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Uniform-in-time bounds for approximate solutions of the drift–diffusion system

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Abstract
In this paper, we consider a numerical approximation of the Van Roosbroeck's drift–diffusion system given by a backward Euler in time and finite volume in space discretization, with Scharfetter–Gummel fluxes. We first propose a proof of existence of a solution to the scheme which does not require any assumption on the time step. The result relies on the application of a topological degree argument which is based on the positivity and on uniform-in-time upper bounds of the approximate densities. Secondly, we establish uniform-in-time lower bounds satisfied by the approximate densities. These uniform-in-time upper and lower bounds ensure the exponential decay of the scheme towards the thermal equilibrium as shown in Bessemoulin-Chatard (Numer Math 25(3):147–168, 2016).

Mathematics Subject Classification 65M08 · 82D37

1 Introduction

1.1 Aim of the paper

The aim of this paper is to establish uniform-in-time positive upper and lower bounds for a finite volume approximation of the linear drift–diffusion system. This system has been introduced by Van Roosbroeck [34] in order to describe the transport of mobile carriers in semiconductor devices. The Van Roosbroeck's drift–diffusion system con-

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sists of two parabolic equations for the electron density N and the hole density P, and a Poisson's equation for the electrostatic potential Ψ.

Let Ω be an open bounded subset of $\mathbb{R}^d$ ($d = 2,\ 3$) corresponding to the geometry of the device and $T > 0$. The drift–diffusion system is then given by:

$$\partial_t N + \mathrm{div}(-\nabla N + N\nabla\Psi) = -R(N, P) \text{ in } \Omega \times (0, T), \tag{1a}$$

$$\partial_t P + \mathrm{div}(-\nabla P - P\nabla\Psi) = -R(N, P) \text{ in } \Omega \times (0, T), \tag{1b}$$

$$-\lambda^2\Delta\Psi = P - N + C \text{ in } \Omega \times (0, T). \tag{1c}$$

It is supplemented with initial conditions:

$$N(x, 0) = N_0(x), \quad P(x, 0) = P_0(x), \quad x \in \Omega, \tag{2}$$

and with mixed Dirichlet–Neumann boundary conditions. More precisely, the boundary $\partial\Omega$ is split into $\partial\Omega = \Gamma^D \cup \Gamma^N$ with $\Gamma^D \cap \Gamma^N = \emptyset$, and the boundary conditions write:

$$N = N^D, P = P^D, \Psi = \Psi^D \quad \text{on } \Gamma^D, \tag{3a}$$

$$\nabla N \cdot \nu = \nabla P \cdot \nu = \nabla\Psi \cdot \nu = 0 \quad \text{on } \Gamma^N, \tag{3b}$$

where ν is the unit normal to $\partial\Omega$ outward to Ω.

The given function $C(x)$ is the doping profile describing fixed background charges and λ is the rescaled Debye length. The recombination–generation rate $R(N, P)$ can usually be written under the form $R(N, P) = R_0(N, P)(NP - 1)$ (see [29]), which includes in particular the Shockley–Read–Hall term:

$$R_{SRH}(N, P) = \frac{NP - 1}{\tau_P N + \tau_N P + \tau_C}, \quad \tau_P,\ \tau_N,\ \tau_C > 0,$$

or the Auger term:

$$R_{AU} = (C_N N + C_P P)(NP - 1).$$

Existence of solutions to the system (1)–(3) has been proved under natural assumptions by Mock [30] and Gajewski and Gröger [21]. The question of uniqueness of the transient solutions has been investigated by the same authors [30] and [20]. Uniform-in-time upper and lower bounds for the densities can be shown by using an approach proposed by Alikakos [1] for nonlinear reaction–diffusion equations, closely related to an iteration technique initially introduced by Moser [31]. Let us also mention that a bound of the internal energy is needed in order to initialize the Moser iteration process and that it is obtained thanks to an energy/energy dissipation relation. The proof of the uniform-in-time upper and lower bounds can be found in [20, Lemmas 3 and 8] for the linear drift–diffusion system (1). In [20], the positive lower bound is obtained by controlling uniformly-in-time the inverse of the densities. The linearity of the diffusion terms in the system (1) is based on the assumption of Boltzmann statistics followed by the charge carriers. Other statistics lead to nonlinear drift–diffusion systems. The case of Fermi–Dirac statistics is considered for instance by Gajewski and Gröger in [21] and existence of solutions, bounds and long-time behavior are also established. In [21], the uniform positive lower bound is proved by bounding the logarithm of the densities. The same type of results have been proved using similar arguments for generalized drift–diffusion systems describing more than two charged species [23].

Many different numerical methods have already been designed for the approximation of the linear drift–diffusion system. It started with 1D finite difference methods and the so-called Scharfetter–Gummel scheme [33]. Finite element methods have been successfully developed in [2,12,32] for instance, as mixed exponential fitting finite element schemes in [7]. Finite volume schemes have also been proposed and studied from different viewpoints: convergence in [10], large time behavior in [3,8,11], study at the quasi-neutral limit $\lambda \to 0$ in [6].

In this paper, we consider a backward Euler in time and finite volume in space scheme with a Scharfetter–Gummel approximation of the convection–diffusion fluxes. One main feature of this scheme is that it preserves the thermal equilibrium (steady-state where the densities of current vanish). It satisfies a discrete energy/energy dissipation estimate as established by Gajewski and Gärtner in [19] and by Chatard [11]. Thanks to this estimate and some functional inequalities, the exponential decay towards the equilibrium of the Scharfetter–Gummel scheme is established in [3]. However, the proof of the exponential decay is also based on uniform-in-time positive upper and lower bounds of the approximate densities. Such a result is easily obtained when the doping profile C vanishes and, in this case, the values of the bounds do only depend on the upper and lower bounds of the initial and boundary densities. With a non-vanishing doping profile, existence of a solution to the scheme is proved in [3] thanks to Brouwer's fixed point theorem, using exponentially growing upper bounds and exponentially decreasing lower bounds on the densities. With this technique of proof, a strong assumption on the time step Δt, $\Delta t \leq \frac{\|C\|_\infty}{\lambda^2}$, is needed in order to get the bounds and the existence result. But, based on this existence result, uniform-in-time upper bounds have been then proved by Bessemoulin-Chatard, Chainais-Hillairet and Jüngel in [5] by application of the Moser iteration process at the discrete level.

Our aim in the current paper is twice: we want first to propose a new proof of existence of a solution to the scheme without any restrictive assumption on Δt. This proof will rely on the application of a topological degree argument. It will use the uniform-in-time upper bounds already proved in [5]. Then, we want to prove the positivity of the approximate densities and some uniform-in-time positive lower bounds.

Throughout the paper, we assume that the domain Ω is an open bounded polygonal (or polyhedral) subset of $\mathbb{R}^d$ $(d = 2,\ 3)$ and that $\partial\Omega = \Gamma^D \cup \Gamma^N$, with $\Gamma^D \cap \Gamma^N = \emptyset$ and Γ^D of positive measure. We assume that the Dirichlet boundary conditions N^D, P^D and Ψ^D are traces of some functions defined on the whole domain Ω, still denoted by N^D, P^D and Ψ^D and that the recombination–generation rate writes

$$R(N, P) = R_0(N, P)(NP - 1). \tag{4}$$

Finally, we consider the following standard assumptions on the data:

(H1) $C \in L^\infty(\Omega)$,
(H2) $N^D,\ P^D \in L^\infty \cap H^1(\Omega)$, $\Psi^D \in H^1(\Omega)$,
(H3) $\exists \alpha^D \in \mathbb{R}$ such that $\log N^D - \Psi^D = \alpha^D$ and $\log P^D + \Psi^D = -\alpha^D$.
(H4) $\exists M,\ m > 0$ such that $m \le N_0,\ P_0,\ N^D,\ P^D \le M$ a.e. on Ω or Γ^D,
(H5) $\exists \bar{R} > 0$ such that $0 \le R_0(N, P) \le \bar{R}(1 + |N| + |P|) \quad \forall N,\ P \in \mathbb{R}$.

Let us just remark that hypothesis (H3) means that the boundary data are in thermal equilibrium. It implies that $N^D P^D = 1$.

1.2 The numerical scheme

In order to introduce the numerical scheme for the drift–diffusion system (1)–(3), we first define the mesh of the domain Ω. It is given by a family $\mathcal{T}$ of open polygonal (or polyhedral in 3D) control volumes, a family $\mathcal{E}$ of edges (or faces), and a family $\mathcal{P} = (x_K)_{K\in\mathcal{T}}$ of points. As it is classical in the finite volume discretization of diffusive terms with two-points flux approximations, we assume that the mesh is admissible in the sense of [16, Definition 9.1]. 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 $\sigma = K|L \in \mathcal{E}_{int}$ and the boundary edges $\sigma \in \mathcal{E}_{ext}$. Within the exterior edges, we distinguish the Dirichlet boundary edges included in Γ^D from the Neumann boundary edges included in Γ^N: $\mathcal{E}_{ext} = \mathcal{E}_{ext}^D \cup \mathcal{E}_{ext}^N$. For a control volume $K \in \mathcal{T}$, we define $\mathcal{E}_K$ the set of its edges, which is also split into $\mathcal{E}_K = \mathcal{E}_{K,int} \cup \mathcal{E}_{K,ext}^D \cup \mathcal{E}_{K,ext}^N$. For each edge $\sigma \in \mathcal{E}$, there exists at least one cell $K \in \mathcal{T}$ such that $\sigma \in \mathcal{E}_K$, which will be denoted K_σ. In the case where $\sigma = K|L \in \mathcal{E}_{int}$, K_σ can be either equal to K or L.

In the sequel, we denote by d the distance in $\mathbb{R}^d$ and m the measure in $\mathbb{R}^d$ or $\mathbb{R}^{d-1}$. For all $\sigma \in \mathcal{E}$, we define $d_\sigma = d(x_K, x_L)$ if $\sigma = K|L \in \mathcal{E}_{int}$ and $d_\sigma = d(x_K, \sigma)$ if $\sigma \in \mathcal{E}_{ext}$, with $\sigma \in \mathcal{E}_K$. Then the transmissibility coefficient is defined by $\tau_\sigma = \mathrm{m}(\sigma)/d_\sigma$, for all $\sigma \in \mathcal{E}$. Notations introduced are illustrated in Fig. 1.

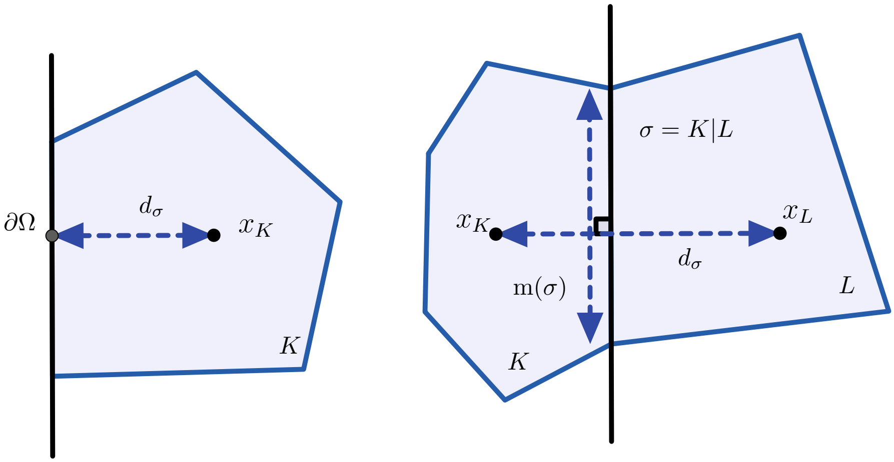


Fig. 1 Admissible mesh

We assume that the mesh satisfies the following regularity constraint:

$$\exists \xi > 0 \text{ such that } d(x_K, \sigma) \geq \xi\, d_\sigma, \quad \forall K \in \mathcal{T}, \quad \forall \sigma \in \mathcal{E}_K. \tag{5}$$

We also assume that the mesh satisfies the following nondegeneracy property:

$$\exists \tau_m > 0 \text{ such that } \tau_\sigma \geq \tau_m, \quad \forall \sigma \in \mathcal{E}. \tag{6}$$

This property is for example fulfilled by meshes satisfying: there exists $\alpha,\ \beta > 0$ such that

$$\begin{aligned} &\alpha\, \mathrm{size}(\mathcal{T})^2 \leq \mathrm{m}(K) \leq \beta\, \mathrm{size}(\mathcal{T})^2 \quad \forall K \in \mathcal{T}, \\ &\alpha\, \mathrm{size}(\mathcal{T}) \leq \mathrm{m}(\sigma) \leq \beta\, \mathrm{size}(\mathcal{T}) \quad \forall \sigma \in \mathcal{E}, \end{aligned} \tag{7}$$

where the size of the mesh is defined by $\mathrm{size}(\mathcal{T}) = \max_{K \in \mathcal{T}} \mathrm{diam}(K)$. Assumptions (7) are rather classical and close to those used within the finite element framework.

Let $\Delta t > 0$ be the time step. For $T > 0$, we set N_T the integer part of $T/\Delta t$ and $t^n = n\Delta t$ for all $n = 0 \ldots N_T$. We denote by $\delta = \max(\Delta t, \mathrm{size}(\mathcal{T}))$ the size of the space–time discretization.

A finite volume scheme with two-point flux approximation provides, for an unknown u, a vector $u_\mathcal{T} = (u_K)_{K \in \mathcal{T}} \in \mathbb{R}^\theta$ (with $\theta = \mathrm{Card}(\mathcal{T})$) of approximate values. A piecewise constant function, still denoted $u_\mathcal{T}$, can be defined by

$$u_\mathcal{T} = \sum_{K \in \mathcal{T}} u_K \mathbf{1}_K,$$

where $\mathbf{1}_K$ denotes the characteristic function of the cell K. However, since there are Dirichlet boundary conditions on a part of the boundary, we also need to define approximate values for u at the corresponding boundary edges: $u_{\mathcal{E}^D} = (u_\sigma)_{\sigma \in \mathcal{E}^D_{ext}} \in \mathbb{R}^{\theta^D}$ (with $\theta^D = \mathrm{Card}(\mathcal{E}^D_{ext})$). Therefore, the vector containing the approximate values both in the control volumes and at the Dirichlet boundary edges is denoted by $u_\mathcal{M} = (u_\mathcal{T}, u_{\mathcal{E}^D})$. We denote by $X(\mathcal{M})$ the set of the discrete functions $u_\mathcal{M}$.

For any vector $u_\mathcal{M} = (u_\mathcal{T}, u_{\mathcal{E}^D})$, we define for all $K \in \mathcal{T}$ and all $\sigma \in \mathcal{E}_K$:

$$u_{K,\sigma} = \begin{cases} u_L & \text{if } \sigma = K|L \in \mathcal{E}_{K,int}, \\ u_\sigma & \text{if } \sigma \in \mathcal{E}^D_{K,ext}, \\ u_K & \text{if } \sigma \in \mathcal{E}^N_{K,ext}, \end{cases} \tag{8}$$

and

$$D_{K,\sigma} u = u_{K,\sigma} - u_K, \quad D_\sigma u = |D_{K,\sigma} u|.$$

Then, we can define the discrete H^1-seminorm $|\cdot|_{1,\mathcal{M}}$ on $X(\mathcal{M})$ by

$$|u_\mathcal{M}|^2_{1,\mathcal{M}} = \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma u)^2, \quad \forall u_\mathcal{M} \in X(\mathcal{M}).$$

Let us now introduce the numerical scheme. We have to define at each time step $n = 0, \dots, N_T$ the approximate solution $u^n_{\mathcal{T}} = (u^n_K)_{K\in\mathcal{T}}$ for $u = N,\ P,\ \Psi$ and the approximate values at the boundary $u^n_{\mathcal{E}^D} = (u^n_\sigma)_{\sigma\in\mathcal{E}^D_{ext}}$ (which in fact do not depend on n since the boundary data do not depend on time). First of all, we discretize the initial and boundary conditions:

$$\left(N^0_K, P^0_K\right) = \frac{1}{\mathrm{m}(K)} \int_K (N_0(x), P_0(x))\, dx, \quad \forall K \in \mathcal{T}, \tag{9}$$

$$\left(N^D_\sigma, P^D_\sigma, \Psi^D_\sigma\right) = \frac{1}{\mathrm{m}(\sigma)} \int_\sigma \left(N^D(\gamma), P^D(\gamma), \Psi^D(\gamma)\right) d\gamma, \quad \forall \sigma \in \mathcal{E}^D_{ext}, \tag{10}$$

and we define

$$N^n_\sigma = N^D_\sigma, \quad P^n_\sigma = P^D_\sigma, \quad \Psi^n_\sigma = \Psi^D_\sigma, \quad \forall \sigma \in \mathcal{E}^D_{ext}, \quad \forall n \geq 0. \tag{11}$$

Then, we consider a backward Euler in time and finite volume in space discretization of the drift–diffusion system (1). The scheme writes:

$$\mathrm{m}(K)\frac{N^{n+1}_K - N^n_K}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \mathcal{F}^{n+1}_{K,\sigma} = -\mathrm{m}(K)\, R(N^{n+1}_K, P^{n+1}_K), \quad \forall K \in \mathcal{T}, \forall n \geq 0, \tag{12}$$

$$\mathrm{m}(K)\frac{P^{n+1}_K - P^n_K}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \mathcal{G}^{n+1}_{K,\sigma} = -\mathrm{m}(K)\, R(N^{n+1}_K, P^{n+1}_K), \quad \forall K \in \mathcal{T}, \forall n \geq 0, \tag{13}$$

$$-\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma}\Psi^n = \mathrm{m}(K)(P^n_K - N^n_K + C_K), \quad \forall K \in \mathcal{T}, \forall n \geq 0. \tag{14}$$

It remains to define the numerical fluxes $\mathcal{F}^{n+1}_{K,\sigma}$ and $\mathcal{G}^{n+1}_{K,\sigma}$. We choose to discretize simultaneously the diffusive part and the convective part of the fluxes by using the Scharfetter–Gummel fluxes: for all $K \in \mathcal{T}$, for all $\sigma \in \mathcal{E}_K$, we set:

$$\mathcal{F}^{n+1}_{K,\sigma} = \tau_\sigma \left[B\left(-D_{K,\sigma}\Psi^{n+1}\right) N^{n+1}_K - B\left(D_{K,\sigma}\Psi^{n+1}\right) N^{n+1}_{K,\sigma} \right], \tag{15}$$

$$\mathcal{G}^{n+1}_{K,\sigma} = \tau_\sigma \left[B\left(D_{K,\sigma}\Psi^{n+1}\right) P^{n+1}_K - B\left(-D_{K,\sigma}\Psi^{n+1}\right) P^{n+1}_{K,\sigma} \right], \tag{16}$$

where B is the Bernoulli function defined by

$$B(0) = 1 \quad \text{and} \quad B(x) = \frac{x}{\exp(x) - 1} \quad \forall x \neq 0. \tag{17}$$

These fluxes have been first introduced by Il'in [26] and Scharfetter and Gummel [33] in a 1D finite difference framework. They are second order accurate in space, as shown by Lazarov et al. [28]. They also preserve steady-states. In [19], the dissipativity of the implicit Scharfetter–Gummel scheme is proved; an energy/energy dissipation relation is also established in [11], leading to the study of the long-time behavior of the Scharfetter–Gummel scheme for the linear drift–diffusion system. The exponential decay towards the thermal equilibrium is obtained in [3] under assumption of uniform-in-time upper and lower bounds for the approximate charge carrier densities. In [24], some bounds for discrete steady-states solutions obtained with the Scharfetter–Gummel scheme are established.

Remark 1 Using definition (8) of $u_{K,\sigma}$ for $\sigma \in \mathcal{E}^N_{K,ext}$ and the fact that $B(0) = 1$, we recover as expected from the continuous framework the zero flux boundary conditions on Γ^N:

$$\mathcal{F}_{K,\sigma} = 0, \quad \mathcal{G}_{K,\sigma} = 0 \quad \forall K \in \mathcal{T},\ \sigma \in \mathcal{E}^N_{K,ext}.$$

In the sequel, we denote by $(\mathcal{S})$ the scheme defined by (9)–(17).

1.3 Main result and outline of the article

In this article, our aim is to adapt the ideas developed by Gajewski and Gröger in [20–22] to the discrete framework in order to obtain uniform-in-time upper and lower bounds for the approximate densities $N^n_{\mathcal{T}}$, $P^n_{\mathcal{T}}$ obtained with the implicit Scharfetter–Gummel scheme $(\mathcal{S})$. In practice, the proof of the bounds will also ensure the existence of a solution to the numerical scheme thanks to a topological degree argument.

In order to get the uniform-in-time L^∞-bounds, we apply a Nash–Moser type iteration method based on L^r bounds [1,31]. This method has already been applied in a discrete framework by Fiebach, Glitzky and Linke in [17] for reaction–diffusion systems arising in electrochemistry.

Our main result is stated in the following theorem.

Theorem 1 *Let (H1)–(H5) be fulfilled. Let $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible mesh of Ω satisfying (5) and (6). We also assume that the time step satisfies $\Delta t \leq 1$.*

Then there exists a solution $(N^n_{\mathcal{T}}, P^n_{\mathcal{T}}, \Psi^n_{\mathcal{T}})_{n\geq 0}$ to the scheme $(\mathcal{S})$, such that the approximate densities satisfy the following uniform-in-time upper and lower bounds:

$\exists D,\ E > 0$ such that

$$0 < D \leq N^n_K,\ P^n_K \leq E \quad \forall K \in \mathcal{T},\ \forall n \geq 0. \tag{18}$$

These constants D and E are independent of the discretization size δ, and depend only on the data, namely the boundary conditions N^D, P^D, Ψ^D, the initial conditions N^0, P^0, the doping profile C, the Debye length λ, the domain Ω and the regularity constraints ξ and τ_m.

This theorem establishes the assumptions needed to prove the exponential decay of approximate solutions given by the scheme $(\mathcal{S})$ towards an approximation of the thermal equilibrium [3, Theorem 3.1].

As mentioned above, the proof of (18) applies a Nash–Moser type iteration method [1,31]. It also follows ideas developed in [15,35,36]. Since we deal here with equations on a bounded domain, we have to take care about the boundary conditions. Therefore, as in [27], we establish the uniform upper bound for $N_M = (N - M)^+$ and $P_M = (P - M)^+$, where M is given in (H4), instead of N and P. Moreover, the positive lower bound is obtained as in [17,21] by establishing a L^∞ bound for an appropriate function of the logarithm of the densities. In both cases, application of the Moser iteration technique needs a convenient initial *a priori* bound in some L^p norm, $p \geq 1$. This starting point of the bootstrapping procedure is provided in the case of the upper bound by an energy/energy dissipation relation which yields uniform-in-time L^1 bound. In the case of the lower bound, we establish an appropriate uniform-in-time L^2 bound to initialize the method.

The outline of the article is as follows. In Sect. 2, we propose a new proof of existence of a solution to the implicit Scharfetter–Gummel scheme which does not necessitate any assumption on the time step. This result is based on a topological degree argument which requires some a priori estimates. We will use and recall the uniform-in-time upper bound for the approximate densities proved in [5]. We will also obtain the positivity of the approximate densities, which allows us to consider the appropriate test functions involving the logarithm of the densities to prove uniform-in-time lower bounds in Sect. 3. The most technical results are detailed in the Appendix to lighten the presentation. We finally present in Sect. 4 some numerical experiments illustrating the presented theoretical results.

2 Existence of a solution to the scheme

We first state the existence of a solution to the scheme, with a uniform-in-time upper bound and the positivity of the approximate densities.

Proposition 1 *Let (H1)–(H5) be fulfilled. Let $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible mesh of Ω satisfying (5) and (6) and let $\Delta t > 0$. Then, for all $T > 0$, there exists a solution $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{0 \leq n \leq N_T}$ to the scheme $(\mathcal{S})$, which satisfies the following L^∞ estimates for the approximate densities:*

$$0 < N_K^n,\ P_K^n \leq E, \quad \forall n = 0, \ldots, N_T, \quad \forall K \in \mathcal{T}, \tag{19}$$

where E is only depending on the data and independent of δ and T.

Proposition 1 will be proved by applying a topological degree argument, similar to Leray–Schauder's fixed point theorem [14,25]. For $\kappa \in [0, 1]$, we introduce a scheme $(\mathcal{S}_\kappa)$ defined by: $\forall K \in \mathcal{T}, \forall n \geq 0$,

$$\mathrm{m}(K) \frac{N_K^{n+1} - N_K^n}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \widehat{\mathcal{F}}_{K,\sigma}^{n+1} = -\kappa \mathrm{m}(K)\, R(N_K^{n+1,+}, P_K^{n+1,+}), \tag{20}$$

$$\mathrm{m}(K) \frac{P_K^{n+1} - P_K^n}{\Delta t} + \sum_{\sigma \in \mathcal{E}_K} \widehat{\mathcal{G}}_{K,\sigma}^{n+1} = -\kappa \mathrm{m}(K)\, R(N_K^{n+1,+}, P_K^{n+1,+}), \tag{21}$$

$$-\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma}\Psi^n = \kappa \mathrm{m}(K)(P_K^n - N_K^n + C_K), \tag{22}$$

where the numerical fluxes $\widehat{\mathcal{F}}_{K,\sigma}^{n+1}$, $\widehat{\mathcal{G}}_{K,\sigma}^{n+1}$ are given by:

$$\widehat{\mathcal{F}}_{K,\sigma}^{n+1} = \tau_\sigma \left[B\left(-D_{K,\sigma}\Psi^{n+1}\right) N_K^{n+1,+} - B\left(D_{K,\sigma}\Psi^{n+1}\right) N_{K,\sigma}^{n+1,+}\right], \tag{23}$$

$$\widehat{\mathcal{G}}_{K,\sigma}^{n+1} = \tau_\sigma \left[B\left(D_{K,\sigma}\Psi^{n+1}\right) P_K^{n+1,+} - B\left(-D_{K,\sigma}\Psi^{n+1}\right) P_{K,\sigma}^{n+1,+}\right], \tag{24}$$

with the notation $x^+ = \max(x, 0)$ for the nonnegative part of x. The scheme is supplemented with the initial and boundary conditions (9), (10) and (11). Let us remark that, in order to lighten the notations, we do not write the dependency of the unknowns with respect to κ: we keep the notation (N_K^n, P_K^n, Ψ_K^n) even if it could be written $(N_K^{n,\kappa}, P_K^{n,\kappa}, \Psi_K^{n,\kappa})$.

The proof of Proposition 1 is split into four steps. Assuming that the scheme $(\mathcal{S}_\kappa)$ has a solution, we first establish the positivity of the densities $(N_K^n, P_K^n)_{K\in\mathcal{T},n\geq 0}$ (Lemmas 1 and 2). It implies that a solution to $(\mathcal{S}_\kappa)$ can be seen as a solution to $(\mathcal{S})$ with κR instead of R and λ^2/κ instead of λ^2 for $\kappa \in (0, 1]$. We then recall a discrete energy/energy dissipation inequality (Proposition 2) and its consequences (Proposition 3). Using these preliminary results, we establish in Sect. 2.3 a uniform-in-time upper bound for the approximate densities. This bound is also uniform with respect to $\kappa \in [0, 1]$. Finally in Sect. 2.4, we apply a topological degree argument based on the a priori estimates to prove the existence of a solution to the initial scheme $(\mathcal{S})$.

2.1 Positivity of the densities

We first prove the nonnegativity of the approximate densities obtained with the scheme $(\mathcal{S}_\kappa)$. It implies that a solution to $(\mathcal{S}_1)$ is necessarily a solution to $(\mathcal{S})$.

Lemma 1 *Under the assumptions of Proposition 1, let assume that there exists a solution $(N_\mathcal{T}^n, P_\mathcal{T}^n, \Psi_\mathcal{T}^n)_{0\leq n\leq N_T}$ to the scheme $(\mathcal{S}_\kappa)$ for $\kappa \in [0, 1]$. Then the obtained approximate densities are nonnegative:*

$$N_K^n,\ P_K^n \geq 0 \quad \forall K \in \mathcal{T}, \forall n = 0, \ldots, N_T.$$

Proof We proceed by induction. The result holds for $n = 0$. We assume it for a given n. Then, multiplying the scheme (20) by $N_K^{n+1,-} = \min(N_K^{n+1}, 0)$ and summing over $K \in \mathcal{T}$, we get:

$$T_1 + T_2 = T_3, \tag{25}$$

with

$$T_1 = \sum_{K \in \mathcal{T}} \mathrm{m}(K) \frac{N_K^{n+1} - N_K^n}{\Delta t} N_K^{n+1,-},$$
$$T_2 = \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \widehat{\mathcal{F}}_{K,\sigma}^{n+1} N_K^{n+1,-},$$
$$T_3 = -\kappa \sum_{K \in \mathcal{T}} \mathrm{m}(K)\, R(N_K^{n+1,+}, P_K^{n+1,+}) N_K^{n+1,-}.$$

Classically, due to the induction hypothesis and since $x^-(x - y) \geq \frac{1}{2}((x^-)^2 - (y^-)^2)$ (with $x^- = \min(x, 0)$), we have

$$T_1 \geq \frac{1}{2} \sum_{K \in \mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t} \left(N_K^{n+1,-}\right)^2.$$

Moreover, using the definition (4) and the nonnegativity of R_0, we have

$$T_3 = \kappa \sum_{K \in \mathcal{T}} \mathrm{m}(K) R_0 \left(N_K^{n+1,+}, P_K^{n+1,+}\right) N_K^{n+1,-} \leq 0.$$

Then, using the definition (23) of the modified numerical flux, and performing a discrete integration by parts, we have

$$\begin{aligned} T_2 = &- \sum_{\sigma \in \mathcal{E}} \tau_\sigma \left[B\left(-D_{K,\sigma}\Psi^{n+1}\right) N_K^{n+1,+} - B\left(D_{K,\sigma}\Psi^{n+1}\right) N_{K,\sigma}^{n+1,+} \right] \\ &\left(N_{K,\sigma}^{n+1,-} - N_K^{n+1,-}\right) \\ = &- \sum_{\sigma \in \mathcal{E}} \tau_\sigma \left[B\left(-D_{K,\sigma}\Psi^{n+1}\right) N_K^{n+1,+} N_{K,\sigma}^{n+1,-} \right. \\ &\left. + B\left(D_{K,\sigma}\Psi^{n+1}\right) N_{K,\sigma}^{n+1,+} N_K^{n+1,-} \right]. \end{aligned}$$

But since $B(x) \geq 0$ for all $x \in \mathbb{R}$ and $x^+ \geq 0$, $x^- \leq 0$ for all x, we finally get that $T_2 \geq 0$. Using this in (25), we obtain that

$$\sum_{K \in \mathcal{T}} \mathrm{m}(K) \left(N_K^{n+1,-}\right)^2 \leq 0,$$

from which we deduce that $N_K^{n+1} \geq 0$ for all $K \in \mathcal{T}$. Finally, we proceed exactly in the same way for P. □

Thanks to the nonnegativity of the approximate densities, we are now able to prove their positivity.

Lemma 2 *Under the assumptions of Proposition 1, let assume that there exists a solution* $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{0\le n\le N_T}$ *to the scheme* $(\mathcal{S}_\kappa)$ *for* $\kappa \in [0,1]$. *Then the approximate densities are positive:*

$$N_K^n,\ P_K^n > 0 \quad \forall n \ge 0, \quad \forall K \in \mathcal{T}. \tag{26}$$

Proof Once again, we proceed by induction. The result holds for $n = 0$. We assume that for a given n, $N_K^n > 0$ and $P_K^n > 0$ for all $K \in \mathcal{T}$. We already know that $N_K^{n+1} \ge 0$ and $P_K^{n+1} \ge 0$ for all $K \in \mathcal{T}$. Let us assume that there is a $K \in \mathcal{T}$ such that $N_K^{n+1} = 0$. Then the scheme (20) yields:

$$-\frac{\mathrm{m}(K)}{\Delta t} N_K^n = \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma B\left(D_{K,\sigma}\Psi^{n+1}\right) N_{K,\sigma}^{n+1,+} + \kappa \mathrm{m}(K) R_0(0, P_K^{n+1,+}) \ge 0,$$

which is in contradiction with the induction assumption. We deduce that $N_K^{n+1} > 0$, and similarly that $P_K^{n+1} > 0$, for all $K \in \mathcal{T}$. □

2.2 Discrete energy/energy dissipation inequality

In all this subsection, we assume that there exists a solution $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{0\le n\le N_T}$ to the scheme $(\mathcal{S}_\kappa)$. Due to the positivity of the densities established in Lemma 2, we note that we can let down the positive parts in the definition of the numerical fluxes (23) and (24) and in the recombination–generation terms.

We now recall an estimate relating the discrete relative energy and its dissipation. To define this discrete relative energy, we need to introduce an approximation of the thermal equilibrium. This equilibrium is a steady state for which electron and hole currents, $\nabla N - N\nabla\Psi$ and $\nabla P + P\nabla\Psi$, vanish, as the recombination–generation term. For the original system (1)–(2), it is defined by

$$\begin{aligned} N^* &= \exp(\alpha^D + \Psi^*)\\ P^* &= \exp(-\alpha^D - \Psi^*)\\ -\lambda^2\Delta\Psi^* &= \exp(-\alpha^D - \Psi^*) - \exp(\alpha^D + \Psi^*) + C\\ \Psi^* &= \Psi^D \quad \text{on } \Gamma^D, \quad \nabla\Psi^*\cdot\nu = 0 \quad \text{on } \Gamma^N, \end{aligned}$$

where α^D is defined by (H3).

For every value of $\kappa \in [0,1]$, we can define the following finite volume scheme: $\forall K \in \mathcal{T}$,

$$-\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma}\Psi^* = \kappa \mathrm{m}(K)\left(\exp(-\alpha^D - \Psi_K^*) - \exp(\alpha^D + \Psi_K^*) + C_K\right), \tag{27}$$

$$N_K^* = \exp(\alpha^D + \Psi_K^*), \tag{28}$$

$$P_K^* = \exp(-\alpha^D - \Psi_K^*). \tag{29}$$

This scheme has been introduced and studied by Chainais-Hillairet and Filbet [8] in the case where $\kappa = 1$: existence and uniqueness of a solution to this nonlinear scheme have been proved. However, the proof still works for $\kappa \in (0, 1]$ and the existence and uniqueness result is still well-known for $\kappa = 0$.

Let $H(x) = x\log(x) - x + 1$. For $\kappa \in [0, 1]$, we define a discrete relative energy functional $(\mathbb{E}^n(\kappa))_{n\geq 0}$ by:

$$\begin{aligned}\mathbb{E}^n(\kappa) = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(&H(N_K^n) - H(N_K^*) - \log(N_K^*)(N_K^n - N_K^*)\\ &+H(P_K^n) - H(P_K^*) - \log(P_K^*)(P_K^n - P_K^*)\big)\\ &+\frac{\lambda^2}{2\kappa}\left|\Psi_{\mathcal{M}}^n - \Psi_{\mathcal{M}}^*\right|_{1,\mathcal{M}}^2, \forall\kappa > 0\end{aligned} \tag{30}$$

and

$$\begin{aligned}\mathbb{E}^n(0) = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(&H(N_K^n) - H(N_K^*) - \log(N_K^*)(N_K^n - N_K^*)\\ &+H(P_K^n) - H(P_K^*) - \log(P_K^*)(P_K^n - P_K^*)\big).\end{aligned} \tag{31}$$

We also define the discrete energy dissipation functional $(\mathbb{I}^n(\kappa))_{n\geq 0}$ by: $\forall\kappa \in [0, 1]$,

$$\begin{aligned}\mathbb{I}^n(\kappa) = \sum_{\sigma\in\mathcal{E}} \tau_\sigma \Big[&\min(N_K^n, N_{K,\sigma}^n)\left(D_\sigma(\log(N^n) - \Psi^n)\right)^2\\ &+ \min(P_K^n, P_{K,\sigma}^n)\left(D_\sigma(\log(P^n) + \Psi^n)\right)^2\Big]\\ &+\kappa\sum_{K\in\mathcal{T}} \mathrm{m}(K)R(N_K^n, P_K^n)\log(N_K^n P_K^n).\end{aligned} \tag{32}$$

We now give the discrete energy/energy dissipation inequality and some first consequences.

Proposition 2 *Let (H1)–(H5) be fulfilled and let $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible mesh of Ω. Let $\kappa \in [0, 1]$ and assume that the scheme $(\mathcal{S}_\kappa)$ has a solution $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{n\geq 0}$. Then, for all $n \geq 0$, we have:*

$$0 \leq \mathbb{E}^{n+1}(\kappa) + \Delta t\,\mathbb{I}^{n+1}(\kappa) \leq \mathbb{E}^n(\kappa). \tag{33}$$

Furthermore, if the mesh satisfies the regularity assumption (5), there exists a constant $C_{\mathbb{E}} > 0$ depending only on the boundary conditions N^D, P^D, Ψ^D, the initial conditions N^0, P^0, the doping profile C, the Debye length λ, the domain Ω and the regularity constraint ξ given in (5) such that for all $n \geq 0$ and for all $\kappa \in [0, 1]$,

$$0 \leq \mathbb{E}^n(\kappa) \leq \mathbb{E}^0(\kappa) \leq C_{\mathbb{E}}. \tag{34}$$

Proof The proof of (33) is given in [11] for the case where $\kappa = 1$. It can be extended to the case $\kappa \in (0, 1]$ just replacing R by κR and λ^2 by λ^2/κ. When $\kappa = 0$, we note that $\Psi^n_{\mathcal{M}} = \Psi^*_{\mathcal{M}}$ for all $n \geq 0$, so that the proof given in [11] also gives (33) in the case $\kappa = 0$.

Summing (33) over $k = 0, \dots, n$, we get that

$$0 \leq \mathbb{E}^{n+1}(\kappa) + \sum_{k=0}^{n} \Delta t \mathbb{I}^{k+1}(\kappa) \leq \mathbb{E}^0(\kappa) \quad \forall n \geq 0.$$

Provided that $\mathbb{E}^0(\kappa)$ is bounded and $\mathbb{I}^k(\kappa)$ is nonnegative for all $k \geq 0$, this gives a uniform-in-time and uniform-in-κ estimate for $\mathbb{E}^n(\kappa)$.

Therefore, it remains to establish the boundedness of $\mathbb{E}^0(\kappa)$. It is proved in [8, Theorem 2.1] that there exists a constant $\mathcal{C} > 0$ only depending on Ψ^D and λ (and in particular not depending on κ) such that:

$$\left|\Psi^*_K\right| \leq \mathcal{C} \quad \forall K \in \mathcal{T}. \tag{35}$$

Then using the definitions (28) and (29), we deduce that there exists $m^* > 0$ and $M^* > 0$ such that

$$m^* \leq N^*_K,\ P^*_K \leq M^* \quad \forall K \in \mathcal{T},$$

and we can choose $m^* \leq m$ and $M^* \geq M$. As the function H satisfies the following inequality:

$$\forall x,\ y > 0, \quad H(y) - H(x) - \log(x)(y - x) \leq \frac{1}{\min(x, y)} \frac{(y - x)^2}{2},$$

we deduce that

$$\sum_{K \in \mathcal{T}} \mathrm{m}(K) \left[H(N^0_K) - H(N^*_K) - \log(N^*_K)(N^0_K - N^*_K) \right] \leq \mathrm{m}(\Omega) \frac{(M^* - m^*)^2}{2m^*},$$

and the same inequality holds for P, which gives a bound for $\mathbb{E}^0(0)$. In order to bound $\mathbb{E}^0(\kappa)$ for $\kappa \in (0, 1]$, it remains to bound

$$\frac{\lambda^2}{2\kappa} \left| \Psi^0_{\mathcal{M}} - \Psi^*_{\mathcal{M}} \right|^2_{1,\mathcal{M}}.$$

But, subtracting the scheme for Ψ^0 and the scheme for Ψ^*, we get:

$$-\lambda^2 \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma}(\Psi^0 - \Psi^*) = \kappa \mathrm{m}(K) \left(P^0_K - N^0_K - P^*_K + N^*_K \right) \quad \forall K \in \mathcal{T}.$$

Then, multiplying this relation by $(\Psi_K^0 - \Psi_K^*)$, summing over $K \in \mathcal{T}$ and using standard techniques like discrete integration by parts, discrete Poincaré inequality (see for instance [4,16]) and the bounds on N^0, P^0, N^* and P^*, we get that there exists $\mathcal{C}$ not depending on κ such that:

$$\frac{\lambda^2}{2\kappa} \left| \Psi_{\mathcal{M}}^0 - \Psi_{\mathcal{M}}^* \right|_{1,\mathcal{M}}^2 \leq \mathcal{C}\kappa \leq \mathcal{C} \quad \forall \kappa \in (0, 1],$$

which concludes the proof. $\square$

From Proposition 2, we can deduce in particular the following result which is useful in what follows:

Proposition 3 *Let (H1)–(H5) be fulfilled, and let $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible mesh of Ω. For $\kappa \in [0, 1]$, we assume that the scheme $(\mathcal{S}_\kappa)$ has a solution $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{K \in \mathcal{T}, n \geq 0}$. If the mesh $\mathcal{M}$ also satisfies (5) and (6), there exists a constant $\gamma \in (0, 1]$ independent of n and κ such that:*

$$B(D_\sigma \Psi^{n+1}) \geq \gamma \quad \forall \sigma \in \mathcal{E}, \quad \forall n \geq 0. \tag{36}$$

Proof From (34), we have $\mathbb{E}^n(\kappa) \leq C_{\mathbb{E}}$ for all $n \geq 0$ and for all $\kappa \in [0, 1]$, and from the definition of the discrete relative energy, this implies that for $\kappa \in (0, 1]$:

$$\frac{\lambda^2}{2} |\Psi_{\mathcal{M}}^{n+1} - \Psi_{\mathcal{M}}^*|_{1,\mathcal{M}}^2 \leq C_{\mathbb{E}}\kappa \leq C_{\mathbb{E}} \quad \forall n \geq 0.$$

Then, thanks to (6), we get that

$$(D_\sigma(\Psi^{n+1} - \Psi^*))^2 \leq \frac{2C_{\mathbb{E}}}{\lambda^2 \tau_m} \quad \forall \sigma \in \mathcal{E}.$$

Using the L^∞ estimate on $\Psi_{\mathcal{T}}^*$, we deduce the existence of C_Ψ depending only on the data N^D, P^D, Ψ^D, N^0, P^0, the doping profile C, the Debye length λ, the domain Ω, the regularity constraints ξ and τ_m, such that

$$0 \leq D_\sigma \Psi^{n+1} \leq C_\Psi \quad \forall \sigma \in \mathcal{E}, \quad \forall n \geq 0. \tag{37}$$

Then the definition of the Bernoulli function ensures (36) with $\gamma \in (0, 1]$ for $\kappa \in (0, 1]$. The result is straightforward for $\kappa = 0$. $\square$

2.3 Uniform-in-time upper bound

We still assume the existence of a solution $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{0 \leq n \leq N_T}$ to the scheme $(\mathcal{S}_\kappa)$ for $\kappa \in [0, 1]$. For $\kappa = 0$, there is a discrete maximum principle for $N_{\mathcal{T}}^n$ and $P_{\mathcal{T}}^n$ for each $n \geq 0$, so that the uniform-in-time upper bound is clearly satisfied.

Let $\kappa \in (0,1]$. We now prove the following uniform-in-time upper bound for the approximate densities $N^n_{\mathcal{T}}$ and $P^n_{\mathcal{T}}$: there exists E as in Proposition 1 such that

$$0 < N^n_K, P^n_K \leq E, \quad \forall K \in \mathcal{T}, \forall n \geq 0, \forall \kappa \in (0,1].$$

This result is established in [5] for $\kappa = 1$. We recall here the guidelines of the proof which still hold for $\kappa \in (0,1]$. The crucial point is that the constants in Proposition 4 do not depend on κ when $\kappa \leq 1$.

Since we have to take care about the boundary conditions, we define

$$N^n_{M,K} = (N^n_K - M)^+,\ P^n_{M,K} = (P^n_K - M)^+, \quad \forall K \in \mathcal{T}, \quad \forall n \geq 0,$$

where M is the upper bound of the initial and boundary conditions given in (H4). Our aim is to prove that $N^n_{M,\mathcal{T}}$ and $P^n_{M,\mathcal{T}}$ are uniformly bounded.

Let us set

$$V^n_q = \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left[(N^n_{M,K})^q + (P^n_{M,K})^q\right], \quad \forall n \geq 0,\ \forall q \geq 1,$$

and

$$W^n_k = V^n_{2^k} \quad \forall n \in \mathbb{N}, \quad \forall k \in \mathbb{N}.$$

The aim is to prove that there is a constant $\overline{\mathcal{M}} > 0$ such that $W^n_k \leq \overline{\mathcal{M}}^{2^k}$, from which we deduce a L^{2^k} bound for the approximate densities which is uniform in k, and finally the L^∞ bound by letting k tend to ∞.

The first step is the following result about the time evolution of V^n_{q+1}, proved in [5].

Proposition 4 *Let (H1)–(H5) be fulfilled, and let $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible mesh satisfying the nondegeneracy assumption* (6)*. Then there exist positive constants μ and ν such that for all $q \geq 1$, for all $n \geq 0$,*

$$\frac{1}{\Delta t}\left(V^{n+1}_{q+1} - V^n_{q+1}\right) + \frac{4q}{q+1}\gamma \sum_{\sigma\in\mathcal{E}}\left[\left(D_\sigma(N^{n+1}_M)^{\frac{q+1}{2}}\right)^2 + (D_\sigma\left(P^{n+1}_M)^{\frac{q+1}{2}}\right)^2\right]$$
$$\leq \mu q V^{n+1}_{q+1} + \nu m(\Omega), \tag{38}$$

where $\gamma \in (0,1]$ is the constant defined in (36).

Then, the aim is to control the term V^{n+1}_{q+1} appearing on the right-hand side of (38). To do this, we use the discrete Nash inequality [4, Corollary 4.5] which reads for functions $\chi_{\mathcal{M}}$ vanishing on a part of the boundary Γ^D as:

$$\left(\sum_{K\in\mathcal{T}} \mathrm{m}(K)\chi_K^2\right)^{1+\frac{2}{d}} \leq \frac{\tilde{C}}{\xi}\left(\sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma\chi)^2\right)\left(\sum_{K\in\mathcal{T}} \mathrm{m}(K)|\chi_K|\right)^{\frac{4}{d}},$$

where ξ is given in (5) and $\tilde{C}$ only depends on Ω and the space dimension d. Thanks to Young's inequality, it follows that for $\varepsilon > 0$, up to a change of the value of $\tilde{C}$,

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K)\chi_K^2 \leq \frac{\tilde{C}}{\varepsilon^{d/2}\xi^{d/2}} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K)|\chi_K|\right)^2 + \varepsilon \left(\sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma \chi)^2\right). \tag{39}$$

Applying this inequality to $\chi = \left(N_M^{n+1}\right)^{\frac{q+1}{2}}$ and $\chi = \left(P_M^{n+1}\right)^{\frac{q+1}{2}}$, we have

$$V_{q+1}^{n+1} \leq \frac{\tilde{C}}{(\varepsilon\xi)^{d/2}} \left(V_{\frac{q+1}{2}}^{n+1}\right)^2 + \varepsilon \sum_{\sigma\in\mathcal{E}} \left[\left(D_\sigma (N_M^{n+1})^{\frac{q+1}{2}}\right)^2 + \left(D_\sigma (P_M^{n+1})^{\frac{q+1}{2}}\right)^2\right]. \tag{40}$$

Arguing similarly as in [15] and using the fact that $\gamma \in (0, 1]$, we can find $A > 0$ depending only on μ such that

$$\frac{\gamma A}{q}\left(\mu q + \frac{\gamma A}{q}\right) \leq \frac{4\gamma q}{q+1}, \quad \forall q \geq 1.$$

Therefore, multiplying (40) by $\mu q + \varepsilon(q)$ with $\varepsilon(q) = \gamma A/q$ and adding the resulting equation to (38), we infer that

$$\frac{V_{q+1}^{n+1} - V_{q+1}^n}{\Delta t} \leq -\varepsilon(q)V_{q+1}^{n+1} + \nu\mathrm{m}(\Omega) + \frac{\tilde{C}}{\varepsilon(q)^{d/2}\xi^{d/2}} (\mu q + \varepsilon(q)) \left(V_{\frac{q+1}{2}}^{n+1}\right)^2. \tag{41}$$

We now use this estimate to prove the uniform bound on the approximate densities by a Moser iteration technique. The definitions of M and the initial condition ensure that $W_k^0 = 0$ for all $k \in \mathbb{N}$. Moreover, the discrete energy/energy dissipation inequality (34) ensures that $\mathbb{E}^n(\kappa) \leq C_{\mathbb{E}}$ for all $n \geq 0$ and applying the inequalities

$$\forall x, y > 0 \quad x \log \frac{x}{y} - x + y \geq (\sqrt{x} - \sqrt{y})^2 \geq \frac{x}{2} - y,$$

we deduce a uniform bound of W_0^n for all $n \geq 0$. With $q = 2^k - 1 = \zeta_k$ and $\varepsilon_k = \gamma A/\zeta_k$, we infer from (41) that

$$\frac{W_k^{n+1} - W_k^n}{\Delta t} \leq -\varepsilon_k W_k^{n+1} + \tilde{B}\left(\zeta_k^{d/2}(\zeta_k + \varepsilon_k)(W_{k-1}^{n+1})^2 + 1\right) \tag{42}$$

with

$$\tilde{B} = \gamma^{-d/2} \max\left\{\nu\mathrm{m}(\Omega), \frac{\tilde{C}}{\xi^{d/2}} A^{-d/2}, \frac{\tilde{C}}{\xi^{d/2}} A^{-d/2}\mu\right\}.$$

Setting $\overline{\mathcal{M}}_k := \sup_{n\geq 0} W_k^n$ and $\delta_k = \widetilde{B}\zeta_k^{d/2}(\zeta_k+\varepsilon_k)/\varepsilon_k$, we then have

$$W_k^n \leq \delta_k(\overline{\mathcal{M}}_{k-1}^2+1) \quad \forall n\geq 0. \tag{43}$$

Since $(W_0^n)_{n\geq 0}$ is uniformly bounded, we then define

$$\overline{\mathcal{M}} = \max(1, \overline{\mathcal{M}}_0) = \max\left(1, \sup_{n\geq 0} W_0^n\right) < +\infty.$$

Using (43), we obtain by induction that for $k\geq 0$,

$$W_k^n \leq 2\delta_k(2\delta_{k-1})^2\dots(2\delta_1)^{2^{k-1}}\overline{\mathcal{M}}^{2^k} \quad \forall n\geq 0,$$

remarking that $\overline{\mathcal{M}}_k = 2\delta_k(2\delta_{k-1})^2\dots(2\delta_1)^{2^{k-1}}\overline{\mathcal{M}}^{2^k} \geq 1$.
We now conclude as in [15] (see also [5]):

$$W_k^n \leq \left(2^{5+d}\frac{\tilde{B}}{A}\overline{\mathcal{M}}\right)^{2^k},$$

and taking the power $\frac{1}{2^k}$ of W_k^n we obtain that

$$\|N_{M,\mathcal{T}}^n\|_{L^{2^k}(\Omega)} \leq 2^{5+d}\frac{\tilde{B}}{A}\overline{\mathcal{M}}, \quad \|P_{M,\mathcal{T}}^n\|_{L^{2^k}(\Omega)} \leq 2^{5+d}\frac{\tilde{B}}{A}\overline{\mathcal{M}}, \quad \forall n\geq 0, \quad \forall k\in\mathbb{N}.$$

Passing to the limit $k\to\infty$ gives

$$\|N_{M,\mathcal{T}}^n\|_{L^\infty(\Omega)} \leq 2^{5+d}\frac{\tilde{B}}{A}\overline{\mathcal{M}}, \quad \|P_{M,\mathcal{T}}^n\|_{L^\infty(\Omega)} \leq 2^{5+d}\frac{\tilde{B}}{A}\overline{\mathcal{M}}, \quad \forall n\geq 0,$$

which concludes the proof of the uniform upper bound.

2.4 Proof of Proposition 1

The existence result exhibited in Proposition 1 is a consequence of the a priori estimates established in the previous sections for the solutions to $(\mathcal{S}_\kappa)$ for all $\kappa\in[0,1]$. To conclude the proof of the existence result, we apply a topological degree argument as presented for instance in [14,25].

Let $(N_K^0, P_K^0)_{K\in\mathcal{T}}$ be given by (9) and $(N_\sigma^n, P_\sigma^n)_{\sigma\in\mathcal{E}_{ext}^D, n\geq 0}$ be given by (11). We define the map $\mathcal{H}$ associated to the scheme $(\mathcal{S}_\kappa)$ in the following way:

$$\begin{aligned}\mathcal{H}:\quad &\mathbb{R}^{\theta\times N_T}\times\mathbb{R}^{\theta\times N_T}\times[0,1] \;\to \mathbb{R}^{\theta\times N_T}\times\mathbb{R}^{\theta\times N_T}\\ &\Big(\big(N_K^n,\ P_K^n\big)_{K\in\mathcal{T},\,1\leq n\leq N_T},\kappa\Big) \mapsto \Big(\big((\mathcal{H}_\kappa N)_K^n,\ (\mathcal{H}_\kappa P)_K^n\big)_{K\in\mathcal{T},\,1\leq n\leq N_T}\Big),\end{aligned}$$

where

$$(\mathcal{H}_\kappa N)_K^n = \mathrm{m}(K)\frac{N_K^{n+1} - N_K^n}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \widehat{\mathcal{F}}_{K,\sigma}^{n+1} + \kappa \mathrm{m}(K) R(N_K^{n+1,+}, P_K^{n+1,+}),$$

$$(\mathcal{H}_\kappa P)_K^n = \mathrm{m}(K)\frac{P_K^{n+1} - P_K^n}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} \widehat{\mathcal{G}}_{K,\sigma}^{n+1} + \kappa \mathrm{m}(K) R(N_K^{n+1,+}, P_K^{n+1,+}),$$

with

$$\widehat{\mathcal{F}}_{K,\sigma}^{n+1} = \tau_\sigma \left[B\left(-D_{K,\sigma}\Psi^{n+1}\right) N_K^{n+1,+} - B\left(D_{K,\sigma}\Psi^{n+1}\right) N_{K,\sigma}^{n+1,+}\right],$$
$$\widehat{\mathcal{G}}_{K,\sigma}^{n+1} = \tau_\sigma \left[B\left(D_{K,\sigma}\Psi^{n+1}\right) P_K^{n+1,+} - B\left(-D_{K,\sigma}\Psi^{n+1}\right) P_{K,\sigma}^{n+1,+}\right],$$

where $\Psi_{\mathcal{T}}^{n+1}$ satisfies:

$$\begin{cases} -\lambda^2 \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma}\Psi^{n+1} = \kappa \mathrm{m}(K)(P_K^{n+1} - N_K^{n+1} + C_K) \quad \forall K \in \mathcal{T}, \\ \Psi_\sigma^n = \Psi_\sigma^D \quad \forall \sigma \in \mathcal{E}_{ext}^D. \end{cases} \tag{44}$$

We define $\mathcal{K} := [0, E+1]^{2\theta\times N_T}$, where E is the uniform upper bound established in the previous section. This subset $\mathcal{K}$ of $\mathbb{R}^{2\theta\times N_T}$ is compact.

The application $\mathcal{H}$ is uniformly continuous on $\mathcal{K}\times[0,1]$, and since we proved that a solution $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{0\le n\le N_T}$ of the scheme $(\mathcal{S}_\kappa)$ satisfies

$$0 < N_K^n,\ P_K^n \le E \quad \forall K \in \mathcal{T}, \quad \forall n = 0, \ldots, N_T,$$

the nonlinear system

$$\mathcal{H}\left((N_K^n)_{K\in\mathcal{T},\,1\le n\le N_T}, (P_K^n)_{K\in\mathcal{T},\,1\le n\le N_T}, \kappa\right) = 0$$

cannot admit any solution on $\partial\mathcal{K}$. Therefore, the corresponding topological degree $\delta(\mathcal{H},\mathcal{K},\kappa)$ is constant with respect to κ.

For $\kappa = 0$, we obtain from (44) that, for all n, $\Psi_{\mathcal{T}}^{n+1}$ does not depend neither on n nor on N or P: it is the solution to the classical scheme for the Laplace equation. Moreover, as the densities are necessarily positive, the fluxes $\widehat{\mathcal{F}}_{K,\sigma}^{n+1}$ (respectively $\widehat{\mathcal{G}}_{K,\sigma}^{n+1}$) are linear combinations of N_K^{n+1} and the $N_{K,\sigma}^{n+1}$ (respectively of P_K^{n+1} and the $P_{K,\sigma}^{n+1}$). Then, the problem

$$\mathcal{H}\left((N_K^n)_{K\in\mathcal{T},\,1\le n\le N_T}, (P_K^n)_{K\in\mathcal{T},\,1\le n\le N_T}, 0\right) = 0$$

reduces to a linear invertible system, so that it admits a unique solution. It implies that $\delta(\mathcal{H},\mathcal{K},0) = 1$ and therefore that $\delta(\mathcal{H},\mathcal{K},1) = 1$. We deduce that the scheme $(\mathcal{S}_1)$ admits a solution and, due to the positivity established for the approximate densities, that $(\mathcal{S})$ admits a solution. This concludes the proof of Proposition 1.

3 Uniform-in-time positive lower bound

In this section, we now prove the uniform lower bound for the approximate densities $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n)_{n\geq 0}$ given by the scheme $(\mathcal{S})$, namely: there exists $D > 0$ as in Theorem 1 such that:

$$0 < D \leq N_K^n,\ P_K^n, \quad \forall K \in \mathcal{T}, \quad \forall n \geq 0. \tag{45}$$

To this end, we adapt to the discrete framework the proof done in [21, Lemma 3.6]. It consists in applying a Moser iteration technique on an appropriate function of the logarithm of the densities.

Let $\overline{m} := \max(-\log m, \log E)$, where E is the uniform upper bound of the approximate densities $(N_{\mathcal{T}}^n)_{n\geq 0}$, $(P_{\mathcal{T}}^n)_{n\geq 0}$. Using the function $w_{\overline{m}}$ defined on $\mathbb{R}_+^*$ by $w_{\overline{m}}(x) = -(\log x + \overline{m})^-$ (where $s^- = \min(s, 0)$), we can define

$$w_{\mathcal{T}}^n = w_{\overline{m}}(N_{\mathcal{T}}^n) = -\left(\log N_{\mathcal{T}}^n + \overline{m}\right)^- .$$

In order to prove that $(N_{\mathcal{T}}^n)_{n\geq 0}$ admits a uniform-in-time positive lower bound, we will in practice prove that $(w_{\mathcal{T}}^n)_{n\geq 0}$ admits a uniform-in-time upper bound. The uniform positive lower bound for $(P_{\mathcal{T}}^n)_{n\geq 0}$ can be established exactly in the same way. We start with the following preliminary result, which will be crucial to apply the Nash–Moser iteration technique.

Proposition 5 *Let (H1)–(H5) be fulfilled. Let $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible mesh of Ω satisfying (5) and (6), and $0 < \Delta t \leq 1$. Let $(N_{\mathcal{T}}^n, P_{\mathcal{T}}^n, \Psi_{\mathcal{T}}^n)_{n\geq 0}$ be a solution to the scheme $(\mathcal{S})$.*

Then there exist two positive constants μ and ν, depending only on the data, such that for all $q \geq 2$, for all $T > 0$:

$$\begin{aligned} &e^{t_{N_T+1}} \sum_{K\in\mathcal{T}} \mathrm{m}(K) \left(w_K^{N_T+1}\right)^q + \frac{q}{(q+1)^2}\gamma \sum_{n=0}^{N_T} \Delta t e^{t_n} \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma (w^{n+1})^{\frac{q+1}{2}}\right)^2 \\ &\quad \leq \mu q^{\frac{d}{2}+1} \sum_{n=0}^{N_T} \Delta t e^{t_n} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) \left(w_K^{n+1}\right)^{q/2}\right)^2 + \nu q \sum_{n=0}^{N_T} \Delta t e^{t_n}, \end{aligned} \tag{46}$$

where $\gamma \in (0, 1]$ is defined in (36).

Proof Multiplying the scheme (12) by $-(w_K^{n+1})^{q-1}\frac{1}{N_K^{n+1}}$ and summing over $K \in \mathcal{T}$, we get $T_1^n + T_2^n = T_3^n$, where

$$T_1^n = -\sum_{K\in\mathcal{T}} \mathrm{m}(K)\frac{N_K^{n+1}-N_K^n}{\Delta t}(w_K^{n+1})^{q-1}\frac{1}{N_K^{n+1}}, \tag{47}$$

$$T_2^n = \sum_{\sigma\in\mathcal{E}} \mathcal{F}_{K,\sigma}^{n+1} D_{K,\sigma}\Big((w^{n+1})^{q-1}\frac{1}{N^{n+1}}\Big), \tag{48}$$

$$T_3^n = \sum_{K\in\mathcal{T}} \mathrm{m}(K) R(N_K^{n+1}, P_K^{n+1})(w_K^{n+1})^{q-1}\frac{1}{N_K^{n+1}}. \tag{49}$$

Using assumption (4) on R, we can rewrite

$$R(N_K^{n+1}, P_K^{n+1})(w_K^{n+1})^{q-1} = R_0(N_K^{n+1}, P_K^{n+1})(N_K^{n+1}P_K^{n+1}-1)(w_K^{n+1})^{q-1}.$$

This term vanishes if $N_K^{n+1} \geq e^{-\overline{m}}$. But, if $N_K^{n+1} \leq e^{-\overline{m}}$, the definition of $\overline{m}$ and the upper bound on $P_{\mathcal{T}}^{n+1}$ ensure that:

$$N_K^{n+1}P_K^{n+1} - 1 \leq e^{-\overline{m}}E - 1 \leq 0.$$

Thanks to (H5), we deduce that $T_3^n \leq 0$.
Applying (69) from Lemma 3, we obtain that

$$T_1^n \geq \sum_{K\in\mathcal{T}} \mathrm{m}(K)\frac{(w_K^{n+1})^q - (w_K^n)^q}{q\Delta t}. \tag{50}$$

Thanks to (74) from Lemma 5, we get:

$$\begin{aligned} T_2^n \geq &\sum_{\sigma\in\mathcal{E}} \tau_\sigma D_{K,\sigma}\Psi^{n+1}\left(D_{K,\sigma}(w^{n+1})^{q-1} + \frac{1}{q}D_{K,\sigma}(w^{n+1})^q\right) \\ &+ \sum_{\sigma\in\mathcal{E}} \tau_\sigma B\left(D_\sigma\Psi^{n+1}\right)\left(\frac{4(q-1)}{q^2}\left(D_\sigma(w^{n+1})^{q/2}\right)^2 + \frac{1}{(q+1)^2}\left(D_\sigma(w^{n+1})^{\frac{q+1}{2}}\right)^2\right). \end{aligned} \tag{51}$$

Performing a discrete integration by parts on the first term of the right-hand-side and using the scheme (14) for Ψ, we obtain:

$$\begin{aligned} T_2^n \geq &\frac{1}{\lambda^2}\sum_{K\in\mathcal{T}} \mathrm{m}(K)\left((w_K^{n+1})^{q-1} + \frac{1}{q}(w_K^{n+1})^q\right)\left(P_K^{n+1} - N_K^{n+1} + C_K\right) \\ &+ \sum_{\sigma\in\mathcal{E}} \tau_\sigma B\left(D_\sigma\Psi^{n+1}\right)\left(\frac{4(q-1)}{q^2}\left(D_\sigma(w^{n+1})^{q/2}\right)^2 + \frac{1}{(q+1)^2}\left(D_\sigma(w^{n+1})^{\frac{q+1}{2}}\right)^2\right). \end{aligned} \tag{52}$$

We may now multiply the inequality $T_1^n + T_2^n \leq 0$ by $q\Delta t e^{t_n}$ and sum over $n \in [\![0, N_T]\!]$. Using that $w_K^0 = 0$, the convexity of $x \mapsto e^x$ and (50), we have:

$$\begin{aligned}
\sum_{n=0}^{N_T} q\Delta t e^{t_n} T_1^n &\geq \sum_{n=0}^{N_T} e^{t_n} \sum_{K\in\mathcal{T}} \mathrm{m}(K) \left((w_K^{n+1})^q - (w_K^n)^q \right) \\
&= \sum_{n=0}^{N_T} \sum_{K\in\mathcal{T}} \mathrm{m}(K) \left[e^{t_{n+1}} (w_K^{n+1})^q - e^{t_n} (w_K^n)^q - (e^{t_{n+1}} - e^{t_n})(w_K^{n+1})^q \right] \\
&\geq e^{t_{N_T+1}} \sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{N_T+1})^q - \sum_{n=0}^{N_T} \Delta t e^{t_{n+1}} \sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{n+1})^q.
\end{aligned} \tag{53}$$

From (52) and the bound (36), we deduce that

$$\begin{aligned}
\sum_{n=0}^{N_T} q\Delta t e^{t_n} T_2^n \geq \frac{1}{\lambda^2} \sum_{n=0}^{N_T} q\Delta t e^{t_n} \sum_{K\in\mathcal{T}} \mathrm{m}(K) &\left((w_K^{n+1})^{q-1} + \frac{1}{q} (w_K^{n+1})^q \right) \\
&\left(P_K^{n+1} - N_K^{n+1} + C_K \right) \\
&+ \gamma \sum_{n=0}^{N_T} q\Delta t e^{t_n} \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(\frac{4(q-1)}{q^2} \left(D_\sigma (w^{n+1})^{q/2} \right)^2 \right. \\
&\left. + \frac{1}{(q+1)^2} \left(D_\sigma (w^{n+1})^{\frac{q+1}{2}} \right)^2 \right).
\end{aligned} \tag{54}$$

But, since $|P_K^{n+1} - N_K^{n+1} + C_K| \leq 2E + \|C\|_\infty$ for all $K \in \mathcal{T}$, for all $n \geq 0$, and

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K) \left((w_K^{n+1})^{q-1} + \frac{1}{q} (w_K^{n+1})^q \right) \leq \sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{n+1})^q + \mathrm{m}(\Omega),$$

we obtain from (53) and (54) the following estimate:

$$\begin{aligned}
&e^{t_{N_T+1}} \sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{N_T+1})^q \\
&\quad + \gamma \sum_{n=0}^{N_T} q\Delta t e^{t_n} \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(\frac{4(q-1)}{q^2} \left(D_\sigma (w^{n+1})^{q/2} \right)^2 + \frac{1}{(q+1)^2} \left(D_\sigma (w^{n+1})^{\frac{q+1}{2}} \right)^2 \right) \\
&\leq \left(e^{\Delta t} + \frac{2E + \|C\|_\infty}{\lambda^2} q \right) \sum_{n=0}^{N_T} \Delta t e^{t_n} \sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{n+1})^q \\
&\quad + q \frac{2E + \|C\|_\infty}{\lambda^2} \mathrm{m}(\Omega) \sum_{n=0}^{N_T} \Delta t e^{t_n}.
\end{aligned}$$

As $\Delta t \leq 1$, let us set

$$\nu = e^1 + \frac{2E + \|C\|_\infty}{\lambda^2} \max(1, \mathrm{m}(\Omega))$$

Using that $q \geq 2$ and applying inequality (39) with $\chi = (w^{n+1})^{q/2}$ and $\varepsilon = \frac{\gamma}{\nu} \frac{4(q-1)}{q^2}$, we finally obtain (46) with

$$\mu = \frac{\nu^{1+\frac{d}{2}} \tilde{C}}{(2\gamma\xi)^{\frac{d}{2}}},$$

independent of q. □

We are now going to apply the Moser iteration technique. Multiplying (46) by $e^{-t_{N_T+1}}$, using that $q^{\frac{d}{2}} \geq 1$ and $x^2 + y^2 \leq (x+y)^2$ for all $x,\ y \geq 0$, we obtain

$$\sum_{K \in \mathcal{T}} \mathrm{m}(K)(w_K^{N_T+1})^q \leq \omega q^{\frac{d}{2}+1} e^{-t_{N_T+1}} \sum_{n=0}^{N_T} \Delta t e^{t_n} \left(\sum_{K \in \mathcal{T}} \mathrm{m}(K)(w_K^{n+1})^{\frac{q}{2}} + 1 \right)^2, \quad (55)$$

with $\omega = \max(\mu, \nu)$.

Let us define

$$Z_k^n := \sum_{K \in \mathcal{T}} \mathrm{m}(K)(w_K^{n+1})^{2^k}, \quad \forall k \geq 1, \quad \forall n \geq 0.$$

We set

$$b_k := \sup_{n \geq 0} Z_k^n + 1.$$

To conclude the proof of the positive lower bound (45), it remains to establish the following result.

Proposition 6 *Under the assumptions of Proposition 5, we have*

$$b_k \leq \left(8\omega 2^d b_1\right)^{2^k}, \quad \forall k \geq 2. \quad (56)$$

Moreover, there exists a constant $\mathcal{Z}$ independent of T and δ such that:

$$b_1 \leq \mathcal{Z} + 1 < +\infty. \quad (57)$$

Proof For all $k \geq 1$, taking $q = 2^k$ in (55) leads to

$$Z_k^{N_T} \leq \omega (2^{\frac{d}{2}+1})^k e^{-t_{N_T+1}} b_{k-1}^2 \sum_{n=0}^{N_T} \Delta t e^{t_n}.$$

Using the convexity of exp, we have

$$\sum_{n=0}^{N_T} \Delta t e^{t_n} \leq \sum_{n=0}^{N_T} (e^{t_{n+1}} - e^{t_n}) \leq e^{t_{N_T+1}},$$

and then we deduce that

$$b_k \leq 2\omega (2^{\frac{d}{2}+1})^k b_{k-1}^2.$$

We finally establish (56) by induction.

It remains now to prove the initialization of the Moser iteration, namely the fact that $b_1 = \sup_{n\geq 0} Z_1^n + 1$ is bounded. We start again from (46), with $q = 2$:

$$e^{t_{N_T+1}} Z_1^{N_T} + \frac{2}{9}\gamma \sum_{n=0}^{N_T} \Delta t e^{t_n} \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma (w^{n+1})^{\frac{3}{2}}\right)^2$$
$$\leq \mu 2^{\frac{d}{2}+1} \sum_{n=0}^{N_T} \Delta t e^{t_n} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) w_K^{n+1}\right)^2 + 2\nu \sum_{n=0}^{N_T} \Delta t e^{t_n}. \tag{58}$$

Using Hölder inequality, we have

$$\left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) w_K^{n+1}\right)^2 \leq \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) (w_K^{n+1})^3\right)^{\frac{2}{3}} \mathrm{m}(\Omega)^{\frac{4}{3}}. \tag{59}$$

Moreover, we can apply the discrete Poincaré inequality [4, Theorem 4.3] since $w_{\mathcal{M}}^{n+1} = 0$ on Γ^D: there exists a constant $C_{\Omega,\xi} > 0$ only depending on Ω and the regularity parameter ξ such that

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{n+1})^3 = \sum_{K\in\mathcal{T}} \mathrm{m}(K) \left((w_K^{n+1})^{\frac{3}{2}}\right)^2 \leq C_{\Omega,\xi} \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma (w^{n+1})^{\frac{3}{2}}\right)^2. \tag{60}$$

Gathering (59) and (60), we obtain

$$\mu 2^{\frac{d}{2}+1} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) w_K^{n+1}\right)^2 \leq \theta \left(\sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma (w^{n+1})^{\frac{3}{2}}\right)^2\right)^{\frac{2}{3}},$$

where $\theta = \mu 2^{\frac{d}{2}+1} \mathrm{m}(\Omega)^{\frac{4}{3}} C_{\Omega,\xi}^{\frac{2}{3}}$, and Young inequality gives

$$\mu 2^{\frac{d}{2}+1} \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) w_K^{n+1}\right)^2 \leq \frac{1}{3}\varepsilon^{-2}\theta^3 + \frac{2}{3}\varepsilon \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma (w^{n+1})^{\frac{3}{2}}\right)^2.$$

Taking $\varepsilon = \gamma/3$, (58) becomes

$$e^{t_{N_T+1}} Z_1^{N_T} \leq \mathcal{Z} \sum_{n=0}^{N_T} \Delta t e^{t_n},$$

with $\mathcal{Z} = 3\theta^3/\gamma^2 + 2\nu$, and finally multiplying by $e^{-t_{N_T+1}}$, we obtain

$$Z_1^{N_T} \leq \mathcal{Z},$$

which gives the desired result (57) since $\mathcal{Z}$ is independent of T and δ. □

Equipped with this result, we can now conclude the proof. Taking the power $1/2^k$ in (56) and using the definition of b_k, we obtain

$$\left(\sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_K^{N_T+1})^{2^k} \right)^{1/2^k} \leq 8\omega 2^d b_1, \quad \forall k \geq 1, \quad \forall N_T \geq 1.$$

Finally, since b_1 is bounded by a constant, we obtain by letting $k \to \infty$ that

$$\|w_{\mathcal{T}}^n\|_\infty \leq 8\omega 2^d b_1 \quad \forall n \geq 0,$$

which gives the uniform-in-time upper bound for $(w_{\mathcal{T}}^n)_{n\geq 0}$ and then the uniform-in-time positive lower bound for $(N_{\mathcal{T}}^n)_{n\geq 0}$. The hole density $(P_{\mathcal{T}}^n)_{n\geq 0}$ can be treated exactly in the same way.

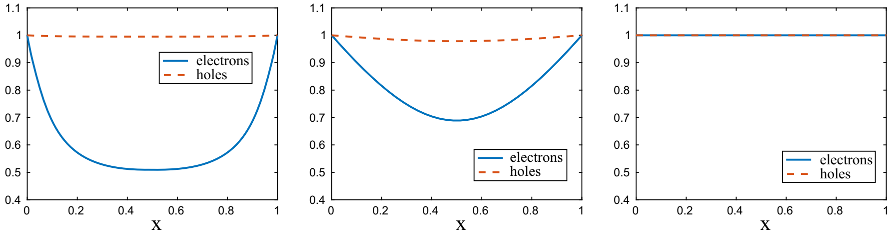
In the end, gathering this with the results established in Sect. 2, the proof of Theorem 1 is achieved.

4 Numerical results

In this section, we present some numerical experiments that illustrate the behavior of the upper and lower bounds of approximate densities for different type of doping profiles. We consider 1D test cases with $\Omega =]0, 1[$. The space step is taken uniform and fixed to $h = 0.01$, and the time step to $\Delta t = 0.01$. In all the simulations, the recombination–generation term is taken equal to 0. We fix $\lambda^2 = 1$ everywhere, except for the last part of Case 1 where we take $\lambda^2 = 10^{-4}$ to illustrate the influence of the Debye length on the upper and lower bounds. The Dirichlet boundary conditions N^D and P^D for the densities are computed from Ψ^D using Hypothesis (H3) with $\alpha^D = 0$.
Case 1 Initial conditions are given by:

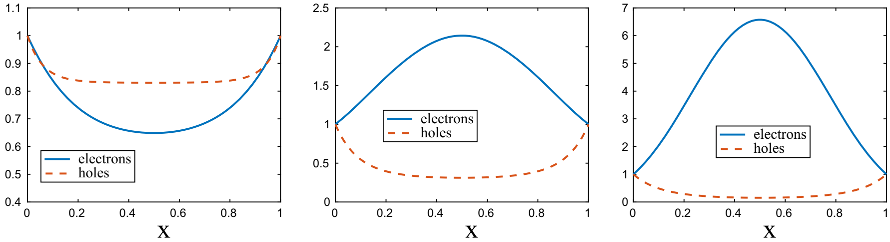
$$N_0(x) = 0.5 \quad \text{and} \quad P_0(x) = 1 \quad \forall x \in]0, 1[,$$

and the Dirichlet boundary conditions for Ψ are $\Psi^D(0) = 0 = \Psi^D(1)$.



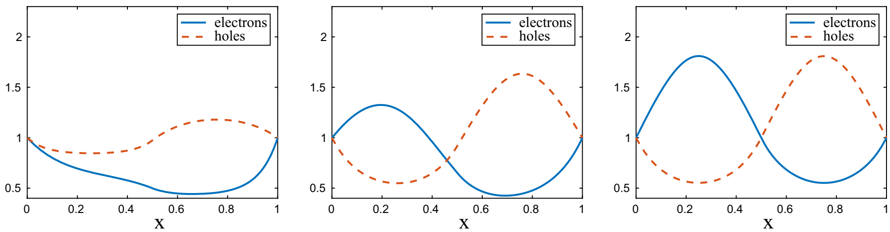
(a) $T = 0.01$ **(b)** $T = 0.07$ **(c)** $T = 5$

Fig. 2 Evolution of approximate densities in Case 1, for $C = 0$



(a) $T = 0.01$ **(b)** $T = 0.07$ **(c)** $T = 5$

Fig. 3 Evolution of approximate densities in Case 1, for $C = 20$



(a) $T = 0.01$ **(b)** $T = 0.07$ **(c)** $T = 5$

Fig. 4 Evolution of approximate densities in Case 1, for C piecewise constant with $\|C\|_\infty = 20$

In Fig. 2, we present the approximate densities of electrons and holes in the case of a zero doping profile, computed at different times: $T = 0.01$, $T = 0.07$ and $T = 5$. As expected, the maximum principle is satisfied in this case.

Figure 3 is devoted to the case of a constant doping profile $C(x) = 20$ and Fig. 4 to the case of a doping profile given by $C(x) = 20$ if $x \in [0, 0.5[$ and $C(x) = -20$ if $x \in [0.5, 1]$. We observe that the maximum principle is no more satisfied in this case. Finally, we investigate the influence of the doping profile on the upper and lower bounds of approximate densities. In Figs. 5 and 6, we present the upper and lower bounds as functions of $\|C\|_\infty$. The lower bound is represented in log scale. Figure 5 corresponds to

$$C(x) = k \quad \text{for } x \in [0, 1], \quad \text{with } k = 0, \ldots, 30, \tag{61}$$

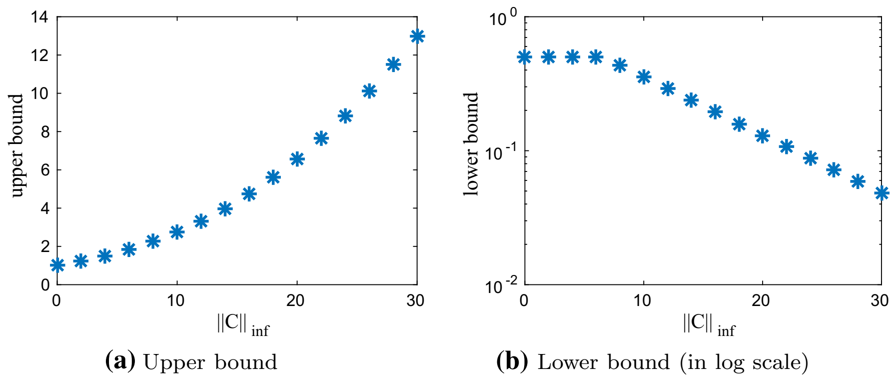


Fig. 5 Upper and lower bounds as functions of $\|C\|_\infty$ in Case 1, with C given by (61)

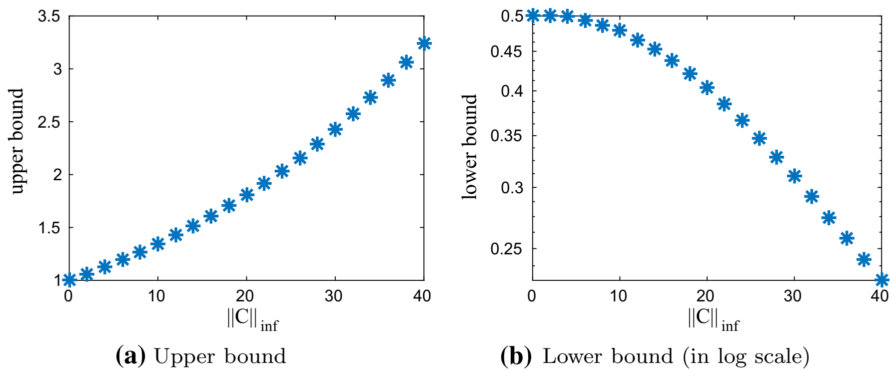


Fig. 6 Upper and lower bounds as functions of $\|C\|_\infty$ in Case 1, with C given by (62)

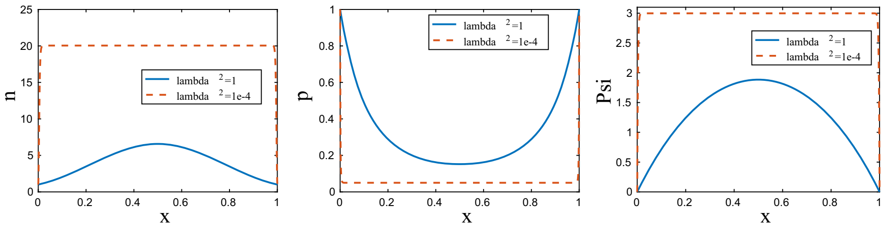
and Fig. 6 to

$$C(x) = \begin{cases} k & \text{for } x \in [0, 0.5[\\ -k & \text{for } x \in [0.5, 1] \end{cases}, \quad \text{with } k = 0, \ldots, 40. \tag{62}$$

Depending on the chosen doping profile, we observe that the obtained upper bound E (resp. lower bound D) can be larger than the upper bound of data $M = 1$ here (resp. lower bound of data $m = 0.5$ here).

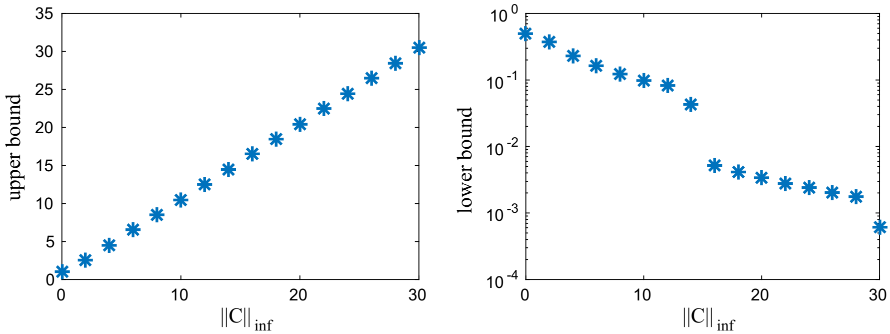
Finally, we consider the same test case but with $\lambda^2 = 10^{-4}$. Due to the stiffness occurring with this choice, we have to choose an adaptative time step to ensure the convergence of the Newton's method used to solve our nonlinear implicit scheme. Indeed, this stiffness comes from the fact that the considered boundary conditions are not compatible with the quasi-neutral limit (the quasi-neutrality relation writes $P - N + C = 0$, which is not satisfied for $C \neq 0$ at the boundary).

We represent in Fig. 7 the solutions obtained at final time $T = 5$ for a constant doping profile $C(x) = 20$ with either $\lambda^2 = 1$ or $\lambda^2 = 10^{-4}$. Finally in Fig. 8, we present the upper and lower bounds obtained with $\lambda^2 = 10^{-4}$ for constant doping



(a) Electron density **(b)** Hole density **(c)** Electrostatic potential

Fig. 7 Comparison of solutions obtained in Case 1 at $T = 5$ with $C = 20$ and $\lambda^2 = 1$ or $\lambda^2 = 10^{-4}$



(a) Upper bound **(b)** Lower bound (in log scale)

Fig. 8 Upper and lower bounds as functions of $\|C\|_\infty$ in Case 1, with C given by (61) and $\lambda^2 = 10^{-4}$

profiles defined by (61). Comparing the results obtained with those presented in Fig. 5, we clearly remark the influence of the Debye length λ^2 on the upper and lower bounds of densities.

Case 2 Initial conditions are now given by

$$N_0(x) = \begin{cases} 0.1 & \text{if } 0 < x \leq 0.8 \\ 1 & \text{if } 0.8 < x < 1 \end{cases}, \quad P_0(x) = \begin{cases} 1 & \text{if } 0 < x \leq 0.7 \\ 0.1 & \text{if } 0.7 < x < 1 \end{cases}.$$

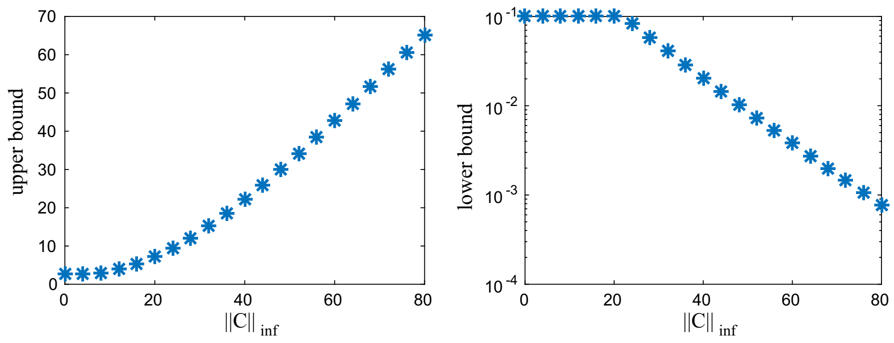
The boundary conditions for Ψ are $\Psi^D(0) = -1$ and $\Psi^D(1) = 1$.

As before, we represent the upper and lower bounds of the densities as functions of $\|C\|_\infty$, in Fig. 9 for a doping profile given by

$$C(x) = 2k \quad \text{for } x \in [0, 1], \quad \text{with } k = 0, \ldots, 40, \tag{63}$$

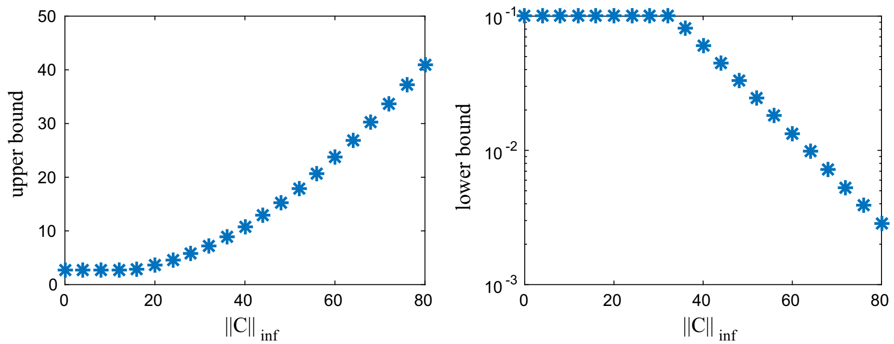
and in Fig. 10 for a doping profile given by

$$C(x) = \begin{cases} 2k & \text{for } x \in [0, 0.7[\\ -2k & \text{for } x \in [0.7, 1] \end{cases}, \quad \text{with } k = 0, \ldots, 40. \tag{64}$$



(a) Upper bound **(b)** Lower bound (in log scale)

Fig. 9 Upper and lower bounds as functions of $\|C\|_\infty$ in Case 2, with C given by (63)



(a) Upper bound **(b)** Lower bound (in log scale)

Fig. 10 Upper and lower bounds as functions of $\|C\|_\infty$ in Case 2, with C given by (64)

We observe that the upper and lower bounds obtained for a same test case depend strongly on the chosen doping profile. The upper bound is a nondecreasing function of $\|C\|_\infty$ whereas the lower bound is a nonincreasing function of $\|C\|_\infty$. The lower bound remains always positive (despite it can be small).

5 Conclusion

In this article, we establish existence of an approximate solution of the Van Roosbroeck's drift–diffusion system obtained with an implicit in time Scharfetter–Gummel scheme. Moreover, we prove that the obtained approximate densities satisfy uniform-in-time positive upper and lower bounds. Our proof relies on the application of a topological degree argument which requires some *a priori* estimates. The discrete energy/energy dissipation inequality (33) is a cornerstone in this work. Such inequality can be obtained for slightly different models and/or discretizations, leading to possible generalizations of our results. We list below some of them.

Models with variable mobilities The original Van Roosbroeck's model [34] includes variable mobilities and can be written, using Einstein relations, as:

$$\begin{cases} \partial_t N + \operatorname{div}\left(\mu_N(-\nabla N + N\nabla\Psi)\right) = -R(N,P), \\ \partial_t P + \operatorname{div}\left(\mu_P(-\nabla P - P\nabla\Psi)\right) = -R(N,P), \\ -\lambda^2\Delta\Psi = P - N + C, \end{cases} \tag{65}$$

where μ_N and μ_P are positive continuous functions of the electric field $\nabla\Psi$. Such variable mobilities model was for example studied in [21], and a semidiscretization in time was also considered in [13]. Our result can be easily generalized to this model. Indeed, using the boundedness of the discrete electric field (37), we obtain that there exists positive constants $\mu_\star$ and $\mu^\star$ such that:

$$0 < \mu_\star \leq \mu_N,\ \mu_P \leq \mu^\star,$$

and then our proofs can be straightforwardly extended to a discretization of this model (65).

Models with nonlinear diffusion In this paper, we only consider the classical drift–diffusion model based on Boltzmann statistics. However, other statistics can be necessary to describe relevantly the behavior of the considered semiconductor device, leading to a modification of the diffusive terms, which become nonlinear. Under some assumptions on the nonlinearity, the discrete energy/energy estimate (33) can be established for a generalized Scharfetter–Gummel scheme [3, Proposition 3.2]. However it seems difficult for the moment to obtain the other results (in particular the technical result given in Lemma 5) in the nonlinear setting.

Other finite volume discretizations In view of [9], extension of our work to a larger class of two-point monotone fluxes seems possible. Indeed, in this paper, a discrete entropy/entropy dissipation estimate is established both for Fokker–Planck equations (Theorem 2.7) and porous media equations (Theorem 3.2), for a family of B-schemes including upwind, centered and Scharfetter–Gummel schemes. The result is not yet proved for the drift–diffusion system, but it could be a natural extension of this work.

Explicit in time discretizations Here we only considered a backward Euler time discretization. In [18, Theorem 4.4], a discrete entropy/entropy dissipation estimate is proved for an explicit in time finite volume scheme discretizing a class of nonlinear parabolic equations, under a CFL condition. However, it seems difficult for the moment to adapt our result to such a time discretization, and even more for high order methods, since it will lead to treat a lot of residual terms coming from the explicit in time discretization.

Appendix: Some technical results

In this Appendix, we detail some technical results which we use in the paper. There are first functional inequalities and then some properties of the numerical fluxes.

We define $x^+ = \max(x, 0)$ and $x^- = \min(x, 0)$ for all $x \in \mathbb{R}$. Let us first recall some elementary inequalities:

$$\forall x, y \in \mathbb{R}, \forall q \geq 1, \quad x\left((x^+)^q - (y^+)^q\right) \geq x^+\left((x^+)^q - (y^+)^q\right), \tag{66}$$

$$\forall x, y \geq 0, \forall \alpha, \beta > 0 \quad (y^\alpha - x^\alpha)(y^\beta - x^\beta) \geq \frac{4\alpha\beta}{(\alpha+\beta)^2}\left(y^{\frac{\alpha+\beta}{2}} - x^{\frac{\alpha+\beta}{2}}\right)^2, \tag{67}$$

$$\forall x, y \geq 0, \forall q \geq 2, \quad y^q - x^q \geq q x^{q-1}(y - x) \tag{68}$$

For $\overline{m} \in \mathbb{R}$, we can define the function $w_{\overline{m}}$ by $w_{\overline{m}}(x) = (\log x + \overline{m})^-$ for all $x \in \mathbb{R}_+^*$. This function is widely used for the proof of the uniform-in-time positive lower bound in Sect. 3. We give in Lemma 3 some properties of the function $w_{\overline{m}}$.

Lemma 3 *Let $\overline{m} \in \mathbb{R}$, the function $w_{\overline{m}}$ defined by $w_{\overline{m}}(x) = -(\log x + \overline{m})^-$ for all $x \in \mathbb{R}_+^*$ verifies the following inequalities:*

- *For all $q \geq 2$, for all $x,\ y > 0$,*

$$-\frac{x-y}{x}\big(w_{\overline{m}}(x)\big)^{q-1} \geq \frac{1}{q}\Big(\big(w_{\overline{m}}(x)\big)^q - \big(w_{\overline{m}}(y)\big)^q\Big). \tag{69}$$

- *For all $q \geq 2$, for all $x,\ y > 0$,*

$$x\left(\frac{(w_{\overline{m}}(y))^{q-1}}{y} - \frac{(w_{\overline{m}}(x))^{q-1}}{x}\right) \geq (w_{\overline{m}}(y))^{q-1} - (w_{\overline{m}}(x))^{q-1} + \frac{1}{q}\left((w_{\overline{m}}(y))^q - (w_{\overline{m}}(x))^q\right). \tag{70}$$

Proof We start with the proof of (69). It is trivial when $x = y$. We consider the case where $x \neq y$. We remark that:

$$\begin{aligned}
&-(x-y)\big(w_{\overline{m}}(x)\big)^{q-1} \\
&\quad = -\frac{x-y}{\log x - \log y}\big(\log x - \log y\big)\big(w_{\overline{m}}(x)\big)^{q-1} \\
&\quad = \frac{x-y}{\log x - \log y}\Big(-(\log x + \overline{m})^+ + w_{\overline{m}}(x) + (\log y + \overline{m})^+ - w_{\overline{m}}(y)\Big)\big(w_{\overline{m}}(x)\big)^{q-1}.
\end{aligned}$$

Therefore,

$$-(x-y)\big(w_{\overline{m}}(x)\big)^{q-1} \geq \frac{x-y}{\log x - \log y}\big(w_{\overline{m}}(x) - w_{\overline{m}}(y)\big)\big(w_{\overline{m}}(x)\big)^{q-1}.$$

But, on one hand the function $w_{\overline{m}}$ is a nonincreasing function and on the other hand, we have:

$$\frac{1}{x}\frac{x-y}{\log x - \log y} > 1 \Longleftrightarrow 0 < x < y.$$

This yields

$$-\frac{x-y}{x}\big(w_{\overline{m}}(x)\big)^{q-1}\geq \big(w_{\overline{m}}(x)-w_{\overline{m}}(y)\big)\big(w_{\overline{m}}(x)\big)^{q-1}.$$

The inequality (69) is then deduced from (68).
Let us now prove (70). We first remark that

$$x\left(\frac{(w_{\overline{m}}(y))^{q-1}}{y}-\frac{(w_{\overline{m}}(x))^{q-1}}{x}\right)=(w_{\overline{m}}(y))^{q-1}-(w_{\overline{m}}(x))^{q-1}+(w_{\overline{m}}(y))^{q-1}\left(\frac{x}{y}-1\right).$$

Thus, we just need to prove:

$$(w_{\overline{m}}(y))^{q-1}\left(\frac{x}{y}-1\right)\geq\frac{1}{q}\Big((w_{\overline{m}}(y))^{q}-(w_{\overline{m}}(x))^{q}\Big),\ \forall x,y>0. \tag{71}$$

If $y\geq e^{-\overline{m}}$, $w_{\overline{m}}(y)=0$ and the result holds for all $x>0$. We consider now the case where $y<e^{-\overline{m}}$. As a direct consequence of (68), we get:

$$\Big(\big(w_{\overline{m}}(y)\big)^{q}-\big(w_{\overline{m}}(x)\big)^{q}\Big)\leq q\big(w_{\overline{m}}(y)\big)^{q-1}\big(w_{\overline{m}}(y)-w_{\overline{m}}(x)\big).$$

But, for all $x>0$, we have:

$$w_{\overline{m}}(y)-w_{\overline{m}}(x)\leq-\log y+\log x\leq\frac{x-y}{y},$$

which yields (71) and therefore (70). □

We now establish some properties satisfied by the numerical fluxes. Lemma 4 is crucial for the proof of Proposition 4, while Lemma 5 is used in the proof of Proposition 5.

Lemma 4 *Let $q\geq 1$. The numerical fluxes defined by (15), (16) and (17) verify that for all $K\in\mathcal{T}$, for all $\sigma\in\mathcal{E}_K$, for all $n\geq 0$,*

$$\begin{aligned}\mathcal{F}_{K,\sigma}^{n+1}D_{K,\sigma}(N_M^{n+1})^q\leq&-\frac{4q}{(q+1)^2}\tau_\sigma B(D_\sigma\Psi^{n+1})\left(D_{K,\sigma}(N_M^{n+1})^{\frac{q+1}{2}}\right)^2\\&+\frac{q}{q+1}\tau_\sigma D_{K,\sigma}\Psi^{n+1}D_{K,\sigma}(N_M^{n+1})^{q+1}\\&+M\tau_\sigma D_{K,\sigma}\Psi^{n+1}D_{K,\sigma}(N_M^{n+1})^q,\end{aligned}\tag{72a}$$

$$\begin{aligned}\mathcal{G}_{K,\sigma}^{n+1}D_{K,\sigma}(P_M^{n+1})^q\leq&-\frac{4q}{(q+1)^2}\tau_\sigma B(D_\sigma\Psi^{n+1})\left(D_{K,\sigma}(P_M^{n+1})^{\frac{q+1}{2}}\right)^2\\&-\frac{q}{q+1}\tau_\sigma D_{K,\sigma}\Psi^{n+1}D_{K,\sigma}(P_M^{n+1})^{q+1}\\&-M\tau_\sigma D_{K,\sigma}\Psi^{n+1}D_{K,\sigma}(P_M^{n+1})^q.\end{aligned}\tag{72b}$$

Proof We prove only inequality (72a) since (72b) can be deduced by replacing $D_{K,\sigma}\Psi^{n+1}$ by $-D_{K,\sigma}\Psi^{n+1}$. Using the property $B(x) - B(-x) = -x$ satisfied by the function B, we can rewrite the fluxes $\mathcal{F}_{K,\sigma}^{n+1}$ under two different forms:

$$\mathcal{F}_{K,\sigma}^{n+1} = \tau_\sigma \left(D_{K,\sigma}\Psi^{n+1} N_K^{n+1} - B(D_{K,\sigma}\Psi^{n+1}) D_{K,\sigma} N^{n+1} \right) \tag{73a}$$

$$= \tau_\sigma \left(D_{K,\sigma}\Psi^{n+1} N_{K,\sigma}^{n+1} - B(-D_{K,\sigma}\Psi^{n+1}) D_{K,\sigma} N^{n+1} \right). \tag{73b}$$

With the formulation (73a), we write:

$$\begin{aligned}\mathcal{F}_{K,\sigma}^{n+1} D_{K,\sigma}(N_M^{n+1})^q = \tau_\sigma \Big(& D_{K,\sigma}\Psi^{n+1}(N_K^{n+1} - M) D_{K,\sigma}(N_M^{n+1})^q \\ & + M D_{K,\sigma}\Psi^{n+1} D_{K,\sigma}(N_M^{n+1})^q \\ & - B(D_{K,\sigma}\Psi^{n+1}) D_{K,\sigma} N^{n+1} D_{K,\sigma}(N_M^{n+1})^q \Big).\end{aligned}$$

But, using (66) and (67), we get:

$$\begin{aligned}(N_K^{n+1} - M) D_{K,\sigma}(N_M^{n+1})^q &\le \frac{q}{q+1} D_{K,\sigma}(N_M^{n+1})^{q+1}, \\ D N_{K,\sigma}^{n+1} D_{K,\sigma}(N_M^{n+1})^q &\ge \frac{4q}{(q+1)^2}\left(D_{K,\sigma}(N_M^{n+1})^{\frac{q+1}{2}} \right)^2.\end{aligned}$$

Moreover, B is a nonnegative function. Then, we deduce (72a) if $D_{K,\sigma}\Psi^{n+1} \ge 0$. The same result is obtained when $D_{K,\sigma}\Psi^{n+1} \le 0$ but starting with (73b) instead of (73a). □

Lemma 5 *Let $q \ge 2$. Let $\overline{m} \in \mathbb{R}$, we set $w_K^{n+1} = w_{\overline{m}}(N_K^{n+1})$ for all $K \in \mathcal{T}$, for all $n \ge 0$. The numerical fluxes defined by (15) and (17) verify that for all $K \in \mathcal{T}$, for all $\sigma \in \mathcal{E}_K$, for all $n \ge 0$,*

$$\begin{aligned}&\mathcal{F}_{K,\sigma}^{n+1} D_{K,\sigma}\left((w^{n+1})^{q-1} \frac{1}{N^{n+1}} \right) \\ &\ge \tau_\sigma D_{K,\sigma}\Psi^{n+1} \left(D_{K,\sigma}(w^{n+1})^{q-1} + \frac{1}{q} D_{K,\sigma}(w^{n+1})^q \right) \\ &\quad + \tau_\sigma B\left(D_\sigma \Psi^{n+1} \right) \left(\frac{4(q-1)}{q^2}\left(D_\sigma (w^{n+1})^{q/2} \right)^2 + \frac{1}{(q+1)^2}\left(D_\sigma (w^{n+1})^{\frac{q+1}{2}} \right)^2 \right).\end{aligned} \tag{74}$$

Proof We first assume that $D_{K,\sigma}\Psi^{n+1} \ge 0$. Using formulation (73a), we write

$$\mathcal{F}_{K,\sigma}^{n+1} D_{K,\sigma}\left((w^{n+1})^{q-1} \frac{1}{N^{n+1}} \right) = R_1 + R_2,$$

with

$$R_1 = -\tau_\sigma B\left(D_\sigma \Psi^{n+1}\right) D_{K,\sigma} N^{n+1} D_{K,\sigma}\left((w^{n+1})^{q-1}\frac{1}{N^{n+1}}\right),$$
$$R_2 = \tau_\sigma D_{K,\sigma}\Psi^{n+1} N_K^{n+1} D_{K,\sigma}\left((w^{n+1})^{q-1}\frac{1}{N^{n+1}}\right).$$

We treat R_1 following the same computations as those used in [17, proof of Theorem 4] for the diffusion term. More precisely, we have

$$R_1 = \tau_\sigma B\left(D_\sigma \Psi^{n+1}\right)(R_{11} + R_{12}),$$

with

$$R_{11} = -D_{K,\sigma} N^{n+1}\frac{1}{2} D_{K,\sigma}\left((w^{n+1})^{q-1}\right)\left(\frac{1}{N_K^{n+1}} + \frac{1}{N_{K,\sigma}^{n+1}}\right),$$
$$R_{12} = -D_{K,\sigma} N^{n+1}\frac{1}{2} D_{K,\sigma}\left(\frac{1}{N^{n+1}}\right)\left((w_K^{n+1})^{q-1} + (w_{K,\sigma}^{n+1})^{q-1}\right).$$

According to [17, Lemma 7], we can rewrite R_{11} and R_{12} respectively as:

$$R_{11} = -f\left(D_{K,\sigma}\left(\log N^{n+1}\right)\right) D_{K,\sigma}\left(\log N^{n+1} + \overline{m}\right) D_{K,\sigma}(w^{n+1})^{q-1},$$
$$R_{12} = g\left(D_{K,\sigma}\left(\log N^{n+1}\right)\right)\left(D_{K,\sigma}\left(\log N^{n+1} + \overline{m}\right)\right)^2 \frac{1}{2}\left((w_K^{n+1})^{q-1} + (w_{K,\sigma}^{n+1})^{q-1}\right),$$

with

$$f(z) = \frac{(e^z - 1)(e^{-z} + 1)}{2z} \geq 1, \quad \forall z \in \mathbb{R},$$
$$g(z) = -\frac{(e^z - 1)(e^{-z} - 1)}{z^2} \geq 1, \quad \forall z \in \mathbb{R}.$$

Moreover, using the definition of $w_{\mathcal{T}}^{n+1}$ and (67) with $\alpha = 1$ and $\beta = q - 1$, we have:

$$\begin{aligned}
-D_{K,\sigma}\left(\log N^{n+1} + \overline{m}\right) D_{K,\sigma}(w^{n+1})^{q-1} &= -D_{K,\sigma}\left((\log N^{n+1} + \overline{m})^+\right) D_{K,\sigma}(w^{n+1})^{q-1} \\
&\quad + D_{K,\sigma}(w^{n+1}) D_{K,\sigma}(w^{n+1})^{q-1} \\
&\geq \frac{4(q-1)}{q^2}\left(D_{K,\sigma}(w^{n+1})^{q/2}\right)^2.
\end{aligned}$$

Then we get

$$R_{11} \geq \frac{4(q-1)}{q^2} \left(D_{K,\sigma} (w^{n+1})^{q/2} \right)^2. \tag{75}$$

We also have

$$R_{12} \geq \frac{1}{2} \left(D_{K,\sigma} w^{n+1} \right)^2 \left((w_K^{n+1})^{q-1} + (w_{K,\sigma}^{n+1})^{q-1} \right),$$

and since for all $x,\ y \geq 0$ we have, as shown in [17, Lemma 6],

$$(x-y)^2 (x^{q-1} + y^{q-1}) \geq \frac{2}{(q+1)^2} \left(x^{\frac{q+1}{2}} - y^{\frac{q+1}{2}} \right)^2,$$

which yields

$$R_{12} \geq \frac{1}{(q+1)^2} \left(D_{K,\sigma} (w^{n+1})^{\frac{q+1}{2}} \right)^2. \tag{76}$$

Gathering (75) and (76), we finally deduce that

$$R_1 \geq \tau_\sigma B \left(D_\sigma \Psi^{n+1} \right) \left(\frac{4(q-1)}{q^2} \left(D_{K,\sigma} (w^{n+1})^{q/2} \right)^2 + \frac{1}{(q+1)^2} \left(D_{K,\sigma} (w^{n+1})^{\frac{q+1}{2}} \right)^2 \right). \tag{77}$$

The term R_2 is now treated using (70) from Lemma 3 with $x = N_K^{n+1}$ and $y = N_{K,\sigma}^{n+1}$ (we still assume that $D_{K,\sigma} \Psi^{n+1} \geq 0$). We get:

$$R_2 \geq \tau_\sigma D_{K,\sigma} \Psi^{n+1} \left(D_{K,\sigma} (w^{n+1})^{q-1} + \frac{1}{q} D_{K,\sigma} (w^{n+1})^q \right). \tag{78}$$

Gathering (77) and (78) yields the result if $D_{K,\sigma} \Psi^{n+1} \geq 0$. The case $D_{K,\sigma} \Psi^{n+1} \leq 0$ can be treated exactly in the same way, starting from the expression (73b) of the flux instead of (73a). □

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