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CONVERGENCE OF A FINITE-VOLUME SCHEME FOR A DEGENERATE-SINGULAR CROSS-DIFFUSION SYSTEM FOR BIOFILMS

ESTHER S. DAUS, ANSGAR JÜNGEL, AND ANTOINE ZUREK

Abstract. An implicit Euler finite-volume scheme for a cross-diffusion system modeling biofilm growth is analyzed by exploiting its formal gradient-flow structure. The numerical scheme is based on a two-point flux approximation that preserves the entropy structure of the continuous model. Assuming equal diffusivities, the existence of nonnegative and bounded solutions to the scheme and its convergence are proved. Finally, we supplement the study by numerical experiments in one and two space dimensions.

1. Introduction

Biofilms are organized, cooperating communities of microorganisms. They can be used for the treatment of wastewater [11, 22], as they help to reduce sulfate and to remove nitrogen. Typically, biofilms consist of several species such that multicomponent fluid models need to be considered. Recently, a multi-species biofilm model was introduced by Rahman, Sudarsan, and Eberl [24], which reflects the same properties as the single-species diffusion model of [16]. The model has a porous-medium-type degeneracy when the local biomass vanishes, and a singularity when the biomass reaches the maximum capacity, which guarantees the boundedness of the total mass. The model was derived formally from a space-time discrete walk on a lattice in [24]. The global existence of weak solutions to the single-species model was proved in [17], while the global existence analysis for the multi-species cross-diffusion system can be found in [15]. The proof of the multi-species model is based on an entropy method which also provides the boundedness of the biomass hidden in its entropy structure. Numerical simulations were performed in [15, 24], but no numerical analysis was given. In this paper, we analyze an implicit Euler finite-volume scheme of the multi-species system that preserves the structure of the continuous model, namely positivity, boundedness, and discrete entropy production.

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The model equations for the proportions of the biofilm species u_i are given by

1.eq (1) $$\partial_t u_i + \operatorname{div} \mathcal{F}_i = 0, \quad \mathcal{F}_i = -\alpha_i p(M)^2 \nabla \frac{u_i q(M)}{p(M)} \quad \text{in } \Omega,\ t>0,\ i=1,\dots,n,$$

where $\Omega \subset \mathbb{R}^d$ $(d \ge 1)$ is a bounded domain, $\alpha_i > 0$ are some diffusion coefficients, and $M = \sum_{i=1}^n u_i$ is the total biomass. The proportions $u_i(x,t)$ are nonnegative and satisfy $M \le 1$. We have assumed for simplicity that the functions p and q only depend on the total biomass and are the same for all species. The function $p \in C^1([0,1])$ represents how favorable the current location is for incoming biofilm species. If the surrounding location is not able to accomodate more biomas, i.e. $M = 1$, then the species cannot move, i.e. $p(M) = 0$. In particular, the function p is decreasing. To recover the single-species model of [16] (see (5) below), we choose

1.q (2) $$q(M) := \frac{p(M)}{M} \int_0^M \frac{s^a}{(1-s)^b} \frac{ds}{p(s)^2}, \quad M > 0,$$

where a, $b \ge 1$ (see the Appendix for details). Equations (1) are complemented by initial and mixed boundary conditions:

1.ic (3) $$u_i(0) = u_i^0 \quad \text{in } \Omega,\ i=1,\dots,n,$$

1.bc (4) $$u_i = u_i^D \quad \text{on } \Gamma^D, \quad \nabla \mathcal{F}_i \cdot \nu = 0 \quad \text{on } \Gamma^N,$$

where $u^D = (u_1^D, \dots, u_n^D)$ is a constant vector such that $\sum_{i=1}^n u_i^D < 1$, Γ^D is the contact boundary part, Γ^N is the union of isolating boundary parts, and $\partial\Omega = \Gamma^D \cup \Gamma^N$. We refer to Appendix A for details on the modeling assumptions and the derivation of the model.

We recover the single-species model of [16] if all species are the same and all diffusivities α_i are equal, $\alpha_i = 1$ for $i = 1, \dots, n$. Indeed, summing (1) over $i = 1, \dots, n$ and using definition (2), it follows that

1.eqM (5) $$\partial_t M = \operatorname{div}\left(p(M)^2 \nabla \frac{M q(M)}{p(M)}\right) = \operatorname{div}\left(\frac{M^a}{(1-M)^b} \nabla M\right),$$

which makes the degenerate-singular structure of the model evident.

Equations (1) can be written as the cross-diffusion system

1.eq2 (6) $$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u) \nabla u_j\right) = 0 \quad \text{in } \Omega,\ t>0,$$

where the nonlinear diffusion coefficients are defined by

1.A (7) $$A_{ij}(u) = \alpha_i \delta_{ij} p(M) q(M) + \alpha_i u_i \big(p(M) q'(M) - p'(M) q(M)\big), \quad i,j = 1,\dots,n.$$

Due to the cross-diffusion structure, standard techniques like the maximum principle and regularity theory cannot be used. Moreover, the diffusion matrix $(A_{ij}(u))$ is generally neither symmetric nor positive definite.

The key of the analysis, already observed in [15], is that system (6)-(7) allows for an entropy or formal gradient-flow structure. Indeed, introduce the (relative) entropy

$$\begin{aligned} H(u) &= \int_\Omega h^*(u|u^D)dx, \quad \text{where} \\ h^*(u|u^D) &= h(u) - h(u^D) - h'(u^D)\cdot(u-u^D), \\ h(u) &= \sum_{i=1}^n \big(u_i(\log u_i - 1) + 1\big) + \int_0^M \log\frac{q(s)}{p(s)}ds, \end{aligned}$$

defined on the set

1.0 (8)
$$\mathcal{O} = \left\{u = (u_1,\ldots,u_n) \in (0,\infty)^n : \sum_{i=1}^n u_i < 1\right\}.$$

A computation gives the entropy identity [15, Theorem 2.1]

$$\frac{dH}{dt} + 2\sum_{i=1}^n \alpha_i \int_\Omega p(M)^2 \left|\nabla\sqrt{\frac{u_i q(M)}{p(M)}}\right|^2 dx = 0.$$

Thus, H is a Lyapunov functional along the solutions to (1). Moreover, under some assumptions on p, the entropy production term (the second term on the left-hand side) can be bounded from below, for some constant $C > 0$, by

1.ineq (9)
$$\begin{aligned} &\sum_{i=1}^n \alpha_i \int_\Omega p(M)^2 \left|\nabla\sqrt{\frac{u_i q(M)}{p(M)}}\right|^2 dx \\ &\qquad \ge C\int_\Omega \frac{M^{a-1}|\nabla M|^2}{(1-M)^{1+b+\kappa}}dx + \sum_{i=1}^n \int_\Omega p(M)q(M)|\nabla\sqrt{u_i}|^2 dx, \end{aligned}$$

yielding suitable gradient estimates. Moreover, it implies that $(1-M)^{1-b-\kappa}$ is integrable for some $\kappa > 0$, showing that $M < 1$ a.e. in Ω, $t > 0$, which excludes biofilm saturation and allows us to define the nonlinear terms.

Another feature of the entropy method is that equations (1), written in the so-called entropy variables $w_i = \partial h^*/\partial u_i$, can be written as the formal gradient-flow system

$$\partial_t u - \operatorname{div}(B(w)\nabla w) = 0,$$

with a positive semidefinite diffusion matrix B. Since the derivative $(h^*)' : \mathcal{O} \to \mathbb{R}^n$ is invertible [15, Lemma 3.3], u can be interpreted as a function of w, $u(w) = [(h^*)']^{-1}(w)$, mapping $\mathbb{R}^n$ to $\mathcal{O}$. This gives automatically $u(w) \in \mathcal{O}$ and consequently L^∞ bounds without the use of a maximum principle. This property, for another volume-filling model, was first observed in [7] and later generalized in [19]. The aim of this paper is to derive and analyze a finite-volume scheme for (1)-(4) which preserves the above-mentioned features of the continuous equations.

In the literature, there exist also other biofilm models. For instance, the authors of [26] proposed a biofilm growth model, surrounded by fluid flow, which takes into account the

growth, decay, detachment, and adhesion of biofilms. Using a finite-volume method, the authors studied numerically the evolution of biofilms for different strengths of the flow. Finite-volume-based schemes were developed in [25] for the simulation of biofilm processes in closed conduits, like a piper. The authors studied numerically the properties of their scheme and in particular its sensitivity to the variation of some numerical (time step, grid size) and physical parameters (length of the piper, initial thickness of the biofilm).

Finite-difference schemes were also proposed in the literature for the discretization of hyperbolic biofilm models. In particular, one-dimensional simulations are presented in [27] for a phase-field model, which takes into account the biofilm growth, its deformation, and the detachment phenomena, while in [28] the authors exhibited some two-dimensional simulations for the same model. We also mention [13], where a nonlinear hyperbolic system for the formation of biofilms was derived. Using an explicit-implicit method in time and a finite-difference method in space, the authors showed simulations of their model in three space dimensions.

Closer to our numerical study is the work [23], where the authors proposed a finite-volume discretization of single-species biofilm models including degenerate, singular, and cross diffusion terms. One of these diffusion effects is given by (5). However, no numerical analysis was performed in [23]. Such an analysis is provided in this paper.

To this end, we propose an implicit Euler scheme in time (with time step size Δt) and a finite-volume discretization in space (with grid size parameter Δx), based on two-point approximations. The challenge is to formulate the discrete fluxes such that the scheme preserves the entropy structure of the model and to design the fluxes such that we are able to establish the upper bound $M < 1$ a.e. in Ω, $t > 0$. We suggest the discrete fluxes (19), where the coefficient $p(M)^2$ is replaced by $(p(M_K)^2 + p(M_L)^2)/2$, and K and L are two neighboring control volumes with a common edge (see Section 2.1 for details). We establish a discrete counterpart of (9) in Lemma 4.3. This result is proved by exploiting the properties of the functions p and q (see Proposition 4.1 and [15, Lemma 3.4]) and distinguishing carefully the cases $M \le 1 - \delta$ and $M > 1 - \delta$ for sufficiently small $\delta > 0$. However, due to the lack of chain rule at the discrete level, we cannot conclude that the "discrete" biomass satisfies $M < 1$. To overcome this issue, we need to assume that the diffusivities are all equal. Then, summing the finite-volume analog of (1) over $i = 1, \ldots, n$, we obtain a discrete analog of the diffusion equation (5) for M that allows us to apply a discrete maximum principle, leading to $M < 1$.

Our results can be sketched as follows (see Section 2.3 for the precise statements):

(i) We prove the existence of finite-volume solutions with nonnegative discrete proportions $u_{i,K}$ and discrete total biomass $M_K < 1$ for all control volumes K.
(ii) The discrete solution satisfies a discrete analog of the entropy equality (which becomes an inequality in (24)) and of the lower bound (9) for the entropy production.
(iii) The discrete solution converges in a certain sense, for mesh sizes $(\Delta x, \Delta t) \to 0$, to a weak solution to (1).

There are several finite-volume schemes for other cross-diffusion systems in the mathematical literature. Most of the works exploit the entropy structure of the equations, except

[21] where the Laplacian structure of a population model is exploited to design a convergent linear finite-volume scheme. For instance, in [2, 3, 4], the sum of the L^2-norm of the population densities is used as a Lyapunov functional to perform a numerical analysis for finite-volume schemes for various cross-diffusion models. Closer to the framework of this paper are the works [1, 8, 10], where the authors used, roughly speaking, a Boltzmann-type entropy functional to prove the convergence of some two-point flux approximation schemes for a seawater intrusion model [1], a model which describes the physical vapor deposition process [10], and an ion transport model [8].

One of the main difference, and also one of the main difficulty, of this work compared to the literature comes from the strategy used for the existence proof. Indeed, in [1, 8, 10] the authors are able to prove the nonnegativity (as in [2, 3, 4]) and upper bounds on the solutions to their schemes thanks to some weak maximum principle, and they deduce the existence of finite-volume solutions via a topological degree argument. Then they established a discrete version of the entropy-dissipation inequality which enables them to obtain uniform estimates needed for their convergence proofs. However, for system (1)-(4), even if the assumption on the diffusion coefficients provides an upper bound for M, no a priori estimates are available to show the nonnegativity of the densities u_i by using a maximum principle.

Instead, we adapt at the discrete level the so-called boundedness-by-entropy method [7, 19]. In this method, we use the (relative) entropy density h^* to prove the nonnegativity *and* the existence of a solution to the scheme thanks to a discrete entropy inequality and the application of a topological degree argument; see Theorem 2.1. The adaptation of this technique to the discrete level represents the first main originality of this work. We remark that this strategy is also applied in [20] to prove the existence (and the convergence) of a finite-volume scheme for a population cross-diffusion system.

The second difficulty is the derivation of suitable discrete gradient estimates by proving a lower bound for the entropy production. We are able to "translate" (9) to the discrete case; see Lemma 4.3. This proof uses a Taylor expansion of $x \mapsto \sqrt{q(x)/p(x)}$ and a monotonicity property of this function. This is the second main originality of the paper.

The paper is organized as follows. The notation and assumptions on the mesh as well as the main theorems are introduced in Section 2. The existence of discrete solutions is proved in Section 3, based on a topological degree argument. We show a gradient estimate, an estimate of the discrete time derivative, and the lower bound for the entropy production in Section 4. These estimates allow us in Section 5 to apply the discrete compactness argument in [5] to conclude the a.e. convergence of the proportions and to show the convergence of the discrete gradient associated to $\nabla(u_i q(M)/p(M))$. The convergence of the scheme is then proved in Section 6. In Section 7, we present some numerical results in one and two space dimensions. They illustrate the L^2-convergence rate in space of the numerical scheme, show the convergence of the solutions to the steady states and the evolution of the relative entropy functional.

2. Numerical scheme and main results

sec.num

In this section, we introduce the numerical scheme and detail our main results.

sec.nota

2.1. **Notation and assumptions.** Let $\Omega \subset \mathbb{R}^2$ be an open, bounded, polygonal domain with $\partial\Omega = \Gamma^D \cup \Gamma^N \in C^{0,1}$, $\Gamma^D \cap \Gamma^N = \emptyset$, and $\mathrm{meas}(\Gamma^D) > 0$. We consider only two-dimensional domains Ω, but the generalization to higher dimensions is straightforward. An admissible mesh $\mathcal{M} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ of Ω is given by a family $\mathcal{T}$ of open polygonal control volumes (or cells), a family $\mathcal{E}$ of edges, and a family $\mathcal{P}$ of points $(x_K)_{K\in\mathcal{T}}$ associated to the control volumes and satisfying Definition 9.1 in [18]. This definition implies that the straight line between two centers of neighboring cells $\overline{x_K x_L}$ is orthogonal to the edge $\sigma = K|L$ between two cells K and L. The condition is satisfied by, for instance, triangular meshes whose triangles have angles smaller than $\pi/2$ [18, Examples 9.1] or Voronoï meshes [18, Example 9.2].

The family of edges $\mathcal{E}$ is assumed to consist of the interior edges $\sigma \in \mathcal{E}_{\mathrm{int}}$ satisfying $\sigma \in \Omega$ and the boundary edges $\sigma \in \mathcal{E}_{\mathrm{ext}}$ fulfilling $\sigma \subset \partial\Omega$. We suppose that each exterior edge is an element of either the Dirichlet or Neumann boundary, i.e. $\mathcal{E}_{\mathrm{ext}} = \mathcal{E}_{\mathrm{ext}}^D \cup \mathcal{E}_{\mathrm{ext}}^N$. For a given control volume $K \in \mathcal{T}$, we denote by $\mathcal{E}_K$ the set of its edges. This set splits into $\mathcal{E}_K = \mathcal{E}_{\mathrm{int},K} \cup \mathcal{E}_{\mathrm{ext},K}^D \cup \mathcal{E}_{\mathrm{ext},K}^N$. For any $\sigma \in \mathcal{E}$, there exists at least one cell $K \in \mathcal{T}$ such that $\sigma \in \mathcal{E}_K$. We denote this cell by K_σ. When σ is an interior cell, $\sigma = K|L$, K_σ can be either K or L.

The admissibility of the mesh and the fact that Ω is two-dimensional implies that

2.estmesh

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \mathrm{m}(\sigma)\mathrm{d}(x_K,\sigma) \le 2\sum_{K\in\mathcal{T}} \mathrm{m}(K) = 2\mathrm{m}(\Omega), \tag{10}$$

where d is the Euclidean distance in $\mathbb{R}^2$ and m the 1 or 2-dimensional Lebesgue measure.

Now, let $\sigma \in \mathcal{E}$ be an edge. We define

$$\mathrm{d}_\sigma = \begin{cases} \mathrm{d}(x_K, x_L) & \text{if } \sigma = K|L \in \mathcal{E}_{\mathrm{int}}, \\ \mathrm{d}(x_K, \sigma) & \text{if } \sigma \in \mathcal{E}_{\mathrm{ext},K}, \end{cases}$$

and the transmissibility coefficient is defined by

2.trans

$$\tau_\sigma = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}, \tag{11}$$

Figure 1 illustrates an admissible mesh of $\Omega = (0,1)^2$ composed of triangles.

We assume that the mesh satisfies the following regularity requirement: There exists $\xi > 0$ such that

2.regmesh

$$\mathrm{d}(x_K,\sigma) \ge \xi \mathrm{d}_\sigma \quad \text{for all } K \in \mathcal{T},\ \sigma \in \mathcal{E}_K. \tag{12}$$

The size of the mesh is denoted by $\Delta x = \max_{K\in\mathcal{T}} \mathrm{diam}(K)$.

Let $N_T \in \mathbb{N}$ be the number of time steps, $\Delta t = T/N_T$ be the time step and set $t_k = k\Delta t$ for $k = 0, \ldots, N_T$. We denote by $\mathcal{D}$ an admissible space-time discretization of $Q_T := \Omega \times (0,T)$ composed of an admissible mesh $\mathcal{M}$ of Ω and the values $(\Delta t, N_T)$. The size of $\mathcal{D}$ is defined by $\eta := \max\{\Delta x, \Delta t\}$.

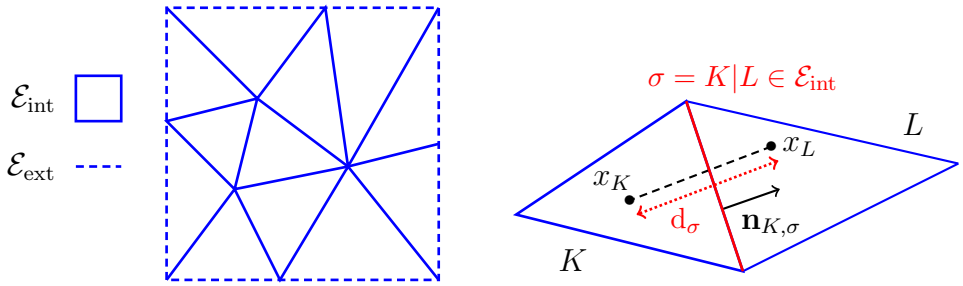

FIGURE 1. Example of an admissible mesh composed of triangles (inspired by an illustration in [9]).

rimal_mesh

As it is usual for the finite-volume method, we introduce functions that are piecewise constant in space and time. A finite-volume scheme provides a vector $v_\mathcal{T} = (v_K)_{K\in\mathcal{T}} \in \mathbb{R}^{\#\mathcal{T}}$ of approximate values of a function v and the associate piecewise constant function, still denoted by $v_\mathcal{T}$,

$$v_\mathcal{T} = \sum_{K\in\mathcal{T}} v_K \mathbf{1}_K,$$

where $\mathbf{1}_K$ is the characteristic function of K. The vector $v_\mathcal{M}$, containing the approximate values in the control volumes and the approximate values on the Dirichlet boundary edges, is written as $v_\mathcal{M} = (v_\mathcal{T}, v_{\mathcal{E}^D})$, where $v_{\mathcal{E}^D} = (v_\sigma)_{\sigma\in\mathcal{E}^D_{\text{ext}}} \in \mathbb{R}^{\#\mathcal{E}^D_{\text{ext}}}$. For a vector $v_\mathcal{M}$, we introduce for $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$ the notation

2.vKsigma

$$v_{K,\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int},K}, \\ v_\sigma & \text{if } \sigma \in \mathcal{E}^D_{\text{ext},K}, \\ v_K & \text{if } \sigma \in \mathcal{E}^N_{\text{ext},K} \end{cases} \tag{13}$$

and the discrete gradient

2.Dsigma

$$D_\sigma v := |D_{K,\sigma} v|, \quad \text{where } D_{K,\sigma} v = v_{K,\sigma} - v_K. \tag{14}$$

The discrete $H^1(\Omega)$ seminorm and the (squared) discrete $H^1(\Omega)$ norm are then defined by

2.norm

$$|v_\mathcal{M}|_{1,2,\mathcal{M}} = \left(\sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma v)^2 \right)^{1/2}, \quad \|v_\mathcal{M}\|^2_{1,2,\mathcal{M}} = \|v_\mathcal{M}\|^2_{0,2,\mathcal{M}} + |v_\mathcal{M}|^2_{1,2,\mathcal{M}}, \tag{15}$$

where $\|\cdot\|_{0,p,\mathcal{M}}$ denotes the $L^p(\Omega)$ norm

$$\|v_\mathcal{M}\|_{0,p,\mathcal{M}} = \left(\sum_{K\in\mathcal{T}} \mathrm{m}(K) |v_K|^p \right)^{1/p}, \quad \forall 1 \le p < \infty.$$

sec.scheme

2.2. **Numerical scheme.** We are now in the position to define the finite-volume discretization of (1)-(4). Let $\mathcal{D}$ be a finite-volume discretization of Q_T. The initial and boundary conditions are discretized by the averages

sch.ic

$$u^0_{i,K} = \frac{1}{\mathrm{m}(K)} \int_K u^0_i(x)dx \quad \text{for } K \in \mathcal{T}, \tag{16}$$

sch.bc (17)
$$u_{i,\sigma}^D = \frac{1}{\mathrm{m}(\sigma)}\int_\sigma u_i^D ds \quad \text{for } \sigma\in\mathcal{E}_{\mathrm{ext}}^D,\ i=1,\dots,n.$$

We suppose for simplicity that the Dirichlet datum is constant on Γ^D such that $u_{i,\sigma}^D = u_i^D$ for $i=1,\dots,n$. Furthermore, we set $u_{i,\sigma}^k = u_{i,\sigma}^D$ for $\sigma\in\mathcal{E}_{\mathrm{ext}}^D$ at time t_k.

Let $u_{i,K}^k$ be an approximation of the mean value of $u_i(\cdot,t_k)$ in the cell K. Then the implicit Euler finite-volume scheme reads as

sch1 (18)
$$\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}^k - u_{i,K}^{k-1}) + \sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{i,K,\sigma}^k = 0,$$

sch2 (19)
$$\mathcal{F}_{i,K,\sigma}^k = -\tau_\sigma\alpha_i(p_\sigma^k)^2 D_{K,\sigma}\left(\frac{u_i^k q(M^k)}{p(M^k)}\right),$$

where $K\in\mathcal{T}$, $\sigma\in\mathcal{E}_K$, $i=1,\dots,n$, and the value p_σ^k is defined by

2.psigma (20)
$$(p_\sigma^k)^2 := \frac{p(M_K^k)^2 + p(M_{K,\sigma}^k)^2}{2},$$

recalling definition (11) for τ_σ and notation (13) for $M_{K,\sigma}^k$.

Observe that definitions (13) and (14) ensure that the discrete fluxes vanish on the Neumann boundary edges, i.e. $\mathcal{F}_{i,K,\sigma}^k = 0$ for all $\sigma\in\mathcal{E}_{\mathrm{ext},K}^N$, $k\in\mathbb{N}$, and $i=1,\dots,n$. This is consistent with the Neumann boundary conditions in (4).

For the convergence result, we need to define the discrete gradients. To this end, let the vector $u_{\mathcal{M}} = (u_{\mathcal{T}}, u_{\mathcal{E}^D})$ as defined before. Then we introduce the piecewise constant approximation $u_{\mathcal{D}} = (u_{1,\mathcal{D}},\dots,u_{n,\mathcal{D}})$ by

reconstruc (21)
$$u_{i,\mathcal{D}}(x,t) = \sum_{K\in\mathcal{T}} u_{i,K}^k \mathbf{1}_K(x) \quad \text{for } x\in\Omega,\ t\in(t_{k-1},t_k],$$

nstrucbord (22)
$$u_{i,\mathcal{D}}(x,t) = u_i^D \quad \text{for } x\in\Gamma^D, i=1,\dots,n.$$

For given $K\in\mathcal{T}$ and $\sigma\in\mathcal{E}_K$, we define the cell $T_{K,\sigma}$ of the dual mesh as follows (see Figure 2):

- If $\sigma = K|L\in\mathcal{E}_{\mathrm{int},K}$, then $T_{K,\sigma}$ is that cell ("diamond") whose vertices are given by x_K, x_L, and the end points of the edge σ.
- If $\sigma\in\mathcal{E}_{\mathrm{ext},K}$, then $T_{K,\sigma}$ is that cell ("triangle") whose vertices are given by x_K and the end points of the edge σ.

An example of a construction of such a dual mesh can be found in [12]. The cells $T_{K,\sigma}$ define a partition of Ω. The definition of the dual mesh implies the following property. As the straight line between two neighboring centers of cells $\overline{x_K x_L}$ is orthogonal to the edge $\sigma = K|L$, it follows that

2.para (23)
$$\mathrm{m}(\sigma)\mathrm{d}(x_K,x_L) = 2\mathrm{m}(T_{K,\sigma}) \quad \text{for all } \sigma = K|L\in\mathcal{E}_{\mathrm{int},K}.$$

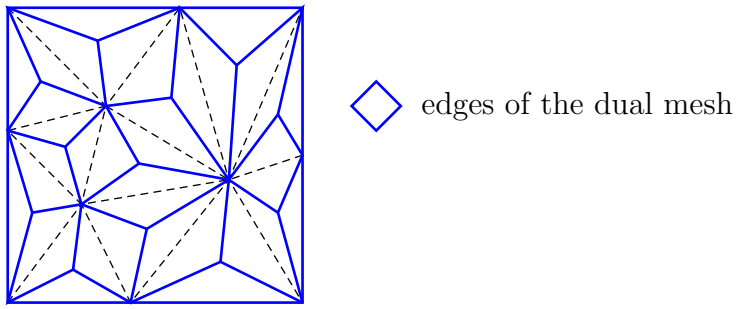

FIGURE 2. The dual mesh associated to the primal mesh of Figure 1 (inspired by an illustration in [9]).

_dual_mesh

We define the approximate gradient of a piecewise constant function $u_{\mathcal{D}}$ in Q_T given by (21)-(22) as follows:

$$\nabla^{\mathcal{D}} u_{\mathcal{D}}(x,t) = \frac{\mathrm{m}(\sigma)}{\mathrm{m}(T_{K,\sigma})} D_{K,\sigma} u^k \, \nu_{K,\sigma} \quad \text{for } x \in T_{K,\sigma},\ t \in (t_{k-1}, t_k],$$

where the discrete operator $D_{K,\sigma}$ is given in (14) and $\nu_{K,\sigma}$ is the unit vector that is normal to σ and points outward of K.

sec.main

2.3. **Main results.** Our first result guarantees that scheme (16)-(20) possesses a solution and that it preserves the entropy dissipation property. Let us collect our assumptions:

(H1) Domain: $\Omega \subset \mathbb{R}^2$ is a bounded polygonal domain with Lipschitz boundary $\partial\Omega = \Gamma^D \cup \Gamma^N$, $\Gamma^D \cap \Gamma^N = \emptyset$, and $\mathrm{meas}(\partial\Gamma^D) > 0$.

(H2) Discretization: $\mathcal{D}$ is an admissible discretization of Q_T satisfying the regularity condition (12).

(H3) Data: $u^0 = (u_1^0, \ldots, u_n^0) \in L^2(\Omega; [0,\infty)^n)$, $u^D = (u_1^D, \ldots, u_n^D) \in (0,\infty)^n$ is a constant vector, $\sum_{i=1}^n u_i^0 < 1$ in Ω, $\sum_{i=1}^n u_i^D < 1$, and $\alpha_1, \ldots, \alpha_n > 0$, a, $b \geq 1$.

(H4) Functions: $p \in C^1([0,1]; [0,\infty))$ is decreasing, $p(1) = 0$, and there exist c, $\kappa > 0$ such that $\lim_{M\to 1}(-(1-M)^{1+\kappa} p'(M)/p(M)) = c$. The function q is defined in (2).

For our main results, we need the following technical assumption:

(A1) The diffusion constants are equal, $\alpha_i = 1$ for $i = 1, \ldots, n$.

Remark 2.1 (Discussion of the hypotheses)**.** The assumption on the behavior of p when $M \to 1$ quantifies how fast this function decreases to zero as $M \to 1$. An integration implies the bound

$$p(M) \leq K_1 \exp(-K_2 (1-M)^{-\kappa}) \quad \text{for } 0 < M < 1,$$

with K_1 and K_2 some positive constants. We imposed this technical assumption to show a discrete version of (9), following the proof of [15, Lemma 3.4]; see Lemma 4.3. The lower bound on the entropy production term is needed to prove the convergence result.

The upper bound for p is also used in [15] to deduce an estimate for $(1-M)^{1-b-\kappa}$ in $L^1(\Omega)$, impliying that $M < 1$ in Ω. Unfortunately, this estimate requires the multiple use of the chain rule which is not available on the discrete level. Therefore, we assume that

the diffusivities α_i are equal and apply a weak maximum principle to the equation for M^k to deduce the bound $M_K^k < 1$ for all $K \in \mathcal{T}$.

In [15], the parameters in the definition (2) of q need to satisfy a, $b > 1$. We are able to allow for the slightly weaker condition a, $b \geq 1$; this is possible since we allow for equal diffusivities (condition (A1)). □

We introduce the discrete entropy

$$H(u_{\mathcal{M}}^k) = \sum_{K\in\mathcal{T}} \mathrm{m}(K) h^*(u_K^k|u^D),$$

where

$$h^*(u_K^k|u^D) = h(u_K^k) - h(u^D) - h'(u^D)\cdot(u_K^k - u^D)$$
$$\text{with } h(u_K^k) = \sum_{i=1}^n \big(u_{i,K}^k(\log u_{i,K}^k - 1) + 1\big) + \int_0^{M_K^k} \log\frac{q(s)}{p(s)}ds$$

is the relative entropy density.

thm.ex **Theorem 2.1** (Existence of discrete solutions)**.** *Let hypotheses (H1)-(H4) and (A1) hold. Then there exists a solution* $(u_K^k)_{K\in\mathcal{T},\,k=0,\ldots,N_T}$ *with* $u_K^k = (u_{1,K}^k,\ldots,u_{n,K}^k)$ *to scheme* (16)-(20) *satisfying*

$$u_{i,K}^k \geq 0, \quad M_K^k = \sum_{i=1}^n u_{i,K}^k \leq M^* \quad \text{for } K\in\mathcal{T},\ k=0,\ldots,N_T,$$

where $M^* = \sup_{x\in\Omega}\{M^D, M^0(x)\} < 1$. *Moreover, the discrete entropy dissipation inequality*

2.edi (24)
$$H(u_{\mathcal{M}}^k) + \Delta t\sum_{i=1}^n I_i(u_{\mathcal{M}}^k) \leq H(u_{\mathcal{M}}^{k-1}), \quad k=1,\ldots,N_T,$$

holds with the entropy dissipation

2.ed (25)
$$I_i(u_{\mathcal{M}}^k) = \sum_{\sigma\in\mathcal{E}} \tau_\sigma (p_\sigma^k)^2 \left(D_\sigma\left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}}\right)\right)^2, \quad i=1,\ldots,n.$$

For the convergence result, we introduce a family $(\mathcal{D}_\eta)_{\eta>0}$ of admissible space-time discretizations of Q_T indexed by the size $\eta = \max\{\Delta x, \Delta t\}$ of the mesh. We denote by $(\mathcal{M}_\eta)_{\eta>0}$ the corresponding meshes of Ω. For any $\eta > 0$, let $u_\eta := u_{\mathcal{D}_\eta}$ be the finite-volume solution constructed in Theorem 2.1 and set $\nabla^\eta := \nabla^{\mathcal{D}_\eta}$.

thm.conv **Theorem 2.2.** *Let the hypotheses of Theorem 2.1 hold. Let* $(\mathcal{D}_\eta)_{\eta>0}$ *be a family of admissible discretizations satisfying* (12) *uniformly in* η. *Furthermore, let* $(u_\eta)_{\eta>0}$ *be a family of finite-volume solutions to scheme* (16)-(20). *Then there exists a function* $u = (u_1,\ldots,u_n)$ *satisfying* $u(x,t) \in \overline{\mathcal{O}}$ *(see* (8)*) such that*

$$u_{i,\eta} \to u_i \quad \text{a.e. in } Q_T,\ i=1,\ldots,n,$$

$$M_\eta = \sum_{i=1}^n u_{i,\eta} \to M = \sum_{i=1}^n u_i < 1 \quad a.e.\ in\ Q_T,$$
$$\nabla^\eta\left(\frac{u_{i,\eta}q(M_\eta)}{p(M_\eta)}\right) \rightharpoonup \nabla\left(\frac{u_i q(M)}{p(M)}\right) \quad weakly\ in\ L^2(Q_T).$$

The limit function satisfies the boundary condition in the sense

$$\frac{u_i q(M)}{p(M)} - \frac{u_i^D q(M^D)}{p(M^D)} \in L^2(0,T;H_D^1(\Omega)),$$

with $H_D^1(\Omega) := \{v \in H^1(\Omega) : v = 0\ on\ \Gamma^D\}$ *and it is a weak solution to* (1)-(4) *in the sense*

.weakformu

$$\sum_{i=1}^n \left(\int_0^T \int_\Omega u_i \partial_t \phi_i dxdt + \int_\Omega u_i^0(x)\phi(x,0)dx\right) = \sum_{i=1}^n \int_0^T \int_\Omega p(M)^2 \nabla\left(\frac{u_i q(M)}{p(M)}\right) \cdot \nabla\phi_i\, dxdt, \tag{26}$$

for all $\phi_i \in C_0^\infty(\Omega \times [0,T))$.

We also need the assumption $\alpha_i = 1$ for $i = 1,\dots,n$ for the proof of Theorem 2.2. Indeed, due to the lack of chain rule at the discrete level, it is not clear how to identify the weak limit of the term $p(M_\eta)^2\nabla^\eta(u_{i,\eta}q(M_\eta)/p(M_\eta))$. Another difficulty comes from the degeneracy of p when $M = 1$, which prevents the proof of a uniform bound on $\nabla^\eta(u_{i,\eta}q(M_\eta)/p(M_\eta))$ from the entropy inequality (24). Our strategy relies on the uniform upper bound satisfied by M_η obtained in Theorem 2.1. Thanks to this bound, the monotonicity of p, and the inequality (24), we can establish a uniform bound on the L^2 norm of $\nabla^\eta(u_{i,\eta}q(M_\eta)/p(M_\eta))$ and identify its weak limit. The numerical experiments in Section 7 seem to indicate that the assumption $\alpha_i = 1$ is purely technical and that the scheme still converges in the case of different diffusivities.

3. Existence of finite-volume solutions

sec.ex

In this section, we prove Theorem 2.1. To this end, we adapt the entropy method used in [15] to the discrete level. The idea is to solve a regularized version of scheme (18)-(19) in the entropy variable which ensures that the proportions u_i of the biofilm species belong to the set $\mathcal{O}$, defined in (8). First, we define a fixed-point operator that provides the solution to the linearized problem. Then the existence of a fixed point is shown by a topological degree argument that is based on a discrete entropy inequality. Finally, we perform the limit when the regularization terms vanish.

3.1. **Proof of Theorem 2.1.** We proceed by induction. For $k = 0$, we have $u^0 \in \overline{\mathcal{O}}$ with $u_i^0 \ge 0$ for $K \in \mathcal{T}$, $i = 1,\dots,n$ by assumption and $M^0 \le M^* = \sup_{x\in\Omega}\{M^D, M^0(x)\}$ by construction. Assume that there exists a solution $u_\mathcal{M}^{k-1}$ for some $k \in \{1,\dots,N_T\}$ such that

$$u_K^{k-1} \ge 0, \quad M_K^{k-1} = \sum_{i=1}^n u_{i,K}^{k-1} \le M^* \quad \text{for } K \in \mathcal{T}.$$

The construction of a solution $u_{\mathcal{M}}^k$ is divided into several steps.

Step 1. Definition of a linearized problem. We introduce the set

$$Z = \big\{w_{\mathcal{M}} = (w_{1,\mathcal{M}}, \ldots, w_{n,\mathcal{M}}) : w_{i,\sigma} = 0 \text{ for } \sigma \in \mathcal{E}_{\text{ext}}^D, \\ \|w_{i,\mathcal{M}}\|_{1,2,\mathcal{M}} < \infty \text{ for } i = 1, \ldots, n\big\}.$$

Let $\varepsilon > 0$. We define the mapping $F_\varepsilon : Z \to \mathbb{R}^{\theta n}$ by $F_\varepsilon(w_{\mathcal{M}}) = w_{\mathcal{M}}^\varepsilon$, with $\theta = \#\mathcal{T} + \#\mathcal{E}^D$, where $w_{\mathcal{M}}^\varepsilon = (w_{1,\mathcal{M}}^\varepsilon, \ldots, w_{n,\mathcal{M}}^\varepsilon)$ is the solution to the linear problem

3.lin (27)
$$\varepsilon\left(-\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma} w_i^\varepsilon + \mathrm{m}(K) w_{i,K}^\varepsilon\right) = -\left(\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K} - u_{i,K}^{k-1}) + \sum_{\sigma\in\mathcal{E}_K} \mathcal{F}_{i,K,\sigma}\right),$$

for $K \in \mathcal{T}$, $i = 1, \ldots, n$ with

3.bc (28)
$$w_{i,\sigma}^\varepsilon = 0 \quad \text{for } \sigma \in \mathcal{E}_{\text{ext}}^D,\ i = 1, \ldots, n.$$

Here, $u_{i,K}$ is a function of $w_{i,K}$, defined by

3.w (29)
$$w_{i,K} = \log\frac{u_{i,K} q(M_K)}{p(M_K)} - \log\frac{u_i^D q(M^D)}{p(M^D)} \quad i = 1, \ldots, n,$$

and $\mathcal{F}_{i,K,\sigma}$ is defined in (19). Note that $\mathcal{F}_{i,K,\sigma}$ depends on $w_{\mathcal{M}}$ via $u_{\mathcal{M}}$ and $M_{\mathcal{M}}$.

It is shown in [15, Lemma 3.3] that the mapping $\mathcal{O} \to \mathbb{R}^n$, $u_K \mapsto w_K$, is invertible. For the convenience of the reader, we recall briefly the argument. We rewrite (29) as

3.inv (30)
$$\frac{u_i^D}{M^D}\exp(w_{i,K}) = \frac{u_{i,K}}{M^D}\frac{q(M_K)/p(M_K)}{q(M^D)/p(M^D)} \quad \text{for all } K \in \mathcal{T},\ i = 1, \ldots, n,$$

sum this identity over $i = 1, \ldots, n$, and introduce the function $\Phi(M) = Mq(M)/p(M)$:

$$\Phi(M_K) = \Phi(M^D)\sum_{i=1}^n \frac{u_i^D}{M^D}\exp(w_{i,K}) \quad \text{for all } K \in \mathcal{T}.$$

Since Φ is increasing, $\Phi(0) = 0$, and $\lim_{M\to 1}\Phi(M) = \infty$, there exists a unique solution $M_K \in (0,1)$ to this nonlinear equation. Using this value in (30), we obtain immediately the invertibility of $\mathcal{O} \to \mathbb{R}^n$, $u_K \mapsto w_K$. This shows that $u_K = u(w_K)$ is well-defined and $u_K \in \mathcal{O}$. We infer that $\mathcal{F}_{i,K,\sigma}$ is well-defined too. Since $M_K = \sum_{i=1}^n u_{i,K}$, we infer that $0 \le u_{i,K} < 1$. Definitions (13) and (14) ensure that $D_{K,\sigma} w_i^\varepsilon = 0$ for all $\sigma \in \mathcal{E}_{\text{ext},K}^N$. The existence of a unique solution w_K^ε to the linear scheme (27)-(28) is now a consequence of [18, Lemma 9.2].

Step 2. Continuity of F_ε. We fix $i \in \{1, \ldots, n\}$. We derive first an a priori estimate for $w_{i,\mathcal{M}}^\varepsilon$. Multiplying (27) by $w_{i,K}^\varepsilon$, summing over $K \in \mathcal{T}$ and using the symmetry of τ_σ with respect to $\sigma = K|L$, we arrive at

$$\varepsilon\sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma w_i^\varepsilon)^2 + \varepsilon\sum_{K\in\mathcal{T}} \mathrm{m}(K)|w_{i,K}^\varepsilon|^2 = -\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(u_{i,K} - u_{i,k}^{k-1})\, w_{i,K}^\varepsilon - \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \mathcal{F}_{i,K,\sigma} w_{i,K}^\varepsilon$$

3.aux1 (31)
$$=: J_1 + J_2,$$

where in the term J_2 the sum is over all edges $\sigma \in \mathcal{E}$, and to each given σ we associate the cell $K = K_\sigma$. For the left-hand side, we use the definition (15) of the discrete $H^1(\Omega)$ norm

$$\varepsilon \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma w_i^\varepsilon)^2 + \varepsilon \sum_{K\in\mathcal{T}} \mathrm{m}(K)|w_{i,K}^\varepsilon|^2 = \varepsilon \|w_{i,\mathcal{M}}^\varepsilon\|_{1,2,\mathcal{M}}^2.$$

By the Cauchy-Schwarz inequality and definition (19) of $\mathcal{F}_{i,K,\sigma}$, we find that

$$\begin{aligned}
|J_1| &\le \frac{1}{\Delta t}\bigg(\sum_{K\in\mathcal{T}} \mathrm{m}(K)(u_{i,K} - u_{i,K}^{k-1})^2\bigg)^{1/2}\bigg(\sum_{K\in\mathcal{T}} \mathrm{m}(K)(w_{i,K}^\varepsilon)^2\bigg)^{1/2} \\
&\le \frac{1}{\Delta t}\|u_{i,\mathcal{M}} - u_{i,\mathcal{M}}^{k-1}\|_{0,2,\mathcal{M}}\, \|w_{i,\mathcal{M}}^\varepsilon\|_{1,2,\mathcal{M}}, \\
|J_2| &\le \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 D_\sigma\bigg(\frac{u_i q(M)}{p(M)}\bigg) D_\sigma w_i^\varepsilon \\
&\le \bigg(\sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(p_\sigma^2\right)^2 \bigg(D_\sigma\bigg(\frac{u_i q(M)}{p(M)}\bigg)\bigg)^2\bigg)^{1/2}\bigg(\sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma w_i^\varepsilon)^2\bigg)^{1/2}.
\end{aligned}$$

Since $M_K \in (0,1)$ for all $K \in \mathcal{T}$, $u_{i,K}\, q(M_K)/p(M_K)$ is bounded. Moreover, $p_\sigma \le p(0)$ as p is decreasing. Hence, there exists a constant $C(M) > 0$ which is independent of $w_{i,\mathcal{M}}^\varepsilon$ such that $|J_2| \le C(M)\|w_{i,\mathcal{M}}^\varepsilon\|_{1,2,\mathcal{M}}$. This constant does not depend on $u_{i,K} \in [0,1)$. Inserting these estimations into (31) yields

3.aux2 (32) $$\sqrt{\varepsilon}\|w_{i,\mathcal{M}}^\varepsilon\|_{1,2,\mathcal{M}} \le C(M),$$

where $C(M) > 0$ is independent of $w_{i,\mathcal{M}}^\varepsilon$.

We turn to the proof of the continuity of F_ε. Let $(w_{\mathcal{M}}^m)_{m\in\mathbb{N}} \in Z$ be such that $w_{\mathcal{M}}^m \to w_{\mathcal{M}}$ as $m \to \infty$. Estimate (32) shows that $w_{\mathcal{M}}^{\varepsilon,m} := F_\varepsilon(w_{\mathcal{M}}^m)$ is bounded uniformly in $m \in \mathbb{N}$. Thus, there exists a subsequence of $(w_{\mathcal{M}}^{\varepsilon,m})$ which is not relabeled such that $w_{\mathcal{M}}^{\varepsilon,m} \to w_{\mathcal{M}}^\varepsilon$ as $m \to \infty$. Passing to the limit $m \to \infty$ in scheme (27)-(28) and taking into account the continuity of the nonlinear functions, we see that $w_{i,\mathcal{M}}^\varepsilon$ is a solution to (27)-(28) and $w_{\mathcal{M}}^\varepsilon = F_\varepsilon(w_{\mathcal{M}})$. Because of the uniqueness of the limit function, the whole sequence converges, which proves the continuity.

Step 3. Existence of a fixed point. We claim that the map F_ε admits a fixed point. We use a topological degree argument [14], i.e., we prove that $\delta(I - F_\varepsilon, Z_R, 0) = 1$, where δ is the Brouwer topological degree and

$$Z_R = \{w_{\mathcal{M}} \in Z : \|w_{i,\mathcal{M}}\|_{1,2,\mathcal{M}} < R \quad \text{for } i = 1,\dots,n\}.$$

Since δ is invariant by homotopy, it is sufficient to prove that any solution $(w_{\mathcal{M}}^\varepsilon, \rho) \in \overline{Z}_R \times [0,1]$ to the fixed-point equation $w_{\mathcal{M}}^\varepsilon = \rho F_\varepsilon(w_{\mathcal{M}}^\varepsilon)$ satisfies $(w_{\mathcal{M}}^\varepsilon, \rho) \notin \partial Z_R \times [0,1]$ for sufficiently large values of $R > 0$. Let $(w_{\mathcal{M}}^\varepsilon, \rho)$ be a fixed point and $\rho \ne 0$, the case $\rho = 0$

being clear. Then $w_{i,\mathcal{M}}^\varepsilon$ solves

3.lin2 (33) $$\varepsilon\bigg(-\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma D_{K,\sigma}w_i^\varepsilon+\mathrm{m}(K)w_{i,K}^\varepsilon\bigg)=-\rho\bigg(\frac{\mathrm{m}(K)}{\Delta t}(u_{i,K}^\varepsilon-u_{i,K}^{k-1})+\sum_{\sigma\in\mathcal{E}_K}\mathcal{F}_{i,K,\sigma}^\varepsilon\bigg),$$

where $\mathcal{F}_{i,K,\sigma}^\varepsilon$ is defined as in (19) with $u_\mathcal{M}$ replaced by $u_\mathcal{M}^\varepsilon$ which is related to $w_\mathcal{M}^\varepsilon$ by (29).

The following discrete entropy inequality is the key argument.

lem.edi **Lemma 3.1** (Discrete entropy inequality)**.** *Let the assumptions of Theorem 2.1 hold. Then for any $\rho\in(0,1]$ and $\varepsilon\in(0,1)$,*

$$\rho H(u_\mathcal{M}^\varepsilon)+\varepsilon\Delta t\sum_{i=1}^n||w_{i,\mathcal{M}}^\varepsilon||_{1,2,\mathcal{M}}^2+\rho\Delta t\sum_{i=1}^n I_i(u_\mathcal{M}^\varepsilon)\le\rho H(u_\mathcal{M}^{k-1}),$$

$$\text{where } I_i(u_\mathcal{M}^\varepsilon)=\sum_{\sigma\in\mathcal{E}}\tau_\sigma(p_\sigma^\varepsilon)^2\bigg(D_\sigma\bigg(\sqrt{\frac{u_i^\varepsilon q(M^\varepsilon)}{p(M^\varepsilon)}}\bigg)\bigg)^2,\quad i=1,\ldots,n,$$

with obvious notations for $(p_\sigma^\varepsilon)^2$ and M^ε.

Proof. We multiply (33) by $\Delta t w_{i,K}^\varepsilon$ and sum over $i=1,\ldots,n$ and $K\in\mathcal{T}$. This gives

$$\varepsilon\Delta t\sum_{i=1}^n\bigg(-\sum_{\substack{\sigma\in\mathcal{E}\\K=K_\sigma}}\tau_\sigma w_{i,K}^\varepsilon D_{K,\sigma}w_i^\varepsilon+\sum_{K\in\mathcal{T}}\mathrm{m}(K)|w_{i,K}^\varepsilon|^2\bigg)+J_3+J_4=0,\quad\text{where}$$

$$J_3=\rho\sum_{i=1}^n\sum_{K\in\mathcal{T}}\mathrm{m}(K)(u_{i,K}^\varepsilon-u_{i,K}^{k-1})w_{i,K}^\varepsilon,$$

$$J_4=\rho\Delta t\sum_{i=1}^n\sum_{\substack{\sigma\in\mathcal{E}\\K=K_\sigma}}\mathcal{F}_{i,K,\sigma}^\varepsilon w_{i,K}^\varepsilon.$$

By the symmetry of τ_σ with respect to $\sigma=K|L$, the first term is written as

$$\varepsilon\Delta t\sum_{i=1}^n\bigg(-\sum_{\substack{\sigma\in\mathcal{E}\\K=K_\sigma}}\tau_\sigma w_{i,K}^\varepsilon D_{K,\sigma}w_i^\varepsilon+\sum_{K\in\mathcal{T}}\mathrm{m}(K)|w_{i,K}^\varepsilon|^2\bigg)=\varepsilon\Delta t\sum_{i=1}^n\|w_{i,\mathcal{M}}^\varepsilon\|_{1,2,\mathcal{M}}^2.$$

Inserting definition (29) of $w_{i,K}^\varepsilon$ and using the convexity of $u\mapsto u(\log u-1)+1$, we obtain

$$\begin{aligned}J_3&=\rho\sum_{i=1}^n\sum_{K\in\mathcal{T}}\mathrm{m}(K)(u_{i,K}^\varepsilon-u_{i,K}^{k-1})\bigg(\log u_{i,K}^\varepsilon+\log\frac{q(M_K^\varepsilon)}{p(M_K^\varepsilon)}\bigg)\\&\quad-\rho\sum_{i=1}^n\sum_{K\in\mathcal{T}}\mathrm{m}(K)(u_{i,K}^\varepsilon-u_{i,K}^{k-1})\bigg(\log u_i^D+\log\frac{q(M^D)}{p(M^D)}\bigg)\\&\ge\rho\sum_{K\in\mathcal{T}}\mathrm{m}(K)\big(h(u_K^\varepsilon)-h(u_K^{k-1})\big)-\rho\sum_{i=1}^n\mathrm{m}(K)(u_{i,K}^\varepsilon-u_{i,K}^{k-1})\frac{\partial h}{\partial u_i}(u^D)\end{aligned}$$

$$
\begin{aligned}
&= \rho \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(h(u_K^\varepsilon) - (u_K^\varepsilon - u^D)\cdot h'(u^D)\big) \\
&\quad - \rho \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(h(u_K^{k-1}) - (u_K^{k-1} - u^D)\cdot h'(u^D)\big) \\
&= \rho \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big(h^*(u_K^\varepsilon|u^D) - h^*(u_K^{k-1}|u^D)\big) = \rho\big(H(u_\mathcal{M}^\varepsilon) - H(u_\mathcal{M}^{k-1})\big).
\end{aligned}
$$

We abbreviate $v_{i,K}^\varepsilon := u_{i,K}^\varepsilon q(M_K^\varepsilon)/p(M_K^\varepsilon)$. Then

$$
\begin{aligned}
J_4 &= -\rho\Delta t \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \mathcal{F}_{i,K,\sigma}^\varepsilon D_{K,\sigma}(w_i^\varepsilon) \\
&= \rho\Delta t \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma(p_\sigma^\varepsilon)^2 (v_{i,K,\sigma}^\varepsilon - v_{i,K}^\varepsilon)(\log v_{i,K,\sigma}^\varepsilon - \log v_{i,K}^\varepsilon).
\end{aligned}
$$

The elementary inequality $(x-y)(\log x - \log y) \ge 4(\sqrt{x}-\sqrt{y})^2$ for any x, $y>0$ implies that

$$
J_4 \ge 4\rho\Delta t \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma(p_\sigma^\varepsilon)^2 \left(D_\sigma\left(\sqrt{\frac{u_i^\varepsilon q(M^\varepsilon)}{p(M^\varepsilon)}}\right)\right)^2.
$$

Putting all the estimations together completes the proof. □

We proceed with the topological degree argument. The previous lemma implies that

$$
\varepsilon\Delta t \sum_{i=1}^n ||w_{i,\mathcal{M}}^\varepsilon||_{1,2,\mathcal{M}}^2 \le \rho H(u_\mathcal{M}^{k-1}) \le H(u_\mathcal{M}^{k-1}).
$$

Then, if we define

$$
R := \left(\frac{H(u_\mathcal{M}^{k-1})}{\varepsilon\Delta t}\right)^{1/2} + 1,
$$

we conclude that $w_\mathcal{M}^\varepsilon \notin \partial Z_R$ and $\delta(I - F_\varepsilon, Z_R, 0) = 1$. Thus, F_ε admits a fixed point.

Step 4. Limit $\varepsilon \to 0$. We recall that $u_\mathcal{M}^\varepsilon \in \overline{\mathcal{O}}$. Thus, up to a subsequence, $u_\mathcal{M}^\varepsilon \to u_\mathcal{M} \in \overline{\mathcal{O}}$ as $\varepsilon \to 0$. We deduce from (32) that there exists a subsequence (not relabeled) such that $\varepsilon w_{i,K}^\varepsilon \to 0$ for any $K \in \mathcal{T}$ and $i = 1,\dots,n$. In order to pass to the limit in the fluxes $\mathcal{F}_{i,K,\sigma}^\varepsilon$, we need to show that $M_K = \sum_{i=1}^n u_{i,K} < 1$ for any $K \in \mathcal{T}$. To this end, we establish the following result:

.borne.sup **Lemma 3.2** (L^2 estimate)**.** *Let the assumptions of Theorem 2.1 hold. Then for all $\varepsilon > 0$, there exists a constant $C > 0$ depending on $H(u_\mathcal{M}^{k-1})$, Ω, Δt, the mesh $\mathcal{T}$, and $M^* = \sup_{x\in\Omega}\{M^D, M^0(x)\}$ such that*

.borne.sup (34)
$$
\sum_{K\in\mathcal{T}} \mathrm{m}(K)\left([M_K^\varepsilon - M^*]^+\right)^2 \le C\sqrt{\varepsilon},
$$

where $z^+ = \max\{z, 0\}$.

Proof. Let $\varepsilon > 0$ be fixed. Then, summing (33) over i, we obtain

$$\varepsilon \sum_{i=1}^n \left(-\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma D_{K,\sigma} w_i^\varepsilon + \mathrm{m}(K) w_{i,K}^\varepsilon \right) + \mathrm{m}(K) \frac{M_K^\varepsilon - M_K^{k-1}}{\Delta t} + \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}_K} \mathcal{F}_{i,K,\sigma}^\varepsilon = 0 \quad \text{for all } K \in \mathcal{T}.$$

Multiplying this equation by $\Delta t[M_K^\varepsilon - M^*]^+$, summing over $K \in \mathcal{T}$, and using $\frac{1}{2}(x^2 - y^2) \le x(x-y)$, we obtain

$$\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{2} \left([M_K^\varepsilon - M^*]_+^2 - [M_K^{k-1} - M^*]_+^2 \right) \le J_5 + J_6 + J_7,$$

where

$$J_5 = -\Delta t \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E} \\ K=K_\sigma}} \mathcal{F}_{i,K,\sigma}^\varepsilon [M_K^\varepsilon - M^*]_+,$$

$$J_6 = \varepsilon \Delta t \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E} \\ K=K_\sigma}} \tau_\sigma D_{K,\sigma} w_i^\varepsilon [M_K^\varepsilon - M^*]^+,$$

$$J_7 = -\varepsilon \Delta t \sum_{i=1}^n \sum_{K\in\mathcal{T}} \mathrm{m}(K) w_{i,K}^\varepsilon [M_K^\varepsilon - M^*]^+.$$

We use discrete integration by parts to rewrite J_5 as

$$J_5 = -\Delta t \sum_{\substack{\sigma\in\mathcal{E} \\ K=K_\sigma}} \tau_\sigma (p_\sigma^\varepsilon)^2 D_{K,\sigma} \left(\frac{M^\varepsilon q(M^\varepsilon)}{p(M^\varepsilon)} \right) D_{K,\sigma} [M^\varepsilon - M^*]^+.$$

We assume that for $\sigma \in \mathcal{E}$ we have $M_{K,\sigma}^\varepsilon \ge M_K^\varepsilon$. Then, since the function $M \mapsto Mq(M)/p(M)$ is increasing (see definition (2)), we deduce that $D_{K,\sigma}(M^\varepsilon q(M^\varepsilon)/p(M^\varepsilon)) \ge 0$. We distinguish the following cases:

- $M^* \ge M_{K,\sigma}^\varepsilon \ge M_K^\varepsilon \Rightarrow D_{K,\sigma}[M^\varepsilon - M^*]^+ = 0$;
- $M_{K,\sigma}^\varepsilon \ge M^* \ge M_K^\varepsilon \Rightarrow D_{K,\sigma}[M^\varepsilon - M^*]^+ = M_{K,\sigma}^\varepsilon - M^* \ge 0$;
- $M_{K,\sigma}^\varepsilon \ge M_K^\varepsilon \ge M^* \Rightarrow D_{K,\sigma}[M^\varepsilon - M^*]^+ = M_{K,\sigma}^\varepsilon - M_K^\varepsilon \ge 0$.

This implies that $D_{K,\sigma}(M^\varepsilon q(M^\varepsilon)/p(M^\varepsilon)) D_{K,\sigma}[M^\varepsilon - M^*]^+ \ge 0$ if $M_{K,\sigma}^\varepsilon \ge M_K^\varepsilon$. A similar argument shows that $D_{K,\sigma}(M^\varepsilon q(M^\varepsilon)/p(M^\varepsilon)) D_{K,\sigma}[M^\varepsilon - M^*]^+ \ge 0$ also in the case $M_K^\varepsilon \ge M_{K,\sigma}^\varepsilon$ and we deduce that $J_5 \le 0$.

For J_6, we apply discrete integration by parts and the Cauchy-Schwarz inequality:

$$|J_6| \le \varepsilon^{1/2} \left(\varepsilon \Delta t \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma w_i^\varepsilon)^2 \right)^{1/2} \left(\Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma (D_\sigma [M^\varepsilon - M^*]^+)^2 \right)^{1/2}.$$

It follows from Lemma 3.1 and the L^∞ bound $M_K^\varepsilon \le 1$ for $K \in \mathcal{T}$ that

$$|J_6| \le 2H(u_{\mathcal{M}}^{k-1})^{1/2}\,(1+M^*)\left(\Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma\right)^{1/2} \varepsilon^{1/2}.$$

Finally, we use the Cauchy-Schwarz inequality together with Lemma 3.1 and then the L^∞ bound $M_K^\varepsilon \le 1$ for $K \in \mathcal{T}$ to estimate J_7:

$$\begin{aligned}|J_7| &\le \varepsilon^{1/2} H(u_{\mathcal{M}}^{k-1})^{1/2}\left(\Delta t \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left([M_K^\varepsilon - M^*]^+\right)^2\right)^{1/2}\\ &\le H(u_{\mathcal{M}}^{k-1})^{1/2}\,(1+M^*)\Delta t^{1/2}\,\mathrm{m}(\Omega)^{1/2}\varepsilon^{1/2}.\end{aligned}$$

Gathering all the previous estimates, we deduce the existence of a constant $C > 0$ such that (34) holds. □

We conclude from Lemma 3.2 that passing to the limit $\varepsilon \to 0$ in (34) that

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K)\left([M_K - M^*]^+\right)^2 \le 0,$$

recall that $M_K^\varepsilon \to M_K$ as $\varepsilon \to 0$ for $K \in \mathcal{T}$. This shows that $M_K \le M^* < 1$ for all $K \in \mathcal{T}$. We can perform the limit $\varepsilon \to 0$ in (33), which completes the proof of Theorem 2.1.

4. A priori estimates

ec.apriori

In this section, we establish some uniform estimates for the solutions to scheme (16)-(20). These estimates are needed to deduce the compactness of the sequence of finite-volume solutions obtained in Theorem 2.1. In particular, we prove a discrete gradient estimate for $\sqrt{u_i^k}$ and an estimate for the discrete time derivative $(u_{i,K}^k - u_{i,K}^{k-1})/\Delta t$.

We first state some technical properties satisfied by the functions p and q.

prop.pq **Proposition 4.1** (Properties of p and q)**.** *The function $M \mapsto \sqrt{q(M)/p(M)}$ is strictly increasing for $M \in (0,1)$. Moreover, there exists a constant C_{pq} such that*

4.Cpq
$$\lim_{M\to 1} \frac{p(M)q(M)}{(1-M)^{1-b+\kappa}} = C_{pq} \in (0,\infty). \tag{35}$$

Proof. The result follows from a meticulous but rather straightforward analysis as done in the proofs of [15, Lemma 3.1, Lemma 3.4] using Hypothesis (H4). □

4.1. **Gradient estimate.** We deduce the following gradient estimate from the entropy inequality (24).

lem.grad **Lemma 4.1** (Gradient estimate)**.** *Let the assumptions of Theorem 2.1 hold. Then there exists a constant $C_1 > 0$ only depending on $H(u_{\mathcal{M}}^0)$, Ω, q, p, and the upper bound M^* defined in Theorem 2.1 such that*

$$\sum_{k=1}^{N_T} \Delta t \left\| \frac{u_{i,\mathcal{M}}^k q(M_{\mathcal{M}}^k)}{p(M_{\mathcal{M}}^k)} \right\|_{1,2,\mathcal{M}}^2 \le C_1 \quad \textit{for all } 1 \le i \le n.$$

Proof. Let $i \in \{1,\ldots,n\}$. Thanks to the uniform L^∞ bound for $u_{\mathcal{M}}^k$, it is sufficient to show that there exists a constant $C>0$ independent of Δx and Δt such that

$$\sum_{k=1}^{N_T} \Delta t \left| \frac{u_{i,\mathcal{M}}^k q(M_{\mathcal{M}}^k)}{p(M_{\mathcal{M}}^k)} \right|_{1,2,\mathcal{M}}^2 \le C.$$

To prove this estimate, we start from the following bound which comes from the discrete entropy inequality (24):

4.aux

$$\sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma \left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}} \right) \right)^2 \le \frac{H(u_{\mathcal{M}}^0)}{p(M^*)^2}. \tag{36}$$

Using the inequality $x^2-y^2 \le 2x(x-y)$ and $u_{i,K,\sigma}^k \le 1$, we can write

$$\begin{aligned}\sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma \left(\frac{u_i^k q(M^k)}{p(M^k)} \right) \right)^2 &\le 4 \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \frac{u_{i,K,\sigma}^k q(M_{K,\sigma}^k)}{p(M_{K,\sigma}^k)} \left(D_\sigma \left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}} \right) \right)^2 \\ &\le 4 \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \frac{q(M_{K,\sigma}^k)}{p(M_{K,\sigma}^k)} \left(D_\sigma \left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}} \right) \right)^2.\end{aligned}$$

By Proposition 4.1 and the bound $M_K^k \le M^*$ for $K\in\mathcal{T}$, we obtain $q(M_{K,\sigma}^k)/p(M_{K,\sigma}^k) \le q(M^*)/p(M^*)$. Therefore,

$$\sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma \left(\frac{u_i^k q(M^k)}{p(M^k)} \right) \right)^2 \le \frac{4q(M^*)}{p(M^*)} \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma \left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}} \right) \right)^2.$$

In view of (36), this shows the lemma. □

4.2. **Estimate for the time difference.** To show the convergence of the scheme, we need an estimate for the time difference $u_{i,K}^k - u_{i,K}^{k-1}$.

lem.time

Lemma 4.2 (Time estimate)**.** *Let the assumptions of Theorem 2.1 hold. Then there exists a constant $C_2>0$ not depending on Δx and Δt such that for all $i\in\{1,\ldots,n\}$ and $\phi\in C_0^\infty(Q_T)$,*

$$\sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} (u_{i,K}^k - u_{i,K}^{k-1}) \phi(x_K,t_k) \le C_2 \Delta t \|\nabla\phi\|_{L^\infty(Q_T)}.$$

Proof. We abbreviate $\phi_K^k := \phi(x_K,t_k)$ and fix $i\in\{1,\ldots,n\}$. We multiply (18) by $\Delta t \phi_K^k$ and sum over $K\in\mathcal{T}$ and $k=1,\ldots,N_T$

$$\sum_{k=1}^{N_T} \sum_{K\in\mathcal{T}} \mathrm{m}(K)(u_{i,K}^k - u_{i,K}^{k-1})\phi_K^k = -\sum_{k=1}^{N_T} \Delta t \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \mathcal{F}_{i,K,\sigma}^k \phi_K^k =: J_8.$$

Inserting the definition of $\mathcal{F}^k_{i,K,\sigma}$ and using the symmetry of τ_σ with respect to $\sigma = K|L$, we find that

$$J_8 = -\sum_{k=1}^{N_T} \Delta t \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma (p^k_\sigma)^2 D_{K,\sigma}\bigg(\frac{u^k_i q(M^k)}{p(M^k)}\bigg) D_{K,\sigma}\phi^k.$$

Using the Cauchy-Schwarz inequality, we obtain $|J_8| \le J_{80}J_{81}$, where

$$J_{80} = \bigg(\sum_{k=1}^{N_T} \Delta t |\phi^k_{\mathcal{M}}|^2_{1,2,\mathcal{M}}\bigg)^{1/2},$$

$$J_{81} = \bigg(\sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \big((p^k_\sigma)^2\big)^2 \bigg[D_\sigma\bigg(\frac{u^k_i q(M^k)}{p(M^k)}\bigg)\bigg]^2\bigg)^{1/2}.$$

It follows from the mesh properties (12) and (10) that

$$\begin{aligned} J_{80} &\le \|\nabla\phi\|_{L^\infty(Q_T)}\bigg(\sum_{k=1}^{N_T}\Delta t\sum_{\sigma\in\mathcal{E}} \mathrm{m}(\sigma)\mathrm{d}_\sigma\bigg)^{1/2} \\ &\le \frac{1}{\xi^{1/2}}\|\nabla\phi\|_{L^\infty(Q_T)}\bigg(\sum_{k=1}^{N_T}\Delta t\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} \mathrm{m}(\sigma)\mathrm{d}(x_K,\sigma)\bigg)^{1/2} \\ &\le \frac{2^{1/2}}{\xi^{1/2}}\|\nabla\phi\|_{L^\infty(Q_T)}\bigg(\sum_{k=1}^{N_T}\Delta t\sum_{K\in\mathcal{T}} \mathrm{m}(K)\bigg)^{1/2} = \sqrt{\frac{2\mathrm{m}(\Omega)T}{\xi}}\|\nabla\phi\|_{L^\infty(Q_T)}. \end{aligned}$$

By Lemma 4.1, $J_{81} \le C_1 p(0)^2$. This shows that $|J_8| \le C_2\Delta t\|\nabla\phi\|_{L^\infty(Q_T)}$, concluding the proof. □

4.3. **Lower bound for the entropy production term.** In this section we establish a discrete counterpart of inequality (9).

lem.lower **Lemma 4.3** (Lower bound for the entropy production)**.** *Let the assumptions of Theorem 2.1 hold. Then there exists a constant $C_3 > 0$ depending on p, q, a, b, and κ such that for $k = 1, \dots, N_T$,*

3.I (37)
$$\sum_{i=1}^n I_i(u^k_{\mathcal{M}}) \ge \frac{1}{2}\sum_{i=1}^n\sum_{\sigma\in\mathcal{E}} \tau_\sigma \beta^k_{K,\sigma}\big(D_\sigma\sqrt{u^k_i}\big)^2 + C_3\sum_{\sigma\in\mathcal{E}}\tau_\sigma\frac{(M^k_\sigma)^{a-1}(D_\sigma M^k)^2}{(1-M^k_\sigma)^{1+b+\kappa}},$$

where $M^k_\sigma = \theta_\sigma M^k_K + (1-\theta_\sigma)M^k_{K,\sigma}$ for some $\theta_\sigma \in (0,1)$,

$$\beta^k_{K,\sigma} = \min\big\{p(M^k_K)q(M^k_K), p(M^k_{K,\sigma})q(M^k_{K,\sigma})\big\},$$

and we recall that $I_i(u^k_{\mathcal{M}})$ is defined in (25)*.*

Proof. To simplify the presentation, we omit the superindex k throughout the proof. Summing definition (25) for $I_i(u_{\mathcal{M}})$ over $i = 1, \dots, n$ and setting $f(x) = \sqrt{q(x)/p(x)}$, we

obtain

$$I := \sum_{i=1}^n I_i(u_{\mathcal{M}}) = \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 \big(D_{K,\sigma}(\sqrt{u_i} f(M))\big)^2.$$

We split the sum into two parts and use the product rule for finite volumes. Then $I = J_{90} + J_{91}$, where

$$J_{90} = \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 \big(\sqrt{u_{i,K,\sigma}} D_{K,\sigma}(f(M)) + D_{K,\sigma}(\sqrt{u_i}) f(M_K)\big)^2 \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}},$$

$$J_{91} = \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 \big(\sqrt{u_{i,K}} D_{K,\sigma}(f(M)) + D_{K,\sigma}(\sqrt{u_i}) f(M_{K,\sigma})\big)^2 \mathbf{1}_{\{M_{K,\sigma}< M_K\}}.$$

A Taylor expansion of f around $M_{K,\sigma}$ gives

$$J_{90} = \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 \big(\sqrt{u_{i,K,\sigma}} D_{K,\sigma}(M) f'(M_\sigma) + D_{K,\sigma}(\sqrt{u_i}) f(M_K)\big)^2 \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}},$$

$$J_{91} = \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 \big(\sqrt{u_{i,K}} D_{K,\sigma}(M) f'(M_\sigma) + D_{K,\sigma}(\sqrt{u_i}) f(M_{K,\sigma})\big)^2 \mathbf{1}_{\{M_{K,\sigma}< M_K\}},$$

where $M_\sigma = \theta_\sigma M_{K,\sigma} + (1-\theta_\sigma) M_K$ for some $\theta_\sigma \in (0,1)$ and for $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$.

We consider the term J_{90} first. Expanding the square gives three terms, $J_{90} = J_{901} + J_{902} + J_{903}$, where

$$J_{901} = \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma p_\sigma^2 f(M_K)^2 \big(D_\sigma(\sqrt{u_i})\big)^2 \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}},$$

$$J_{902} = 2\sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 \sqrt{u_{i,K,\sigma}} D_{K,\sigma}(\sqrt{u_i}) f'(M_\sigma) f(M_K) D_{K,\sigma}(M) \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}},$$

$$\begin{aligned} J_{903} &= \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma p_\sigma^2 u_{i,K,\sigma} f'(M_\sigma)^2 (D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}} \\ &= \sum_{\sigma\in\mathcal{E}} \tau_\sigma p_\sigma^2 M_{K,\sigma} f'(M_\sigma)^2 (D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}}, \end{aligned}$$

and in the last equality we used the identity $\sum_{i=1}^n u_{i,K,\sigma} = M_{K,\sigma}$.

Definition (20) of p_σ^2 implies that $p_\sigma^2 \ge p(M_K)^2/2$. Then, by definition of f,

$$J_{901} = \frac{1}{2} \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma p(M_K) q(M_K) \big(D_\sigma(\sqrt{u_i})\big)^2 \mathbf{1}_{\{M_{K,\sigma}\ge M_K\}}.$$

By Proposition 4.1, the function f is increasing. Together with $x(x-y) \geq \frac{1}{2}(x^2-y^2)$, this gives

$$\begin{aligned} J_{902} &\geq \sum_{i=1}^n \sum_{\substack{\sigma\in\mathcal{E}\\ K=K_\sigma}} \tau_\sigma p_\sigma^2 (u_{i,K,\sigma}-u_{i,K}) f'(M_\sigma) f(M_K) D_{K,\sigma}(M) \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}} \\ &= \sum_{\sigma\in\mathcal{E}} \tau_\sigma p_\sigma^2 (D_\sigma M)^2 f'(M_\sigma) f(M_K) \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}} \geq 0. \end{aligned}$$

It remains to estimate J_{903}. For this, we set $J_{903} = \sum_{\sigma\in\mathcal{E}} J_{903}(\sigma)$, where

$$J_{903}(\sigma) = \tau_\sigma p_\sigma^2 M_{K,\sigma} f'(M_\sigma)^2 (D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}.$$

Thanks to Proposition 4.1, there exists $\delta\in(0,1/2)$ such that for all $M_\sigma > 1-\delta$,

4.pq

$$\frac{p(M_\sigma)q(M_\sigma)}{(1-M_\sigma)^{1-b+\kappa}} \geq \frac{C_{pq}}{2}, \tag{38}$$

where the constant $C_{pq}>0$ is defined in (35). We distinguish the cases (i) $0\leq M_\sigma\leq 1-\delta$ and (ii) $1-\delta < M_\sigma < 1$.

Consider first case (i). Modifying slightly the proof of [15, Lemma 3.4], it holds that for all $0\leq M_\sigma \leq 1-\delta$,

$$f'(M_\sigma) \geq \frac{a}{2M_\sigma} f(M_\sigma), \quad p(M_\sigma)q(M_\sigma) \geq \frac{p(1-\delta)^2 M_\sigma^a}{p(0)^2(a+1)}.$$

On the set $\{M_{K,\sigma}\geq M_K\}$ we have $M_{K,\sigma}\geq M_\sigma \geq M_K$, and thus, $p_\sigma^2 \geq p(M_K)^2/2 \geq p(M_\sigma)^2/2$. Therefore, taking into account the definition of f,

$$\begin{aligned} J_{903}(\sigma) &\geq \tau_\sigma \frac{p(M_\sigma)^2}{2} M_{K,\sigma} \frac{a^2}{4M_\sigma^2} f(M_\sigma)^2 (D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}} \\ &= \frac{a^2}{8}\tau_\sigma p(M_\sigma)q(M_\sigma)\frac{M_{K,\sigma}}{M_\sigma^2}(D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}} \\ &\geq \frac{a^2 p(1-\delta)^2}{8(a+1)p(0)^2}\tau_\sigma M_\sigma^{a-1}\frac{M_{K,\sigma}}{M_\sigma}(D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}} \\ &\geq \frac{a^2 p(1-\delta)^2}{8(a+1)p(0)^2}\tau_\sigma M_\sigma^{a-1}(D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}, \end{aligned}$$

where we used $M_{K,\sigma}\geq M_\sigma$ in the last inequality. Since $M_\sigma\leq 1-\delta$, we have $(1-M_\sigma)^{1+b+\kappa}\geq \delta^{1+b+\kappa}$ and consequently,

$$J_{903}(\sigma) \geq \frac{a^2 p(1-\delta)^2\delta^{1+b+\kappa}}{8(a+1)p(0)^2}\frac{\tau_\sigma M_\sigma^{a-1}}{(1-M_\sigma)^{1+b+\kappa}}(D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}.$$

In case (ii), using $M_{K,\sigma}\geq M_\sigma > 1-\delta$ and $p_\sigma^2 \geq p(M_K)^2/2 \geq p(M_\sigma)^2/2$, we find that

$$J_{903}(\sigma) \geq \frac{1}{2}(1-\delta)\tau_\sigma p(M_\sigma)^2 f'(M_\sigma)^2 (D_\sigma M)^2 \mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}$$

$$\geq \frac{1}{2}(1-\delta)\tau_\sigma p(M_\sigma)q(M_\sigma)\left(\frac{f'(M_\sigma)}{f(M_\sigma)}\right)^2(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}.$$

The proof of [15, Lemma 3.4] shows that there exists a constant $C_4>0$ such that

$$\frac{f'(x)}{f(x)}\geq\frac{C_4}{(1-x)^{1+\kappa}}\quad\text{for }\frac{1}{2}<x<1.$$

Hence, together with (38), we infer that

$$\begin{aligned}J_{903}(\sigma)&\geq\frac{1}{2}(1-\delta)C_4^2\tau_\sigma\frac{p(M_\sigma)q(M_\sigma)}{(1-M_\sigma)^{1-b+\kappa}}(1-M_\sigma)^{-1-b-\kappa}(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}\\&\geq\frac{1}{4}(1-\delta)C_{pq}C_4^2\tau_\sigma(1-M_\sigma)^{-1-b-\kappa}(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}\\&\geq\frac{1}{4}(1-\delta)C_{pq}C_4^2\tau_\sigma\frac{M_\sigma^{a-1}}{(1-M_\sigma)^{1+b+\kappa}}(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}\geq M_K\}},\end{aligned}$$

where in the last step we used $M_\sigma\leq 1$ and $a\geq 1$. We have proved that in both cases (i) and (ii), there exists a constant $C_5>0$ such that

$$J_{903}\geq C_5\sum_{\sigma\in\mathcal{E}}\tau_\sigma\frac{M_\sigma^{a-1}}{(1-M_\sigma)^{1+b+\kappa}}(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}\geq M_K\}}.$$

Similarly, we expand the square in J_{91} such that $J_{91}=J_{911}+J_{912}+J_{913}$, where

$$\begin{aligned}J_{911}&=\sum_{i=1}^n\sum_{\sigma\in\mathcal{E}}\tau_\sigma p_\sigma^2 f(M_{K,\sigma})^2(D_\sigma(\sqrt{u_i}))^2\mathbf{1}_{\{M_{K,\sigma}<M_K\}},\\J_{912}&=2\sum_{i=1}^n\sum_{\substack{\sigma\in\mathcal{E}\\K=K_\sigma}}\tau_\sigma p_\sigma^2\sqrt{u_{i,K}}D_{K,\sigma}(\sqrt{u_i})f'(M_\sigma)f(M_{K,\sigma})D_{K,\sigma}(M)\mathbf{1}_{\{M_{K,\sigma}<M_K\}},\\J_{913}&=\sum_{i=1}^n\sum_{\sigma\in\mathcal{E}}\tau_\sigma p_\sigma^2 u_{i,K}f'(M_\sigma)^2(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}<M_K\}}.\end{aligned}$$

Arguing as for the expressions J_{901} and J_{902}, we obtain $J_{912}\geq 0$ and

$$J_{911}=\frac{1}{2}\sum_{i=1}^n\sum_{\sigma\in\mathcal{E}}\tau_\sigma p(M_{K,\sigma})q(M_{K,\sigma})(D_\sigma(\sqrt{u_i}))^2\mathbf{1}_{\{M_{K,\sigma}<M_K\}}.$$

The terms in J_{913} are studied as before for the cases $0\leq M_\sigma\leq 1-\delta$ and $M_\sigma>1-\delta$. Similar computations lead to the existence of a constant $C_6>0$ such that

$$J_{913}\geq C_6\sum_{\sigma\in\mathcal{E}}\tau_\sigma\frac{M_\sigma^{a-1}}{(1-M_\sigma)^{1+b+\kappa}}(D_\sigma M)^2\mathbf{1}_{\{M_{K,\sigma}<M_K\}}.$$

We put together the estimates for J_{901} and J_{911},

J91J101 (39) $$J_{901}+J_{911}\geq\frac{1}{2}\sum_{\sigma\in\mathcal{E}}\tau_\sigma\min\big\{p(M_K)q(M_K),p(M_{K,\sigma})q(M_{K,\sigma})\big\}(D_\sigma\sqrt{u_i})^2.$$

and add J_{903} and J_{913},

J93J103 (40)
$$J_{903} + J_{913} \geq \min\{C_5, C_6\} \sum_{\sigma\in\mathcal{E}} \tau_\sigma \frac{M_\sigma^{a-1}}{(1-M_\sigma)^{1+b+\kappa}} (D_\sigma M)^2.$$

Note that $J_{902} + J_{912} \geq 0$. Then $I \geq (J_{901} + J_{911}) + (J_{903} + J_{913})$ and inserting estimates (39) and (40), we finish the proof. □

5. Convergence of solutions

ec.convsol

Before proving the convergence of the scheme, we show some compactness properties for the solutions to scheme (16)-(20). More precisely, we deduce from the compactness criterion of [5] the almost everywhere convergence of $u_{i,\eta}$. This criterion can be seen as a discrete "compensated compactness" result in the framework of Tartar and Murat. Then we establish the weak convergence of (a subsequence of) the discrete gradient of $u_{i,\eta}q(M_\eta)/p(M_\eta)$ in $L^2(Q_T)$ and the convergence for the traces in a weak sense.

prop.conv **Proposition 5.1** (Almost everywhere convergence)**.** *Let the assumptions of Theorem 2.2 hold and let $(u_\eta)_{\eta>0}$ be a family of discrete solutions to scheme* (16)-(20) *constructed in Theorem 2.1. Then there exists a subsequence of $(u_\eta)_{\eta>0}$, which is not relabeled, and a function $u = (u_1, \ldots, u_n) \in L^\infty(Q_T)^n$ such that, as $\eta \to 0$,*

$$u_{i,\eta} \to u_i \geq 0 \quad \text{a.e. in } Q_T,\ i = 1, \ldots, n.$$

Moreover, there exists $M \in L^\infty(Q_T)$ such that

$$M_\eta = \sum_{i=1}^n u_{i,\eta} \to M = \sum_{i=1}^n u_i < 1 \quad \text{a.e. in } Q_T.$$

Proof. Assumptions (A_x1) and (A_x3) in [5, Theorem 3.9] are satisfied due to the choice of finite volumes. Assumption (A_t) is always fulfilled for one-step methods like the implicit Euler discretization. Assumptions (a) and (b) are a consequence of the L^∞ bound, while Lemma 4.2 ensures assumption (c). Thus, the result follows directly from [5, Theorem 3.9]. □

The gradient estimate in Lemma 4.1 shows that the discrete gradient of $u_{i,\eta}q(M_\eta)/p(M_\eta)$ converges weakly in $L^2(Q_T)$ (up to a subsequence) to some function. The following lemma shows that the limit can be identified with $\nabla(u_i q(M)/p(M))$.

m.convgrad **Lemma 5.1** (Convergence of the gradient)**.** *Let the assumptions of Theorem 2.2 hold and let $(u_\eta)_{\eta>0}$ be a family of discrete solutions to scheme* (16)-(20) *constructed in Theorem 2.1. Then, up to a subsequence, as $\eta \to 0$,*

$$\nabla^\eta\left(\frac{u_{i,\eta}q(M_\eta)}{p(M_\eta)}\right) \rightharpoonup \nabla\left(\frac{u_i q(M)}{p(M)}\right) \quad \text{weakly in } L^2(Q_T),$$

where u_i and M are the limit functions obtained in Proposition 5.1.

Proof. The goal is to establish the limit

$$\int_{Q_T} \nabla^\eta \left(\frac{u_{i,\eta} q(M_\eta)}{p(M_\eta)} \right) \cdot \phi \, dxdt + \int_{Q_T} \frac{u_{i,\eta} q(M_\eta)}{p(M_\eta)} \operatorname{div} \phi \, dxdt \to 0 \quad \text{as } \eta \to 0$$

for all $\phi \in C_0^\infty(Q_T)$ and $i = 1, \ldots, n$. Thanks to the proof of [12, Lemma 4.4], this result is a direct consequence of the definition of the discrete gradient operator ∇^η defined in Section 2.2 and Lemma 4.1, which guarantees uniform estimates on the discrete $L^2(0,T;H^1(\Omega))$ norm of $u_{i,\eta} q(M_\eta)/p(M_\eta)$ for $i = 1, \ldots, n$. □

Finally, we verify that the limit function u satisfies the Dirichlet boundary condition in a weak sense.

lem.trace **Lemma 5.2** (Convergence of the traces)**.** *Let the assumptions of Theorem 2.2 hold and let $(u_\eta)_{\eta>0}$ be a family of discrete solutions to scheme* (16)-(20) *constructed in Theorem 2.1 such that $u_\eta \to u$ and $M_\eta \to M$ a.e. in Q_T as $\eta \to 0$. Then*

$$\frac{u_i q(M)}{p(M)} - \frac{u_i^D q(M^D)}{p(M^D)} \in L^2(0,T;H_D^1(\Omega)).$$

Proof. Let us define $v_{i,\eta} := u_{i,\eta} q(M_\eta)/p(M_\eta)$ for $i = 1, \ldots, n$. Then, using [6, Lemma 4.7] and [6, Lemma 4.8], we can prove, thanks to Lemma 4.1 and the L^∞-estimate, that up to a subsequence, for all $1 \le p < +\infty$ as $\eta \to 0$,

$$v_{i,\eta} \to v_i = \frac{u_i \, q(M)}{p(M)} \quad \text{strongly in } L^p(\Gamma^D \times (0,T)), \ i = 1, \ldots, n,$$

see for instance the proof of [6, Proposition 4.9]. Then, up to a subsequence,

convtrace (41) $$v_{i,\eta} \to v_i \quad \text{a.e. in } \Gamma^D \times (0,T), \ i = 1, \ldots, n.$$

Moreover, by construction (21)-(22),

$$v_{i,\eta}(x,t) = \frac{u_i^D \, q(M^D)}{p(M^D)} \quad \text{for } (x,t) \in \Gamma^D \times (0,T), \ i = 1, \ldots, n.$$

Thus, we deduce from (41) that

$$v_i = \frac{u_i^D \, q(M^D)}{p(M^D)} \quad \text{a.e. in } \Gamma^D \times (0,T), \ i = 1, \ldots, n,$$

which concludes the proof. □

6. Convergence of the scheme

ec.convsch

In this section, we identify, under the assumptions of Theorem 2.2, the limit function $u = (u_1, \ldots, u_n)$ obtained in Proposition 5.1 as a weak solution to (1)-(4). For this, we follow some ideas developed in [8, 12]. Roughly speaking, this approach consists of replacing in the weak formulation (26) the weak solution by $u_\eta = (u_{1,\eta}, \ldots, u_{n,\eta})$. Then, applying the convergence results proved in the previous section and passing to the limit $\eta \to 0$, we identify the function u as a weak solution. Finally, using the uniqueness result obtained

in [15, Theorem 2.3], if $\alpha_i = 1$ for $i = 1, \dots, n$, we conclude that the whole sequence u_η converges towards the weak solution of (1)-(4) when $\eta \to 0$.

6.1. **Convergence towards the weak solution.** Let $\phi \in C_0^\infty(\Omega \times [0,T))$ and choose $\eta = \max\{\Delta x, \Delta t\}$ sufficiently small such that $\mathrm{supp}(\phi) \subset \{x \in \Omega : \mathrm{d}(x, \partial\Omega) > \eta\} \times [0,T)$. In particular, ϕ vanishes in any cell $K \in \mathcal{T}$ with $K \cap \partial\Omega \neq \emptyset$. Again, we abbreviate $\phi_K^k = \phi(x_K, t_k)$ and we fix $i \in \{1, \dots, n\}$. Let

$$\begin{aligned}
&\varepsilon(\eta) = F_{10}^\eta + F_{20}^\eta, \quad \text{where} \\
&F_{10}^\eta = -\int_0^T \int_\Omega u_{i,\eta} \partial_t \phi dx dt - \int_\Omega u_{i,\eta}(x,0)\phi(x,0)dx, \\
&F_{20}^\eta = \int_0^T \int_\Omega p(M_\eta)^2 \nabla^\eta \left(\frac{u_{i,\eta} q(M_\eta)}{p(M_\eta)} \right) \cdot \nabla\phi dx dt.
\end{aligned}$$

Proposition 5.1 and Lemma 5.1 allow us to perform the limit $\eta \to 0$ in these integrals, leading to

$$\begin{aligned}
\lim_{\eta\to 0} \varepsilon(\eta) = &-\int_0^T \int_\Omega u_i \partial_t \phi dx dt - \int_\Omega u_i(x,0)\phi(x,0)dx \\
&+ \int_0^T \int_\Omega p(M)^2 \nabla \left(\frac{u_i q(M)}{p(M)} \right) \cdot \nabla\phi dx dt.
\end{aligned}$$

Therefore, it remains to prove that $\varepsilon(\eta) \to 0$ as $\eta \to 0$.

To this end, we multiply (18) by $\Delta t \phi_K^{k-1}$ and sum over $K \in \mathcal{T}$ and $k = 1, \dots, N_T$, giving

$$\begin{aligned}
&F_1^\eta + F_2^\eta = 0, \quad \text{where} \\
&F_1^\eta = \sum_{k=1}^{N_T} \sum_{K\in\mathcal{T}} \mathrm{m}(K)(u_{i,K}^k - u_{i,K}^{k-1})\phi_K^{k-1}, \\
&F_2^\eta = \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \mathcal{F}_{i,K,\sigma}^k \phi_K^{k-1}.
\end{aligned}$$

For the proof of $\varepsilon(\eta) \to 0$ as $\eta \to 0$, it is sufficient to show that $F_{j0}^\eta - F_j^\eta \to 0$ as $\eta \to 0$ for $j = 1, 2$.

The arguments in [8, Section 5.2] show that

$$|F_{10}^\eta - F_1^\eta| \le CT\mathrm{m}(\Omega)\|\phi\|_{C^1(\overline{Q_T})}\, \eta \to 0 \quad \text{as } \eta \to 0.$$

The remaining convergence for $|F_{20}^\eta - F_2^\eta|$ is more involved. First, we rewrite F_2^η. By the conservation of the numerical fluxes $\mathcal{F}_{i,K,\sigma} + \mathcal{F}_{i,L,\sigma} = 0$ for all the edges $\sigma = K|L \in \mathcal{E}_{\mathrm{int}}$ and the definition of $\mathcal{F}_{i,K,\sigma}^k$, we infer that

$$F_2^\eta = -\sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \mathcal{F}_{i,K,\sigma}^k D_{K,\sigma}\phi^{k-1}$$

$$
\begin{aligned}
&= \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} p(M_K^k)^2 \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \tau_\sigma D_{K,\sigma}\bigg(\frac{u_i^k q(M^k)}{p(M^k)}\bigg) D_{K,\sigma}\phi^{k-1} \\
&\quad + \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \tau_\sigma\big((p_\sigma^k)^2 - p(M_K^k)^2\big) D_{K,\sigma}\bigg(\frac{u_i^k q(M^k)}{p(M^k)}\bigg) D_{K,\sigma}\phi^{k-1} \\
&=: F_{21}^\eta + F_{22}^\eta.
\end{aligned}
$$

Inserting the definition of the discrete gradient $\nabla^\eta = \nabla^{\mathcal{D}^\eta}$, we can reformulate F_{20}^η as

$$
F_{20}^\eta = \sum_{k=1}^{N_T} \sum_{K\in\mathcal{T}} p(M_K^k)^2 \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} D_{K,\sigma}\bigg(\frac{u_i^k q(M^k)}{p(M^k)}\bigg) \frac{\mathrm{m}(\sigma)}{\mathrm{m}(T_{K,\sigma})} \int_{t_{k-1}}^{t_k} \int_{T_{K,\sigma}} \nabla\phi\cdot\nu_{K,\sigma} dx dt.
$$

Thus, using the monotonicity of p, we have

$$
\begin{aligned}
|F_{20}^\eta - F_{21}^\eta| &\le p(0)^2 \sum_{k=1}^{N_T} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \mathrm{m}(\sigma) D_\sigma\bigg(\frac{u_i^k q(M^k)}{p(M^k)}\bigg) \\
&\qquad \times \bigg| \int_{t_{k-1}}^{t_k} \bigg(\frac{D_{K,\sigma}\phi^k}{\mathrm{d}_\sigma} - \frac{1}{\mathrm{m}(T_{K,\sigma})} \int_{T_{K,\sigma}} \nabla\phi\cdot\nu_{K,\sigma} dx\bigg) dt\bigg|.
\end{aligned}
$$

In view of the proof of Theorem 5.1 in [12], there exists a constant $C_{\mathrm{cons}} > 0$ such that

$$
\bigg| \int_{t_{k-1}}^{t_k} \bigg(\frac{D_{K,\sigma}\phi^k}{\mathrm{d}_\sigma} - \frac{1}{\mathrm{m}(T_{K,\sigma})} \int_{T_{K,\sigma}} \nabla\phi\cdot\nu_{K,\sigma} dx\bigg) dt\bigg| \le C_{\mathrm{cons}} \Delta t \eta.
$$

Applying this inequality and the Cauchy-Schwarz inequality, we obtain

$$
|F_{20}^\eta - F_{21}^\eta| \le p(0)^2 C_{\mathrm{cons}} \eta \bigg(\sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \mathrm{m}(\sigma)\mathrm{d}_\sigma\bigg)^{1/2} \bigg(\sum_{k=1}^{N_T} \Delta t \bigg|\frac{u_i^k q(M^k)}{p(M^k)}\bigg|_{1,2,\mathcal{M}}^2\bigg)^{1/2}.
$$

It remains to use the mesh regularity (12), property (23), and the gradient estimate given by Lemma 4.1 to conclude that, for some constant $C > 0$,

F20F21 (42) $$|F_{20}^\eta - F_{21}^\eta| \le C(\xi, C_3) p(0)^2 \eta \to 0 \quad \text{as } \eta \to 0.$$

We turn to the estimate of F_{22}^η. To this end, we use the definition of $(p_\sigma^k)^2$ to rewrite F_{22}^η as $F_{22}^\eta = F_{220}^\eta + F_{221}^\eta$, where

$$
\begin{aligned}
F_{220}^\eta &= \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \tau_\sigma \frac{p(M_{K,\sigma}^k)^2 - p(M_K^k)^2}{2} D_{K,\sigma}\bigg(\frac{u_i^k q(M^k)}{p(M^k)}\bigg) D_{K,\sigma}\phi^{k-1} \mathbf{1}_{\{M_K^k > M_{K,\sigma}^k\}}, \\
F_{221}^\eta &= \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \tau_\sigma \frac{p(M_{K,\sigma}^k)^2 - p(M_K^k)^2}{2} D_{K,\sigma}\bigg(\frac{u_i^k q(M^k)}{p(M^k)}\bigg) D_{K,\sigma}\phi^{k-1} \mathbf{1}_{\{M_K^k \le M_{K,\sigma}^k\}}.
\end{aligned}
$$

It follows from $p(M_K^k) \le p(M_{K,\sigma}^k)$ and the inequality $x^2 - y^2 \le 2x(x-y)$ that

$$|F_{220}^\eta| \le 2\eta \|\phi\|_{C^1(\overline{Q_T})} \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \tau_\sigma$$
$$\times \left| \frac{p(M_{K,\sigma}^k)^2 - p(M_K^k)^2}{2} \sqrt{\frac{u_{i,K,\sigma}^k q(M_{K,\sigma}^k)}{p(M_{K,\sigma}^k)}} D_{K,\sigma}\left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}}\right) \mathbf{1}_{\{M_K^k > M_{K,\sigma}^k\}} \right|.$$

A Taylor expansion, for $\widetilde{M}_\sigma^k = \tilde\theta_\sigma M_K^k + (1-\tilde\theta_\sigma) M_{K,\sigma}^k$ for some $\tilde\theta_\sigma \in (0,1)$,

$$p(M_{K,\sigma}^k)^2 - p(M_K^k)^2 = 2p'(\widetilde{M}_\sigma^k) p(\widetilde{M}_\sigma^k)(M_{K,\sigma}^k - M_K^k),$$

and the Cauchy-Schwarz inequality gives

F22 (43) $$|F_{220}^\eta| \le 2\eta \|\phi\|_{C^1(\overline{Q_T})} F_{2200}^\eta F_{2201}^\eta, \quad \text{where}$$

$$F_{2200}^\eta = p(0) \left\{ \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \left(D_\sigma \left(\sqrt{\frac{u_i^k q(M^k)}{p(M^k)}} \right) \right)^2 \right\}^{1/2},$$

$$F_{2201}^\eta = \left\{ \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma p'(\widetilde{M}_\sigma^k)^2 \frac{u_{i,K,\sigma}^k q(M_{K,\sigma}^k)}{p(M_{K,\sigma}^k)} (D_\sigma M)^2 \mathbf{1}_{\{M_K^k > M_{K,\sigma}^k\}} \right\}^{1/2}.$$

Inequality (36) shows that $F_{2200}^\eta \le p(0) H(u_{\mathcal{M}}^0)^{1/2}/p(M^*)$.

For the estimate of F_{2201}^η, we use $u_{i,K,\sigma}^k \le 1$ and $C_7 := \sup_{0\le x\le M^*} p'(x)^2/p(x) < \infty$ (this is finite since $M^* < 1$) to infer that

$$F_{2201}^\eta \le C_7 \left\{ \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma q(M_{K,\sigma}^k)(D_\sigma M)^2 \mathbf{1}_{\{M_K^k > M_{K,\sigma}^k\}} \right\}^{1/2}$$
$$= C_7 \left\{ \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma (M_{K,\sigma}^k)^{1-a} (1 - M_{K,\sigma}^k)^{1+b+\kappa} q(M_{K,\sigma}^k) \right.$$
$$\left. \times \frac{(M_{K,\sigma}^k)^{a-1}}{(1-M_{K,\sigma}^k)^{1+b+\kappa}} (D_\sigma M)^2 \mathbf{1}_{\{M_K^k > M_{K,\sigma}^k\}} \right\}^{1/2}.$$

Set $M_\sigma^k = \theta_\sigma M_K^k + (1-\theta_\sigma) M_{K,\sigma}^k$ as in the proof of Lemma 4.3. Using the inequality $(1-M_{K,\sigma}^k)^{1+b+\kappa} \le 1$ together with the monotonicity of $x \mapsto x^{a-1}/(1-x)^{-1-b-\kappa}$, we obtain

$$F_{2201}^\eta \le C_7 \left\{ \sum_{k=1}^{N_T} \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma (M_{K,\sigma}^k)^{1-a} q(M_{K,\sigma}^k) \frac{(M_\sigma^k)^{a-1}}{(1-M_\sigma^k)^{1+b+\kappa}} (D_\sigma M)^2 \mathbf{1}_{\{M_K^k > M_{K,\sigma}^k\}} \right\}^{1/2}.$$

By (37) and the bound

$$(M_{K,\sigma}^k)^{1-a}\, q(M_{K,\sigma}^k) \le \frac{M^*}{(a+1)\, p(M^*)^2\, (1-M^*)^b} \quad \text{for all } \sigma \in \mathcal{E},$$

this expression is bounded by the entropy production which is uniformly bounded due to the entropy inequality. We have shown that F_{2200}^η and F_{2201}^η are bounded uniformly in η such that (43) implies that $F_{220}^\eta \to 0$ as $\eta \to 0$.

Now we rewrite $|F_{221}^\eta|$ as

$$|F_{221}^\eta| \le 2\eta \|\phi\|_{C^1(\overline{Q_T})} \sum_{k=1}^{N_T} \Delta t \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}} \tau_\sigma \left| \frac{p(M_K^k)^2 - p(M_{K,\sigma}^k)^2}{2} \sqrt{\frac{u_{i,K}^k q(M_K^k)}{p(M_K^k)}} \right.$$
$$\left. \times \left(\sqrt{\frac{u_{i,K}^k q(M_K^k)}{p(M_K^k)}} - \sqrt{\frac{u_{i,K,\sigma}^k q(M_{K,\sigma}^k)}{p(M_{K,\sigma}^k)}} \right) \mathbf{1}_{\{M_K^k \le M_{K,\sigma}^k\}} \right|.$$

Arguing as for the term $|F_{220}^\eta|$, we see that $F_{221}^\eta \to 0$ as $\eta \to 0$.

The previous convergences and (42) imply that

$$|F_{20}^\eta - F_2^\eta| \le |F_{20}^\eta - F_{21}^\eta| + |F_{22}^\eta| \to 0 \quad \text{as } \eta \to 0.$$

To conclude the proof of Theorem 2.2, it remains to apply [15, Theorem 2.3] which shows the uniqueness of the weak solution to (1)-(4) (in the case $\alpha_i = 1$ for $i = 1, \dots, n$) and which implies in particular that the whole sequence $(u_\eta)_{\eta>0}$ converges to the weak solution.

7. Numerical experiments

ec.exp.num

We present some numerical experiments in one and two space dimensions, when the biofilm is composed of $n = 2$ different species of bacteria and the function p satisfies hypothesis (H4) (case 1) or not (case 2).

7.1. **Implementation of the scheme.** The finite-volume scheme (16)-(20) is implemented in MATLAB. Since the numerical scheme is implicit in time, one has to solve a nonlinear system of equations at each time step. In the one-dimensional case, we use a plain Newton method. Starting from $u^{k-1} = (u_1^{k-1}, u_2^{k-1})$, we apply a Newton method with precision $\varepsilon = 10^{-10}$ to approximate the solution to the scheme at time step k. In the two-dimensional case, we use a Newton method complemented by an adaptive time step strategy to approximate the solution of the scheme at time k. More precisely, starting again from $u^{k-1} = (u_1^{k-1}, u_2^{k-1})$, we launch a Newton method. Then, if the method did not converge with precision $\varepsilon = 10^{-10}$ after at most 50 steps, we half the time step and restart the Newton method. At the beginning of each time step, we double the previous time step. Moreover, we impose the condition $10^{-8} \le \Delta t_{k-1} \le 10^{-2}$ with an initial time step set to $\Delta t_0 = 10^{-5}$.

7.2. **Test case 1.** We introduce a function p that satisfies hypothesis (H4),

p.1

$$p(x) = \exp(-1/(1-x)) \quad \text{for all } x \in [0,1), \tag{44}$$

and we choose $a = b = 2$. In this case $\kappa = 1$ and

$$\lim_{M\to 1} (-(1-M)^2) \frac{p'(M)}{p(M)} = 1.$$

This definition of p allows us to compute explicitly the value of $q(M)/p(M)$:

qsurptest1

$$\frac{q(M)}{p(M)} = \frac{1}{M}\left(e^{2/(1-M)}\left(M - \frac{1}{2}\right) + \frac{e^2}{2}\right). \tag{45}$$

We consider a one-dimensional test case on $\Omega = (0,1)$ with $\Gamma^D = \{0\}$, $\Gamma^N = \{1\}$, $u_1^D = u_2^D = 0.1$, and the following initial data:

$$u_1^0(x) = u_1^D + u_1^D \mathbf{1}_{[0.2,0.5]}(x), \quad u_2^0(x) = u_2^D + u_2^D \mathbf{1}_{[0.5,0.8]}(x).$$

In Figure 3, we illustrate the order of convergence in space of the scheme. Since exact solutions to the biofilm model are not explicitly known, we compute a reference solution on a uniform mesh composed of 5120 cells and with $\Delta t = (1/5120)^2$. We use this rather small value of Δt because the Euler discretization in time exhibits a first-order convergence rate, while we expect a second-order convergence rate in space for scheme (16)-(20), due to the approximation of $p(M)^2$ in the numerical fluxes. We compute approximate solutions on uniform meshes made of respectively 40, 80, 160, 320, 640, 1280, and 2560 cells. Finally, we compute the L^2 norm of the difference between the approximate solution and the average of the reference solution over 40, 80, 160, 320, 640, and 1280 cells at the final time $T = 10^{-3}$. Figure 3 shows the results for p defined in (44) and with different choices of the diffusivities α_1 and α_2. We observe that the scheme converges, even when $\alpha_1 \neq \alpha_2$, with an order around two.

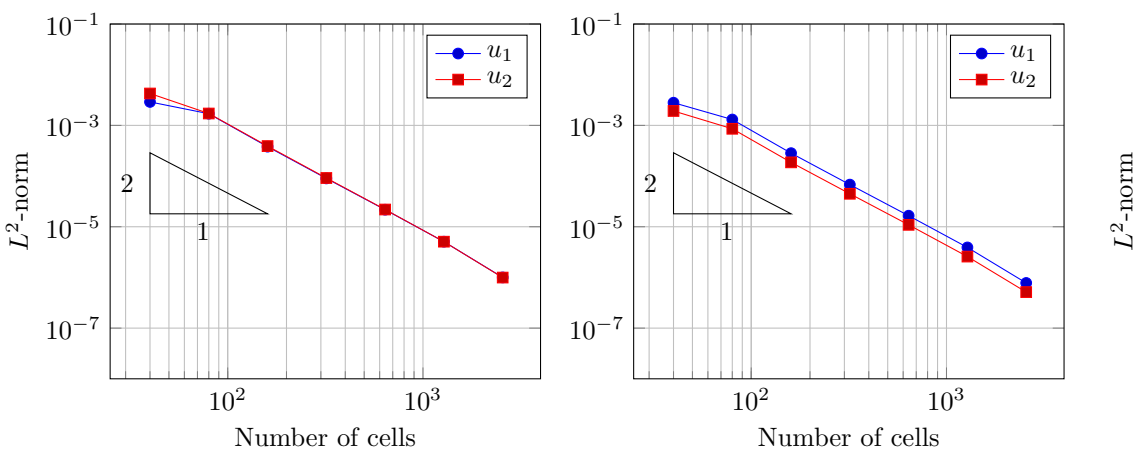

FIGURE 3. L^2 norm of the error in space with $\alpha_1 = \alpha_2 = 1$ (left) and $\alpha_1 = 1$ and $\alpha_2 = 10$ (right); p is defined in (44).

Fig1

Next, we consider a two-dimensional test case on $\Omega = (0,1) \times (0,1)$ with $\Gamma^D = \{y = 1\}$, $\Gamma^N = \partial\Omega \setminus \Gamma^D$, $u_1^D = u_2^D = 0.1$, $\alpha_1 = 1$, $\alpha_2 = 5$, and the initial data

$$u_1^0(x,y) = u_1^D + u_1^D\, \mathbf{1}_{[0.2,0.5]}(x)\mathbf{1}_{[0,0.4]}(y), \quad u_2^0(x,y) = u_2^D + 2\, u_2^D\, \mathbf{1}_{[0.5,0.8]}(x)\mathbf{1}_{[0,0.4]}(y).$$

The mesh of $\Omega = (0,1)^2$ is composed of 3584 triangles.

In Figure 4, we show the evolution of the biomass M at different times, illustrating the convergence to the steady state. It is proved in [15, Theorem 2.2] that the convergence in the L^2 norm is of order $1/t$. Figure 5 (left) shows in logarithmic scale and for $T = 110$ that the convergence is slightly faster than $1/t$. Numerically, we observe a convergence of order $1/t^\alpha$ with $\alpha = 1.7$. For larger times, the solution is close to the steady state and the linear regime dominates.

We plot in Figure 5 (right) the behavior of the relative entropy functional $H(u)$ versus time. We approximate the integral between 0 and M_K^k of $\log(q(s)/p(s))$, which appears in the definition of H, by the midpoint quadrature rule according to

$$\int_0^{M_K^k} \log\frac{q(s)}{p(s)}\,ds \approx M_K^k \log\left(e^{4/(2-M_K^k)}\,(M_K^k-1)+e^2\right) - M_K^k\left(\log M_K^k + \log 2 - 1\right),$$

for all $K \in \mathcal{T}$ and $k \geq 0$. The use of such a quadrature formula could explain why $k \mapsto H(u^k)$ does not converge to zero but stays "far away" from zero even for large times.

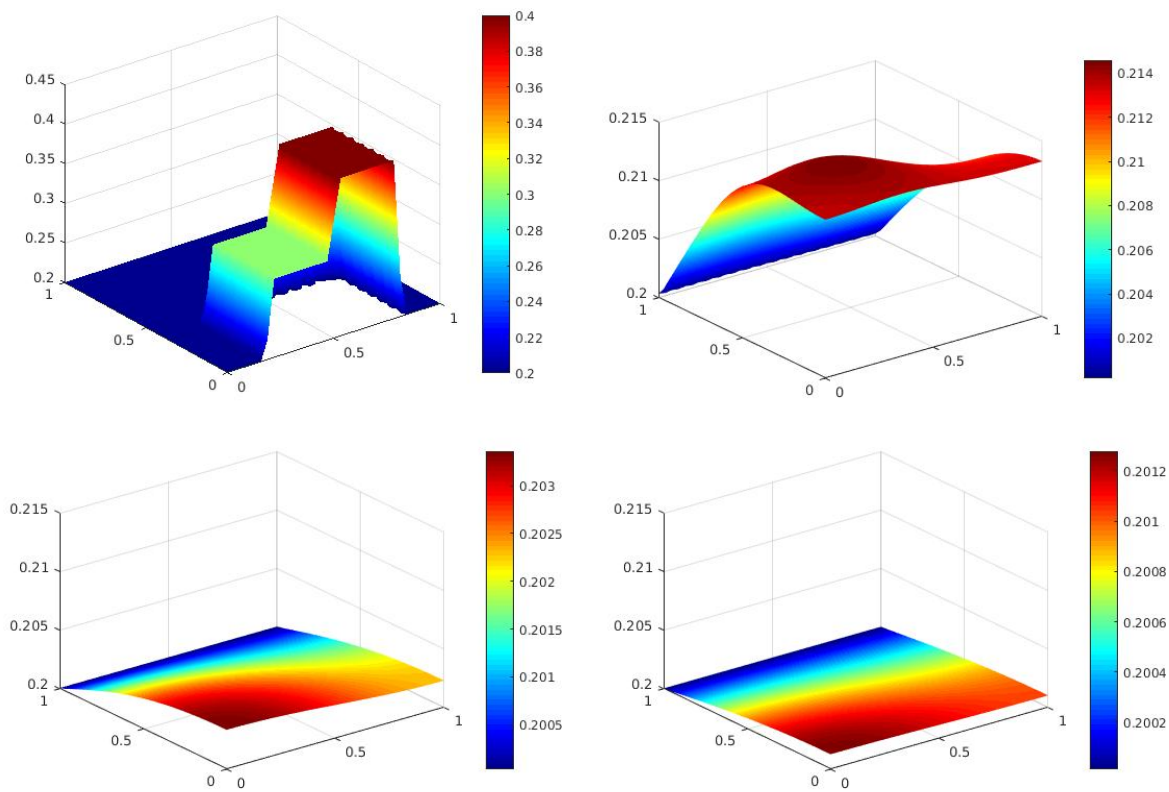

FIGURE 4. Evolution of the biomass M at different times with p defined in (44). Top left: $t = 0$, top right: $t = 1$, bottom left: $t = 5$, bottom right: $t = 10$.

Fig2

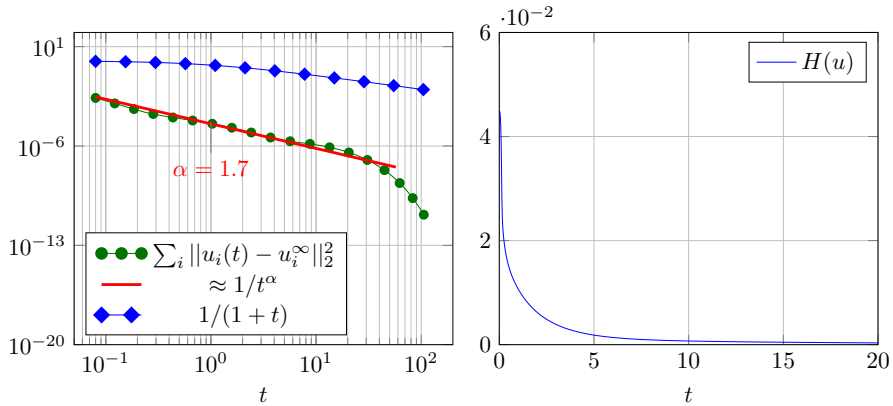

FIGURE 5. Convergence of the solution to the steady state in the L^2 norm (left) and evolution of the relative entropy versus time (right) with p defined by (44).

ntropTest1

7.3. **Test case 2.** We use a function p that does *not* satisfy hypothesis (H4):

p.2

$$p(x) = 1 - x \quad \text{for all } x \in [0,1] \tag{46}$$

and take $a = b = 1$. Also here, we can also compute explicitly $q(M)/p(M)$:

$$\frac{q(M)}{p(M)} = \frac{M}{2(1-M)^2}.$$

As before, we consider first a one-dimensional test case on $\Omega = (0,1)$ with $\Gamma^D = \{0\}$, $\Gamma^N = \{1\}$, $u_1^D = u_2^D = 0.1$, and the initial data

$$u_1^0(x) = u_1^D + u_1^D \mathbf{1}_{[0.2,0.5]}(x), \quad u_2^0(x) = u_2^D + u_2^D \mathbf{1}_{[0.5,0.8]}(x).$$

We investigate the L^2-convergence rate in space of the scheme for different values of α_1 and α_2; see Figure 6. We use the same strategy as described in the previous section. In particular, the scheme converges with an order around two.

Finally, we consider a two-dimensional test case on $\Omega = (0,1)\times(0,1)$ with $\Gamma^D = \{y = 1\}$, $\Gamma^N = \partial\Omega \setminus \Gamma^D$, $u_1^D = u_2^D = 0.01$, $\alpha_1 = 1$, $\alpha_2 = 5$, and the initial data

$$u_1^0(x,y) = u_1^D + \max\left\{1 - 8^2\left(x - \frac{3}{8}\right)^2 - 8^2\left(y - \frac{1}{2}\right) - u_1^D, 0\right\},$$
$$u_2^0(x,y) = u_2^D + \max\left\{1 - 8^2\left(x - \frac{5}{8}\right)^2 - 8^2\left(y - \frac{1}{2}\right) - 2u_2^D, 0\right\},$$

which is close to one in the interior of the domain; see Figure 7 (top left). Again, we choose a mesh of $\Omega = (0,1)^2$ consisting of 3584 triangles.

In Figure 7, we show the evolution of the biomass M at different times. We observe even in this case and with different diffusivities that the discrete biomass M stays strictly

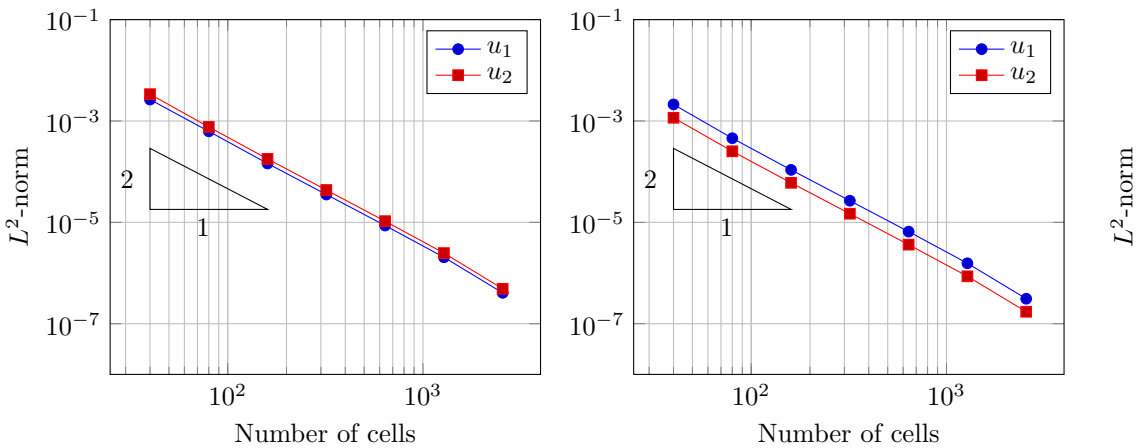

FIGURE 6. L^2 norm of the error in space with $\alpha_1 = \alpha_2 = 1$ (left) and $\alpha_1 = 1$ and $\alpha_2 = 10$ (right); p is defined in (46).

Fig4

smaller than one. This is not surprising since the equation for the biomass is of fast-diffusion type when $1 - M \approx 0$ such that the diffusion is very fast. Because of the mixed boundary conditions, the biomass converges to a nonconstant steady state.

In Figure 8 (left), we investigate the rate of convergence of the solution to the steady state $u_1^\infty = u_1^D$ and $u_2^\infty = u_2^D$. We show the (squared) L^2 norm of the difference between u_i and u_i^∞ in logarithmic scale with final time $T = 130$. Similarly to the previous case, the rate of convergence in the L^2 norm seems to be better than that one obtained analytically in [15, Theorem 2.2], which is of order $1/t$. Numerically, we observe a convergence of order $1/t^\alpha$ with $\alpha = 1.6$.

Finally, for $T = 2$, we illustrate the behavior of the relative entropy functional H; see Figure 8 (right). The relative entropy can be computed explicitly thanks to

$$\int_0^{M_K^k} \log \frac{q(s)}{p(s)} ds = M_K^k \log\left(\frac{M_K^k}{2} + 1\right) - 2(M_K^k - 1)\log(1 - M_K^k),$$

where $K \in \mathcal{T}$ and $k \geq 0$. The numerical results indicate that H is also a Lyapunov functional for system (1)-(4), even if the assumptions of [15] are not satisfied, and that scheme (16)-(20) preserves the entropy structure of the model, even when the assumptions of Theorem 2.1 do not hold.

APPENDIX A. MODELING

app

We briefly recall the modeling assumptions and the derivation of equations (1) from a lattice model. For details and references, we refer to [15, Appendix A]. We consider the evolution of the proportions u_i^j of biofilm species on a one-dimensional spatial lattice with the uniform cell distance $h > 0$, where $i = 1, \ldots, n$ denotes the species number and $j \in \mathbb{Z}$ the number of the grid cell. In particular, the total biomass $M^j = \sum_{i=1}^n u_i^j$ in the jth cell is bounded by one. Assuming that the particles of the ith species in cell j move to one of

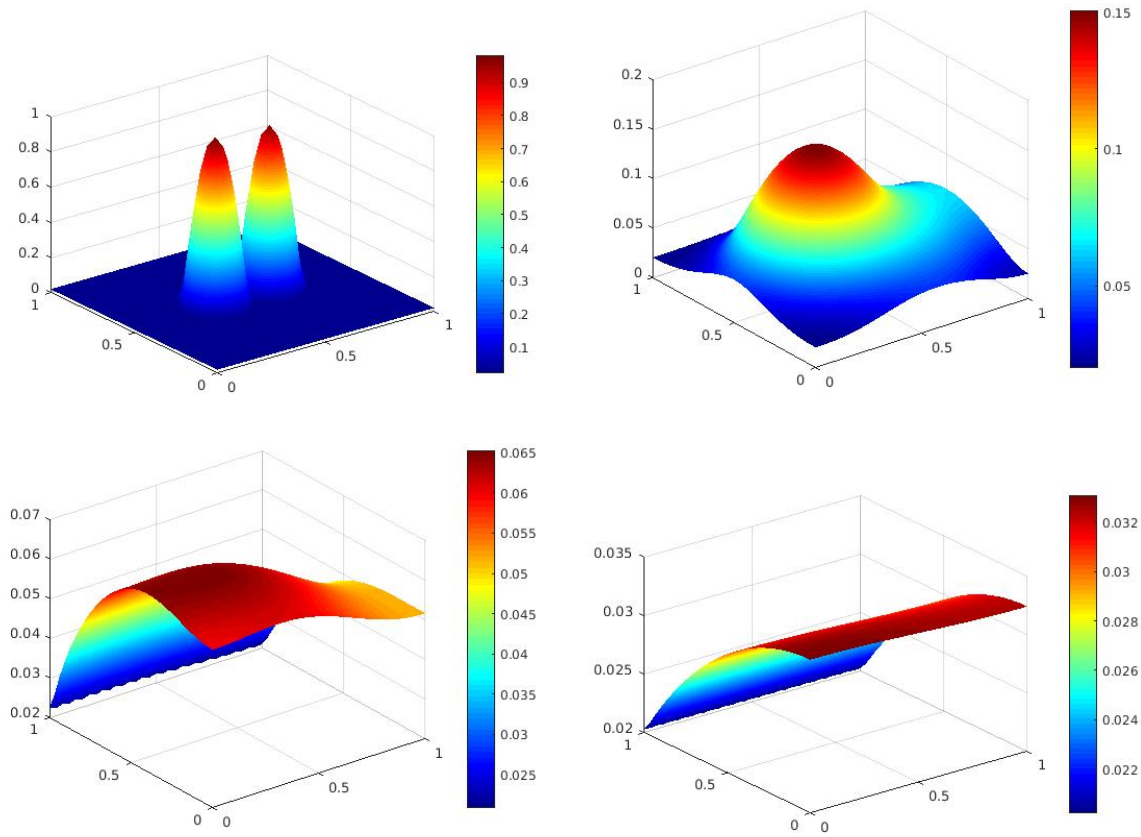

FIGURE 7. Evolution of the biomass M at different times with p defined in (46). Top left: $t = 0$, top right: $t = 0.1$, bottom left: $t = 1$, bottom right: $t = 10$.

Fig5

the neighboring cells with transition rate $T_i^{(j-1)+}$ and $T_i^{(j+1)-}$, respectively, and that the particles from the neighboring cells move to the cell j with transition rates $T_i^{j\pm}$, the master equations read as

$$\partial_t u_i^j = T_i^{(j-1)+} u_i^{j-1} + T_i^{(j+1)-} u_i^{j+1} - (T_i^{j+} + T_i^{j-}) u_i^j.$$

The transition rates are supposed to be of the form

$$T_i^{j\pm} = \alpha_i q_i(u_1^j, \ldots, u_n^j) p_i(u_1^{j\pm 1}, \ldots, u_n^{j\pm 1}),$$

where $\alpha_i = \alpha_i(h)$ measures how fast populations move between neighboring cells and the nonnegative functions p_i and q_i describe the local movement of the species.

Macroscopic equations are derived in the (formal) limit $h \to 0$. We assume that $\lim_{h\to 0} \alpha_i(h) h^2 = \alpha_i^0 > 0$, and we introduce functions u_i that interpolate the grid functions, $u_i(jh, t) = u_i^j(t)$. Performing a Taylor expansion of u_i, inserting these expressions into the master equations, and passing to the formal limit $h \to 0$ (see [29] for details), we

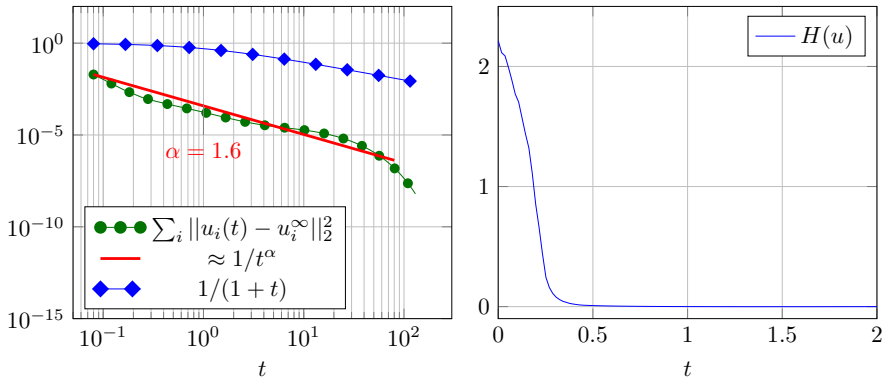

FIGURE 8. Convergence of the solutions to the steady state in the L^2 norm (left) and evolution of the relative entropy versus time (right) with p defined by (46).

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arrive at

$$\partial_t u_i = \alpha_i^0 \frac{\partial}{\partial x}\left(\sum_{j=1}^n A_{ij}(u)\frac{\partial u_j}{\partial x}\right), \quad i = 1, \ldots, n,$$

where

$$A_{ij}(u) = \delta_{ij} p_i(u) q_i(u) + u_i\left(p_i(u)\frac{\partial q_i}{\partial u_j}(u) - q_i(u)\frac{\partial p_i}{\partial u_j}(u)\right).$$

The same procedure can be applied in the case of several space dimensions, leading to the same equations as above, replacing $\partial/\partial x$ by ∇.

Our model is supposed to describe volume-filling effects. This means that the motivation of the particles to leave a cell is small if the target cell is crowded and large if the departure cell is crowded, i.e., if the total biomass $M = \sum_{i=1}^n u_i$ is close to the maximal cell capacity (normalized to one). Thus, we assume that the functions p_i and q_i only depend on the total biomass, p_i is decreasing with $p_i(1) = 0$, and q_i is increasing. A further assumption is that the biomass species have similar properties such that $p = p_i$ and $q = q_i$ for $i = 1, \ldots, n$. Then we can write

$$\sum_{j=1}^n A_{ij}(u)\nabla u_j = p(M)^2 \nabla\left(\frac{u_i q(M)}{p(M)}\right),$$

which leads to (1).

The functions p and q are chosen in such a way that the evolution equation for the total biomass M is consistent with the single-species biofilm model of [16] (without reaction terms),

app.M

$$\partial_t M = \operatorname{div}\left(\frac{M^a}{(1-M)^b}\nabla M\right), \tag{47}$$

where a, $b \geq 1$. Thus, we choose p and q such that

$$p(M)^2 \nabla \left(\frac{Mq(M)}{p(M)} \right) = \frac{M^a}{(1-M)^b} \nabla M.$$

This leads to

$$q(M) = \frac{p(M)}{M} \int_0^M \frac{s^a}{(1-s)^b} \frac{ds}{p(s)^2}, \quad M > 0,$$

defined in (2). For instance, assuming a linear dependency of the transition rate to leave the cell with respect to the total biomass, we may choose $p(M) = 1 - M$, yielding

$$q(M) = \frac{1-M}{M} \int_0^M \frac{s^a ds}{(1-s)^{b+2}}.$$

Equation (47) is a degenerate-singular parabolic equation first suggested in [16]. It acts as a porous-medium equation when the total biomass is small, $M \ll 1$, and as a fast-diffusion equation when the total biomass is close to ist maximal value. The analysis in [15] and our numerical results show that the singular value in fact is not reached, i.e. $M < 1$ (if the initial total biomass is smaller than one). In real biofilms, the saturation case $M = 1$ may occur but this is not covered by our model. The value $M = 1$ is reached in finite time in the model of [17, Prop. 7] in the case of pure Neumann conditions and for suitably chosen source terms.

Model equations (1) are solved in a bounded domain with suitable boundary conditions. We may assume that the biofilm fraction u_i is fixed on the boundary Γ^D and that the remaining boundary part Γ^N is insulating, i.e., no biofilm species can exit or enter through this boundary part. This leads to Dirichlet boundary conditions on Γ^D and homogeneous Neumann conditions on Γ^N; see (4). Pure Neumann conditions represent the evolution of the biofilm mixture in a closed container.

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