ANALYSIS OF A FINITE-VOLUME SCHEME FOR A SINGLE-SPECIES BIOFILM MODEL

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ABSTRACT. An implicit Euler finite-volume scheme for a parabolic reaction-diffusion system modeling biofilm growth is analyzed and implemented. The system consists of a degenerate-singular diffusion equation for the biomass fraction, which is coupled to a diffusion equation for the nutrient concentration, and it is solved in a bounded domain with Dirichlet boundary conditions. By transforming the biomass fraction to an entropy-type variable, it is shown that the numerical scheme preserves the lower and upper bounds of the biomass fraction. The existence and uniqueness of a discrete solution and the convergence of the scheme are proved. Numerical experiments in one and two space dimensions illustrate, respectively, the rate of convergence in space of our scheme and the temporal evolution of the biomass fraction and the nutrient concentration.

1. INTRODUCTION

Biofilms are accumulations of microorganisms that grow on surfaces in liquids and can be prevalent in natural, industrial, and hospital environments [26]. They can form, for instance, on teeth as dental plaque and on inert surfaces of implanted devices like catheters. Another example are biofilms grown on filters, which may extract and digest organic compounds and help to clean wastewater. A biofilm growth model that well describes the spatial spreading mechanism for biomass and the dependency on the nutrient was suggested in [14]. The model was analyzed in [15, 21] and numerically solved in [2, 11]. Up to our knowledge, there does not exist any analysis for the numerical approximations in the literature. In this paper, we provide such an analysis for an implicit Euler finite-volume scheme for the model in [15].

The biofilm is modeled by the biomass fraction $M(x,t)$ and the nutrient concentration $S(x,t)$, satisfying the diffusion equations

$$\partial_t S - d_1 \Delta S = g(S, M), \tag{1}$$

$$\partial_t M - d_2 \operatorname{div}(f(M) \nabla M) = h(S, M) \quad \text{in } \Omega, \ t > 0, \tag{2}$$

and the initial and boundary conditions

(3) $\qquad S(0) = S^0, \ M(0) = M^0 \quad \text{in } \Omega, \quad S = 1, \ M = M^D \quad \text{on } \partial\Omega, \ t > 0,$

where $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) is a bounded domain and $0 < M^D < 1$. Other boundary conditions can also be considered; see Remark 1.

The nutrients are consumed with the Monod reaction rate $g(S, M)$, while biomass is produced by the production rate $h(S, M)$ that is the sum of a Monod reaction term and a wastage term,

(4) $\qquad g(M, S) = -\kappa_1 \dfrac{SM}{\kappa_4 + S}, \quad h(M, S) = \kappa_3 \dfrac{SM}{\kappa_4 + S} - \kappa_2 M,$

where $\kappa_i \geq 0$ for $i = 1, 2, 3$ and $\kappa_4 > 0$. The diffusion coefficients d_1 and d_2 are assumed to be positive numbers. Postulating that there is a sharp biomass front, spatial spreading occurs only when there is a significant amount of biomass, and the biomass fraction cannot exceed the maximum bound $M_{\max} = 1$, the authors of [14] have suggested the density-dependent diffusion term

(5) $\qquad f(M) = \dfrac{M^b}{(1 - M)^a}, \quad \text{where } a > 1, \ b > 0.$

The diffusion operator in (2) can be written as $\operatorname{div}(f(M)\nabla M) = \Delta F(M)$, where

(6) $\qquad F(M) = \displaystyle\int_0^M f(s)\,ds, \quad M \geq 0,$

which gives a porous-medium degeneracy for M close to zero. This degeneracy leads to a finite speed of propagation and is responsible for the formation of a sharp interface between the biofilm and the surrounding liquid. The superdiffusion singularity forces the biomass fraction to be smaller than the maximal amount $M_{\max} = 1$.

The aim of this paper is to analyze an implicit Euler finite-volume scheme for (1)–(5) that preserves the bounds $0 \leq S \leq 1$ and $0 \leq M < 1$. We show the existence of a discrete solution, prove the convergence of the scheme, and present some numerical tests in one and two space dimensions. The main difficulty of the analysis is the degenerate-singular diffusion term. On the continuous level, if $M^0 \leq 1 - \varepsilon_0$ in Ω and $M^D \leq 1 - \varepsilon_0$ for some $\varepsilon_0 \in (0, 1)$ then the comparison principle implies that there exists $\delta(\varepsilon_0) > 0$ such that $M \leq 1 - \delta(\varepsilon_0)$ in Ω [15, Prop. 6]. Unfortunately, we have not found any suitable comparison principle on the discrete level.

We overcome this issue by using two ideas. First, we formulate equation (2) for the biomass in terms of the approximate "entropy variable" [22]

$$W_K^\varepsilon := F(M_K^\varepsilon) - F(M^D) + \varepsilon \log \frac{M_K^\varepsilon}{M^D},$$

where $K \subset \Omega$ denotes a control volume and $\varepsilon > 0$ is a regularization parameter. For given $W_K^\varepsilon \in \mathbb{R}$, the biomass fraction is defined implicitly by the invertible mapping $(0, 1) \to \mathbb{R}$, $M^\varepsilon \mapsto W^\varepsilon$. The advantage is that the bounds $0 < M_K^\varepsilon < 1$ are guaranteed by this definition. In fact, the singularity in F provides the upper bound, while the ε-regularization

gives the lower bound. Second, we prove an ε-uniform bound for $F(M^\varepsilon)$ in $L^1(\Omega)$, which shows that the a.e. limit $M_K = \lim_{\varepsilon \to 0} M_K^\varepsilon$ satisfies $0 \le M_K < 1$ for all control volumes K.

The original biofilm model of [14] contains the transport term $u \cdot \nabla M$ in the equation for the biofilm fraction. The flow velocity u is assumed to satisfy the incompressible Navier–Stokes equations in the region $\{M = 0\}$, while $u = 0$ in $\{M > 0\}$. Thus, model (1)–(2) implicitly assumes that $M > 0$. We do not require this condition but we prove in Theorem 2 below that this property is fulfilled if M^0 and M^D are strictly positive.

The existence and uniqueness of a global weak solution to (1)–(5) was shown in [15], while the original model was analyzed in [21] by formulating it as a system of variational inequalities. The model of [14] was extended in [13] by taking into account nutrient taxis, which forces the biofilm to move up a nutrient concentration gradient. In that work, a fast-diffusion exponent $a \in (0, 1)$ instead of a superdiffusive value $a > 1$ (like in [14]) was considered. Equations (1)–(5) were numerically solved using finite differences [14] or finite volumes [2] but without any analysis. Some properties of the semi-implicit Euler finite-difference scheme were shown in [12]. A finite-element approximation for (2) with linear diffusion $f(M) = 1$ but a constraint on the upper bound for the biomass was suggested in [1].

Local mixing effects between different biofilm species can be described by multispecies biofilm models [24]. The resulting cross-diffusion system for the biofilm proportions (without nutrient equation) was analyzed in [9] and numerically investigated in [8]. A nutrient equation was included in a two-species biofilm system in [20], where a time-adaptive scheme was suggested to deal with biomasses close to the maximal value. A finite-volume method was proposed in [23] for a biofilm system for the active and inert biomasses, completed by equations for the nutrient and biocide concentrations, but without performing a numerical analysis.

Let us mention also related biofilm models. The first model was suggested by Wanner and Gujer [27] and consists of a one-dimensional transport equation for the biofilm species together with a differential equation for the biofilm thickness. A nonlinear hyperbolic system for the formation of biofilms was derived in [7]. Other works were concerned with diffusion equations coupled to a fluiddynamical model as in [14]. For instance, the paper [25] provides a formal derivation of the diffusion equations for the biomass and nutrient, coupled to the Darcy–Stokes equation for the fluid velocity. Numerical simulations of a gradient-flow system for the dead and live biofilm bacteria, coupled to the incompressible Navier–Stokes equations for the fluid velocity, were presented in [28], based on a Crank–Nicolson discretization and an upwinding scheme.

With the exception of [1, 8], these mentioned works do not contain any analysis of the numerical scheme. The paper [1] is concerned with a finite-element method and assumes linear diffusion, while [8] does not contain an equation for the nutrient. In this paper, we provide a numerical analysis of a finite-volume scheme to (1)–(2) for the first time. Our results can be sketched as follows:

- We prove the existence of a finite-volume solution (S_K^k, M_K^k), where K denotes a control volume and k is the time step, satisfying the bounds $0 \leq S_M^k \leq 1$ and $0 \leq M_K^k < 1$ for all control volumes K and all time steps k.
- If the initial and boundary biomass are strictly positive, we obtain the uniqueness of a discrete solution.
- The discrete solution converges in a certain sense, for mesh sizes $(\Delta x, \Delta t) \to 0$, to a weak solution to (1)–(6).

The paper is organized as follows. The numerical scheme and the main results are formulated in Section 2. Section 3 is concerned with the existence proof (Theorem 2), while the uniqueness result (Theorem 3) is shown in Section 4. The convergence of the scheme requires uniform estimates which are proved in Section 5. The convergence result (Theorem 4) is then shown in Section 6. Numerical simulations are presented in Section 7.

2. NUMERICAL SCHEME AND MAIN RESULTS

2.1. **Notation and assumptions.** Let $\Omega \subset \mathbb{R}^2$ be an open, bounded, polygonal domain. We consider only two-dimensional domains, but the generalization to higher space dimensions is straightforward. An admissible mesh 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 $\overline{x_K x_L}$ between two centers of neighboring cells is orthogonal to the edge $\sigma = K|L$ between two cells. The condition is satisfied, for instance, by triangular meshes whose triangles have angles smaller than $\pi/2$ [18, Example 9.1] or by Voronoï meshes [18, Example 9.2].

The family of edges $\mathcal{E}$ is assumed to consist of interior edges $\mathcal{E}_{\text{int}}$ satisfying $\sigma \subset \Omega$ and boundary edges $\sigma \in \mathcal{E}_{\text{ext}}$ fulfilling $\sigma \subset \partial\Omega$. For a given control volume $K \in \mathcal{T}$, we denote by $\mathcal{E}_K$ the set of edges of K. This set splits into $\mathcal{E}_K = \mathcal{E}_{\text{int},K} \cup \mathcal{E}_{\text{ext},K}$. For any $\sigma \in \mathcal{E}$, there exists at least one cell $K \in \mathcal{T}$ such that $\sigma \in \mathcal{E}_K$. 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 imply that

$$(7) \qquad \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \mathrm{m}(\sigma) \mathrm{d}(x_K, \sigma) \leq 2 \sum_{K \in \mathcal{T}} \mathrm{m}(K) = 2\,\mathrm{m}(\Omega),$$

where d is the Euclidean distance in $\mathbb{R}^2$ and m is the one- or two-dimensional Lebesgue measure. Let $\sigma \in \mathcal{E}$ be an edge. We define the distance

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

and introduce the transmissibility coefficient by

$$(8) \qquad \tau_\sigma = \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}.$$

We assume that the mesh satisfies the following regularity assumption: There exists $\xi > 0$ such that for all $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$,

$$(9) \qquad \mathrm{d}(x_K, \sigma) \geq \xi \mathrm{d}_\sigma.$$

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

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

As it is usual for the finite-volume method, we introduce functions that are piecewise constant in space and time. The finite-volume scheme yields a vector $v_{\mathcal{T}} = (v_K)_{K \in \mathcal{T}} \in \mathbb{R}^{\#\mathcal{T}}$ of approximate values of a piecewise constant function v such that $v = \sum_{K \in \mathcal{T}} v_K \mathbf{1}_K$, where $\mathbf{1}_K$ is the characteristic function of K. We write $v_{\mathcal{M}} = (v_{\mathcal{T}}, v_{\mathcal{E}})$ for the vector that contains the approximate values in the control volumes and on the boundary edges, where $v_{\mathcal{E}} := (v_\sigma)_{\sigma \in \mathcal{E}_{\mathrm{ext}}} \in \mathbb{R}^{\#\mathcal{E}_{\mathrm{ext}}}$. For such a vector, we use the notation

$$(10) \qquad v_{K,\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \in \mathcal{E}_{\mathrm{int},K}, \\ v_\sigma & \text{if } \sigma \in \mathcal{E}_{\mathrm{ext},K} \end{cases}$$

for $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$ and introduce the discrete gradient

$$(11) \qquad \mathrm{D}_\sigma v := |\mathrm{D}_{K,\sigma} v|, \quad \text{where } \mathrm{D}_{K,\sigma} v = v_{K,\sigma} - v_K.$$

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

$$(12) \qquad |v|_{1,2,\mathcal{M}} = \left(\sum_{\sigma \in \mathcal{E}} \tau_\sigma (\mathrm{D}_\sigma v)^2 \right)^{1/2}, \quad \|v\|_{1,2,\mathcal{M}} = \left(\|v\|_{0,2,\mathcal{M}}^2 + |v|_{1,2,\mathcal{M}}^2 \right)^{1/2},$$

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

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

Then, for a given family of vectors $v^k = (v_{\mathcal{T}}^k, v_{\mathcal{E}}^k)$ for $k = 1, \ldots, N_T$ and a given nonnegative constant v^D such that $v_\sigma^k = v^D$ for all $\sigma \in \mathcal{E}_{\mathrm{ext}}$, we define the piecewise constant in space and time function v by

$$(13) \qquad v(x, t) = \sum_{K \in \mathcal{T}} v_K^k \mathbf{1}_K(x) \quad \text{for } x \in \Omega, \ t \in (t_{k-1}, t_k], \ k = 1, \ldots, N_T.$$

For the definition of an approximate gradient for such functions, we need to introduce a dual mesh. Let $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$. The cell $T_{K,\sigma}$ of the dual mesh is defined as follows:

- 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 ("half-diamond") whose vertices are given by x_K and the end points of the edge σ.

An example of a construction of a dual mesh can be found in [6]. The cells $T_{K,\sigma}$ define, up to a negligible set, 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

$$(14) \qquad \mathrm{m}(\sigma)\mathrm{d}(x_K, x_L) = 2\,\mathrm{m}(T_{K,\sigma}) \quad \text{for all } \sigma = K|L \in \mathcal{E}_{\mathrm{int},K}.$$

The approximate gradient of a piecewise constant function v in Ω_T is given by

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

where the discrete operator $\mathrm{D}_{K,\sigma}$ is given in (11) and $\nu_{K,\sigma}$ is the unit vector that is normal to σ and that points outward of K.

2.2. **Numerical scheme.** We are now in the position to formulate the finite-volume discretization of (1)–(3). Let $\mathcal{D}$ be an admissible discretization of Ω_T. The initial conditions are discretized by the averages

$$(15) \qquad S_K^0 = \frac{1}{\mathrm{m}(K)} \int_K S^0(x)dx, \quad M_K^0 = \frac{1}{\mathrm{m}(K)} \int_K M^0(x)dx \quad \text{for } K \in \mathcal{T}.$$

On the Dirichlet boundary, we set $S_\sigma^k = 1$ and $M_\sigma^k = M^D$ for $\sigma \in \mathcal{E}_{\mathrm{ext}}$ at time t_k.

Let S_K^k and M_K^k be some approximations of the mean values of $S(\cdot, t_k)$ and $M(\cdot, t_k)$, respectively, in the cell K. Then the elements S_K^k and M_K^k are solutions to

$$(16) \qquad \frac{\mathrm{m}(K)}{\Delta t}(S_K^k - S_K^{k-1}) + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{S,K,\sigma}^k = \mathrm{m}(K)g(S_K^k, M_K^k),$$

$$(17) \qquad \frac{\mathrm{m}(K)}{\Delta t}(M_K^k - M_K^{k-1}) + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{M,K,\sigma}^k = \mathrm{m}(K)h(S_K^k, M_K^k),$$

the numerical fluxes are defined as

$$(18) \qquad \mathcal{F}_{S,K,\sigma}^k = -\tau_\sigma d_1 \mathrm{D}_{K,\sigma} S^k, \quad \mathcal{F}_{M,K,\sigma}^k = -\tau_\sigma d_2 \mathrm{D}_{K,\sigma} F(M^k),$$

where $K \in \mathcal{T}$, $\sigma \in \mathcal{E}_K$, $k \in \{1, \ldots, N_T\}$, and we recall definitions (4) for g and h, (6) for F, and (8) for τ_σ.

For the convenience of the reader, we recall the discrete integration-by-parts formula for piecewise constant functions $v = (v_{\mathcal{T}}, v_{\mathcal{E}})$:

$$(19) \qquad \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{K,\sigma} v_K = -\sum_{\sigma \in \mathcal{E}} \mathcal{F}_{K,\sigma} \mathrm{D}_{K,\sigma} v + \sum_{\sigma \in \mathcal{E}_{\mathrm{ext}}} \mathcal{F}_{K,\sigma} v_\sigma,$$

where $\mathcal{F}_{K,\sigma}$ is a numerical flux like in (18).

2.3. **Main results.** We impose the following hypotheses:

(H1) Domain: $\Omega \subset \mathbb{R}^2$ is a bounded polygonal domain.

(H2) Discretization: $\mathcal{D}$ is an admissible discretization of $\Omega_T := \Omega \times (0, T)$ satisfying the regularity condition (9).

(H3) Initial data: S^0, $M^0 \in L^2(\Omega)$ satisfy $0 \le S^0 \le 1$ and $0 \le M^0 < 1$ in Ω.

(H4) Dirichlet datum: $0 < M^D < 1$.

(H5) Parameters: d_1, $d_2 > 0$, $\kappa_i \ge 0$ for $i = 1, 2, 3$, $\kappa_4 > 0$, $a \ge 1$, and $b \ge 0$.

Remark 1 (Discussion of the hypotheses). Conditions $M^0 < 1$ and $M^D < 1$ allow for the proof of $M_K^k < 1$ for all $K \in \mathcal{T}$ and $k = 1, \ldots, N_T$, thus avoiding quenching of the solution, i.e. the occurrence of regions with $M_K^k = 1$. We assume that M^D is positive to be able to introduce an entropy variable. This condition can be relaxed by introducing an approximation procedure. The assumption that the boundary biomass is constant is imposed for simplicity. It can be generalized to piecewise constant or time-dependent boundary data, for instance. Moreover, mixed Dirichlet–Neumann boundary conditions for the biomass could be imposed as well; see [15, Section 4]. On the other hand, pure Neumann boundary conditions for M may lead, in the continuous case, to a quenching phenomenon in finite time, as shown in [15]. We may assume that the diffusion coefficients d_1 and d_2 depend on the spatial variable if $d_1(x)$ and $d_2(x)$ are strictly positive. The condition $a \ge 1$ corresponds to "very fast diffusion". In numerical simulations, usually the values $a = b = 4$ are chosen [14, Table 1]. $\qquad\square$

Our first main result concerns the existence of solutions to the numerical scheme. We introduce the function

$$(20) \qquad Z(M) := \int_{M^D}^{M} F(s)ds - F(M^D)(M_K - M^D), \quad M \in [0, 1).$$

Theorem 2 (Existence of discrete solutions). *Assume that Hypotheses (H1)–(H5) hold. Then, for every $k = 1, \ldots, N_T$, there exists a solution (S^k, M^k) to scheme (15)–(18) satisfying*

$$(21) \qquad 0 \le S_K^k \le 1, \quad 0 \le M_K^k < 1 \quad \text{for all } K \in \mathcal{T},$$

and there exist positive constants C_1 and C_2 independent of Δx and Δt such that

$$(22) \qquad \|Z(M^k)\|_{0,1,\mathcal{M}} + \Delta t C_1 \|F(M^k)\|_{1,2,\mathcal{M}}^2 \le \|Z(M^{k-1})\|_{0,1,\mathcal{M}} + \Delta t C_2.$$

Moreover, if $M^0 \ge m_0$ in Ω and $M_D \ge m_0$ for some $m_0 > 0$ then

$$(23) \qquad M_K^k \ge m_0 \exp(-\kappa_2 t_k) \quad \text{for all } K \in \mathcal{T}, \ k = 1, \ldots, N_T.$$

The existence result is proved by a fixed-point argument based on a topological degree result. The main difficulty is to approximate the equations in such a way that the singular point $M = 1$ is avoided. This can be done, as in [15], by introducing a cut-off approximation $f_\varepsilon(M)$ of $f(M)$. Then, by the comparison principle, it is possible to show the bound $M^\varepsilon \le 1 - \delta(\varepsilon)$ for the approximate biomass M^ε, where $\delta(\varepsilon) \in (0, 1)$. Since the comparison principle cannot be easily extended to the discrete case, we have chosen another approach.

We introduce the "entropy variable" $W_K^\varepsilon := Z_\varepsilon'(M_K^\varepsilon)$, where Z_ε is the sum of $Z(M_K^\varepsilon)$ and ε times the Boltzmann entropy (see (26)). Then $0 < M_K^\varepsilon < 1$ by definition and we can derive a uniform estimate similar to (22). The uniform bound for $F(M^\varepsilon)$ allows us to infer that the a.e. limit function $M_K = \lim_{\varepsilon \to 0} M_K^\varepsilon$ satisfies $M_K < 1$ for all $K \in \mathcal{T}$. The positive lower bound for M^k comes from the fact that the source term $h(S_K^k, M_K^k)$ is bounded from below by the linear term $-\kappa_2 M_K^k$, and it is proved by a Stampacchia truncation method.

Theorem 3 (Uniqueness of discrete solutions). *Assume that Hypotheses (H1)–(H5) hold and that there exists a constant $m_0 > 0$ such that $M^0(x) \geq m_0$ for $x \in \Omega$ and $M^D \geq m_0$. Then there exists $\gamma^* > 0$, depending on the data, the mesh, and m_0, such that for all $0 < \Delta t < \gamma^*$, there exists a unique solution to scheme (15)–(18).*

The proof of the theorem is based on a discrete version of the dual method. On the continuous level, the idea is to choose test functions ψ and ϕ solving $-\Delta\psi = S_1 - S_2$ and $-\Delta\phi = M_1 - M_2$ with homogeneous Dirichlet boundary data, where (S_1, M_1) and (S_2, M_2) are two solutions to (1)–(2) with the same initial data, and to exploit the monotonicity of the nonlinearity $F(M)$. On the discrete level, we replace the diffusion equations for ψ and ϕ by the corresponding finite-volume schemes and estimate similarly as in the continuous case. The restriction on the time step size is due to $L^2(\Omega)$ estimates coming from the source terms.

We also prove that our scheme converges to the continuous model, up to a subsequence. For this result, we introduce a family $(\mathcal{D}_m)_{m \in \mathbb{N}}$ of admissible space-time discretizations of Ω_T indexed by the size $\eta_m = \max\{\Delta x_m, \Delta t_m\}$ of the mesh, satisfying $\eta_m \to 0$ as $m \to \infty$. We denote by $\mathcal{M}_m$ the corresponding meshes of Ω and by Δt_m the corresponding time step sizes. Finally, we set $\nabla^m := \nabla^{\mathcal{D}_m}$.

Theorem 4 (Convergence of the scheme). *Assume that the Hypotheses (H1)–(H5) hold. Let $(\mathcal{D}_m)_{m \in \mathbb{N}}$ be a family of admissible meshes satisfying (9) uniformly and let $(S_m, M_m)_{m \in \mathbb{N}}$ be a corresponding sequence of finite-volume solutions to scheme (15)–(18) constructed in Theorem 2. Then there exist $(S, M) \in L^\infty(\Omega_T; \mathbb{R}^2)$ and a subsequence of (S_m, M_m) (not relabeled) such that, as $m \to \infty$,*

$$S_m \to S, \quad M_m \to M \quad \text{a.e. in } \Omega_T,$$

$$\nabla^m S_m \rightharpoonup \nabla S, \quad \nabla^m F(M_m) \rightharpoonup \nabla F(M) \quad \text{weakly in } L^2(\Omega_T).$$

The functions $S - 1$ and $F(M) - F(M^D)$ belong to the space $L^2(0, T; H_0^1(\Omega))$. Moreover, the limit (S, M) is a weak solution to (1)–(3), i.e., for all $\psi, \phi \in C_0^\infty(\Omega \times [0, T))$,

$$(24) \qquad -\int_0^T \int_\Omega S \partial_t \psi \, dx \, dt - \int_\Omega S^0(x)\psi(x, 0)\, dx + d_1 \int_0^T \int_\Omega \nabla S \cdot \nabla \psi \, dx \, dt$$

$$= \int_0^T \int_\Omega g(S, M)\psi \, dx \, dt,$$

$$(25) \qquad -\int_0^T \int_\Omega M \partial_t \phi \, dx \, dt - \int_\Omega M^0(x)\phi(x, 0)\, dx + d_2 \int_0^T \int_\Omega \nabla F(M) \cdot \nabla \phi \, dx \, dt$$

$$= \int_0^T \int_\Omega h(S, M)\phi dx dt.$$

The convergence proof is based on the uniform estimates derived for the proof of Theorem 2 and a discrete compensated compactness technique [3] needed to identify the nonlinear limits. For the limit $m \to \infty$, we use the techniques of [6]. If uniqueness for the limiting model holds in the class of weak solutions, the whole sequence (S_m, M_m) converges. Uniqueness in a smaller class of functions is proved [15, Theorem 3.2], but we have been unable to show the required regularity of the limit (S, M) from our approximate system, since the time discretization is not compatible with the technique of [15].

Remark 5. We could adapt the construction of scheme (15)–(18) and the proofs of our main results, Theorem 2 and Theorem 4, for the approximation of the solution to a quorum-sensing-induced biofilm dispersal model introduced in [16], which can be seen as a generalization of (1)–(6). $\qquad\square$

3. Existence of solutions

For the proof of Theorem 2, we proceed by induction. By Hypothesis (H3), $0 \le S_K^0 \le 1$, $0 \le M_K^0 < 1$ holds for $K \in \mathcal{T}$. Let (S^{k-1}, M^{k-1}) satisfy $0 \le S_K^{k-1} \le 1$, $0 \le M_K^{k-1} < 1$ for all $K \in \mathcal{T}$ and some $k \in \{1, \dots, N_T\}$. We use the function $Z_\varepsilon : [0, 1) \to \mathbb{R}$, defined by

$$(26) \qquad Z_\varepsilon(M) = \int_0^M F(s)ds - F(M^D)(M - M^D) + \varepsilon\left(M \log \frac{M}{M^D} + M^D - M\right),$$

where $\varepsilon > 0$ and $F(M)$ is given in (6).

Step 1: Definition of a linearized problem. Let $R > 0$ and set

$$\mathcal{K}_R := \left\{(S, W) \in \mathbb{R}^{2\theta} : \|S\|_{0,2,\mathcal{M}} < R, \ \|W\|_{1,2,\mathcal{M}} < R, \ S_\sigma = 1, \ W_\sigma = 0 \text{ for } \sigma \in \mathcal{E}_{\text{ext}}\right\},$$

where $\theta = \#\mathcal{T} + \#\mathcal{E}_{\text{ext}}$. We define the fixed-point mapping $Q : \mathcal{K}_R \to \mathbb{R}^{2\theta}$ by $Q(S, W) = (S^\varepsilon, W^\varepsilon)$, where $(S^\varepsilon, W^\varepsilon)$ solves

$$(27) \qquad \frac{\mathrm{m}(K)}{\Delta t}(S_K^\varepsilon - S_K^{k-1}) + \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{S,K,\sigma} = \mathrm{m}(K)g([S_K]_+, M_K),$$

$$(28) \qquad \varepsilon\left(\mathrm{m}(K)W_K^\varepsilon - \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}W^\varepsilon\right)$$

$$= -\frac{\mathrm{m}(K)}{\Delta t}(M_K - M_K^{k-1}) - \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{M,K,\sigma} + \mathrm{m}(K)h([S_K]_+, M_K),$$

the fluxes are as in (18), $[z]_+ := \max\{0, z\}$, and we impose the Dirichlet boundary conditions $S_\sigma^\varepsilon = 1$, $W_\sigma^\varepsilon = 0$ for $\sigma \in \mathcal{E}_{\text{ext}}$. The value M_K is a function of W_K, implicitly defined by

$$(29) \qquad W_K = Z_\varepsilon'(M_K) = F(M_K) - F(M^D) + \varepsilon \log \frac{M_K}{M^D}, \quad K \in \mathcal{T}.$$

The map $(0,1) \to \mathbb{R}$, $M_K \mapsto W_K$ is invertible because the function Z'_ε is increasing. This shows that M_K is well defined and $M_K \in (0,1)$ for $K \in \mathcal{T}$. The existence of a unique solution $(S^\varepsilon, W^\varepsilon)$ to (27)–(28) is a consequence of [18, Lemma 9.2].

We claim that Q is continuous. To show this, we first multiply (28) by W_K^ε, sum over $K \in \mathcal{T}$, and use the discrete integration-by-parts formula (19):

$$\varepsilon \|W^\varepsilon\|_{1,2,\mathcal{M}}^2 = \varepsilon \sum_{K \in \mathcal{T}} \left(\mathrm{m}(K)(W_K^\varepsilon)^2 - \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}(W^\varepsilon) W_K^\varepsilon \right) = J_1 + J_2 + J_3, \quad \text{where}$$

$$J_1 = - \sum_{K \in \mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t}(M_K - M_K^{k-1}) W_K^\varepsilon,$$

$$J_2 = - \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{M,K,\sigma} W_K^\varepsilon,$$

$$J_3 = \sum_{K \in \mathcal{T}} \mathrm{m}(K) \left(\frac{\kappa_3 [S_K]_+}{\kappa_4 + [S_K]_+} - \kappa_2 \right) M_K W_K^\varepsilon.$$

By the Cauchy–Schwarz inequality and the bound $0 < M_K < 1$, we find that

$$|J_1| \leq \frac{2}{\Delta t} \mathrm{m}(\Omega)^{1/2} \|W^\varepsilon\|_{0,2,\mathcal{M}},$$

$$|J_2| \leq \left(\sum_{K \in \mathcal{T}} \frac{1}{\mathrm{m}(K)} \sum_{\sigma \in \mathcal{E}_K} |\mathcal{F}_{M,K,\sigma}|^2 \right)^{1/2} \|W^\varepsilon\|_{0,2,\mathcal{M}},$$

$$|J_3| \leq \left(\frac{\kappa_3}{\kappa_4 + 1} + \kappa_2 \right) \mathrm{m}(\Omega)^{1/2} \|W^\varepsilon\|_{0,2,\mathcal{M}}.$$

Because of the assumption $\|W\|_{1,2,\mathcal{M}} < R$, the flux $|\mathcal{F}_{M,K,\sigma}|$ is bounded from above by a constant depending on R. This implies that $|J_2| \leq C(R) \|W^\varepsilon\|_{0,2,\mathcal{M}}$, where $C(R) > 0$ is some constant. (Here and in the following, we denote by C, $C_i > 0$ generic constants whose value change from line to line.) This shows that $\varepsilon \|W^\varepsilon\|_{1,2,\mathcal{M}} \leq C(R)$ for (another) constant $C(R) > 0$. Using similar arguments, we obtain the existence of $C(R) > 0$ such that $\|S^\varepsilon\|_{0,2,\mathcal{M}} \leq C(R)$.

Next, let $(S_n, W_n)_{n \in \mathbb{N}} \subset \mathcal{K}_R$ be a sequence satisfying $(S_n, W_n) \to (S, W)$ as $n \to \infty$. The previous uniform estimates for $(S_n^\varepsilon, W_n^\varepsilon) := Q(S_n, W_n)$ show that $(S_n^\varepsilon, W_n^\varepsilon)$ is bounded uniformly in $n \in \mathbb{N}$. Therefore, there exists a subsequence which is not relabeled such that $(S_n^\varepsilon, W_n^\varepsilon) \to (S^\varepsilon, W^\varepsilon)$ as $n \to \infty$. Taking the limit $n \to \infty$ in (27)–(28), we see that $(S^\varepsilon, W^\varepsilon) = Q(S, W)$. We deduce from the uniqueness of the limit that the whole sequence converges, which means that Q is continuous.

Step 2: Definition of the fixed-point operator. We claim that Q admits a fixed point. We use a topological degree argument [10, Chap. 1] and prove that $\deg(I - Q, \mathcal{K}_R, 0) = 1$, where deg is the Brouwer topological degree. Since deg is invariant by homotopy, it is sufficient to show that any solution $(S^\varepsilon, W^\varepsilon, \rho) \in \overline{\mathcal{K}}_R \times [0,1]$ to the fixed-point equation $(S^\varepsilon, W^\varepsilon) = \rho Q(S^\varepsilon, W^\varepsilon)$ satisfies $(S^\varepsilon, W^\varepsilon, \rho) \notin \partial \mathcal{K}_R \times [0,1]$ for sufficiently large values of $R > 0$. Let $(S^\varepsilon, W^\varepsilon, \rho)$ be a fixed point and assume that $\rho \neq 0$, the case $\rho = 0$ being clear.

Then $(S^\varepsilon, W^\varepsilon)$ solves

$$
(30) \qquad \frac{\mathrm{m}(K)}{\Delta t}(S_K^\varepsilon - \rho S_K^{k-1}) + \rho \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{S,K,\sigma}^\varepsilon = \rho\,\mathrm{m}(K) g([S_K^\varepsilon]_+, M_K^\varepsilon),
$$

$$
(31) \qquad \varepsilon\left(\mathrm{m}(K) W_K^\varepsilon - \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma} W^\varepsilon \right)
$$

$$
= -\rho \frac{\mathrm{m}(K)}{\Delta t}(M_K - M_K^{k-1}) - \rho \sum_{\sigma \in \mathcal{E}_K} \mathcal{F}_{M,K,\sigma} + \rho\,\mathrm{m}(K) h([S_K^\varepsilon]_+, M_K^\varepsilon)
$$

for $K \in \mathcal{T}$ with the boundary conditions $S_\sigma^\varepsilon = 1$, $W_\sigma^\varepsilon = 0$ for $\sigma \in \mathcal{E}_K$, the fluxes are given by (18) with (S, M) replaced by $(S^\varepsilon, M^\varepsilon)$, and M_K^ε is the unique solution to (29) with W_K replaced by W_K^ε.

Step 3: A priori estimates. We establish some a priori estimates for the fixed points $(S^\varepsilon, W^\varepsilon)$ of Q, which are uniform in R. Definition (29) immediately gives the bound $0 < M_K^\varepsilon < 1$ for all $K \in \mathcal{T}$.

Lemma 6 (Pointwise bounds for S^ε). *The following bounds hold:*

$$
0 \le S_K^\varepsilon \le 1 \quad \text{for } K \in \mathcal{T}.
$$

Proof. First, we multiply (30) by $\Delta t[S_K^\varepsilon]_-$, where $[z]_- = \min\{0, z\}$, and sum over $K \in \mathcal{T}$. Then, after a discrete integration by parts,

$$
\sum_{K \in \mathcal{T}} \mathrm{m}(K)[S_K^\varepsilon]_-^2 + \rho d_1 \Delta t \sum_{\sigma \in \mathcal{E}} \tau_\sigma \mathrm{D}_{K,\sigma}(S^\varepsilon) \mathrm{D}_{K,\sigma}[S^\varepsilon]_- = \rho \sum_{K \in \mathcal{T}} \mathrm{m}(K) S_K^{k-1}[S_K^\varepsilon]_- \le 0,
$$

since $g([S_K^\varepsilon]_+, M_K^\varepsilon)[S_K^\varepsilon]_- = 0$ and $S_K^{k-1} \ge 0$ by the induction hypothesis. The second term on the left-hand side is nonnegative, since $z \mapsto [z]_-$ is monotone. This implies that the first term must be nonpositive, showing that $[S_K^\varepsilon]_- = 0$ and hence $S_K^\varepsilon \ge 0$ for all $K \in \mathcal{T}$.

To verify the upper bound for S^ε, we multiply (30) by $\Delta t[S_K^\varepsilon - 1]_+$, sum over $K \in \mathcal{T}$, and use discrete integration by parts:

$$
\sum_{K \in \mathcal{T}} \mathrm{m}(K)\big((S_K^\varepsilon - 1) - (\rho S_K^{k-1} - 1)\big)[S_K^\varepsilon - 1]_+ + \rho d_1 \Delta t \sum_{\sigma \in \mathcal{E}} \mathrm{D}_{K,\sigma}(S^\varepsilon - 1) \mathrm{D}_{K,\sigma}[S^\varepsilon - 1]_+
$$

$$
(32) \qquad = \rho \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K) g\big(S_K^\varepsilon, M_K^\varepsilon\big)[S_K^\varepsilon - 1]_+ \le 0,
$$

since we have always $g(S_K^\varepsilon, M_K^\varepsilon) \le 0$. It follows from the induction hypothesis and $\rho \le 1$ that $\rho S_K^{k-1} \le 1$, and the first term on the left-hand side can be estimated according to

$$
\sum_{K \in \mathcal{T}} \mathrm{m}(K)\big((S_K^\varepsilon - 1) - (\rho S_K^{k-1} - 1)\big)[S_K^\varepsilon - 1]_+ \ge \sum_{K \in \mathcal{T}} \mathrm{m}(K)[S_K^\varepsilon - 1]_+^2.
$$

We deduce from the monotonicity of $z \mapsto [z]_+$ that the second term on the left-hand side of (32) is nonnegative as well. Hence, $\sum_{K \in \mathcal{T}} \mathrm{m}(K)[S_K^\varepsilon - 1]_+^2 \le 0$ and consequently $S_K^\varepsilon \le 1$ for all $K \in \mathcal{T}$. $\qquad\square$

Lemma 7 (Estimate for $F(M_K^\varepsilon)$). *There exist constants C_1, $C_2 > 0$, only depending on the given data, such that*

$$(33) \qquad \varepsilon\Delta t\|W^\varepsilon\|_{1,2,\mathcal{M}}^2 + \rho\|Z(M^\varepsilon)\|_{0,1,\mathcal{M}} + \rho\Delta t C_1\|F(M^\varepsilon) - F(M^D)\|_{1,2,\mathcal{M}}^2$$

$$\leq \Delta t C_2 + \|Z_\varepsilon(M^{k-1})\|_{0,1,\mathcal{M}}.$$

Proof. We multiply (31) by $\Delta t W_K^\varepsilon$, sum over K, and use discrete integration by parts:

$$(34) \qquad\qquad \varepsilon\Delta t\|W^\varepsilon\|_{1,2,\mathcal{M}}^2 + J_4 + J_5 = J_6, \quad \text{where}$$

$$J_4 = \rho \sum_{K\in\mathcal{T}} \mathrm{m}(K)(M_K^\varepsilon - M_K^{k-1})W_K^\varepsilon,$$

$$J_5 = \rho\Delta t d_2 \sum_{\sigma\in\mathcal{E}} \tau_\sigma \mathrm{D}_{K,\sigma}F(M^\varepsilon)\mathrm{D}_{K,\sigma}W^\varepsilon,$$

$$J_6 = \rho\Delta t \sum_{K\in\mathcal{T}} \mathrm{m}(K)h(S_K^\varepsilon, M_K^\varepsilon)W^\varepsilon.$$

By the convexity of Z_ε, $(M_K^\varepsilon - M_K^{k-1})Z_\varepsilon'(M_K^\varepsilon) \geq Z(M_K^\varepsilon) - Z_\varepsilon(M_K^{k-1})$ such that

$$J_4 \geq \rho \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left\{Z(M_K^\varepsilon) + \varepsilon\left(M_K^\varepsilon \log\frac{M_K^\varepsilon}{M^D} + M^D - M_K^\varepsilon\right) - Z_\varepsilon(M_K^{k-1})\right\}$$

$$\geq \rho\|Z(M_K^\varepsilon)\|_{0,1,\mathcal{M}} - \rho\|Z_\varepsilon(M_K^{k-1})\|_{0,1\mathcal{M}}.$$

The definition of W_K^ε and the monotonicity of the functions F and $\log$ imply that

$$(35) \qquad J_5 = \rho\Delta t d_2 \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left([\mathrm{D}_{K,\sigma}(F(M^\varepsilon) - F(M^D))]^2 + \varepsilon\mathrm{D}_{K,\sigma}F(M^\varepsilon)\mathrm{D}_{K,\sigma}\log M^\varepsilon\right)$$

$$\geq \rho\Delta t d_2|F(M^\varepsilon) - F(M^D)|_{1,2,\mathcal{M}}^2 \geq \rho\Delta t d_2 C(\xi)\|F(M^\varepsilon) - F(M^D)\|_{1,2\mathcal{M}}^2,$$

where the last step follows from the discrete Poincaré inequality [4, Theorem 3.2]. Finally, by the Young inequality and taking into account the bounds $S_K^\varepsilon \leq 1$ and $M_K^\varepsilon < 1$, we find that

$$J_6 \leq \rho\Delta t\left(\kappa_2 + \frac{\kappa_3}{\kappa_4+1}\right) \sum_{K\in\mathcal{T}} \mathrm{m}(K)\left(|F(M_K^\varepsilon) - F(M^D)| + \varepsilon M_K^\varepsilon\left|\log\frac{M_K^\varepsilon}{M^D}\right|\right)$$

$$\leq \frac{\eta}{2}\rho\Delta t\left(\kappa_2 + \frac{\kappa_3}{\kappa_4+1}\right)\|F(M^\varepsilon) - F(M^D)\|_{1,2,\mathcal{M}}^2 + \frac{\Delta t}{2\eta}\left(\kappa_2 + \frac{\kappa_3}{\kappa_4+1}\right)\mathrm{m}(\Omega)$$

$$+ \varepsilon\Delta t C(\Omega),$$

where $\eta > 0$. Inserting the estimates for J_4, J_5, and J_6 into (34) yields

$$\varepsilon\Delta t\|W^\varepsilon\|_{1,2,\mathcal{M}}^2 + \rho\Delta t\left(d_2 C(\xi) - \frac{\eta}{2}\left(\kappa_2 + \frac{\kappa_3}{\kappa_4+1}\right)\right)\|F(M^\varepsilon) - F(M^D)\|_{1,2,\mathcal{M}}^2$$

$$+ \rho\|Z(M^\varepsilon)\|_{0,1,\mathcal{M}} \leq \rho\|Z_\varepsilon(M^{k-1})\|_{0,1,\mathcal{M}} + \Delta t C(\eta).$$

Then, choosing $\eta > 0$ sufficiently small shows the conclusion. $\square$

Step 4: Topological degree argument. We deduce from the estimates of Lemmas 6–7 that

$$\|S^\varepsilon\|_{0,2,\mathcal{M}} \le \mathrm{m}(\Omega)^{1/2}, \quad \|W^\varepsilon\|_{1,2,\mathcal{M}} \le \frac{1}{\sqrt{\varepsilon\Delta t}}(\|Z_\varepsilon(M^{k-1})\|_{0,1,\mathcal{M}} + \Delta t C)^{1/2}.$$

Thus, choosing

$$R = \max\left\{ \mathrm{m}(\Omega)^{1/2}, \frac{1}{\sqrt{\varepsilon\Delta t}}(\|Z_\varepsilon(M^{k-1})\|_{0,1,\mathcal{M}} + \Delta t C)^{1/2}\right\} + 1,$$

we see that $(S^\varepsilon, W^\varepsilon) \notin \partial\mathcal{K}_R$ and $\deg(I - Q, \mathcal{K}_R, 0) = 1$. We conclude that Q admits a fixed point, i.e. a solution $(S^\varepsilon, W^\varepsilon)$ to (30)–(31).

Step 5: Limit $\varepsilon \to 0$. Thanks to Lemmas 6–7 and the bound $0 < M_K^\varepsilon < 1$, there exist subsequences, which are not relabeled, such that $S_K^\varepsilon \to S_K^k$, $M_K^\varepsilon \to M_K^k$, and $\varepsilon W_K^\varepsilon \to 0$ as $\varepsilon \to 0$, where $0 \le S_K^k \le 1$ and $0 \le M_K^k \le 1$ for all $K \in \mathcal{T}$. Passing to the limit $\varepsilon \to 0$ in (33) and taking into account the lower semicontinuity of F, we find that

$$\Delta t C_1 \|F(M^k) - F(M^D)\|_{0,2,\mathcal{M}}^2 \le \|Z(M^{k-1})\|_{0,1,\mathcal{M}} + \Delta t C < \infty.$$

Thus, $F(M_K^k)$ is finite, which implies that $M_K^k < 1$ for any $K \in \mathcal{T}$. We can perform the limit $\varepsilon \to 0$ in (30)–(31) to deduce the existence of a solution (S^k, M^k) to scheme (15)–(18).

Step 6: Positive lower bound for M^k. Again, we proceed by induction. Let $M^0 \ge m_0$ in Ω and $M^D \ge m_0$. Then $M_K^0 \ge m_0$ for all $K \in \mathcal{T}$. Set $m^k = m_0(1+\kappa_2\Delta t)^{-k}$. The induction hypothesis reads as $M_K^{k-1} \ge m^{k-1}$ for $K \in \mathcal{T}$. We multiply (17) by $\Delta t[M_K^k - m^k]_-$, sum over $K \in \mathcal{T}$, and use discrete integration by parts:

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K)(M_K^k - M_K^{k-1})[M_K^k - m^k]_- = J_7 + J_8, \quad \text{where}$$

$$J_7 = -\Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \mathrm{D}_{K,\sigma}F(M^k)\mathrm{D}_{K,\sigma}[M_K^k - m^k]_-,$$

$$J_8 = \Delta t \sum_{K\in\mathcal{T}} \mathrm{m}(K)h(S^k, M^k)[M_K^k - m^k]_-.$$

Taking into account that $M_K^{k-1} - m^{k-1} \ge 0$ and $m^k - m^{k-1} = -\kappa_2\Delta t m^k$, we estimate the left-hand side according to

$$\sum_{K\in\mathcal{T}} \mathrm{m}(K)(M_K^k - M_K^{k-1})[M_K^k - m^k]_-$$

$$= \sum_{K\in\mathcal{T}} \mathrm{m}(K)\big((M_K^k - m^k) - (M_K^{k-1} - m^{k-1})\big)[M_K^k - m^k]_-$$

$$+ \sum_{K\in\mathcal{T}} \mathrm{m}(K)(m^k - m^{k-1})[M_K^k - m^k]_-$$

$$\ge \sum_{K\in\mathcal{T}} \mathrm{m}(K)[M_K^k - m^k]_-^2 - \kappa_2\Delta t m^k \sum_{K\in\mathcal{T}} \mathrm{m}(K)[M_K^k - m^k]_-.$$

Since F and $z \mapsto [z - m^k]_-$ are monotone, we have $J_7 \leq 0$. Furthermore,

$$J_8 = \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K) \left(\frac{\kappa_3 S_K^k}{\kappa_4 + S_K^k} - \kappa_2 \right) M_K^k [M_K^k - m^k]_-$$

$$\leq -\kappa_2 \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K) M_K^k [M_K^k - m^k]_- \leq -\kappa_2 \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K) m^k [M_K^k - m^k]_-.$$

The terms involving κ_2 cancel and we end up with

$$\sum_{K \in \mathcal{T}} \mathrm{m}(K) [M_K^k - m^k]_-^2 \leq 0.$$

It follows that $[M_K^k - m^k]_- = 0$ and hence $M_K^k \geq m^k \geq m_0 \exp(-\kappa_2 k \Delta t)$.

4. Uniqueness of solutions

We proceed by induction. Let $k \in \{1, \ldots, N_T\}$, let (S_1^k, M_1^k) and (S_2^k, M_2^k) be two solutions to scheme (15)–(18), and assume that $S_1^{k-1} = S_2^{k-1}$, $M_1^{k-1} = M_2^{k-1}$. We wish to show that $S_1^k = S_2^k$, $M_1^k = M_2^k$. The functions $S_1^k - S_2^k$ and $M_1^k - M_2^k$ are solutions, respectively, to

$$(36) \qquad \frac{\mathrm{m}(K)}{\Delta t}(S_{1,K}^k - S_{2,K}^k) - d_1 \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}(S_1^k - S_2^k) = \mathrm{m}(K) G_K^k,$$

$$(37) \qquad \frac{\mathrm{m}(K)}{\Delta t}(M_{1,K}^k - M_{2,K}^k) - d_2 \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}(F(M_1^k) - F(M_2^k)) = \mathrm{m}(K) H_K^k$$

for $K \in \mathcal{T}$, where

$$G_K^k = -\frac{\kappa_1 S_{1,K}^k}{\kappa_4 + S_{1,K}^k}(M_{1,K}^k - M_{2,K}^k) - \frac{\kappa_1 \kappa_4 M_{2,K}^k}{(\kappa_4 + S_{1,K}^k)(\kappa_4 + S_{2,K}^k)}(S_{1,K}^k - S_{2,K}^k),$$

$$H_K^k = \left(\frac{\kappa_3 S_{1,K}^k}{\kappa_4 + S_{1,K}^k} - \kappa_2 \right)(M_{1,K}^k - M_{2,K}^k) + \frac{\kappa_3 \kappa_4 M_{2,K}^k}{(\kappa_4 + S_{1,K}^k)(\kappa_4 + S_{2,K}^k)}(S_{1,K}^k - S_{2,K}^k).$$

Now, let the vectors $(\psi_\mathcal{T}^k, \psi_\mathcal{E}^k)$ and $(\phi_\mathcal{T}^k, \phi_\mathcal{E}^k)$ be the unique solutions to

$$-\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma} \psi^k = \mathrm{m}(K)(S_{1,K}^k - S_{2,K}^k),$$

$$-\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma} \phi^k = \mathrm{m}(K)(M_{1,K}^k - M_{2,K}^k)$$

for $K \in \mathcal{T}$, where we impose the boundary conditions $\psi_\sigma^k = \phi_\sigma^k = 0$ for $\sigma \in \mathcal{E}_{\mathrm{ext}}$. The existence and uniqueness of these solutions is a direct consequence of [18, Lemma 9.2]. We multiply (37) by ϕ_K^k and sum over $K \in \mathcal{T}$:

$$(38) \qquad \frac{1}{\Delta t} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(M_{1,K}^k - M_{2,K}^k)\phi_K^k = I_1 + I_2, \quad \text{where}$$

$$I_1 = d_2 \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}(F(M_{1,K}^k) - F(M_{2,K}^k))\phi_K^k, \quad I_2 = \sum_{K \in \mathcal{T}} \mathrm{m}(K) H_K^k \phi_K^k.$$

Inserting the equation for ϕ^k and using discrete integration by parts gives

$$\sum_{K \in \mathcal{T}} \mathrm{m}(K)(M_{1,K}^k - M_{2,K}^k)\phi_K^k = -\sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}(\phi^k)\phi_K^k = \sum_{\sigma \in \mathcal{E}} \tau_\sigma (\mathrm{D}_{K,\sigma}\phi^k)^2 = |\phi^k|_{1,2,\mathcal{M}}^2.$$

Concerning the sum I_1, we use the equation for ϕ^k again, apply discrete integration by parts twice, and take into account the positive lower bound for M_i^k from Theorem 2:

$$I_1 = d_2 \sum_{K \in \mathcal{T}} (F(M_{1,K}^k) - F(M_{2,K}^k)) \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \mathrm{D}_{K,\sigma}\phi^k$$

$$= -d_2 \sum_{K \in \mathcal{T}} \mathrm{m}(K)(F(M_{1,K}^k) - F(M_{2,K}^k))(M_{1,K}^k - M_{2,K}^k)$$

$$\leq -d_2 c_0 \sum_{K \in \mathcal{T}} \mathrm{m}(K)(M_{1,K}^k - M_{2,K}^k)^2,$$

where $c_0 > 0$ depends on the minimum of M_1^k or M_2^k. Finally, because of the bounds $0 \leq S_K^k \leq 1$ and $0 \leq M_K^k < 1$ from Theorem 2, the Young inequality and the discrete Poincaré inequality [4, Theorem 3.2],

$$I_2 \leq -\kappa_2 |\phi^k|_{1,2,\mathcal{M}}^2 + \sum_{K \in \mathcal{T}} \mathrm{m}(K)\left(\frac{\kappa_3}{\kappa_4 + 1}|M_{1,K}^k - M_{2,K}^k| + \frac{\kappa_3}{\kappa_4}|S_{1,K}^k - S_{2,K}^k|\right)|\phi_K^k|$$

$$\leq \frac{\delta}{2}\left(\frac{\kappa_3^2}{(\kappa_4 + 1)^2}\|M_1^k - M_2^k\|_{0,2,\mathcal{M}}^2 + \frac{\kappa_3^2}{\kappa_4^2}\|S_1^k - S_2^k\|_{0,2,\mathcal{M}}^2\right) + \frac{C}{\delta\xi}|\phi^k|_{1,2,\mathcal{M}}^2,$$

where $\delta > 0$ is arbitrary. Collecting these estimates, we infer from (38) that

$$\left(\frac{1}{\Delta t} - \frac{C}{\delta\xi}\right)|\phi^k|_{1,2,\mathcal{M}}^2 + \frac{1}{2}d_2 c_0\|M_1^k - M_2^k\|_{0,2,\mathcal{M}}^2$$

$$\leq \frac{\delta}{2}\left(\frac{\kappa_3^2}{(\kappa_4 + 1)^2}\|M_1^k - M_2^k\|_{0,2,\mathcal{M}}^2 + \frac{\kappa_3^2}{\kappa_4^2}\|S_1^k - S_2^k\|_{0,2,\mathcal{M}}^2\right).$$

Arguing similarly for equation (36), we arrive to

$$\left(\frac{1}{\Delta t} - \frac{C}{\delta\xi}\right)|\psi^k|_{1,2,\mathcal{M}}^2 + \frac{1}{2}d_1\|S_1^k - S_2^k\|_{0,2,\mathcal{M}}^2$$

$$\leq \frac{\delta}{2}\left(\frac{\kappa_1^2}{(\kappa_4 + 1)^2}\|M_1^k - M_2^k\|_{0,2,\mathcal{M}}^2 + \frac{\kappa_1^2}{\kappa_4^2}\|S_1^k - S_2^k\|_{0,2,\mathcal{M}}^2\right).$$

We set $R^k := \|S_1^k - S_2^k\|_{0,2,\mathcal{M}}^2 + \|M_1^k - M_2^k\|_{0,2,\mathcal{M}}^2$. Then an addition of the previous two inequalities yields

$$\left(\frac{1}{\Delta t} - \frac{C}{\delta\xi}\right)\left(|\phi^k|_{1,2,\mathcal{M}}^2 + |\psi^k|_{1,2,\mathcal{M}}^2\right) + \frac{1}{2}\left(\min\{d_1, d_2 c_0\} - \delta\frac{\kappa_1^2 + \kappa_3^2}{\kappa_4^2}\right)R^k \leq 0.$$

Choosing $\delta \leq \kappa_4^2/(\kappa_1^2 + \kappa_3^2)\min\{d_1, d_2 c_0\}$ and $\Delta t < C/(\delta \xi)$, both terms are nonnegative, and we infer that $\phi_K^k = \psi_K^k = 0$ and consequently $M_{1,K}^k - M_{2,K}^k = S_{1,K}^k - S_{2,K}^k = 0$ for all $K \in \mathcal{T}$.

5. UNIFORM ESTIMATES

We establish some estimates that are uniform with respect to Δx and Δt. The first bounds follow from the results of the previous section.

Lemma 8 (Uniform estimates I). *There exists a constant $C > 0$ independent of Δx and Δt such that*

$$0 \leq S_K^k \leq 1, \quad 0 \leq M_K^k < 1 \quad for \ K \in \mathcal{T},$$

$$\sum_{k=1}^{N_T} \Delta t \big(\|F(M^k)\|_{1,2,\mathcal{M}}^2 + \|S^k\|_{1,2,\mathcal{M}}^2\big) \leq C.$$

Proof. The L^∞ bounds follow directly from Theorem 2, while the discrete gradient bound for $F(M^k)$ is a consequence of Lemma 7. It remains to show the discrete gradient bound for S^k. We multiply (16) by $\Delta t(S_K^k - 1)$, sum over $K \in \mathcal{T}$, and use discrete integration by parts:

$$(39) \qquad \sum_{K \in \mathcal{T}} \mathrm{m}(K)(S_K^k - S_K^{k-1})(S_K^k - 1) = -\Delta t \sum_{\sigma \in \mathcal{E}} \tau_\sigma \mathrm{D}_{K,\sigma}(S^k)\mathrm{D}_{K,\sigma}(S^k - 1)$$

$$+ \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K)g(S_K^k, M_K^k)(S_K^k - 1)$$

$$\leq -\Delta t \sum_{\sigma \in \mathcal{E}} \tau_\sigma (\mathrm{D}_{K,\sigma}(S^k - 1))^2 + \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K)\frac{\kappa_1 S_K^k M_K^k}{\kappa_4 + S_K^k}.$$

The left-hand side is bounded from below by

$$\sum_{K \in \mathcal{T}} \mathrm{m}(K)\big((S_K^k - 1) - (S_K^{k-1} - 1)\big)(S_K^k - 1) \geq \frac{1}{2} \sum_{K \in \mathcal{T}} \mathrm{m}(K)\big((S_K^k - 1)^2 - (S_K^{k-1} - 1)^2\big).$$

In view of the upper bounds for S_K^k and M_K^k, the last term on the right-hand side of (39) is bounded by $\Delta t\,\mathrm{m}(\Omega)\kappa_1/(\kappa_4 + 1)$. Therefore, it follows from (39) that

$$\frac{1}{2} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(S_K^k - 1)^2 + \Delta t|S_K^k - 1|_{1,2,\mathcal{M}}^2 \leq \frac{1}{2} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(S_K^{k-1} - 1)^2 + C\Delta t.$$

Summing this inequality from $k = 1, \ldots, N_T$, we find that

$$\frac{1}{2}\|S^{N_T} - 1\|_{0,2,\mathcal{M}}^2 + \sum_{k=1}^{N_T} \Delta t|S_K^k - 1|_{1,2,\mathcal{M}}^2 \leq \frac{1}{2}\|S^0 - 1\|_{0,2,\mathcal{M}}^2 + CT.$$

This yields the desired estimate.   □

We also need an estimate for the time translates of the solution. For this, let $\phi \in C_0^\infty(\Omega_T)$ be given and define $\phi^k = (\phi_\mathcal{T}^k, \phi_\mathcal{E}^k) \in \mathbb{R}^\theta$ (recall that $\theta = \#\mathcal{T} + \#\mathcal{E}$) for $k = 1, \ldots, N_T$ by

$$\phi_K^k = \frac{1}{\mathrm{m}(K)} \int_K \phi(x, t_k)dx, \quad \phi_\sigma^k = \frac{1}{\mathrm{m}(\sigma)} \int_\sigma \phi(s, t_k)ds = 0,$$

where $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_{\mathrm{ext}}$.

Lemma 9 (Uniform estimates II). *For any $\phi \in C_0^\infty(\Omega_T)$, there exist constants $C_3, C_4 > 0$, only depending on the data and the mesh, such that*

$$\sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(M_K^k - M_K^{k-1})\phi_K^k \leq C_3 \|\nabla\phi\|_{L^\infty(\Omega_T)},$$

$$\sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(S_K^k - S_K^{k-1})\phi_K^k \leq C_4 \|\nabla\phi\|_{L^\infty(\Omega_T)}.$$

Proof. We multiply (17) by $\Delta t \phi_K^k$, sum over $K \in \mathcal{T}$ and $k = 1, \ldots, N_T$, and use discrete integration by parts. Then

(40)
$$\sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(M_K^k - M_K^{k-1})\phi_K^k = I_3 + I_4, \quad \text{where}$$

$$I_3 = -d_2 \sum_{k=1}^{N_T} \Delta t \sum_{\sigma \in \mathcal{E}} \tau_\sigma \mathrm{D}_{K,\sigma} F(M^k) \mathrm{D}_{K,\sigma} \phi^k,$$

$$I_4 = \sum_{k=1}^{N_T} \Delta t \sum_{K \in \mathcal{T}} \mathrm{m}(K)\left(\frac{\kappa_3 S_K^k}{\kappa_4 + S_K^k} - \kappa_2\right) M_K^k \phi_K^k.$$

It follows from the Cauchy–Schwarz inequality, Lemma 8, and the mesh regularity (9) that

$$|I_3| \leq d_2 C \|\nabla\phi\|_{L^\infty(\Omega_T)}\left(\sum_{k=1}^{N_T} \Delta t \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \mathrm{m}(\sigma)\mathrm{d}_\sigma\right)^{1/2}$$

$$\leq d_2 C \xi^{-1/2} \|\nabla\phi\|_{L^\infty(\Omega_T)}\left(\sum_{k=1}^{N_T} \Delta t \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \mathrm{m}(\sigma)\mathrm{d}(x_K, \sigma)\right)^{1/2}$$

$$= d_2 C \sqrt{2\,\mathrm{m}(\Omega)T\xi^{-1}} \|\nabla\phi\|_{L^\infty(\Omega_T)},$$

where we used (7) in the last step. Next, using similar arguments and the discrete Poincaré inequality [4, Theorem 3.2],

$$|I_4| \leq \left(\kappa_2 + \frac{\kappa_3}{\kappa_4 + 1}\right)\sqrt{T\,\mathrm{m}(\Omega)}\left(\sum_{k=1}^{N_T} \Delta t \|\phi^k\|_{0,2,\mathcal{M}}^2\right)^{1/2}$$

$$\leq \left(\kappa_2 + \frac{\kappa_3}{\kappa_4 + 1}\right)\sqrt{T\,\mathrm{m}(\Omega)C\xi^{-1}}\left(\sum_{k=1}^{N_T} \Delta t |\phi^k|_{1,2,\mathcal{M}}^2\right)^{1/2}$$

$$\leq \left(\kappa_2 + \frac{\kappa_3}{\kappa_4 + 1} \right) \sqrt{T \, \mathrm{m}(\Omega) C \xi^{-1}} \|\nabla \phi\|_{L^\infty(\Omega_T)} \left(\sum_{k=1}^{N_T} \Delta t \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \mathrm{m}(\sigma) \mathrm{d}_\sigma \right)^{1/2}$$

$$\leq C(T, \Omega, \xi) \xi^{-1} \left(\kappa_2 + \frac{\kappa_3}{\kappa_4 + 1} \right) \|\nabla \phi\|_{L^\infty(\Omega_T)}.$$

Inserting these estimates into (40) shows the first statement of the lemma. The second statement is proved in a similar way. $\qquad\square$

6. Convergence of the scheme

The compactness follows from the uniform estimates proved in the previous section and the discrete compensated compactness result obtained in [3, Theorem 3.9].

Lemma 10 (Compactness). *Let $(S_m, M_m)_{m \in \mathbb{N}}$ be a sequence of solutions to scheme* (15)–(18) *constructed in Theorem 2. Then there exists $(S, M) \in L^\infty(\Omega_T; \mathbb{R}^2)$ satisfying $F(M)$, $S \in L^2(0, T; H^1(\Omega))$ such that, up to a subsequence, as $m \to \infty$,*

$$M_m \to M, \quad S_m \to S \quad a.e. \ in \ \Omega_T,$$

$$F(M_m) \to F(M) \quad strongly \ in \ L^r(\Omega_T) \ for \ 1 \leq r < 2,$$

$$\nabla^m F(M_m) \rightharpoonup \nabla F(M), \quad \nabla^m S_m \rightharpoonup \nabla S \quad weakly \ in \ L^2(\Omega_T).$$

Proof. The a.e. convergence for M_m is a consequence of [3, Theorem 3.9]. Indeed, the estimates in Lemmas 8–9 correspond to conditions (a)–(c) in [3, Prop. 3.8], while assumptions (A_t1), (A_x1)–(A_x3) are satisfied for our implicit Euler finite-volume scheme. We infer that there exists a subsequence which is not relabeled such that $M_m \to M$ and $F(M_m) \to F(M)$ a.e. in Ω_T. In view of Lemma 8, the sequence $(F(M_m))$ is bounded in $L^2(\Omega_T)$, and thanks to the Vitali's lemma, we conclude that $F(M_m) \to F(M)$ strongly in $L^r(\Omega_T)$ for all $1 \leq r < 2$.

As a consequence of the gradient estimate in Lemma 7, there exists a subsequence of $(\nabla^m F(M_m))$ (not relabeled) such that $\nabla^m F(M_m) \rightharpoonup \Psi$ weakly in $L^2(\Omega_T)$ as $m \to \infty$. The limit Ψ can be identified with $F(M)$ by following the arguments in the proof of [6, Lemma 4.4]. Indeed, the idea is to prove that for all $\phi \in C_0^\infty(\Omega_T; \mathbb{R}^2)$,

$$A_m := \int_0^T \int_\Omega \nabla^m F(M_m) \cdot \phi \, dx dt + \int_0^T \int_\Omega F(M_m) \, \mathrm{div} \, \phi \, dx dt \to 0$$

as $m \to \infty$. This is done by reformulating the two integrals:

$$\int_\Omega \nabla^m F(M_m) \cdot \phi \, dx = -\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\mathrm{int},K}} \frac{\mathrm{m}(\sigma)}{\mathrm{m}(T_{K,\sigma})} \mathrm{D}_{K,\sigma} F(M_m) \int_{T_{K,\sigma}} \phi(s, t) \cdot \nu_{K,\sigma} dx,$$

$$\int_\Omega F(M_m) \, \mathrm{div} \, \phi \, dx = \frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\mathrm{int},K}} \mathrm{D}_{K,\sigma} F(M_m) \int_\sigma \phi(s, t) \cdot \nu_{K,\sigma} ds.$$

Because of the property (see [6, Lemma 4.4])

$$\left| \frac{1}{\mathrm{m}(T_{K,\sigma})} \int_{T_{K,\sigma}} \phi(t, s) \cdot \nu_{K,\sigma} dx - \frac{1}{\mathrm{m}(\sigma)} \int_\sigma \phi(s, t) \cdot \nu_{K,\sigma} ds \right| \leq \eta_m \|\phi\|_{C^1(\overline{\Omega})}$$

and the uniform estimates for $F(M_m)$ from Lemma 8, it follows that

$$|A_m| \leq \frac{1}{2} \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\text{int},K}} \text{m}(\sigma) \text{D}_{K,\sigma} F(M^k)$$

$$\times \left| \frac{1}{\text{m}(T_{K,\sigma})} \int_{T_{K,\sigma}} \phi(t,s) \cdot \nu_{K,\sigma} dx - \frac{1}{\text{m}(\sigma)} \int_\sigma \phi(s,t) \cdot \nu_{K,\sigma} ds \right|$$

$$\leq \eta_m C \|\phi\|_{C^1(\overline{\Omega})} \to 0 \quad \text{as } m \to \infty.$$

This implies that $\Psi = \nabla F(M)$. Finally, similar arguments as above show the convergence results for S_m and $\nabla^m S_m$. $\qquad \square$

Lemma 11 (Convergence of the traces). *Let $(S_m, M_m)_{m \in \mathbb{N}}$ be a sequence of solutions to scheme (15)–(18) constructed in Theorem 2. Then the limit function (S, M) obtained in Lemma 10 satisfies*

$$S - 1, \quad F(M) - F(M^D) \in L^2(0, T; H_0^1(\Omega)).$$

Proof. The proof for S is a direct consequence of [5, Prop. 4.9]. For $F(M)$, we follow the proof of [5, Prop. 4.11]. In particular, we aim to prove that

$$(41) \qquad \int_0^T \int_{\partial\Omega} (F(M_m) - F(M))\psi dx dt \to 0 \quad \text{as } m \to \infty$$

for every $\psi \in C_0^\infty(\partial\Omega \times (0, T))$. If this result holds then, as $M_m = M^D$ on $\partial\Omega \times (0, T)$, we obtain

$$\int_0^T \int_{\partial\Omega} (F(M) - F(M^D))\psi dx dt = \lim_{m \to \infty} \left(\int_0^T \int_{\partial\Omega} (F(M) - F(M_m))\psi dx dt \right.$$

$$\left. + \int_0^T \int_{\partial\Omega} (F(M_m) - F(M^D))\psi dx dt \right) = 0,$$

which implies that $F(M) = F(M^D)$ a.e. on $\partial\Omega \times (0, T)$.

To prove (41), we choose a fixed $m \in \mathbb{N}$ and introduce another definition of the trace of M_m, denoted by $\widetilde{M}_m$, such that $\widetilde{M}_m(x, t) = M_K^k$ if $(x, t) \in \sigma \times (t_{k-1}, t_k]$ with $\sigma \in \mathcal{E}_{\text{ext,K}}$. Following [5], we notice that the property (41) is equivalent to

$$(42) \qquad \int_0^T \int_{\partial\Omega} (F(\widetilde{M}_m) - F(M))\psi dx dt \to 0 \quad \text{as } m \to \infty$$

for all $\psi \in C_0^\infty(\partial\Omega \times (0, T))$. Indeed, we have, by the Cauchy–Schwarz inequality,

$$\int_0^T \int_{\partial\Omega} |F(M_m) - F(\widetilde{M}_m)| dx dt = \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\text{ext},K}} \text{m}(\sigma)|F(M^D) - F(M_K^k)|$$

$$\leq \left(\sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\text{ext},K}} \tau_\sigma |F(M^D) - F(M_K^k)|^2 \right)^{1/2}$$

$$\times \left(\sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\mathrm{ext},K}} \mathrm{m}(\sigma) \mathrm{d}_\sigma \right)^{1/2}.$$

Hence, thanks to Lemma 8 and the fact that $\mathrm{d}_\sigma = \mathrm{d}(x_K, \sigma) \leq \mathrm{diam}(K) \leq \eta_m$ for every $\sigma \in \mathcal{E}_{\mathrm{ext},K}$, it follows that

$$\int_0^T \int_{\partial\Omega} |F(M_m) - F(\widetilde{M}_m)| dx dt \leq C(T\, \mathrm{m}(\partial\Omega)\eta_m)^{1/2} \to 0 \quad \text{as } m \to \infty,$$

which proves the claim.

Now, as Ω is assumed to be a polygonal domain, $\partial\Omega$ consists of a finite number of faces denoted by $(\Gamma_i)_{1 \leq i \leq I}$. Similarly to [5, 19], we define for $\varepsilon > 0$ the subset $\Omega_{i,\varepsilon}$ of Ω such that every $x \in \Omega_{i,\varepsilon}$ satisfies $\mathrm{d}(x, \Gamma_i) < \varepsilon$ and $\mathrm{d}(x, \Gamma_i) < \mathrm{d}(x, \Gamma_j)$ for all $j \neq i$. We also define the subset $\omega_{i,\varepsilon} \subset \Omega_{i,\varepsilon}$ as the largest cylinder of width ε generated by Γ_i. Let ν_i be the unit vector that is normal to Γ_i, i.e., more precisely, we introduce the set

$$\omega_{i,\varepsilon} := \big\{ x - h\nu_i \in \Omega_i : x \in \Gamma_i,\ 0 < h < \varepsilon \text{ and } [x, x - h\nu_i] \subset \overline{\Omega}_{i,\varepsilon} \big\} \quad \text{for all } 1 \leq i \leq I.$$

Finally, we also introduce the subset $\Gamma_{i,\varepsilon} := \partial\omega_{i,\varepsilon} \cap \Gamma_i$, which fulfills $\mathrm{m}(\Gamma_i \setminus \Gamma_{i,\varepsilon}) \leq C\varepsilon$ for some constant $C > 0$ only depending on Ω.

Let $i \in \{1, \ldots, I\}$ be fixed and let $\psi \in C_0^\infty(\Gamma_i \times (0, T))$. Then there exists $\varepsilon^* = \varepsilon^*(\psi) > 0$ such that for every $\varepsilon \in (0, \varepsilon^*)$, we have $\mathrm{supp}(\psi) \subset \Gamma_{i,\varepsilon} \times (0, T)$. We write

$$\int_0^T \int_{\Gamma_i} (F(\widetilde{M}_m) - F(M))\psi\, dx dt = B_{1,m,\varepsilon} + B_{2,m,\varepsilon} + B_{3,\varepsilon}, \quad \text{where}$$

$$B_{1,m,\varepsilon} = \int_0^T \frac{1}{\varepsilon} \int_{\Gamma_{i,\varepsilon}} \int_0^\varepsilon \big(F(\widetilde{M}_m(x, t)) - F(M_m(x - h\nu_i, t)) \big) \psi(x, t) dh dx dt,$$

$$B_{2,m,\varepsilon} = \int_0^T \frac{1}{\varepsilon} \int_{\Gamma_{i,\varepsilon}} \int_0^\varepsilon \big(F(M_m(x - h\nu_i, t)) - F(M(x - h\nu_i, t)) \big) \psi(x, t) dh dx dt,$$

$$B_{3,\varepsilon} = \int_0^T \frac{1}{\varepsilon} \int_{\Gamma_{i,\varepsilon}} \int_0^\varepsilon \big(F(M(x - h\nu_i, t)) - F(M) \big) \psi(x, t) dh dx dt.$$

We apply the Cauchy–Schwarz inequality to the first term and then use [5, Lemma 4.8] and Lemma 8 to find that

$$|B_{1,m,\varepsilon}| \leq \left(\int_0^T \frac{1}{\varepsilon} \int_{\Gamma_{i,\varepsilon}} \int_0^\varepsilon \big(F(\widetilde{M}_m(x, t)) - F(M_m(x - h\nu_i, t)) \big)^2 dh dx dt \right)^{1/2}$$

$$\times \left(\int_0^T \int_{\Gamma_i} \psi(x, t)^2 dx dt \right)^{1/2} \leq \sqrt{\varepsilon + \eta_m} \|F(M_m)\|_{1,2,\mathcal{M}} \|\psi\|_{L^2(\Gamma_i \times (0,T))}.$$

Taking into account that Lemma 10 implies that $F(M_m) \to F(M)$ strongly in $L^r(\Omega_T)$ for $1 \leq r < 2$, we infer that the second term $B_{2,m,\varepsilon}$ converges to zero as $m \to \infty$. This shows that

$$\lim_{m \to \infty} \left| \int_0^T \int_{\Gamma_i} (F(\widetilde{M}_m) - F(M))\psi\, dx dt \right| \leq C\sqrt{\varepsilon} + |B_{3,\varepsilon}|.$$

Since $F(M) \in L^2(0, T; H^1(\Omega))$, the function $F(M)$ has a trace in $L^2(\partial\Omega \times (0, T))$ such that $B_{3,\varepsilon} \to 0$ as $\varepsilon \to 0$. Hence, performing the limit $\varepsilon \to 0$, we conclude that (42) holds, finishing the proof. $\qquad \square$

It remains to verify that the limit function (S, M) obtained in Lemma 10 is a weak solution to (1)–(5). We follow the ideas of [6] and prove that M solves (25), as the proof of (24) is analogous. Let $\phi \in C_0^\infty(\Omega \times [0, T))$ and let $\eta_m = \max\{\Delta x_m, \Delta t_m\}$ be sufficiently small such that $\mathrm{supp}(\phi) \subset \{x \in \Omega : \mathrm{d}(x, \partial\Omega) > \eta_m\} \times (0, T)$. The aim is to prove that $F_{10}^m + F_{20}^m + F_{30}^m \to 0$ as $m \to \infty$, where

$$F_{10}^m = -\int_0^T \int_\Omega M_m \partial_t \phi \, dx \, dt - \int_\Omega M_m(x, 0)\phi(x, 0)dx,$$

$$F_{20}^m = d_2 \int_0^T \int_\Omega \nabla^m F(M_m) \cdot \nabla\phi \, dx \, dt,$$

$$F_{30}^m = -\int_0^T \int_\Omega h(S_m, M_m)\phi \, dx \, dt.$$

The convergence results from Lemma 10 allow us to perform the limit $m \to \infty$ in these integrals, leading to

$$F_{10}^m + F_{20}^m + F_{30}^m \to -\int_0^T \int_\Omega M \partial_t \phi \, dx \, dt - \int_\Omega M^0(x)\phi(x, 0)dx$$
$$+ d_2 \int_0^T \int_\Omega \nabla F(M) \cdot \nabla\phi \, dx \, dt - \int_0^T \int_\Omega h(S, M)\phi \, dx \, dt.$$

Now we set $\phi_K^k = \phi(x_K, t_k)$, multiply (17) by $\Delta t \phi_K^{k-1}$, and sum over $K \in \mathcal{T}$ and $k = 1, \ldots, N_T$:

$$(43) \qquad F_1^m + F_2^m + F_3^m = 0, \quad \text{where}$$

$$F_1^m = \sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}} \mathrm{m}(K)(M_K^k - M_K^{k-1})\phi_K^{k-1},$$

$$F_2^m = -d_2 \sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_{\mathrm{int}, K}} \tau_\sigma \mathrm{D}_{K,\sigma} F(M^k)\phi_K^{k-1},$$

$$F_3^m = -\sum_{k=1}^{N_T} \Delta t_m \sum_{K \in \mathcal{T}} \mathrm{m}(K)h(S_K^k, M_K^k)\phi_K^{k-1}.$$

We claim that $F_{j0}^m - F_j^m \to 0$ as $m \to \infty$ for $j = 1, 2, 3$. Then (43) implies that $F_{10}^m + F_{20}^m + F_{30}^m \to 0$ for $m \to \infty$, finishing the proof.

For the first limit, we argue as in [6, Theorem 5.2]:

$$F_{10}^m = -\sum_{k=1}^{N_T} \sum_{K \in \mathcal{T}} \mathrm{m}(K)M_{m,K}^k(\phi_K^k - \phi_K^{k-1}) - \sum_{K \in \mathcal{T}} \mathrm{m}(K)M_{m,K}^0\phi_K^0$$

$$= -\sum_{k=1}^{N_T}\sum_{K\in\mathcal{T}}\int_{t_{k-1}}^{t_k}\int_K M_{m,K}^k\partial_t\phi(x_K,t)dxdt - \sum_{K\in\mathcal{T}}\int_K M_{m,K}^0\phi(x_K,0)dx.$$

This shows that $|F_{10}^m - F_1^m| \le C\|\phi\|_{C^2(\overline{\Omega_T})}\eta_m \to 0$ as $m \to \infty$.

Next, we use discrete integration by parts to rewrite F_2^m:

$$F_2^m = d_2\sum_{k=1}^{N_T}\Delta t_m\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}}\tau_\sigma D_{K,\sigma}F(M^k)D_{K,\sigma}\phi^{k-1}.$$

By the definition of the discrete gradient, we can also rewrite F_{20}^m:

$$F_{20}^m = d_2\sum_{k=1}^{N_T}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_{int,K}}D_{K,\sigma}F(M^k)\frac{\mathrm{m}(\sigma)}{\mathrm{m}(T_{K,\sigma})}\int_{t_{k-1}}^{t_k}\int_{T_{K,\sigma}}\nabla\phi\cdot\nu_{K,\sigma}dxdt.$$

Hence, using [6, Theorem 5.1] and the Cauchy–Schwarz inequality, we find that

$$|F_{20}^m - F_2^m| \le d_2\sum_{k=1}^{N_T}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}}\mathrm{m}(\sigma)D_\sigma F(M^k)$$

$$\times\left|\int_{t_{k-1}}^{t_k}\left(\frac{1}{\mathrm{m}(T_{K,\sigma})}\int_{T_{K,\sigma}}\nabla\phi\cdot\nu_{K,\sigma}dx - \frac{1}{\mathrm{d}_\sigma}D_{K,\sigma}\phi^{k-1}dx\right)dt\right|$$

$$\le d_2\sum_{k=1}^{N_T}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_{\mathrm{int},K}}\mathrm{m}(\sigma)D_\sigma F(M^k)\times C\Delta t_m\eta_m$$

$$\le C\eta_m d_2\left(\sum_{k=1}^{N_T}\Delta t_m\sum_{\sigma\in\mathcal{E}}\mathrm{m}(\sigma)\mathrm{d}_\sigma\right)^{1/2}\left(\sum_{k=1}^{N_T}\Delta t_m|F(M^k)|_{1,2,\mathcal{M}}^2\right)^{1/2}$$

$$\le C\eta_m d_2\xi^{-1/2}\left(\sum_{k=1}^{N_T}\Delta t_m\sum_{\sigma\in\mathcal{E}}\mathrm{m}(\sigma)\mathrm{d}(x_K,\sigma)\right)^{1/2},$$

where we used the mesh regularity (9) in the last step. Taking into account the estimate for $F(M_m)$ from Lemma 7 and the property (7), we infer that $F_{20}^m - F_2^m \to 0$.

Finally, using the regularity of ϕ, we obtain

$$|F_{30}^m - F_3^m| \le \sum_{k=1}^{N_T}\sum_{K\in\mathcal{T}}\mathrm{m}(K)|h(S_K^k,M_K^k)|\left|\int_{t_{k-1}}^{t_k}\left(\phi_K^{k-1} - \frac{1}{\mathrm{m}(K)}\int_K\phi dx\right)dt\right|$$

$$\le\left(\kappa_2 + \frac{\kappa_3}{\kappa_4}\right)\sum_{k=1}^{N_T}\sum_{K\in\mathcal{T}}\mathrm{m}(K)\left|\int_{t_{k-1}}^{t_k}\left(\phi_K^{k-1} - \frac{1}{\mathrm{m}(K)}\int_K\phi dx\right)dt\right|$$

$$\le\left(\kappa_2 + \frac{\kappa_3}{\kappa_4}\right)\mathrm{m}(\Omega)T\|\nabla\phi\|_{L^\infty(\Omega_T)}\eta_m \to 0.$$

This finishes the proof.

7. Numerical experiments

We present in this section some numerical experiments for the biofilm model (15)–(18) in one and two space dimensions.

7.1. Implementation of the scheme.

The finite-volume scheme (15)–(18) is implemented in MATLAB. Since the numerical scheme is implicit in time, we have to solve a nonlinear system of equations at each time step. In the one-dimensional case, we use Newton's method. Starting from (S^{k-1}, M^{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-stepping strategy to approximate the solution of the scheme at time t_k. More precisely, starting again from (S^{k-1}, M^{k-1}), we launch a Newton method. If the method does not converge with precision $\varepsilon = 10^{-8}$ after at most 50 steps, we multiply the time step by a factor 0.2 and restart the Newton method. At the beginning of each time step, we increase the value of the previous time step size by multiplying it by 1.1. Moreover, we impose the condition $10^{-8} \leq \Delta t_k \leq 10^{-2}$ with an initial time step size equal to 10^{-5}. Our adaptive time-step strategy aims to improve the numerical performance of our scheme in terms of number of time steps, CPU time, etc. However, this strategy is not mandatory and, as in our one-dimensional test case, we can always implement our scheme with a constant time step with a reasonable size.

7.2. Test case 1: Rate of convergence in space.

We illustrate the order of convergence in space for the biofilm model in one space dimension with $\Omega = (0, 1)$. To this purpose, we choose the coefficients $d_1 = 4.1667$, $d_2 = 4.2$, $\kappa_1 = 793.65$, $\kappa_2 = 0.067$, $\kappa_3 = 1$, $\kappa_4 = 0.4$ and $M^D = 0$. These values are close to those used in [16]. We take $a = 2$ and $b = 1$ such that, after elementary computations,

$$F(M) = \log(1 - x) + \frac{1}{1 - x} - 1.$$

Finally, we impose the initial data $S^0(x) = 1 - 0.2 \sin(\pi x)$ and

$$M^0(x) = 0.2 \, g(x - 0.38) + 0.9 \, g(x - 0.62),$$

$$\text{where } g(x) = \max\{1 - 9^2 x^2, 0\}.$$

Since exact solutions to the biofilm model are not explicitly known, we compute a reference solution $(S_{\text{ref}}, M_{\text{ref}})$ on a uniform mesh composed of $20,480$ cells and with $\Delta t = (1/20,480)^2$. 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 (15)-(18), due to to two-point flux approximation scheme used in this work. We compute approximate solutions on uniform meshes made of 80, 160, 320, 640, 1280 and 2560 cells, respectively. In Figure 1, we present the $L^1(\Omega)$ norm of the difference between the approximate solutions and the average of the reference solution $(S_{\text{ref}}, M_{\text{ref}})$ at the final time $T = 10^{-3}$. As expected, we observe a second-order convergence rate in space.
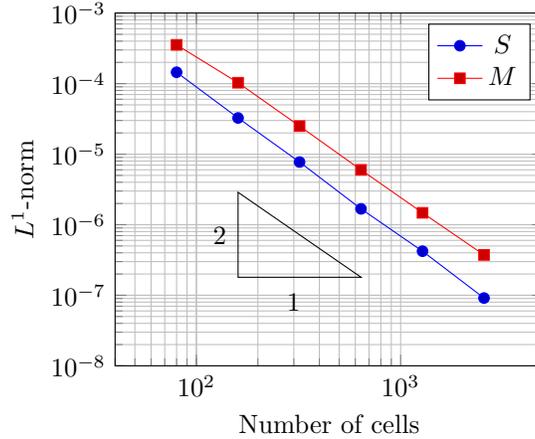
FIGURE 1. Test case 1: L^1 norm of the error between the reference solution and the solutions computed on coarser grids at final time $T = 10^{-3}$.

7.3. **Test case 2: Microbial floc.** We investigate the behavior of S and M in two space dimensions with domain $\Omega = (0,1) \times (0,1)$ and final time $T = 2$. As in the first test case, we choose the coefficients $d_1 = 4.1667$, $d_2 = 4.2$, $\kappa_1 = 793.65$, $\kappa_2 = 0.067$, $\kappa_3 = 1$, $\kappa_4 = 0.4$ and $M^D = 0$. Here, we take $a = b = 4$ such that

$$F(M) = -\frac{18x^2 - 30x + 13}{3(x-1)^3} + x + 4\log(1-x) - \frac{13}{3}$$

and the initial data $S^0(x,y) = 1$ and

$$M^0(x,y) = 0.3\, p(x - 0.4, y - 0.5) + 0.9\, p(x - 0.6, y - 0.5),$$
$$\text{where } p(x,y) = \max\{1 - 8^2 x^2 - 8^2 y^2, 0\}.$$

The initial data models a microbial floc, i.e. a biofilm without substratum. This situation plays an important role in wastewater treatment.

In Figure 2, we illustrate the behavior of S and M along time for a mesh of $\Omega = (0,1)^2$ composed of 3584 triangles. We observe, as in [14, 15, 16], that after a transient time, the two colonies merge. After this stage, we observe an expansion of the region $\{M > 0\}$ due to the porous-medium type degeneracy for the equation of M, which implies a finite speed of propagation of the interface between $\{M > 0\}$ and $\{M = 0\}$. With the chosen parameters, the production rate of the biofilm is positive if and only if $S > \kappa^* := \kappa_2 \kappa_4 / (\kappa_3 - \kappa_2) \approx 0.029$, and the biomass fraction is increasing in $\{S > \kappa^*\}$, which is confirmed by the numerical experiments.

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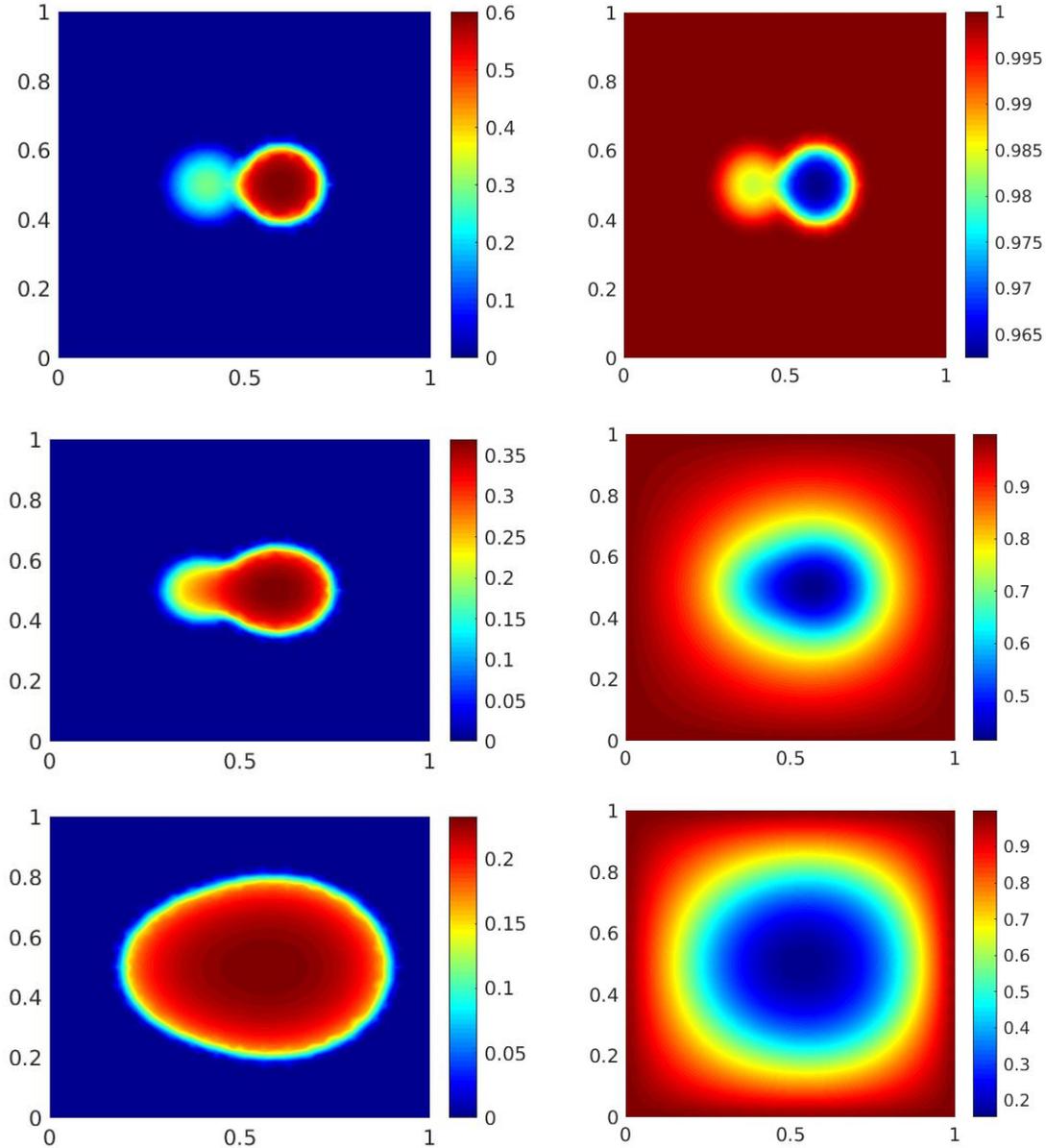
FIGURE 2. Test case 2: Evolution of M (left column) and S (right column) for $t = 10^{-4}$ (top row), $t = 10^{-2}$ (middle row) and $t = 2$ (bottom row).

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