the scheme by $[V_K - V^D_K]$ and summing over $K\in\mathscr{T}$, we get:

$$-\sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}_K} \tau_\sigma\,DV_{K,\sigma}\,[V_K-V^D_K] = -\sum_{K\in\mathscr{T}} \mathrm{m}(K)\,G_K(V_K)\,[V_K-V^D_K]. \tag{3.11}$$

On the one hand, we have the following lower bound for the left hand side:

$$\begin{aligned} -\sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}_K} \tau_\sigma\,DV_{K,\sigma}\,[V_K-V^D_K] &= \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma\,[V_K-V_L]\left([V_K-V_L]-[V^D_K-V^D_L]\right) +\\ &\quad \sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma\,[V_K-V_\sigma]\left([V_K-V_\sigma]-[V^D_K-V^D_\sigma]\right)\\ &\geqslant \frac{1}{2}|V|^2_{1,\Omega} - \frac{1}{2}|V^D|^2_{1,\Omega} \end{aligned} \tag{3.12}$$

On the other hand, applying successively the L^∞-estimate (3.7) and Young inequality with $\varepsilon>0$ on the right hand side of (3.11), there exists a constant $\mathscr{C}>0$ such that

$$\left|\mathrm{m}(K)\,G_K(V_K)\,[V_K-V^D_K]\right| \leqslant \mathscr{C}\left(\frac{\mathrm{m}(K)}{\varepsilon} + \varepsilon\,\mathrm{m}(K)\,[V_K-V^D_K]^2\right).$$

Therefore, summing over $K \in \mathscr{T}$ and applying the discrete Poincaré inequality (3.9), we get:

$$\begin{aligned}\sum_{K\in\mathscr{T}} \mathrm{m}(K)\,|G_K(V_K)|\,|V_K - V_K^D| \;&\leqslant\; \mathscr{C}\left(\frac{\mathrm{m}(\Omega)}{\varepsilon} + \varepsilon\|V - V^D\|_{0,\Omega}^2\right)\\ &\leqslant\; \mathscr{C}\left(\frac{\mathrm{m}(\Omega)}{\varepsilon} + \varepsilon\,|V - V^D|_{1,\Omega}^2\right),\\ &\leqslant\; \mathscr{C}\left(\frac{\mathrm{m}(\Omega)}{\varepsilon} + 2\,\varepsilon\,(|V|_{1,\Omega}^2 + |V^D|_{1,\Omega}^2)\right) \qquad (3.13)\end{aligned}$$

It remains to choose ε small enough to deduce (3.10) from (3.12) and (3.13). □

4. Asymptotic behavior of the time dependent approximate solution

4.1 *Classical a priori estimates*

We do not detail here the proof of the convergence of the scheme (2.8)-(2.12) when space and time steps go to 0. Indeed, this scheme is very close to the scheme studied in (5): the only difference is the discretization of the diffusive fluxes. Therefore the proof of the convergence of the scheme towards a weak solution of the problem (1.1)-(1.6) is similar to the proof done in(5). Let us recall the required hypotheses:

$(H1)$ $N^0, P^0 \in L^\infty(\Omega)$, $N^D, P^D \in L^2(\Omega_T)\cap H^1(\Omega_T)$ and $V^D \in L^\infty(\mathbb{R}^+;H^1(\Omega))$;

$(H2)$ there exist two constants m and M such that

$$0 < m < N^0, P^0 < M, \quad \text{in } \Omega, \quad \text{and } m < N^D, P^D < M, \quad \text{in } \Omega_T;$$

$(H3)$ $r \in C^2(\mathbb{R})$ is strictly increasing on $(0,+\infty)$;

$(H4)$ $C \in L^\infty(\Omega_T)$ with $\overline{C} = \|C\|_\infty$.

The result is the following. We insist on the *a priori* estimates which will be used in the proof of Theorem 2.2.

THEOREM 4.1 Let $(H1)-(H4)$ hold and $\mathscr{T}$ be an admissible mesh of Ω. Assume that the following stability condition is fulfilled

$$\Delta t\, D_T \;<\; 1, \quad \text{where } D_T := M\exp(\overline{C}\,T) + \overline{C}. \tag{4.1}$$

Then, there exists a unique approximate solution $(N_\delta, P_\delta, V_\delta)$ to the scheme (2.8)-(2.12), which satisfies for all $K \in \mathscr{T}$ and all $n = 0,1,...,M_T$,

$$m\exp(-\overline{C}\,T) \;\leqslant\; N_K^n,\, P_K^n \;\leqslant\; M\exp(\overline{C}\,T).$$

In particular, if $C = 0$, the maximum principle holds for N_δ and P_δ, *i.e.*;

$$m \;\leqslant\; N_K^n,\, P_K^n \;\leqslant M, \quad \forall (n,K) \in \mathbb{N}\times\mathscr{T}. \tag{4.2}$$

and

$$\|V^n\|_{1,\Omega}^2 \;=\; \|V^n\|_{0,\Omega}^2 + |V^n|_{1,\Omega}^2 \;\leqslant\; 4\,\mathrm{m}(\Omega)^2 M^2, \quad \forall n \in \mathbb{N}. \tag{4.3}$$

Moreover, the approximate solution $(N_\delta, P_\delta, V_\delta)$ converges to (N,P,V) as space and time steps go to 0, where (N,P,V) is a weak solution to (1.1)-(1.6).

4.2 *Preliminary results*

As in the continuous case, see (19), the study of the large time behavior of the scheme (2.8)-(2.12) is based on an energy estimate with the control of the energy dissipation.

First, let us recall some notations. We denote by (N_K, P_K, V_K) the solution to the discrete thermal equilibrium. This means that (V_K) is the solution to (2.3)-(2.7) and

$$N_K = g(\alpha_N + V_K), \quad \text{and } P_K = g(\alpha_P - V_K),$$

which is equivalent to

$$h(N_K) - V_K \;=\; \alpha_N, \quad h(P_K) + V_K \;=\; \alpha_P.$$

The solution to the time-dependent scheme (2.8)-(2.12) is denoted (N_K^n, P_K^n, V_K^n).

For the sequel, we need to define

$$H(s) = \int_1^s h(\tau)\, d\,\tau, \quad 0 \;\leqslant\; s$$

(with the convention $h(0) = h(0^+)$). Then we can introduce the discrete version of the deviation of the total energy (sum of the internal energies for the electron and hole densities and the energy due to the electrostatic potential) from the thermal equilibrium, see (19): for $n \geqslant 0$,

$$\begin{aligned} \mathscr{E}^n \quad := \quad & \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, [H(N_K^n) - H(N_K) - h(N_K)\,(N_K^n - N_K)] \\ & + \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, [H(P_K^n) - H(P_K) - h(P_K)\,(P_K^n - P_K)] \\ & + \frac{1}{2}\, |V^n - V|^2_{1,\Omega}. \end{aligned}$$

As H is a convex function, we have $\mathscr{E}^n \geqslant 0$ for $n \geqslant 0$. We also introduce the energy dissipation $\mathscr{I}(N^{n+1}, P^{n+1}, V^n)$:

$$\begin{aligned} \mathscr{I}(N^{n+1}, P^{n+1}, V^n) \quad := \quad & \sum_{\substack{\sigma\in\mathscr{E}_{int} \\ \sigma=K|L}} \tau_\sigma \min(N_K^{n+1}, N_L^{n+1}) \left[D\left(h(N^{n+1}) - V^n\right)_{K,\sigma}\right]^2 \\ & + \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}} \tau_\sigma \min(N_K^{n+1}, N_\sigma) \left[D\left(h(N^{n+1}) - V^n\right)_{K,\sigma}\right]^2 \\ & + \sum_{\substack{\sigma\in\mathscr{E}_{int} \\ \sigma=K|L}} \tau_\sigma \min(P_K^{n+1}, P_L^{n+1}) \left[D\left(h(P^{n+1}) + V^n\right)_{K,\sigma}\right]^2 \\ & + \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}} \tau_\sigma \min(P_K^{n+1}, P_\sigma) \left[D\left(h(P^{n+1}) + V^n\right)_{K,\sigma}\right]^2 \end{aligned}$$

The proof of Theorem 2.2 relies on the control of energy and energy dissipation given by the following Proposition.

PROPOSITION 4.2 Let $(H1)-(H4)$ hold and $\mathscr{T}$ be an admissible mesh of Ω. Then, for $n \geqslant 1$,

$$\mathscr{E}^{n+1} \;+\; \left(1 - \frac{M^2}{m}\Delta t\right)\; \Delta t\; \mathscr{I}(N^{n+1}, P^{n+1}, V^n) \;\leqslant\; \mathscr{E}^n. \tag{4.4}$$

The proof of Proposition 4.2 will be given later. First, we give a result to estimate the energy due to the elecrostatic potential.

LEMMA 4.1 Let $(H1)-(H4)$ hold and $\mathscr{T}$ be an admissible mesh of Ω. Then, for $n \geqslant 0$,

$$\frac{1}{2}|V^{n+1}-V|^2_{1,\Omega} - \frac{1}{2}|V^n-V|^2_{1,\Omega} \leqslant -\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(N_K^{n+1}-N_K^n-P_K^{n+1}+P_K^n\right)[V_K^n-V_K] + \frac{M^2}{m}\Delta t^2\,\mathscr{I}(N^{n+1},P^{n+1},V^n). \tag{4.5}$$

and

$$\frac{1}{2}|V^{n+1}-V^n|_{1,\Omega} \leqslant \frac{M^2}{m}\Delta t^2\,\mathscr{I}(N^{n+1},P^{n+1},V^n). \tag{4.6}$$

Proof. Substituting the discrete Poisson equation (2.10) at time t^{n+1} and t^n, we easily obtain for $K\in\mathscr{T}$

$$\sum_{\sigma\in\mathscr{E}_K}\tau_\sigma\left[DV^{n+1}_{K,\sigma}-DV^n_{K,\sigma}\right] = \mathrm{m}(K)\left(N_K^{n+1}-N_K^n-P_K^{n+1}+P_K^n\right). \tag{4.7}$$

Next, we multiply the latter equality by $-[V_K^n-V_K]$ and sum over $K\in\mathscr{T}$. Performing a discrete integration by part, we classically have

$$\begin{aligned}&\sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}}\tau_\sigma\left([V_L^{n+1}-V_K^{n+1}]-[V_L^n-V_K^n]\right)[D(V^n-V)_{K,\sigma}]\\ &+\sum_{K\in\mathscr{T}}\sum_{\sigma\in\mathscr{E}^D_{ext,K}}\tau_\sigma\left([V_\sigma-V_K^{n+1}]-[V_\sigma-V_K^n]\right)[D(V^n-V)_{K,\sigma}]\\ \leqslant\ &-\sum_{K\in\mathscr{T}}\mathrm{m}(K)\left(N_K^{n+1}-N_K^n-P_K^{n+1}+P_K^n\right)[V_K^n-V_K].\end{aligned}$$

Thus, using the following equality

$$[a-b]\,b = \frac{a^2}{2}-\frac{b^2}{2}-\frac{1}{2}[a-b]^2,$$

we take $a=D(V^{n+1}-V)_{K,\sigma}$, $b=D(V^n-V)_{K,\sigma}$ and set $W=V^{n+1}-V^n$, which give the following inequality

$$\begin{aligned}&\frac{1}{2}\left(|V^{n+1}-V|^2_{1,\Omega}-|V^n-V|^2_{1,\Omega}\right)-\frac{1}{2}|W|^2_{1,\Omega}\\ \leqslant\ &-\sum_{K\in\mathscr{T}}\mathrm{m}(K)\left(N_K^{n+1}-N_K^n-P_K^{n+1}+P_K^n\right)[V_K^n-V_K].\end{aligned} \tag{4.8}$$

Now, the main step consists in the control of the residual term $|W|^2_{1,\Omega}$. To this aim, we start again from (4.7), multiply it by $-W_K$ and sum over $K\in\mathscr{T}$. We get

$$|W|^2_{1,\Omega} = -\sum_{K\in\mathscr{T}}\mathrm{m}(K)\left(N_K^{n+1}-N_K^n-P_K^{n+1}+P_K^n\right)W_K \leqslant \Delta t\,[I_1+I_2+I_3+I_4],$$

where I_α, $\alpha\in\{1,..,4\}$ are obtained using the finite volume scheme (2.11), (2.12) for N^{n+1} and P^{n+1}. More precisely,

$$I_1 = \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}}\tau_\sigma\left|\min(N_K^{n+1},N_L^{n+1})\,Dh(N^{n+1})_{K,\sigma}-(DV^n_{K,\sigma})^+N_K^{n+1}-(DV^n_{K,\sigma})^-N_L^{n+1}\right|\,|DW_{K,\sigma}|$$

$$I_2 = \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \left|\min(N_K^{n+1}, N_\sigma)\, Dh(N^{n+1})_{K,\sigma} - (DV^n_{K,\sigma})^+ N_K^{n+1} - (DV^n_{K,\sigma})^- N_\sigma\right| |DW_{K,\sigma}|$$

$$I_3 = \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \left|\min(P_K^{n+1}, P_L^{n+1})\, Dh(P^{n+1})_{K,\sigma} + (DV^n_{K,\sigma})^+ P_L^{n+1} + (DV^n_{K,\sigma})^- P_K^{n+1}\right| |DW_{K,\sigma}|$$

$$I_4 = \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \left|\min(P_K^{n+1}, P_\sigma)\, Dh(P^{n+1})_{K,\sigma} + (DV^n_{K,\sigma})^+ P_\sigma + (DV^n_{K,\sigma})^- P_K^{n+1}\right| |DW_{K,\sigma}|.$$

On the one hand, using that h is a nondecreasing function the following estimate holds for $N = N_L^{n+1}$ and N_σ

$$\begin{aligned}\left|\min(N_K^{n+1}, N)\, Dh(N^{n+1})_{K,\sigma} - (DV^n_{K,\sigma})^+ N_K^{n+1} - (DV^n_{K,\sigma})^- N\right| \\ \leqslant \max(N_K^{n+1}, N) \left| d\left(h(N^{n+1}) - V^n\right)_{K,\sigma}\right|.\end{aligned}$$

Then, we easily check that

$$I_1 \leqslant \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \max(N_K^{n+1}, N_L^{n+1}) \left|D\left(h(N^{n+1}) - V^n\right)_{K,\sigma}\right| |DW_{K,\sigma}|$$

and

$$I_2 \leqslant \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \max(N_K^{n+1}, N_\sigma) \left|D\left(h(N^{n+1}) - V^n\right)_{K,\sigma}\right| |DW_{K,\sigma}|,$$

On the other hand, performing the same kind of computation, we also get

$$I_3 \leqslant \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \max(P_K^{n+1}, P_L^{n+1}) \left|D\left(h(P^{n+1}) + V^n\right)_{K,\sigma}\right| |DW_{K,\sigma}|$$

and

$$I_4 \leqslant \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \max(P_K^{n+1}, P_\sigma) \left|D\left(h(P^{n+1}) + V^n\right)_{K,\sigma}\right| |DW_{K,\sigma}|.$$

Then, applying the Cauchy-Schwarz inequality to the latter inequalities, it yields

$$|W|^2_{1,\Omega} \leqslant \frac{2M^2}{m} \Delta t^2\, \mathscr{I}(N^{n+1}, P^{n+1}, V^n),$$

and gathering the latter result with (4.8), it finally yields

$$\begin{aligned}\frac{1}{2}|V^{n+1} - V|^2_{1,\Omega} - \frac{1}{2}|V^n - V|^2_{1,\Omega} \quad \leqslant \quad & -\sum_{K\in\mathscr{T}} \mathrm{m}(K) \left(N_K^{n+1} - N_K^n - P_K^{n+1} + P_K^n\right) [V_K^n - V_K] \\ & + \frac{M^2}{m} \Delta t^2\, \mathscr{I}(N^{n+1}, P^{n+1}, V^n).\end{aligned}$$

which concludes the proof of Lemma 4.1. □

Next, we prove another entropy type inequality for the two densities N and P, which will be useful later.

LEMMA 4.2 Let $(H1)-(H4)$ hold and $\mathscr{T}$ be an admissible mesh of Ω. Then, for $n \geqslant 0$,

$$\begin{aligned}
&\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(N_K^{n+1}-N_K^n\right)\left[h(N_K^{n+1})-V_K^n-\alpha_N\right] \\
&\leqslant \ -\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \min(N_K^{n+1},N_L^{n+1})\left[D(h(N^{n+1})-V^n)_{K,\sigma}\right]^2 \\
&\quad -\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}^D} \tau_\sigma \min(N_K^{n+1},N_\sigma)\left[D(h(N^{n+1})-V^n)_{K,\sigma}\right]^2. \qquad (4.9)
\end{aligned}$$

and

$$\begin{aligned}
&\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(P_K^{n+1}-P_K^n\right)\left[h(P_K^{n+1})+V_K^n-\alpha_P\right] \\
&\leqslant \ -\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \min(P_K^{n+1},P_L^{n+1})\left[D(h(P^{n+1})+V^n)_{K,\sigma}\right]^2 \\
&\quad -\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}^D} \tau_\sigma \min(P_K^{n+1},P_\sigma)\left[D(h(P^{n+1})+V^n)_{K,\sigma}\right]^2.
\end{aligned}$$

Proof. First, we multiply the scheme (2.11) by $\Delta t\left[h(N_K^{n+1})-V_K^n-\alpha_N\right]$ and sum over $K\in\mathscr{T}$. Then, we obtain

$$T_1+T_2+T_3=0,$$

with

$$T_1 = \sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(N_K^{n+1}-N_K^n\right)\left[h(N_K^{n+1})-V_K^n-\alpha_N\right],$$

$$\begin{aligned}
T_2 = &-\Delta t \sum_{K\in\mathscr{T}} \sum_{\substack{\sigma\in\mathscr{E}_K\\ \sigma=K|L}} \tau_\sigma\left[\min(N_K^{n+1},N_L^{n+1})Dh(N^{n+1})_{K,\sigma}\right]\left[h(N_K^{n+1})-V_K^n-\alpha_N\right] \\
&-\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}^D} \tau_\sigma\left[\min(N_K^{n+1},N_\sigma)Dh(N^{n+1})_{K,\sigma}\right]\left[h(N_K^{n+1})-V_K^n-\alpha_N\right],
\end{aligned}$$

$$\begin{aligned}
T_3 = &+\Delta t \sum_{K\in\mathscr{T}} \sum_{\substack{\sigma\in\mathscr{E}_K\\ \sigma=K|L}} \tau_\sigma\left[(DV_{K,\sigma}^n)^+N_K^{n+1}+(DV_{K,\sigma}^n)^-N_L^{n+1}\right]\left[h(N_K^{n+1})-V_K^n-\alpha_N\right] \\
&+\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}^D} \tau_\sigma\left[(DV_{K,\sigma}^n)^+N_K^{n+1}+(DV_{K,\sigma}^n)^-N_\sigma\right]\left[h(N_K^{n+1})-V_K^n-\alpha_N\right].
\end{aligned}$$

Now, we perform a discrete integration by part (using the symmetry of τ_σ) and estimate the term T_2

$$\begin{aligned}
T_2 = &+\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \min(N_K^{n+1},N_L^{n+1})Dh(N^{n+1})_{K,\sigma}\left[D(h(N^{n+1})-V^n)_{K,\sigma}\right] \\
&+\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}_{ext,K}^D} \tau_\sigma \min(N_K^{n+1},N_\sigma)Dh(N^{n+1})_{K,\sigma}\left[D(h(N^{n+1})-V^n)_{K,\sigma}\right]
\end{aligned}$$

and next the term T_3

$$T_3 \;=\; -\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \left[(DV^n_{K,\sigma})^+ N^{n+1}_K - (DV^n_{K,\sigma})^- N^{n+1}_L\right] \left[D(h(N^{n+1})-V^n)_{K,\sigma}\right] \\ -\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \left[(DV^n_{K,\sigma})^+ N^{n+1}_K - (DV^n_{K,\sigma})^- N_\sigma\right] \left[D(h(N^{n+1})-V^n)_{K,\sigma}\right].$$

Then, we introduce the term $T_3^\star$

$$T_3^\star \;=\; -\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \min(N^{n+1}_K, N^{n+1}_L)\, DV^n_{K,\sigma} \left[D(h(N^{n+1})-V^n)_{K,\sigma}\right] \\ -\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \min(N^{n+1}_K, N_\sigma)\, DV^n_{K,\sigma} \left[D(h(N^{n+1})-V^n)_{K,\sigma}\right]$$

and want to prove that $T_3 \geqslant T_3^\star$.

Let us estimate the difference $T_3 - T_3^\star$. On the one hand, using that the function h is nondecreasing, we show that for $N = N^{n+1}_L, N_\sigma$

$$(DV^n_{K,\sigma})^+ \left[h(N^{n+1}_K) - h(N)\right] \left[N^{n+1}_K - \min(N^{n+1}_K, N)\right] \geqslant 0$$

and for $N = N^{n+1}_L, N_\sigma$

$$(DV^n_{K,\sigma})^- \left[h(N^{n+1}_K) - h(N)\right] \left[N - \min(N^{n+1}_K, N)\right] \geqslant 0.$$

On the other hand, using the property of $u \to u^\pm$, we have for $N = N^{n+1}_L, N_\sigma$

$$(DV^n_{K,\sigma})^+ DV^n_{K,\sigma} \left[N_K - \min(N^{n+1}_K, N)\right] \geqslant 0$$

and for $N = N^{n+1}_L, N_\sigma$

$$(DV^n_{K,\sigma})^- DV^n_{K,\sigma} \left[N - \min(N^{n+1}_K, N)\right] \geqslant 0.$$

Thus, from these classical inequalities we easily conclude that $T_3 - T_3^\star \geqslant 0$.

Finally, it follows that

$$T_1 \;\leqslant\; -T_2 - T_3^\star.$$

More precisely, we have

$$\sum_{K\in\mathscr{T}} \mathrm{m}(K) \left(N^{n+1}_K - N^n_K\right) \left[h(N^{n+1}_K) - V^n_K - \alpha_N\right] \\ \leqslant\; -\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \min(N^{n+1}_K, N^{n+1}_L) \left[D(h(N^{n+1})-V^n)_{K,\sigma}\right]^2 \\ -\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \min(N^{n+1}_K, N_\sigma) \left[D(h(N^{n+1})-V^n)_{K,\sigma}\right]^2.$$

Using the scheme (2.12), we also prove in the same way that

$$\begin{aligned}
&\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(P_K^{n+1}-P_K^n\right)\left[h(P_K^{n+1})+V_K^n-\alpha_P\right] \\
&\leqslant \quad -\Delta t \sum_{\substack{\sigma\in\mathscr{E}_{int}\\ \sigma=K|L}} \tau_\sigma \min(P_K^{n+1},P_L^{n+1})\left[D(h(P^{n+1})+V^n)_{K,\sigma}\right]^2 \\
&\qquad -\Delta t \sum_{K\in\mathscr{T}} \sum_{\sigma\in\mathscr{E}^D_{ext,K}} \tau_\sigma \min(P_K^{n+1},P_\sigma)\left[D(h(P^{n+1})+V^n)_{K,\sigma}\right]^2.
\end{aligned}$$

□

Now, we give the proof of Proposition 4.2. *Proof.* We introduce the nonnegative and convex functions Φ_1 and Φ_2

$$\Phi_1(x) := H(x) - H(N_K) - h(N_K)\,[x-N_K]$$

and

$$\Phi_2(x) := H(x) - H(P_K) - h(P_K)\,[x-P_K]$$

such that

$$\Phi_1'(x) = h(x)-h(N_K),\ \Phi_2'(x) = h(x)-h(P_K),\ \text{ and }\ \Phi_1''(x) = \Phi_2''(x) = h'(x) \geqslant 0.$$

Therefore, using the convexity of H, it yields

$$\begin{aligned}
&\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left[\Phi_1(N_K^{n+1})-\Phi_1(N_K^n)\right] \\
=\ &\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left[H(N_K^{n+1})-H(N_K^n)-h(N_K)\left(N_K^{n+1}-N_K^n\right)\right] \\
\leqslant\ &\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(N_K^{n+1}-N_K^n\right)\left[h(N_K^{n+1})-h(N_K)\right]
\end{aligned}\tag{4.10}$$

and

$$\begin{aligned}
&\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left[\Phi_2(P_K^{n+1})-\Phi_2(P_K^n)\right] \\
&\qquad\leqslant \sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(P_K^{n+1}-P_K^n\right)\left[h(P_K^{n+1})-h(P_K)\right].
\end{aligned}\tag{4.11}$$

Now, we apply the result of Lemma 4.1, *i.e.*;

$$\begin{aligned}
&\frac{1}{2}|V^{n+1}-V|^2_{1,\Omega} - \frac{1}{2}|V^n-V|^2_{1,\Omega} \\
\leqslant\ &\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left[\left[N_K^{n+1}-N_K^n\right]-\left[P_K^{n+1}-P_K^n\right]\right][V_K-V_K^n] \\
&+\frac{M^2}{m}\,\Delta t^2\,\mathscr{I}(N^{n+1},P^{n+1},V^n).
\end{aligned}$$

Adding the two latter inequalities and using that $h(N_K)-V_K=\alpha_N$ and $h(P_K)+V_K=\alpha_P$, it yields

$$\begin{aligned}
\mathscr{E}^{n+1}-\mathscr{E}^n \quad\leqslant\quad &\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(N_K^{n+1}-N_K^n\right)\left[h(N_K^{n+1})-V_K^n-\alpha_N\right]. \\
&+\sum_{K\in\mathscr{T}} \mathrm{m}(K)\left(P_K^{n+1}-P_K^n\right)\left[h(P_K^{n+1})+V_K^n-\alpha_P\right] \\
&+\frac{M^2}{m}\,\Delta t^2\,\mathscr{I}(N^{n+1},P^{n+1},V^n).
\end{aligned}$$

Finally a straighforward application of Lemma 4.2 gives an upper bound of the right hand side

$$\mathscr{E}^{n+1} - \mathscr{E}^{n} \quad \leqslant \quad -\Delta t \left(1 - \frac{M^2}{m}\Delta t\right) \mathscr{I}(N^{n+1}, P^{n+1}, V^n).$$

Thus, under a smallness condition on the time step $\Delta t < m/M^2$ the total energy is decreasing with respect to n. □

4.3 *Proof of Theorem 2.2*

Now we are ready to achieve the proof of Theorem 2.2. On the one hand, from the convexity of the functional H, we show that $\mathscr{E}^{n+1}$ is nonnegative and then applying Proposition 4.2, it yields

$$0 \leqslant \mathscr{E}^{n+1} + \left(1 - \frac{M^2}{m}\Delta t\right) \sum_{k=0}^{n} \Delta t\, \mathscr{I}(N^{k+1}, P^{k+1}, V^k) \leqslant \mathscr{E}^0.$$

Thus, the series $\sum_{n\in\mathbb{N}} \mathscr{I}(N^{n+1}, P^{n+1}, V^n)$ is bounded and $\mathscr{I}(N^{n+1}, P^{n+1}, V^n)$ is nonnegative, which means that

$$\mathscr{I}(N^{n+1}, P^{n+1}, V^n) \to 0, \qquad \text{as } n \to \infty, \tag{4.12}$$

and since on the boundary Γ_D, we have $h(N_\sigma^{n+1}) - V_\sigma^n = h(N_\sigma) - V_\sigma = \alpha_N$ and $h(P_\sigma^{n+1}) + V_\sigma^n = h(P_\sigma) + V_\sigma = \alpha_P$, it yields

$$h(N_K^{n+1}) - V_K^n \to \alpha_N, \qquad h(P_K^{n+1}) + V_K^n \to \alpha_P, \qquad n \to \infty.$$

Moreover, applying Lemma 4.1 and using the bound (4.6) on $V^{n+1} - V^n$, we also get

$$|V^{n+1} - V^n|_{1,\Omega} \to 0, \qquad \text{as } n \to \infty. \tag{4.13}$$

On the other hand, we have

$$(x-y)\,(h(x) - h(y)) \leqslant c\,(x-y)^2, \qquad \forall\,(x,y) \in [m, M].$$

Hence, applying the Young inequality, we get for any $\delta > 0$

$$\begin{aligned}
&\frac{\delta}{2} \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, |N_K^{n+1} - N_K|^2 + \frac{1}{2\delta} \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, |h(N_K^{n+1}) - V_K^{n+1} - \alpha_N|^2 \\
&\geqslant \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, \left[N_K^{n+1} - N_K\right] \left[h(N_K^{n+1}) - V_K^{n+1} - \alpha_N\right] \\
&\geqslant c \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, \left[N_K^{n+1} - N_K\right]^2 + \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, \left[N_K^{n+1} - N_K\right] [V_K - V_K^{n+1}].
\end{aligned}$$

and

$$\begin{aligned}
&\frac{\delta}{2} \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, |P_K^{n+1} - P_K|^2 + \frac{1}{2\delta} \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, |h(P_K^{n+1}) + V_K^{n+1} - \alpha_P|^2 \\
&\geqslant c \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, \left[P_K^{n+1} - P_K\right]^2 - \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, \left[P_K^{n+1} - P_K\right] [V_K - V_K^{n+1}].
\end{aligned}$$

Thus, adding the two latter inequalities and using the scheme (2.10) at time t^{n+1}, it yields for $\delta < 2c$

$$
\begin{aligned}
&(c-\frac{\delta}{2}) \sum_{K\in\mathscr{T}} \mathrm{m}(K) \left(\left[N_K^{n+1}-N_K\right]^2 + \left[P_K^{n+1}-P_K\right]^2 \right) + |V^{n+1}-V|_{1,\Omega} \\
\leqslant\ & \frac{1}{2\delta} \left(\sum_{K\in\mathscr{T}} \mathrm{m}(K)\, |h(N_K^{n+1}) - V_K^{n+1} - \alpha_N|^2 + \sum_{K\in\mathscr{T}} \mathrm{m}(K)\, |h(P_K^{n+1}) + V_K^{n+1} - \alpha_P|^2 \right) \\
\leqslant\ & \frac{C_\Omega}{2\delta} \left(|h(N^{n+1}) - V^n - \alpha_N|_{1,\Omega} + |h(P^{n+1}) + V^n - \alpha_P|_{1,\Omega} + 2\, |V^n - V^{n+1}|_{1,\Omega} \right).
\end{aligned}
$$

Therefore, passing to the limit in $n \to \infty$ and using (4.12) and (4.13), we finally get the result

$$N_K^n \to N_K, \quad P_K^n \to P_K, \quad V_K^n \to V_K, \quad \text{as } n \to \infty,$$

where (N_K, P_K, V_K) is given by (1.10) and (2.3).

5. Numerical results

In this section, we give numerical results in one and two dimensions, obtained by the finite volume scheme (2.10)-(2.12).

5.1 *Thermal equilibrium at the boundary in 1-D*

We consider the following initial data for $x \in (0,1)$

$$N^0(x) = N_0 + (N_1 - N_0)\, x^{1/2}, \quad P^0(x) = P_0 + (P_1 - P_0)\, x^{1/2}$$

with the boundary condition

$$N(t,0) = 0.1, \quad P(t,0) = 0.9, \quad V(t,0) = \frac{h(N(t,0)) - h(P(t,0))}{2},$$

$$N(t,1) = 0.9, \quad P(t,1) = 0.1, \quad V(t,1) = \frac{h(N(t,1)) - h(P(t,1))}{2},$$

where $h(x) = \log(x)$. The doping profile is taken equal to zero. In this case, we have proven that the numerical solution converges to a steady state and the energy $\mathscr{E}^n$ is decreasing with respect to n. In Figures 1, we clearly observe that the energy is decreasing and converges to zero when times goes to infinity. Moreover, the dissipation $\mathscr{I}(N^n, P^n, V^{n-1})$ also converges to zero when n goes to infinity. In Figures 2, the density $(N(t^n), P(t^n))$ converges to the steady state obtained from the scheme (2.3)-(2.6) for the steady state problem.

5.2 *Thermal equilibrium at the boundary in 1-D with doping*

In this second example, we consider the system (1.1) where the doping profile C is given by

$$C(x) = \begin{cases} +1 & \text{if} x \in [0,1/2), \\ -1 & \text{else} \end{cases}$$

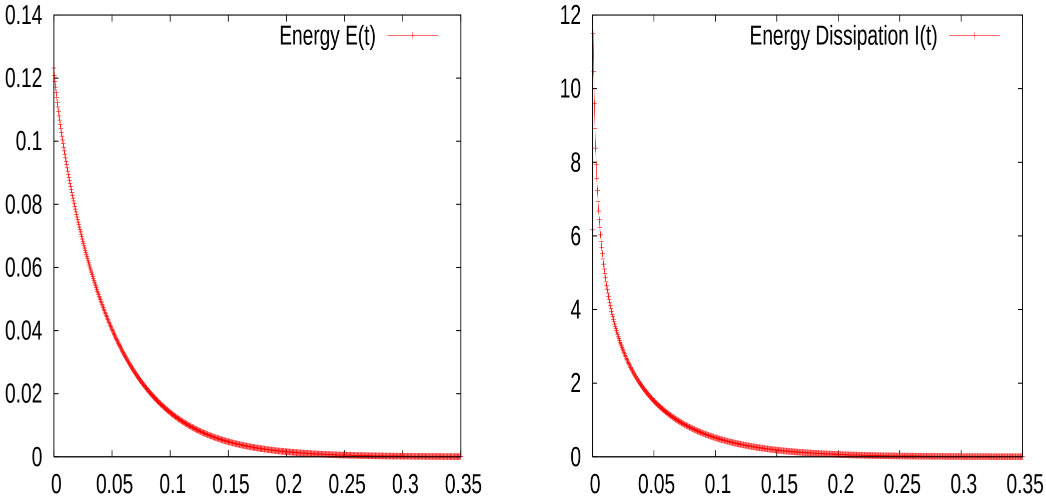

FIG. 1. Thermal equilibrium at the boundary 1-D: *evolution of the numerical energy* $\mathscr{E}^n$ *and its numerical dissipation* $\mathscr{I}(N^n, P^n, V^{n-1})$, $n \geqslant 1$.

and the pressure law is $r(s) = s^{5/3}$. Moreover, Dirichlet boundary conditions are prescribed

$$N(t,0) = P(t,1) = 0.1, \quad P(t,0) = N(t,1) = 0.9$$

and the potential $V(t,0)$ and $V(t,1)$ such that thermal equilibrium occurs

$$V(t,\sigma) = \frac{h(N(t,\sigma)) - h(P(t,\sigma))}{2}, \text{ for } \sigma = \{0,1\}.$$

In this case, we can apply the entropy method to prove that the solution converges to an equilibrium even if the L^∞ estimates on (N,P) are not valid. We perform numerical simulations using our algorithm and observe that the density (N,P) converges to a stationary solution given by solving the corresponding discrete steady state problem. In Figure 3, we observe that the energy converges to zero, whereas the density (N,P) goes to the equilibrium.

5.3 *Thermal equilibrium at the boundary in 2-D*

We present here a test case for a geometry corresponding to a PN-junction in 2D. The geometry is shown in Figure 4. The doping profile is piecewise constant, equal to +1 in the N-region and -1 in the P-region.

The Dirichlet boundary conditions are

$$N^D = 0.1,\ P^D = 0.9,\ V^D = \frac{h(N^D) - h(P^D)}{2} \quad \text{on } y = 1,\ 0 \leqslant x \leqslant 0.25$$
$$N^D = 0.9,\ P^D = 0.1,\ V^D = \frac{h(N^D) - h(P^D)}{2} \quad \text{on } y = 0$$

Elsewhere, we put Neumann boundary conditions.

We compute the numerical approximation of the thermal equilibrium and of the transient drift-diffusion system on a mesh made of 599 triangles. Figures 5 and 6 are devoted to the case where the pressure is linear

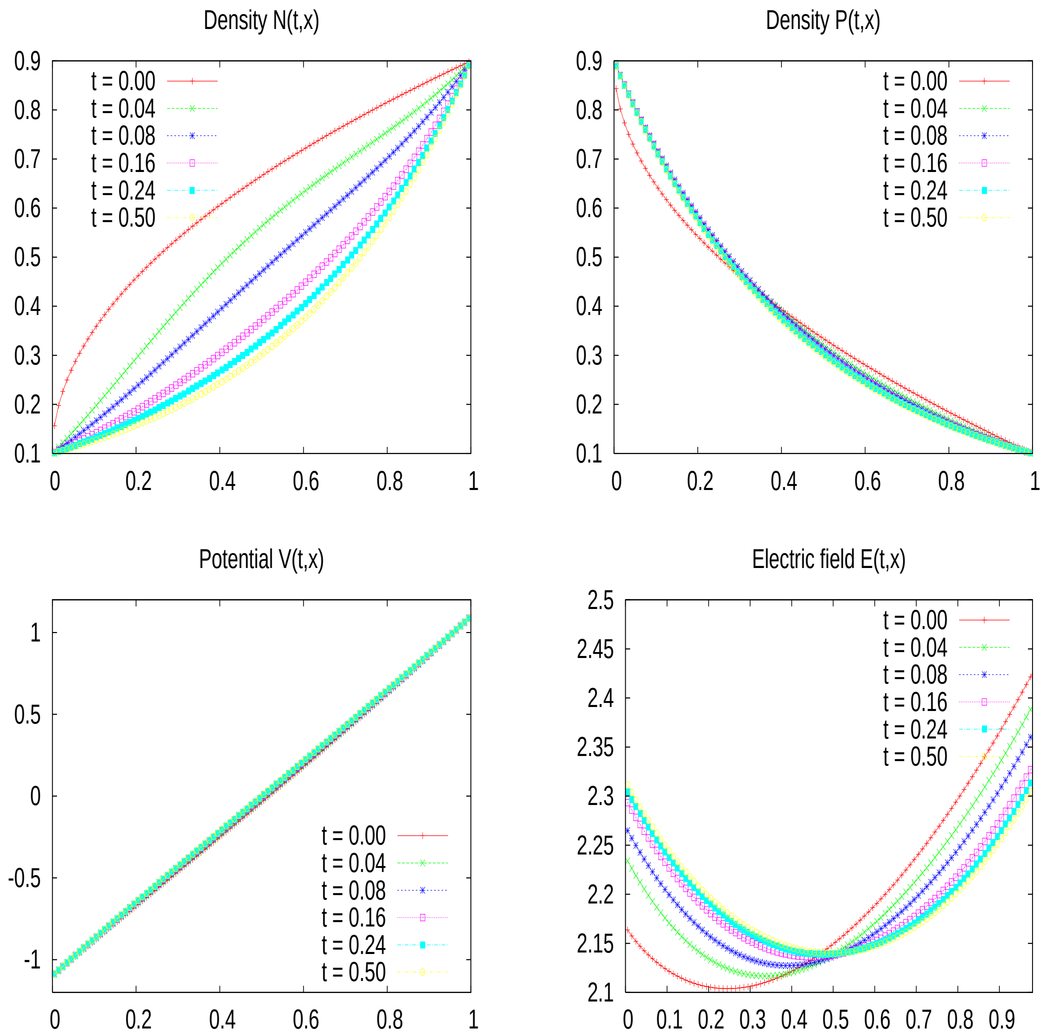

FIG. 2. Thermal equilibrium at the boundary 1-D: *evolution of the numerical density* (N,P), *the potential* V *and the electric field* DV, $n \geqslant 1$.

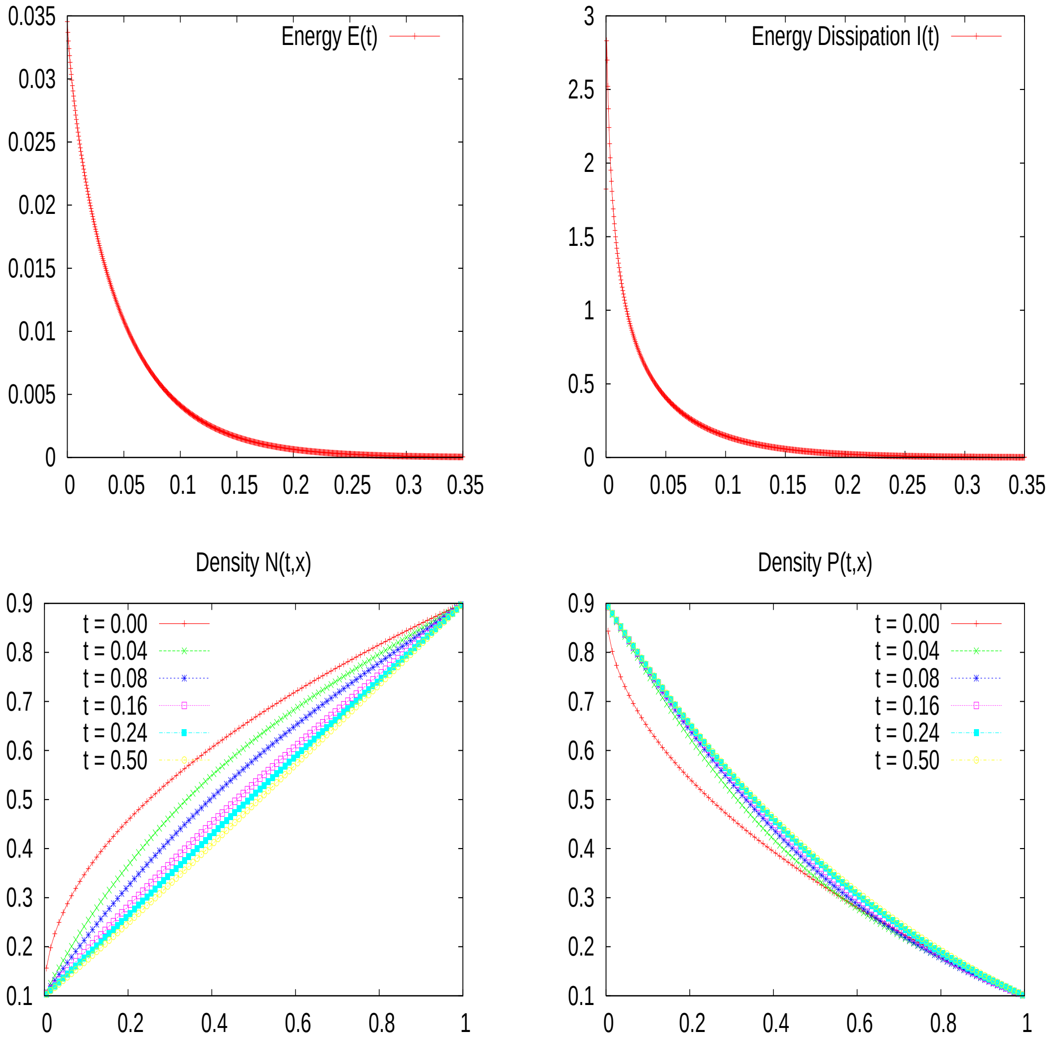

FIG. 3. Thermal equilibrium at the boundary 1-D with doping: *evolution of the numerical energy and its dissipation, and the density* (N,P), $n \geqslant 1$.

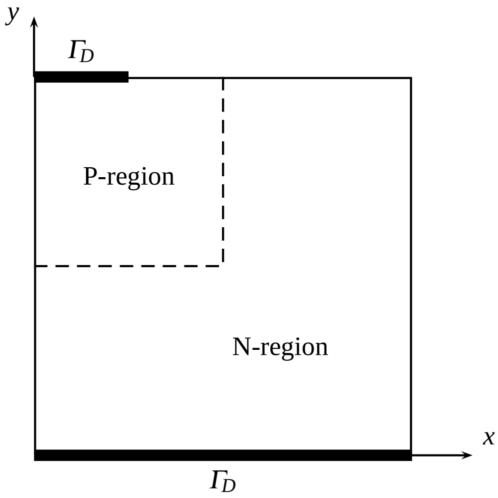

FIG. 4. Geometry of the PN-junction diode

$(r(s) = s)$. Figure 5 presents the evolution of the density of holes P computed with the time-dependent scheme at three different times $t = 0.04$, $t = 0.2$ and $t = 0.6$ and the approximation of P at the thermal equilibrium. Figure 6 shows the evolution of the energy and of its dissipation.

Figures 7 and 8 are devoted to the case where the pressure is nonlinear ($r(s) = s^\alpha$ with $\alpha = 5/3$). Figure 7 presents the evolution of the density of electrons N computed with the time-dependent scheme at three different times $t = 0.02$, $t = 0.1$ and $t = 0.6$ and the approximation of N at the thermal equilibrium. Figure 8 shows the evolution of the energy and of its dissipation.

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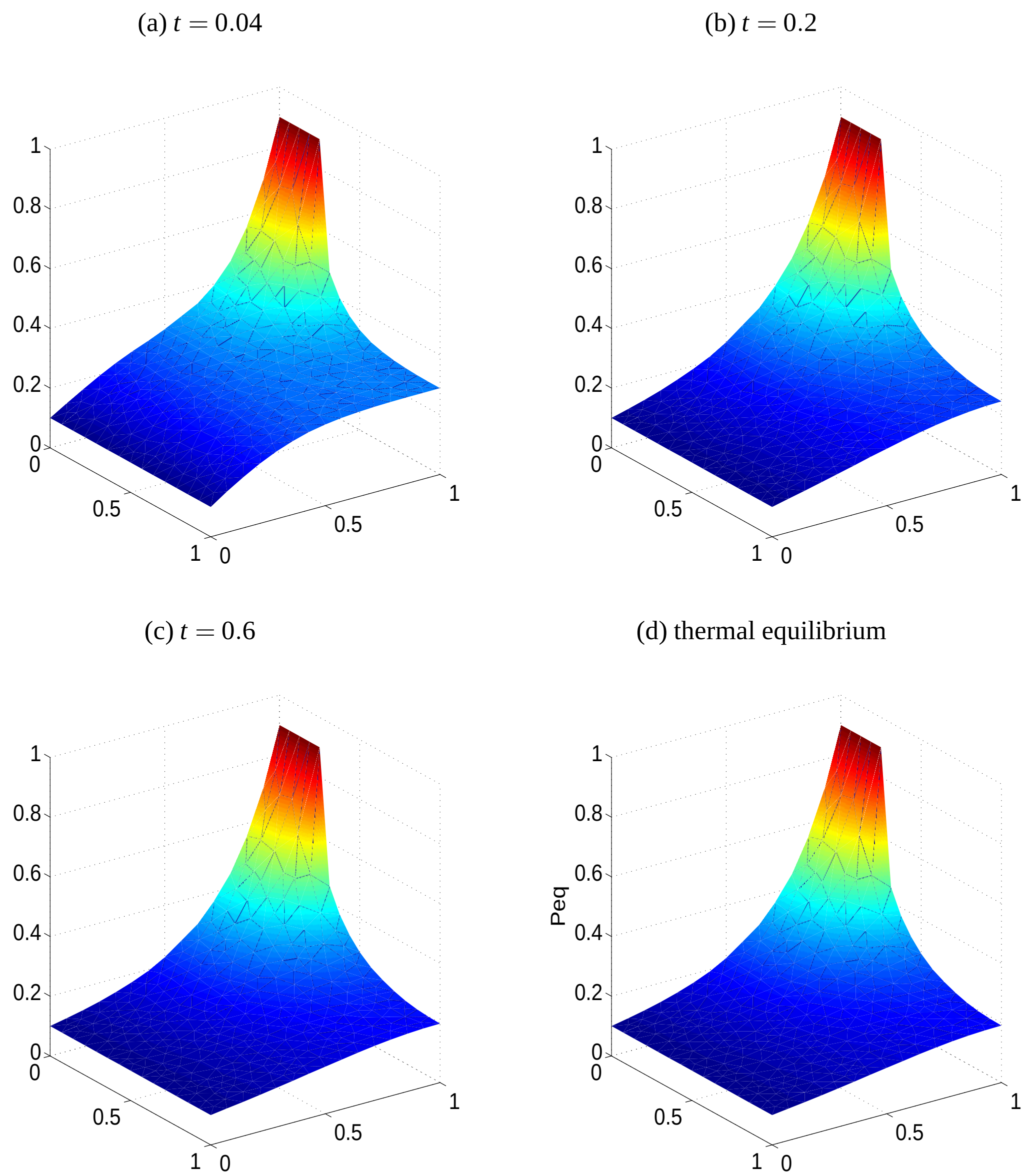

FIG. 5. Thermal equilibrium at the boundary in 2-D: *evolution of the density of holes and thermal equilibrium in the linear case*

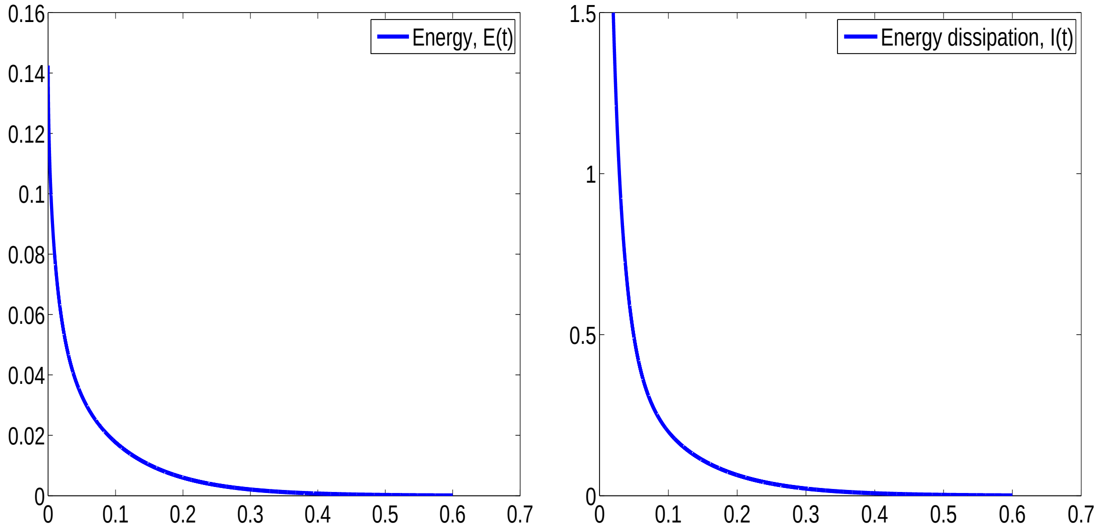

FIG. 6. Thermal equilibrium at the boundary in 2-D: *evolution of the numerical energy and its numerical dissipation in the linear case*

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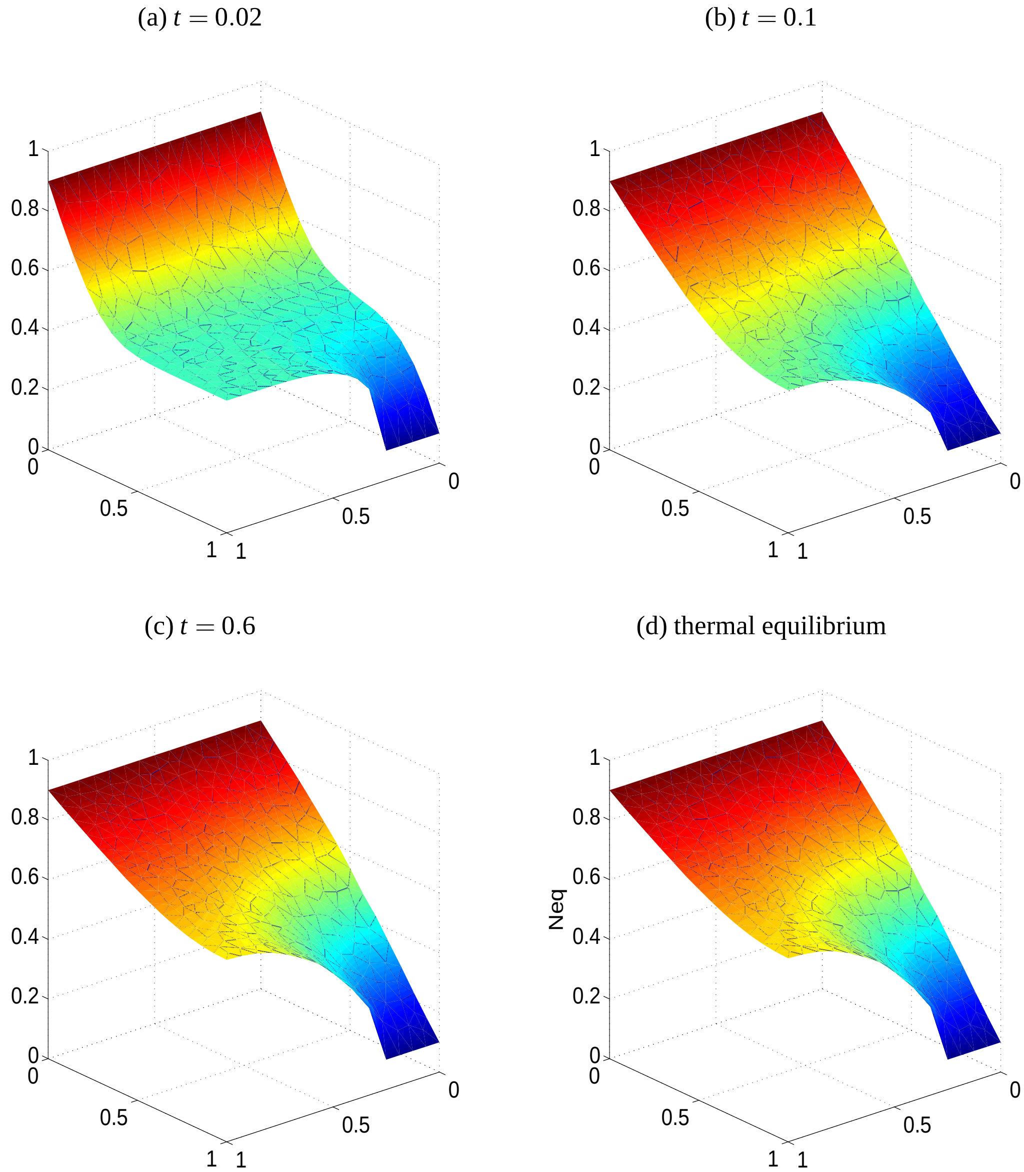

FIG. 7. Thermal equilibrium at the boundary in 2-D: *evolution of the density of electrons and thermal equilibrium in the non linear case*

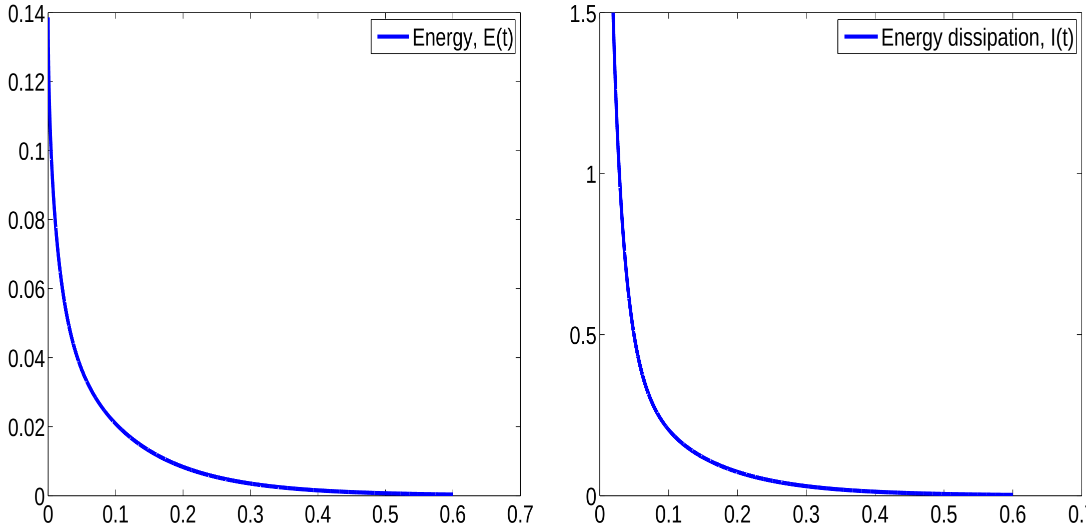

FIG. 8. Thermal equilibrium at the boundary in 2-D: *evolution of the numerical energy and its numerical dissipation in the nonlinear case*

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