EXISTENCE ANALYSIS FOR A REACTION-DIFFUSION CAHN-HILLIARD-TYPE SYSTEM WITH DEGENERATE MOBILITY AND SINGULAR POTENTIAL MODELING BIOFILM GROWTH

CHRISTOPH HELMER AND ANSGAR JÜNGEL

ABSTRACT. The global existence of bounded weak solutions to a diffusion system modeling biofilm growth is proven. The equations consist of a reaction-diffusion equation for the substrate concentration and a fourth-order Cahn–Hilliard-type equation for the volume fraction of the biomass, considered in a bounded domain with no-flux boundary conditions. The main difficulties are coming from the degenerate diffusivity and mobility, the singular potential arising from a logarithmic free energy, and the nonlinear reaction rates. These issues are overcome by a truncation technique and a Browder–Minty trick to identify the weak limits of the reaction terms. The qualitative behavior of the solutions is illustrated by numerical experiments in one space dimension, using a BDF2 (second-order backward Differentiation Formula) finite-volume scheme.

1. INTRODUCTION

Biofilms are prevalent in nature and occur, for instance, in lakes, on rocks, and in sediments. They play an important rule in medicine, where they attach surfaces of biomedical devices like catheters, and in wastewater treatment, where they convert organic matter in the water into bacterial biomass. Biofilms consist of microorganisms that are embedded in extracellular polymeric stubstances (EPS), which are produced by the bacteria within the biofilm. In this paper, we analyze a variant of the model derived in [24] from kinetic equations. The model consists of a reaction-diffusion equation for the substrate concentration and a Cahn–Hilliard-type equation for the volume fraction of the biomass, composed of the EPS and bacteria. The particular feature of this model is that it contains a degenerate diffusivity and mobility, a singular potential, and nonlinear production rates.

1.1. Model setting. The dynamics of the biofilm is given by the volume fraction of the biomass u(x, t) and the substrate concentration v(x, t):

(1)
$$\partial_t v - \operatorname{div}((1-u)\nabla v) = g(u,v),$$

(2)
$$\partial_t u - \operatorname{div}(M(u)\nabla\mu) = h(u, v),$$

Date: February 15, 2023.

Key words and phrases. Biofilms, reaction-diffusion equation, Cahn–Hilliard equation, degenerate mobility, singular potential, existence of solutions, logarithmic free energy.

The authors acknowledge partial support from the Austrian Science Fund (FWF), grants P33010 and F65. This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme, ERC Advanced Grant no. 101018153.

²⁰⁰⁰ Mathematics Subject Classification. 35K35, 35K65, 35K67, 35Q92, 92C17.

C. HELMER AND A. JÜNGEL

(3)
$$\mu = -\Delta u + f'(u) \quad \text{in } \Omega, \ t > 0,$$

where $\Omega \subset \mathbb{R}^d$ $(d \ge 1)$ is a bounded domain. Denoting by u_s the solvent concentration, we impose the volume-filling condition $u_s + u = 1$ [23, Section 5.2]. Equations (1)–(3) are scaled, and we have set the scaled physical parameters equal to one; see Section 5.1 for the physical values. The initial and boundary conditions read as

(4)
$$u(0) = u^0, \quad v(0) = v^0 \quad \text{in } \Omega,$$

(5)
$$(1-u)\nabla v \cdot \nu = M(u)\nabla \mu \cdot \nu = \nabla u \cdot \nu = 0 \quad \text{on } \partial\Omega, \ t > 0$$

The diffusion of the concentration vanishes if there is no solvent, which means that equation (1) is degenerate with a nonstandard degeneracy. We suppose that the dynamics of the biomass is a gradient flow with the chemical potential μ and the mobility M(u). The mobility vanishes if the biomass or the solvent vanish, M(0) = M(1) = 0, and we choose

$$M(u) = u(1-u)$$

More general choices are possible; see Remark 13. The chemical potential $\mu = -\Delta u + f'(u)$ is the variational derivative of the phase-separation gradient energy and the Flory-Huggins mixing free energy [14, 19], given by its (nonconvex) density

(7)
$$f(u) = \frac{1}{N}u\log u + (1-u)\log(1-u) + \lambda u(1-u).$$

where N > 0 is the generalized polymerisation index and $\lambda > 0$ the Flory–Huggins mixing parameter. The reaction terms are given by

(8)
$$g(u,v) = -ug_0(v), \quad h(u,v) = u(1-u)h_0(v),$$

where g_0 and h_0 are continuous functions. Examples are $g_0(v) = v$ and $h_0(c) = v/(K+v)$ with K > 0 [23]. This means that the substrate is consumed by the EPS, such that the consumption rate g(u, v) is proportional to both the substrate concentration and the biomass fraction, and the polymer production rate $h_0(u)$ is modeled by Monod kinetics with half-saturation rate K. Here, we allow for more general reaction functions; see Assumption (A3) below.

Compared to the model in [24], we have modified the equations. First, we neglected the velocities of the biomass and the solvent. Assuming that both are given by the same average velocity, it may be a given function or be determined by the incompressible Navier– Stokes equations, see [27, (5)–(6)]. Our analysis works if we add a given velocity with bounded divergence. Second, we added the solvent fraction $u_s = 1 - u$ as a factor to the production rate and the mobility in equation (2). This is needed to guarantee the bound $u \leq 1$ and to derive the entropy inequality associated to the system (see Section 1.3 for details). Third, we neglect the elastic energy which simplifies the definition of the chemical potential. Fourth, and most importantly, we have simplified the time derivative in equation (1) for the solvent concentration. Wang and Zhang [24] suggested the twophase equation $\partial_t(u_s v) - \operatorname{div}(u_s \nabla v) = g(u, v)$. However, the derivative $\partial_t(u_s v)$ introduces another degeneracy at $u_s = 0$, which we are not able to treat. A two-phase model with such a degeneracy was analyzed in [1], but in this work, the bounds for the volume fractions are a consequence of the assumptions on the nonlinearities, which do not hold in the present situation.

1.2. State of the art. In the literature, many models for biofilm growth have been presented. One of the first models was suggested in [25], consisting of a transport equation for the biofilm mass and a differential equation for the biofilm thickness. This model, extended to multispecies biofilms with an equation for the free boundary, was analyzed in [6] and refined in [7] (to describe biofilm attachment). A different approach, based on diffusion equations coupled to fluiddynamical models, was proposed in [10] and mathematically analyzed in [11]; also see the extensions in [9, 12] and the numerical analysis in [8, 18]. The model of [10] describes the dynamics of the biomass density and nutrient concontration, coupled with the incompressible homogeneous Navier–Stokes equations. The mobility in the biomass equation is assumed to vanish if the biomass vanishes and blows up if the biomass reaches its maximal value. In this way, the existence of a "sharp front" of biomass at the fluid/solid transition and significant biomass spreading close to the maximum biomass value can be achieved. Another idea is to formulate the biofilm growth as a free-boundary problem, modeling an incompressible viscous Stokes fluid in one phase and a mixture of viscous fluid and the polymeric network in the other phase [15]. Another free-boundary problem was suggested in [5], taking into account surface forces, frictional drag generated by the EPS, hydrostatic pressure, and osmotic pressure that is modeled by the potential f'(u) in the framework of the Flory-Huggins theory (see (7)).

This approach was extended in [28, 29] by assuming that the biomass is driven by the chemical potential given by a free energy density that includes the Flory–Huggins mixing term and a gradient energy density. Then the diffusion equation for the biomass becomes of fourth order and is similar to the Cahn–Hilliard equation, which was introduced to study phase separation in binary alloys [3]. Since fourth-order equations generally do not allow for a maximum principle, the assumption that the mobility vanishes at the minimal and maximal value of the mass variable guarantees lower and upper bounds. The first existence analysis of Cahn–Hilliard equations was given in [26] in one space dimension and in [13] in several space dimensions. Most of the analytical results on the Cahn–Hilliard equations do not contain reaction terms. Moreover, if reaction terms are included in the Cahn–Hilliard model, nondegenerate mobilities are required; see, e.g., [2, 4, 17]. When the gradient term in the free energy is replaced by a nonlocal spatial interaction energy, degenerate mobilities (and singular potentials) can be treated [16, 20]. Up to our knowledge, there are no papers considering degenerate mobilities and singular potentials together with reaction terms. In this paper, we are able to analyze such a situation.

1.3. Main result and key ideas. We impose the following assumptions:

- (A1) Domain: $\Omega \subset \mathbb{R}^d$ $(d \ge 1)$ is a bounded domain with Lipschitz continuous boundary. Set $\Omega_T = \Omega \times (0, T)$.
- (A2) Initial data: $u^0 \in H^1(\Omega)$ satisfies $0 < u_* \le u^0 \le u^*$ in Ω for some $u_*, u^* > 0$ and $v^0 \in L^2(\Omega)$ satisfying $0 \le v^0 \le 1$ in Ω .

(A3) Source terms: $g_0 \in C^0([0,1])$ is nondecreasing and satisfies $g_0(0) = 0$, and $h_0 \in C^1([0,1])$ is nondecreasing.

Our main result is the global existence of bounded weak solutions.

Theorem 1 (Global existence). Let Assumptions (A1)–(A3) hold. Then there exists a weak solution (u, v) to (1)–(5) with the constitutive relations (6)–(8), satisfying $0 \le u \le 1$, $0 \le v \le 1$ in Ω_T ,

$$u \in L^{2}(0,T; H^{2}(\Omega)) \cap C^{0}([0,T]; H^{1}(\Omega)),$$

(1-u)\(\nabla v, \(\partial_{t}u, \(\partial_{t}v) \in L^{2}(0,T; H^{1}(\Omega)'), \)

and the weak formulation for all $\phi_1, \phi_2 \in L^2(0,T; H^2(\Omega))$,

$$\int_0^T \langle \partial_t v, \phi_1 \rangle dt + \int_0^T \langle (1-u) \nabla v, \nabla \phi_1 \rangle dt = \int_0^T \int_\Omega g(u, v) \phi_1 dx dt,$$
$$\int_0^T \langle \partial_t u, \phi_2 \rangle dt + \int_0^T \langle J, \nabla \phi_2 \rangle dt = \int_0^T \int_\Omega h(u, v) \phi_2 dx dt,$$

where $\langle \cdot, \cdot \rangle$ is the dual product between $H^1(\Omega)'$ and $H^1(\Omega)$ and $J = -\nabla(M(u)\Delta u) + M'(u)\nabla u + M(u)f''(u)\nabla u$ as well as $(1-u)\nabla v = \nabla((1-u)v) + v\nabla u$ are understood in the sense of $L^2(0,T; H^1(\Omega)')$.

The proof of Theorem 1 is based on a suitable approximation scheme, truncating the nonlinearities and using a Galerkin method similarly as in [13]. Uniform estimates are obtained from the energy and entropy equalities, proved in Lemma 7 for the sequence of approximate solutions,

(9)
$$\frac{d}{dt} \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + f(u) \right) dx + \int_{\Omega} M(u) |\nabla \mu|^2 dx = \int_{\Omega} h(u, v) \mu dx,$$

(10)
$$\frac{d}{dt} \int_{\Omega} \Phi(u) dx + \int_{\Omega} \left((\Delta u)^2 + f''(u) |\nabla u|^2 \right) dx = \int_{\Omega} h(u, v) \Phi'(u) dx$$

where Φ is defined by $\Phi''(u) = 1/M(u)$ and $\Phi(1/2) = \Phi'(1/2) = 0$. This function can be interpreted as the thermodynamic entropy of the system, since a computation shows that, with M(u) given by (6),

$$\Phi(u) = u \log u + (1 - u) \log(1 - u) + \log 2 \ge 0 \quad \text{for } 0 < u < 1.$$

Since $f''(u)|\nabla u|^2 \ge -2\lambda |\nabla u|^2$ for 0 < u < 1, the corresponding integral in (10) can be bounded by Gronwall's lemma and the energy bound (9).

The difficulty is to estimate the right-hand sides of (9)-(10). The term h(u, v) contains the factor u(1-u) which cancels the singularity from $\Phi'(u)$, such that $\int_{\Omega} h(u, v) \Phi'(u) dx$ is bounded. For the other integral, we include the definition of μ and integrate by parts:

$$\int_{\Omega} h(u,v)\mu dx = \int_{\Omega} \left((1-2u)|\nabla u|^2 + u(1-u)h'_0(v)\nabla v \cdot \nabla u + h(u,v)f'(u) \right) dx.$$

The last term is bounded since h(u, v) cancels the singularity of the potential f'(u). The first term can be treated by Gronwall's lemma since u is bounded. For the second term, we use Young's inequality:

$$\int_{\Omega} u(1-u)h'_0(v)\nabla v \cdot \nabla u dx \le C \int_{\Omega} |\nabla u|^2 dx + C \int_{\Omega} (1-u)|\nabla v|^2 dx,$$

where we use the property $0 \le v \le 1$. The last integral can be absorbed by the energy bound for v:

(11)
$$\frac{1}{2}\frac{d}{dt}\int_{\Omega}v^{2}dx + \int_{\Omega}(1-u)|\nabla v|^{2}dx = \int_{\Omega}g(u,v)vdx \le C.$$

There is another difficulty: Because of the degeneracy in the equation for v, we do not obtain an estimate for ∇v (see (11)) and therefore we cannot expect strong convergence for (a subsequence of) the approximate solutions (v_{δ}) with $\delta > 0$ being an approximation parameter, but only weak^{*} convergence in $L^{\infty}(\Omega_T)$. Surprisingly, the weak convergence of (v_{δ}) is enough to pass to the limit $\delta \to 0$ in $(1 - u_{\delta})\nabla v_{\delta}$, since this expression can be written as $\nabla((1 - u_{\delta})v_{\delta}) + v_{\delta}\nabla u_{\delta}$, which converges weakly in the sense of distributions, since (∇u_{δ}) converges strongly (up to a subsequence). However, the weak convergence is not sufficient to perform the limit in the reaction rates. The idea is to use the duality of $H^1(\Omega)'$ and $H^1(\Omega)$ as well as a Minty-Browder trick. Indeed, since h_0 is nondecreasing, we have for $y \in C_0^{\infty}(\Omega_T)$,

$$0 \leq \int_0^T \int_\Omega u_\delta (1 - u_\delta) (v_\delta - y) (h_0(v_\delta) - h(y)) dx dt$$
$$= \int_0^T \langle v_\delta - y, u_\delta (1 - u_\delta) (h_0(v_\delta) - h_0(y)) \rangle dt.$$

(Observe that we need to truncate the factor $u_{\delta}(1-u_{\delta})$, since we cannot expect that $0 \leq u_{\delta} \leq 1$; see Section 2.1.) By the Aubin–Lions lemma, $v_{\delta} \to v$ strongly in $L^2(0,T; H^1(\Omega))$ and $u_{\delta} \to u$ strongly in $L^2(0,T; H^1(\Omega))$. Hence, a computation shows that the limit $\delta \to 0$ in the previous inequality leads to

$$0 \le \int_0^T \left\langle v - y, u(1 - u)(h_1 - h(y)) \right\rangle dt,$$

where h_1 is the weak $L^2(\Omega_T)$ -limit of $(h_0(v_\delta))$. A Minty-Browder argument, made precise in Lemma 12, shows that $h_1 = h_0(v)$, implying that $h(u_\delta, v_\delta) \rightharpoonup h(u, v)$ weakly in $L^2(\Omega_T)$.

The paper is organized as follows. We formulate and prove the existence of a solution to a truncated regularized system in Section 2. We truncate the mobility and the mixing free energy using the parameter δ , add the regularization $\kappa > 0$ in the equation for v (because of the degeneracy), and introduce the Galerkin dimension $L \in \mathbb{N}$. First estimates allow us to perform the limit $L \to \infty$. Estimates uniform in (δ, κ) are derived from the energy and entropy inequalities in Section 3. In Section 4, we pass to the limit $\delta = \kappa \to 0$. Finally, we present some numerical experiments in one space dimension in Section 5 to compare our model with that one of [24].

2. Existence for the approximate system

2.1. Truncated regularized system. We truncate the functions M(u), f(u), and the source terms. Let $\delta > 0$ and set $[u]_{+} = \max\{0, u\}$ and $[u]_{+}^{1} = \min\{1, \max\{0, u\}\}$ for $u \in \mathbb{R}$. We introduce for $u \in \mathbb{R}$

$$M_{\delta}(u) = \begin{cases} M(\delta) & \text{if } u \leq \delta, \\ M(u) & \text{if } \delta < u < 1 - \delta, \\ M(1 - \delta) & \text{if } u \geq 1 - \delta. \end{cases}$$

Then $M_{\delta}(u) \geq M(u)$ for $u \in \mathbb{R}$. Furthermore, we set

$$D_+(u) = [1-u]^1_+.$$

We approximate the singular part $f_1(u) = N^{-1}u \log u + (1-u) \log(1-u)$ of the free energy by setting

$$\begin{aligned} f_{1,\delta}(u) &= f_1(u) & \text{if } \delta < u < 1 - \delta, \\ f_{1,\delta}(u) &= f_1(\delta) + f_1'(\delta)(u - \delta) + \frac{1}{2}f_1''(\delta)(u - \delta)^2 & \text{if } u \le \delta, \\ f_{1,\delta}(u) &= f_1(1 - \delta) + f_1'(1 - \delta)(u - (1 - \delta)) + \frac{1}{2}f_1''(1 - \delta)(u - (1 - \delta))^2 & \text{if } u \ge 1 - \delta. \end{aligned}$$

This means that

(12)
$$f_{1,\delta}''(u) = \begin{cases} f_1''(\delta) & \text{if } u \le \delta, \\ f_1''(u) & \text{if } \delta < u < 1 - \delta, \\ f_1''(1 - \delta) & \text{if } u \ge 1 - \delta. \end{cases}$$

The regular (nonvex) part $f_2(u) = \lambda u(1-u)$ $(0 \le u \le 1)$ of the free energy is extended to \mathbb{R} such that $|f_2(u)| \le C$ for $u \in \mathbb{R}$. Furthermore, we set $f_{\delta} = f_{1,\delta} + f_2$, and this function is defined for all $u \in \mathbb{R}$. We also need to truncate the source terms:

$$g_+(u,v) = -[u]_+^1 g_0([v]_+^1), \quad h_+(u,v) = [u]_+[1-u]_+h_0([v]_+^1).$$

Finally, let $\kappa > 0$. We wish to find a solution to the truncated and regularized system

(13)
$$\partial_t v - \operatorname{div}(D_+(u)\nabla v) - \kappa \Delta v = g_+(u,v)$$

(14)
$$\partial_t u - \operatorname{div}(M_\delta(u)\nabla\mu) = h_+(u,v),$$

(15)
$$\mu = -\Delta u + f'_{\delta}(u) \quad \text{in } \Omega, \ t > 0,$$

subject to the initial conditions (4) and the Neumann boundary conditions

(16)
$$\nabla v \cdot \nu = \nabla \mu \cdot \nu = \nabla u \cdot \nu = 0 \quad \text{on } \partial \Omega, \ t > 0.$$

2.2. Galerkin approximation. To solve (4), (13)–(16), we use the Galerkin method (as in [13]). Let $(\phi_{\ell})_{\ell \in \mathbb{N}}$ be the orthonormal eigenfunctions of the Laplace operator with homogeneous Neumann boundary conditions. We can assume that $\lambda_1 = 0$ and $\phi_1 = \text{const.}$ Let $L \in \mathbb{N}$. We wish to find solutions

$$v_L(x,t) = \sum_{\ell=1}^{L} A_\ell(t)\phi_\ell(x), \quad u_L(x,t) = \sum_{\ell=1}^{L} B_\ell(t)\phi_\ell(x), \quad \mu_L(x,t) = \sum_{\ell=1}^{L} C_\ell(t)\phi_\ell(x)$$

to the finite-dimensional system

(17)
$$\int_{\Omega} \partial_t v_L \phi dx = -\int_{\Omega} (D_+(u_L) + \kappa) \nabla v_L \cdot \nabla \phi dx + \int_{\Omega} g_+(u_L, v_L) \phi dx,$$

(18)
$$\int_{\Omega} \partial_t u_L \phi dx = -\int_{\Omega} M_{\delta}(u_L) \nabla \mu_L \cdot \nabla \phi dx + \int_{\Omega} h_+(u_L, v_L) \phi dx,$$

(19)
$$\int_{\Omega} \mu_L \phi dx = \int_{\Omega} \nabla u_L \cdot \nabla \phi dx + \int_{\Omega} f'_{\delta}(u_L) \phi dx$$

for all $\phi \in \text{span}(\phi_1, \ldots, \phi_L)$, with the initial conditions

$$v_L(0) = \sum_{\ell=1}^N (v^0, \phi_\ell)_{L^2(\Omega)} \phi_\ell dx, \quad u_L(0) = \sum_{\ell=1}^N (u^0, \phi_\ell)_{L^2(\Omega)} \phi_\ell dx.$$

This gives an initial-value problem for a system of ordinary differential equations for (A_1, \ldots, A_L) and (B_1, \ldots, B_N) :

$$\partial_t A_\ell = -\int_{\Omega} ([u_L]^1_+ + \kappa) \nabla v_L \cdot \nabla \phi_\ell dx + \int_{\Omega} g_+(u_L, v_L) \phi_\ell dx,$$

$$\partial_t B_\ell = -\int_{\Omega} M_\delta(u_L) \nabla \mu_L \cdot \nabla \phi_\ell dx + \int_{\Omega} h_+(u_L, v_L) \phi_\ell dx,$$

$$C_\ell = \int_{\Omega} \nabla u_L \cdot \nabla \phi_\ell dx + \int_{\Omega} f'_\delta(u_L) \phi_\ell dx \quad \text{for } \ell = 1, \dots, L,$$

with the initial conditions $A_{\ell}(0) = (v^0, \phi_{\ell})_{L^2(\Omega)}$ and $B_{\ell}(0) = (u^0, \phi_{\ell})_{L^2(\Omega)}$. As the righthand side of this system is continuous in (A_1, \ldots, A_L) and (B_1, \ldots, B_N) , the Peano theorem ensures the existence of a local solution. To extend this solution globally, we prove some a priori estimates.

Lemma 2 (Energy estimate for the Galerkin approximation). There exists a constant $C(\delta) > 0$ independent of L such that for all $t \in (0,T)$,

$$\frac{1}{2} \|\nabla u_L(t)\|_{L^2(\Omega)}^2 + \int_{\Omega} f_{\delta}(u_L(t)) dx + \frac{1}{2} M(\delta) \int_0^t \|\nabla \mu_L\|_{L^2(\Omega)}^2 ds \\
\leq \frac{1}{2} \|\nabla u_L(0)\|_{L^2(\Omega)}^2 + \int_{\Omega} f_{\delta}(u_L(0)) dx + C(\delta),$$

and because of Assumption (A2), the right-hand side can be bounded independently of L. Proof. We choose $\phi = \mu_L$ in (18) and $\phi = \partial_t u_L$ in (19):

$$\begin{split} \int_{\Omega} \partial_t u_L \mu_L dx &= -\int_{\Omega} M_{\delta}(u_L) |\nabla \mu_L|^2 dx + \int_{\Omega} h_+(u_L, v_L) \mu_L dx \\ &\leq -M(\delta) \int_{\Omega} |\nabla \mu_L|^2 dx + C \|\mu_L\|_{L^1(\Omega)}, \\ \int_{\Omega} \mu_L \partial_t u_L dx &= \int_{\Omega} \nabla u_L \cdot \nabla \partial_t u_L dx + \int_{\Omega} f_{\delta}'(u_L) \partial_t u_L dx \end{split}$$

C. HELMER AND A. JÜNGEL

$$= \frac{d}{dt} \left(\frac{1}{2} \int_{\Omega} |\nabla u_L|^2 dx + \int_{\Omega} f_{\delta}(u_L) dx \right),$$

since $|h_+(u_L, v_L)| \leq C$ because of our truncations. Here and in the following, C > 0 denotes a generic constant with values changing from line to line. Equating both expressions and integrating over (0, t) gives

(20)
$$\frac{1}{2} \int_{\Omega} \|\nabla u_L(t)\|_{L^2(\Omega)}^2 + \int_{\Omega} f_{\delta}(u_L(t)) dx \leq \frac{1}{2} \int_{\Omega} |\nabla u_L(0)|^2 dx + \int_{\Omega} f_{\delta}(u_L(0)) dx \\ - M(\delta) \int_0^t \int_{\Omega} |\nabla \mu_L|^2 dx ds + C \int_0^t \|\mu_L\|_{L^1(\Omega)} ds.$$

The choice $\phi_1 = \text{const.}$ in (19) shows that

$$\left|\int_{\Omega} \mu_L dx\right| \leq \int_{\Omega} |f_{\delta}'(u_L)| dx \leq C(\delta).$$

Set $\bar{\mu}_L = |\Omega|^{-1} \int_{\Omega} \mu_L dx$. By the Poincaré–Wirtinger inequality, the previous estimate provides a bound for the $L^2(\Omega)$ norm of μ_L :

$$\|\mu_L\|_{L^2(\Omega)} \le \|\mu_L - \bar{\mu}_L\|_{L^2(\Omega)} + \|\bar{\mu}_L\|_{L^2(\Omega)} \le C_P \|\nabla\mu_L\|_{L^2(\Omega)} + C(\delta).$$

Applying Young's inequality, we have

$$\int_0^t \|\mu_L\|_{L^1(\Omega)} ds \le C(\Omega) \int_0^t \|\mu_L\|_{L^2(\Omega)} ds \le \frac{1}{2} M(\delta) \int_0^t \|\nabla\mu_L\|_{L^2(\Omega)}^2 ds + C(\delta, \Omega, T).$$

Inserting this estimate into (20) finishes the proof.

Lemma 3 (Estimates for u_L and μ_L). There exists $C(\delta) > 0$ independent of L such that

$$\|u_L\|_{L^{\infty}(0,T;H^1(\Omega))} + \|\mu_L\|_{L^2(0,T;H^1(\Omega))} \le C(\delta).$$

Proof. The proof of Lemma 2 shows that $(\nabla \mu_L)$ and (μ_L) are bounded in $L^2(\Omega_T)$ and that (∇u_L) is bounded in $L^{\infty}(0,T;L^2(\Omega))$. We choose $\phi_1 = \text{const.}$ in (18):

$$\frac{d}{dt}\int_{\Omega}u_L dx = \int_{\Omega}h_+(u_L, v_L)dx \le C(\Omega).$$

Consequently, $\int_{\Omega} u_L(t) dx$ is uniformly bounded, at least on finite time intervals. This allows us to apply the Poincaré–Wirtinger inequality to deduce an $L^2(\Omega)$ bound for $u_L(t)$ uniformly in time.

We also need a priori estimates for the substrate concentration.

Lemma 4 (Estimates for v_L). There exists $C(v^0) > 0$ only depending on the initial datum v^0 such that

$$\|v_L\|_{L^{\infty}(0,T;L^2(\Omega))} + \|D_+(u_L)^{1/2}\nabla v_L\|_{L^2(\Omega_T)} + \kappa^{1/2}\|\nabla v^L\|_{L^2(\Omega_T)} \le C(v^0).$$

Proof. We choose the test function $\phi = v_L$ in (17) and take into account that $g_0(0) = 0$:

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega}v_{L}^{2}dx + \int_{\Omega}(D_{+}(u_{L}) + \kappa)|\nabla v_{L}|^{2}dx = -\int_{\Omega}[u_{L}]_{+}^{1}g_{0}([v_{L}]_{+}^{1})v_{L}dx \le 0.$$

An integration over (0, T) yields the result.

The uniform estimates for u_L in $L^{\infty}(0,T; H^1(\Omega))$ and v_L in $L^{\infty}(0,T; L^2(\Omega))$ show that the coefficients (A_ℓ) and (B_ℓ) are bounded in (0,T). Thus, we infer the global existence of solutions to the Galerkin system (17)–(19). To pass to the limit $L \to \infty$, we need an estimate for the time derivatives.

Lemma 5 (Estimates for the time derivatives). There exist $C_1(\delta) > 0$ depending on δ and $C_2 > 0$ independent of δ such that

$$\|\partial_t u_L\|_{L^2(0,T;H^1(\Omega)')} \le C_1(\delta), \quad \|\partial_t v_L\|_{L^2(0,T;H^1(\Omega)')} \le C_2.$$

Proof. Let $\psi \in L^2(0,T; H^1(\Omega))$ and let $\Pi_L \psi$ be the projection of ψ on span (ϕ_1, \ldots, ϕ_L) . We infer from (17) and the bounds of Lemma 4 that

$$\begin{split} \left| \int_{0}^{T} \int_{\Omega} \partial_{t} v_{L} \psi dx dt \right| &= \left| \int_{0}^{T} \int_{\Omega} \partial_{t} v_{L} \Pi_{L} \psi dx dt \right| \\ &\leq \int_{0}^{T} \| D_{+} (u_{L})^{1/2} \|_{L^{\infty}(\Omega)} \| D_{+} (u_{L})^{1/2} \nabla v_{L} \|_{L^{2}(\Omega)} \| \nabla \Pi_{L} \psi \|_{L^{2}(\Omega)} dt \\ &+ \int_{0}^{t} \| g_{+} (u_{L}, v_{L}) \|_{L^{2}(\Omega)} \| \Pi_{L} \psi \|_{L^{2}(\Omega)} dt \leq C_{2} \| \psi \|_{L^{2}(0,T;H^{1}(\Omega))}. \end{split}$$

Furthermore, using $M_{\delta}(u_L) \leq C_M$ and the bounds of Lemma 3,

$$\left| \int_0^T \int_\Omega \partial_t u_L \psi dx dt \right| = \left| \int_0^T \int_\Omega \partial_t u_L \Pi_L \psi dx dt \right|$$

$$\leq C_M \int_0^T \|\nabla \mu_L\|_{L^2(\Omega)} \|\nabla \Pi_L \psi\|_{L^2(\Omega)} dt$$

$$+ \int_0^T \|h_+(u_L, v_L)\|_{L^2(\Omega)} \|\Pi_L \psi\|_{L^2(\Omega)} dt \leq C_1(\delta) \|\psi\|_{L^2(0,T;H^1(\Omega))}.$$

This concludes the proof.

The estimates of Lemmas 3–5 allow us to apply the Aubin–Lions lemma [22, Corollary 4] to find subsequences (not relabeled) such that, as $L \to \infty$,

$$u_L \to u, \quad v_L \to v \quad \text{strongly in } L^2(\Omega_T),$$

 $u_L \to u, \quad v_L \to v, \quad \mu_L \to \mu \quad \text{weakly in } L^2(0,T;H^1(\Omega)),$
 $\partial_t u_L \to \partial_t u, \quad \partial_t v_L \to \partial_t v \quad \text{weakly in } L^2(0,T;H^1(\Omega)').$

Since M_{δ} , D_+ , f'_{δ} , g_+ , and h_+ are bounded functions, we have

 $M_{\delta}(u_L) \to M_{\delta}(u), \quad D_+(u_L) \to D_+(u), \quad f'_{\delta}(u_L) \to f'_{\delta}(u),$

C. HELMER AND A. JÜNGEL

$$h_+(u_L, v_L) \to h_+(u, v), \quad g_+(u_L, v_L) \to g_+(u, v) \quad \text{strongly in } L^2(\Omega_T).$$

Thus, we can perform the limit $L \to \infty$ in the Galerkin system (17)–(19), which yields the existence of a solution (u, v, μ) to

(21)
$$\int_{0}^{t} \langle \partial_{t} u, \phi_{1} \rangle ds = -\int_{0}^{t} \int_{\Omega} M_{\delta}(u) \nabla \mu \cdot \nabla \phi_{1} dx ds + \int_{0}^{t} \int_{\Omega} h_{+}(u, v) \phi_{1} dx ds,$$

(22)
$$\int_{0}^{t} \langle \partial_{t} v, \phi_{2} \rangle ds = -\int_{0}^{t} \int_{\Omega} (D_{+}(u) + \kappa) \nabla v \cdot \nabla \phi_{2} dx ds + \int_{0}^{t} \int_{\Omega} g_{+}(u, v) \phi_{2} dx ds,$$

(23)
$$\int_0^t \int_{\Omega} \mu \phi_3 dx ds = \int_0^t \int_{\Omega} \nabla u \cdot \nabla \phi_3 dx ds + \int_0^t \int_{\Omega} f_{\delta}'(u) \phi_3 dx ds$$

for all $\phi_i \in L^2(0,T; H^1(\Omega))$, i = 1, 2, 3, and all 0 < t < T, recalling that $\langle \cdot, \cdot \rangle$ is the dual product between $H^1(\Omega)'$ and $H^1(\Omega)$.

3. UNIFORM ESTIMATES

We need some estimates uniform in δ and κ as well as lower and upper bounds to remove the truncation.

Lemma 6 (Uniform estimates for v). There exists $C(v^0) > 0$ only depending on v^0 such that

$$\|v\|_{L^{\infty}(0,T;L^{2}(\Omega))} + \|D_{+}(u)^{1/2}\nabla v\|_{L^{2}(\Omega_{T})} + \kappa^{1/2}\|\nabla v\|_{L^{2}(\Omega_{T})} \leq C(v^{0}).$$

Furthermore, it holds that $0 \leq v(t) \leq 1$ in Ω for $0 < t < T$.

Because of the lower and upper bounds for v, we can remove the truncation in $g_+(u,v) = -[u]_+^1 g_0(v)$ and $h_+(u,v) = [u]_+[1-u]_+h_0(v)$.

Proof. We start with the lower and upper bounds for v. We use the test function $[v]_{-} = \min\{0, v\}$ in (22) and use the assumption $v(0) \ge 0$ in Ω :

$$\int_{\Omega} [v(t)]_{-}^{2} dx + \int_{0}^{t} \int_{\Omega} (D_{+}(u) + \kappa) |\nabla[v]_{-}|^{2} dx ds = \int_{0}^{t} \int_{\Omega} g_{+}(u, v) [v]_{-} dx ds = 0,$$

since $g_0(0) = 0$ implies that $g_+(u, v)[v]_- = -[u]_+^1 g_0(0)[v]_- = 0$. This implies that $v(t) \ge 0$ in Ω , t > 0. The property $v(t) \le 1$ is proved in a similar way using the test function $[v-1]_+$ and the fact that $g_+(u, v)[v-1]_+ = -[u]_+^1 g_0(1)[v-1]_+ \le 0$. The remaining estimates can be shown as in Lemma 4.

Next, we show some uniform estimates for u. For this, we introduce the entropy density

(24)
$$\Phi_{\delta}(u) = \int_{1/2}^{u} \int_{1/2}^{s} \frac{drds}{M_{\delta}(r)} \ge 0.$$

Lemma 7 (Energy and entropy estimates). There exists C(T) > 0 independent of δ and κ such that for all t > 0 and all sufficiently small $\delta > 0$,

(25)
$$\sup_{0 < t < T} \int_{\Omega} \left(\frac{1}{2} |\nabla u(t)|^2 dx + f_{\delta}(u(t)) \right) dx + \int_0^T \int_{\Omega} M_{\delta}(u) |\nabla \mu|^2 dx ds \le C(T),$$

A DIFFUSION SYSTEM FOR BIOFILM GROWTH

(26)
$$\sup_{0 < t < T} \int_{\Omega} \Phi_{\delta}(u(t)) dx + \int_{0}^{T} \int_{\Omega} (\Delta u)^{2} dx ds \leq C(T).$$

Since f_{δ} is bounded from below (by construction), the energy inequality provides uniform bounds for u.

Proof. We first prove the energy inequality and then the entropy inequality.

Step 1: Energy inequality. We know from Section 2.2 that $u \in L^{\infty}(0, T; H^{1}(\Omega))$ and $\mu \in L^{2}(0, T; H^{1}(\Omega))$. Then we infer from the boundedness of f'_{δ} that $\Delta u = f'_{\delta}(u) - \mu \in L^{2}(0, T; L^{2}(\Omega))$. By elliptic regularity theory, $u \in L^{2}(0, T; H^{2}(\Omega))$. Moreover, $\nabla \Delta u = f''_{\delta}(u) \nabla u - \nabla \mu \in L^{2}(\Omega_{T})$, which implies that $u \in L^{2}(0, T; H^{3}(\Omega))$ (this regularity is not uniform in (δ, κ)). Consequently, $\Delta u \in L^{2}(0, T; H^{1}(\Omega))$ and

$$0 = \int_0^t \langle \partial_t u, \mu + \Delta u - f_{\delta}'(u) \rangle ds$$

=
$$\int_0^t \langle \partial_t u, \mu \rangle ds - \frac{1}{2} \int_{\Omega} (|\nabla u(t)|^2 - |\nabla u(0)|^2) ds - \int_{\Omega} (f_{\delta}(u(t)) - f_{\delta}(u(0)) ds.$$

On the other hand, we use $\phi_2 = \mu \in L^2(0, T; H^1(\Omega))$ as a test function in (21):

$$\int_0^t \langle \partial_t u, \mu \rangle ds + \int_0^t \int_\Omega M_\delta(u) |\nabla \mu|^2 dx ds = \int_0^t \int_\Omega h_+(u, v) \mu dx.$$

This shows that, using the definition of μ ,

$$(27) \qquad \frac{1}{2} \int_{\Omega} |\nabla u(t)|^2 dx + \int_{\Omega} f_{\delta}(u(t)) dx + \int_0^t \int_{\Omega} M_{\delta}(u) |\nabla \mu|^2 dx ds = \frac{1}{2} \int_{\Omega} |\nabla u^0|^2 dx + \int_{\Omega} f_{\delta}(u^0) dx + \int_0^t \int_{\Omega} \nabla h_+(u,v) \cdot \nabla u dx ds + \int_0^t \int_{\Omega} h_+(u,v) f_{\delta}'(u) dx ds.$$

It remains to estimate the last two integrals. For the last but one integral, we insert the definition of $h_+(u, v)$ and apply Young's inequality:

$$\begin{split} \int_0^t \int_\Omega \nabla h_+(u,v) \cdot \nabla u dx ds \\ &= \int_0^t \int_\Omega \mathbf{1}_{\{0 < u < 1\}} \big((1-2u)h_0(v) |\nabla u|^2 + u(1-u)h_0'(v)\nabla v \cdot \nabla u \big) dx ds \\ &\leq C \int_0^t \int_\Omega |\nabla u|^2 dx ds + C \int_0^t \int_\Omega \mathbf{1}_{\{0 < u < 1\}} (1-u) |\nabla v|^2 dx ds \\ &\leq C \int_0^t \int_\Omega |\nabla u|^2 dx ds + C, \end{split}$$

where the last step follows from Lemma 6, and C > 0 denotes here and in the following a constant independent of δ and κ .

For the last integral in (27), we observe that the function $s \mapsto -s(1-s)(N^{-1}\log s - \log(1-s) + N^{-1} - 1)$ is bounded in [0, 1]. We insert the definition of $f'_{\delta}(u)$ and distinguish

three cases. First, let $u \leq \delta$. Then

$$\begin{aligned} h_{+}(u,v)f_{\delta}'(u) &= [u]_{+}[1-u]_{+}\left(f_{\delta}'(\delta) + f_{1}''(\delta)(u-\delta) + \lambda(1-2u)\right) \\ &= [u]_{+}[1-u]_{+}\left(\frac{1}{N}\log\delta - \log(1-\delta) + \frac{1}{N} - 1\right) \\ &+ [u]_{+}[1-u]_{+}(u-\delta)\left(\frac{1}{N\delta} + \frac{1}{1-\delta}\right) + \lambda[u]_{+}[1-u]_{+}(1-2u) \\ &\leq \delta(1-\delta)\left(|\log(1-\delta)| + \frac{1}{N}\right) + \lambda\delta(1-\delta) \leq C, \end{aligned}$$

using $[u]_+[1-u]_+ \leq \delta(1-\delta)$ and $u-\delta \leq 0$. Second, let $\delta < u < 1-\delta$. We have

$$h_{+}(u,v)f_{\delta}'(u) = u(1-u)\left(\frac{1}{N}\log u - \log(1-u) + \frac{1}{N} - 1\right) + \lambda u(1-u)(1-2u) \le C,$$

since $z \mapsto z \log z$ is bounded in [0, 1]. Finally, let $u \ge 1 - \delta$ (and $\delta \le 1/2$). We obtain

$$\begin{aligned} h_{+}(u,v)f_{\delta}'(u) &= [u]_{+}[1-u]_{+}\left(\frac{1}{N}\log(1-\delta) - \log\delta + \frac{1}{N} - 1\right) \\ &+ [u]_{+}[1-u]_{+}(u-\delta)\left(\frac{1}{N(1-\delta)} + \frac{1}{\delta}\right) + \lambda[u]_{+}[1-u]_{+}(1-2u) \\ &\leq \delta(1-\delta)\left(|\log\delta| + \frac{1}{N}\right) + (1-\delta)\delta(1-2\delta)\left(\frac{1}{N(1-\delta)} + \frac{1}{\delta}\right) + \lambda \leq C. \end{aligned}$$

This proves that, for 0 < t < T,

$$\int_0^t \int_{\Omega} h_+(u,v) f'_{\delta}(u) dx ds \le C(\Omega,T).$$

Therefore, we infer from (27) that

$$\frac{1}{2} \int_{\Omega} |\nabla u(t)|^2 dx + \int_{\Omega} f_{\delta}(u(t)) dx + \int_0^t \int_{\Omega} M_{\delta}(u) |\nabla \mu|^2 dx ds$$
$$= \frac{1}{2} \int_{\Omega} |\nabla u^0|^2 dx + \int_{\Omega} f_{\delta}(u^0) dx + C \int_0^t \int_{\Omega} |\nabla u|^2 dx ds + C.$$

Since u^0 is strictly positive and bounded away from one, there exists $\delta_0 > 0$ such that $f_{\delta}(u^0) = f(u^0)$ for $0 < \delta \leq \delta_0$. An application of Gronwall's lemma shows (25).

Step 2: Entropy inequality. Because of the truncation, we have $\nabla \Phi'_{\delta}(u) = \nabla u/M_{\delta}(u) \in L^2(\Omega_T)$, where Φ_{δ} is defined in (24). Thus, we can use $\phi_1 = \Phi'_{\delta}(u)$ as a test function in (21):

(28)
$$\int_{\Omega} \Phi_{\delta}(u(t)) dx - \int_{\Omega} \Phi_{\delta}(u(0)) dx = \int_{0}^{t} \langle \partial_{t}u, \Phi_{\delta}'(u) \rangle ds$$
$$= -\int_{0}^{t} \int_{\Omega} M_{\delta}(u) \nabla \mu \cdot \nabla \Phi_{\delta}'(u) dx ds + \int_{0}^{t} \int_{\Omega} h_{+}(u, v) \Phi_{\delta}'(u) dx ds$$

$$\leq -\int_0^t \int_{\Omega} \nabla(-\Delta u + f_{\delta}'(u)) \cdot \nabla u dx ds + \int_0^t \int_{\Omega} [u]_+ [1-u]_+ h_0(v) \Phi_{\delta}'(u) dx ds.$$

The first integral on the right-hand side can be written as

$$-\int_0^t \int_\Omega \nabla(-\Delta u + f_\delta'(u)) \cdot \nabla u dx ds = -\int_0^t \int_\Omega (\Delta u)^2 dx ds - \int_0^t \int_\Omega f_\delta''(u) |\nabla u|^2 dx ds.$$

Because of $f_{1,\delta}''(u) \ge 0$ by (12) and $f_2''(u) \ge -C$, we obtain

$$-\int_0^t \int_{\Omega} \nabla (-\Delta u + f_{\delta}'(u)) \cdot \nabla u dx ds \leq -\int_0^t \int_{\Omega} (\Delta u)^2 dx ds + C \int_0^t \int_{\Omega} |\nabla u|^2 dx ds.$$

We claim that the integrand of the last integral in (28) is bounded, i.e. $[u]_+[1-u]_+\Phi'_{\delta}(u)$ is bounded uniformly in $u \in [0, 1]$ and $\delta \in (0, 1/2)$. Indeed, if $\delta \leq u \leq 1 - \delta$, we can compute

$$|[u]_{+}[1-u]_{+}\Phi_{\delta}'(u)| = \left|u(1-u)\int_{1/2}^{u} \frac{ds}{s(1-s)}\right| = \left|u(1-u)\log\frac{u}{1-u}\right| \le 1.$$

If $0 < u < \delta$, we find that

$$\begin{split} |[u]_{+}[1-u]_{+}\Phi_{\delta}'(u)| &= \left| u(1-u) \left(\int_{1/2}^{\delta} \frac{ds}{s(1-s)} + \int_{\delta}^{u} \frac{ds}{\delta(1-\delta)} \right) \right| \\ &= u(1-u) \log \frac{\delta}{1-\delta} + u(1-u) \frac{\delta-u}{\delta(1-\delta)}. \end{split}$$

The first term is uniformly bounded since $|u \log \delta| \le |\delta \log \delta| \le 1$ and $|(1-u) \log(1-\delta)| \le 1$. This holds also true for the second term because of $u(1-u) < \delta(1-\delta)$. The final case $1-\delta < u < 1$ is treated in a similar way:

$$\begin{split} |[u]_{+}[1-u]_{+}\Phi_{\delta}'(u)| &= \left| u(1-u) \left(\int_{1/2}^{1-\delta} \frac{ds}{s(1-s)} + \int_{1-\delta}^{u} \frac{ds}{\delta(1-\delta)} \right) \right| \\ &= u(1-u) \log \frac{1-\delta}{\delta} + u(1-u) \frac{u-(1-\delta)}{\delta(1-\delta)}. \end{split}$$

The first term is uniformly bounded since $|(1-u)\log \delta| \le |\delta \log \delta| \le 1$ and $|u \log(1-\delta)| \le 1$, and the second term is bounded too. We conclude from (28) that

$$\int_{\Omega} \Phi_{\delta}(u(t))dx + \int_{0}^{t} \int_{\Omega} (\Delta u)^{2} dx ds \leq \int_{\Omega} \Phi_{\delta}(u^{0})dx + C \int_{0}^{t} \int_{\Omega} |\nabla u|^{2} dx ds,$$

and the energy bound (25) leads to (26).

Finally, we derive a bound for the time derivatives of u and v.

Lemma 8 (Bounds for the time derivatives). There exists C > 0 independent of δ and κ such that

$$\|\partial_t u\|_{L^2(0,T;H^1(\Omega)')} + \|\partial_t v\|_{L^2(0,T;H^1(\Omega)')} \le C.$$

Proof. The proof is similar to that one of Lemma 5; we just have to estimate the reaction terms. Since $0 \le v \le 1$, we have the pointwise bounds $g_+(u,v) = -[u]_+^1 g_0(v) \le \max_{0 \le v \le 1} g_0(v)$ and $h_+(u,v) = [u]_+[1-u]_+h_0(v) \le \max_{0 \le v \le 1} h_0(v)$. Consequently, $||g_+(u,v)||_{L^2(\Omega_T)}$ and $||h_+(u,v)||_{L^2(\Omega_T)}$ are uniformly bounded, concluding the proof.

4. The limit
$$(\delta, \kappa) \to 0$$

Set $\kappa = \delta$ and let $(u_{\delta}, v_{\delta}, \mu_{\delta})$ be a weak solution to (21)–(23). Lemmas 6–8 give the following uniform bounds:

$$0 \le v_{\delta} \le 1 \quad \text{in } \Omega_{T},$$

$$\|D_{+}(u_{\delta})^{1/2} \nabla v_{\delta}\|_{L^{2}(\Omega_{T})} + \delta^{1/2} \|v_{\delta}\|_{L^{2}(0,T;H^{1}(\Omega))} + \|\partial_{t}v_{\delta}\|_{L^{2}(0,T;H^{1}(\Omega)')} \le C,$$

$$\|u_{\delta}\|_{L^{\infty}(0,T;H^{1}(\Omega))} + \|u_{\delta}\|_{L^{2}(0,T;H^{2}(\Omega))} + \|\partial_{t}u_{\delta}\|_{L^{2}(0,T;H^{1}(\Omega)')} \le C,$$

$$\|M_{\delta}(u_{\delta})^{1/2} \nabla \mu_{\delta}\|_{L^{2}(\Omega_{T})} \le C.$$

The Aubin–Lions lemma [22, Corollary 4] implies the existence of a subsequence, which is not relabeled, such that, as $\delta \to 0$,

$$u_{\delta} \to u$$
 strongly in $L^2(0,T; H^1(\Omega))$ and $C^0([0,T]; L^2(\Omega))$.

We also have the weak convergences

$$v_{\delta} \rightarrow v \quad \text{weakly* in } L^{\infty}(0,T;L^{\infty}(\Omega)),$$

$$\partial_{t}u_{\delta} \rightarrow \partial_{t}u, \quad \partial_{t}v_{\delta} \rightarrow \partial_{t}v \quad \text{weakly in } L^{2}(0,T;H^{1}(\Omega)'),$$

$$D_{+}(u_{\delta})\nabla v_{\delta} \rightarrow I, \quad M_{\delta}(u_{\delta})^{1/2}\nabla \mu_{\delta} \rightarrow J \quad \text{weakly in } L^{2}(\Omega_{T}),$$

where $I, J \in L^2(\Omega_T)$, and it holds that $\delta \nabla v_{\delta} \to 0$ strongly in $L^2(\Omega_T)$. Before we identify the limits I and J, we show that the limit u is bounded from below and above.

Lemma 9 (L^{∞} bounds for u). It holds that $0 \le u \le 1$ in Ω_T .

Proof. We proceed as in the proofs of [13, Lemma 2] or [21, Theorem 5]. Let $\alpha > 0$ and introduce the set $V_{\alpha,\delta} = \{(x,t) \in \Omega_T : u_{\delta}(x,t) \ge 1 + \alpha\}$. Integrating $\Phi''_{\delta}(u_{\delta}(x,t)) = 1/M_{\delta}(1-\delta) = 1/(\delta(1-\delta))$ for $(x,t) \in V_{\alpha,\delta}$ twice gives

$$\Phi_{\delta}(u_{\delta}(x,t)) = \int_{1/2}^{u_{\delta}(x,t)} \int_{1/2}^{s} \frac{drds}{M_{\delta}(r)} = \frac{(u_{\delta} - 1/2)^{2}}{2\delta(1-\delta)} \quad \text{for } (x,t) \in V_{\alpha,\delta}.$$

The entropy estimate (26) shows that

$$\frac{\alpha^2 |V_{\alpha,\delta}|}{2\delta(1-\delta)} \le \int_{V_{\alpha,\delta}} \frac{(u_\delta - 1/2)^2}{2\delta(1-\delta)} d(x,t) = \int_{V_{\alpha,\delta}} \Phi_\delta(u_\delta) d(x,t) \le C(T).$$

Then we deduce from the a.e. pointwise limit $u_{\delta}(x,t) \to u(x,t)$ as $\delta \to 0$ and Fatou's lemma that

$$|\{u(x,t) \ge 1+\alpha\}| = \lim_{\delta \to 0} |V_{\alpha,\delta}| \le \lim_{\delta \to 0} \frac{2C(T)}{\alpha^2} \delta(1-\delta) = 0,$$

implying that $u(x,t) \leq 1 + \alpha$ a.e. in Ω_T for all $\alpha > 0$. Therefore, $u(x,t) \leq 1$ in Ω_T .

A similar argument proves that $u \ge 0$ in Ω_T . Indeed, let $W_{\alpha,\delta} = \{(x,t) : u_{\delta}(x,t) \le -\alpha\}$ for $\alpha > 0$. It follows from $\Phi_{\delta}''(u_{\delta}(x,t)) = 1/\delta(1-\delta)$ for $(x,t) \in W_{\alpha,\delta}$ that $\Phi_{\delta}(u_{\delta}(x,t)) \le (1/2 - u_{\delta}(x,t))^2/(2\delta(1-\delta))$. Hence,

$$\frac{\alpha^2 |W_{\alpha,\delta}|}{2\delta(1-\delta)} \le \int_{W_{\alpha,\delta}} \frac{(1/2 - u_{\delta})^2}{2\delta(1-\delta)} d(x,t) = \int_{W_{\alpha,\delta}} \Phi_{\delta}(u_{\delta}) d(x,t) \le C(T)$$

and proceeding as before gives $|\{u(x,t) \leq -\alpha\}| = 0$ in the limit $\delta \to 0$ for all $\alpha > 0$ and therefore $u \geq 0$ in Ω_T .

We continue by identifying I. We conclude from $[1-u_{\delta}]^1_+v_{\delta} \rightharpoonup (1-u)v$ and $v_{\delta}\nabla u_{\delta} \rightharpoonup v\nabla u$ weakly in $L^2(\Omega_T)$ that

$$D_+(u_{\delta})\nabla v_{\delta} = \nabla([1-u_{\delta}]^1_+v_{\delta}) + v_{\delta}1_{\{0 < u_{\delta} < 1\}}\nabla u_{\delta} \rightarrow \nabla((1-u)v) + v\nabla u = (1-u)\nabla v$$

weakly in $L^2(0,T; H^1(\Omega)')$. This shows that $I = (1-u)\nabla v$ in $L^2(0,T; H^1(\Omega)')$.

Lemma 10 (Identification of J). It holds that $J = -\nabla(M(u)\Delta u) + \nabla M(u)\Delta u + M(u)\nabla f'(u)$ in the sense of $L^2(0,T; H^1(\Omega)')$.

Proof. We proceed as in [13, Section 3]. It holds for $\phi \in C_0^{\infty}(\Omega_T)$ that

$$\int_{0}^{T} \int_{\Omega} M_{\delta}(u_{\delta}) \nabla \mu_{\delta} \cdot \nabla \phi dx dt = \int_{0}^{T} \int_{\Omega} M_{\delta}(u_{\delta}) \nabla \left(-\Delta u_{\delta} + f_{\delta}'(u_{\delta}) \right) \cdot \nabla \phi dx dt$$
$$= \int_{0}^{T} \int_{\Omega} M_{\delta}(u_{\delta}) \Delta u_{\delta} \Delta \phi dx dt + \int_{0}^{T} \int_{\Omega} M_{\delta}'(u_{\delta}) \Delta u_{\delta} \nabla u_{\delta} \cdot \nabla \phi dx dt$$
$$+ \int_{0}^{T} \int_{\Omega} M_{\delta}(u_{\delta}) f_{\delta}''(u_{\delta}) \nabla u_{\delta} \cdot \nabla \phi dx dt =: J_{1} + J_{2} + J_{3}.$$

First, we consider J_1 . We observe that $M_{\delta} \to M$ uniformly, since by the mean-value theorem,

$$|M_{\delta}(z) - M(z)| \leq \sup_{0 < z < \delta} |M(\delta) - M(z)| + \sup_{1 - \delta < z < 1} |M(1 - \delta) - M(z)|$$
$$\leq M'(\xi_{\delta})\delta + M'(\eta_{\delta})\delta \to 0,$$

where $\xi_{\delta} \in (z, \delta)$ and $\eta_{\delta} \in (1 - \delta, z)$. This implies that $M_{\delta}(u_{\delta}) \to M(u)$ a.e. in Ω_T and, as M_{δ} is uniformly bounded, also strongly in $L^2(\Omega_T)$. Together with the convergence $\Delta u_{\delta} \rightharpoonup \Delta u$ weakly in $L^2(\Omega_T)$, we find that

$$J_1 \to \int_0^T \int_\Omega M(u) \Delta u \Delta \phi dx dt.$$

For the integral J_2 , we claim that $M'_{\delta}(u_{\delta})\nabla u_{\delta} \to M'(u)\nabla u$ strongly in $L^2(\Omega_T)$. This limit is not trivial since M'_{δ} is discontinuous at δ and $1 - \delta$. We consider the integrals

$$\int_0^T \int_\Omega |M'_\delta(u_\delta)\nabla u_\delta - M'(u)\nabla u|^2 dx dt = \int_0^T \int_{\{0 < u < 1\}} |M'_\delta(u_\delta)\nabla u_\delta - M'(u)\nabla u|^2 dx dt$$

$$+\int_0^T\int_{\{u=0\}}|M_{\delta}'(u_{\delta})\nabla u_{\delta}-M'(u)\nabla u|^2dxdt+\int_0^T\int_{\{u=1\}}|M_{\delta}'(u_{\delta})\nabla u_{\delta}-M'(u)\nabla u|^2dxdt.$$

On the set $\{0 < u < 1\}$, we know that $M'_{\delta}(u_{\delta}) \to M'(u)$ a.e. in Ω_T and, because of the strong convergence of (∇u_{δ}) , also $M'_{\delta}(u_{\delta})\nabla u_{\delta} \to M'(u)\nabla u$ a.e. in Ω_T (possibly for a subsequence). Moreover, $|M'_{\delta}(u_{\delta})\nabla u_{\delta}|^2$ is uniformly bounded on $\{0 < u < 1\}$. Therefore, by dominated convergence,

$$\int_0^T \int_{\{0 < u < 1\}} |M'_{\delta}(u_{\delta})\nabla u_{\delta} - M'(u)\nabla u|^2 dx dt \to 0.$$

It follows from $\nabla u = 0$ on $\{u = 0\} \cup \{u = 1\}$ and the uniform bound for M'_{δ} that

$$\int_{0}^{T} \int_{\{u=0\}} |M_{\delta}'(u_{\delta})\nabla u_{\delta} - M'(u)\nabla u|^{2} dx dt = \int_{0}^{T} \int_{\{u=0\}} |M_{\delta}'(u_{\delta})\nabla u_{\delta}|^{2} dx dt$$
$$\leq C \int_{0}^{T} \int_{\{u=0\}} |\nabla u_{\delta}|^{2} dx dt \to \int_{0}^{T} \int_{\{u=0\}} |\nabla u|^{2} dx dt = 0.$$

The limit in the remaining integral over $\{u = 1\}$ vanishes in the same way. This shows that

$$J_2 \to \int_0^T \int_{\Omega} M'(u) \Delta u \nabla u \cdot \nabla \phi dx dt.$$

Finally, for the limit in J_3 , we observe that $M_{\delta}(z)f_{\delta}''(z) = M_{\delta}(z)(f_{1,\delta}''(z) + f_2''(z))$ is uniformly bounded, since the singularities as $\delta \to 0$ in $f_{1,\delta}''$ are canceled by the factor $M_{\delta}(z)$. Thus, it remains to show that $M_{\delta}(u_{\delta})f_{\delta}''(u_{\delta}) \to M(u)f''(u)$ in $\Omega_T \setminus N$, where N is a set of measure zero. To this end, we distinguish several cases.

Let $(x,t) \in \Omega_T \setminus N$ and 0 < u(x,t) < 1. For given $\varepsilon > 0$, there exists $0 < \delta < \varepsilon$ such that $\delta < \varepsilon \leq u_{\delta}(x,t) \leq 1 - \varepsilon < 1 - \delta$. At this point, we have $M_{\delta}(u_{\delta}(x,t))f''_{\delta}(u_{\delta}(x,t)) = M(u_{\delta}(x,t))f''(u_{\delta}(x,t)) \to M(u(x,t))f''(u(x,t))$. Next, if u(x,t) = 1, we choose $\delta > 0$ such that $u_{\delta}(x,t) \geq 1 - \delta$. Then

$$M_{\delta}(u_{\delta}(x,t))f_{\delta}''(u_{\delta}(x,t)) = M(\delta)(f_{1}''(\delta) + f_{2}(u_{\delta}))$$

= $N^{-1}\delta + (1-\delta) + \delta(1-\delta)f_{2}(u_{\delta}) \to 1 = (Mf'')(1).$

On the other hand, if $u_{\delta}(x,t) < 1 - \delta$ and $u_{\delta}(x,t) \rightarrow 1$,

$$M_{\delta}(u_{\delta}(x,t))f_{\delta}''(u_{\delta}(x,t)) = M(u_{\delta}(x,t))f''(u_{\delta}(x,t))$$

= $N^{-1}(1 - u_{\delta}(x,t)) + u_{\delta}(x,t) + u_{\delta}(1 - u_{\delta})f_{0}''u_{\delta} \to 1 = (Mf'')(1).$

The case u(x,t) = 0 is treated in a similar way. We conclude that $M_{\delta}(u_{\delta})f_{\delta}''(u_{\delta}) \rightarrow M(u)f''(u)$ strongly in $L^{2}(\Omega_{T})$. Then, in view of the strong convergence of (∇u_{δ}) ,

$$J_3 \to \int_0^T \int_\Omega M(u) f''(u) \nabla u \cdot \nabla \phi dx dt.$$

Summarizing, we have shown that

$$\int_0^T \int_\Omega M_\delta(u_\delta) \nabla \mu_\delta \cdot \nabla \phi dx dt \to \int_0^T \int_\Omega \left(M(u) \Delta u \Delta \phi + M'(u) \Delta u \nabla u \cdot \nabla \phi \right) \\ + M(u) f''(u) \nabla u \cdot \nabla \phi \right) dx dt,$$

and the right-hand side can be identified as the weak formulation of J.

Remark 11. Choosing the mobility such that $\Phi(0) = \Phi(1) = \infty$, one can show that $\{u = 0\} \cup \{u = 1\}$ has measure zero, which means that 0 < u < 1 holds a.e. in Ω_T , and we can write $J = M(u)\nabla(-\Delta u + f'(u))$ in the sense of distributions. The claim that $\{u = 0\} \cup \{u = 1\}$ has measure zero can be proved as in [13, Corollary]. It follows from the entropy bound $\int_{\Omega} \Phi_{\delta}(u_{\delta}(t))dx \leq C(T)$ and the fact that $\liminf_{\delta \to 0} \Phi_{\delta}(u_{\delta}) = \Phi(u)$ if 0 < u < 1 and $\liminf_{\delta \to 0} \Phi_{\delta}(u_{\delta}) = \infty$ else.

It remains to pass to the limit $\delta \to 0$ in the reaction terms. Since (v_{δ}) is only converging weakly, this limit is not trivial. The idea is to use the Browder–Minty trick, which is possible since (u_{δ}) converges strongly in $L^2(0, T; H^1(\Omega))$.

Lemma 12. It holds that $g_+(u_{\delta}, v_{\delta}) \rightharpoonup g(u, v)$ and $h_+(u_{\delta}, v_{\delta}) \rightharpoonup h(u, v)$ weakly in $L^2(\Omega_T)$ as $\delta \to 0$.

Proof. We only show the limit in $h_+(u_{\delta}, v_{\delta})$ as the proof in $g_+(u_{\delta}, v_{\delta})$ is similar. We know that $(\partial_t v_{\delta})$ is bounded in $L^2(0, T; H^1(\Omega)')$ and (v_{δ}) is bounded in $L^2(\Omega_T)$. Since the embedding $L^2(\Omega) \hookrightarrow H^1(\Omega)'$ is compact, we infer from the Aubin–Lions lemma that, up to a subsequence, $v_{\delta} \to v$ strongly in $L^2(0, T; H^1(\Omega)')$. Moreover, $([1 - u_{\delta}]^{1/2}_+ \nabla v_{\delta})$ is bounded in $L^2(\Omega_T)$. Furthermore, we know that (u_{δ}) is bounded in $L^{\infty}(0, T; H^1(\Omega))$ and $L^2(0, T; H^2(\Omega))$, and $u_{\delta} \to u$ strongly in $L^2(0, T; H^1(\Omega))$.

Let $y \in C_0^{\infty}(\Omega_T)$. It follows from the monotonicity of h_0 that

(29)
$$0 \leq \int_{0}^{T} \int_{\Omega} [u_{\delta}]_{+} [1 - u_{\delta}]_{+} (v_{\delta} - y) (h_{0}(v_{\delta}) - h_{0}(y)) dx dt$$
$$= \int_{0}^{T} \langle v_{\delta} - y, [u_{\delta}]_{+} [1 - u_{\delta}]_{+} (h_{0}(v_{\delta}) - h_{0}(y)) \rangle dt,$$

recalling that $\langle \cdot, \cdot \rangle$ is the dual product between $H^1(\Omega)'$ and $H^1(\Omega)$. This formulation is possible if $[u_{\delta}]_+[1-u_{\delta}]_+h_0(v_{\delta}) \in L^2(0,T; H^1(\Omega))$. To verify this statement, we observe that $\nabla u_{\delta} \in L^2(0,T; H^1(\Omega))$ implies that $(1-2u_{\delta})1_{\{0 < u_{\delta} < 1\}} \nabla u_{\delta} \in L^2(0,T; L^2(\Omega))$. Moreover, $[u_{\delta}]_+[1-u_{\delta}]^{1/2}_+ \in L^{\infty}(\Omega_T)$ and $[1-u_{\delta}]^{1/2}_+ \nabla v_{\delta} \in L^2(\Omega_T)$. This shows that

$$\nabla ([u_{\delta}]_{+}[1-u_{\delta}]_{+}h_{0}(v_{\delta})) = [u_{\delta}]_{+}[1-u_{\delta}]_{+}h_{0}'(v_{\delta})\nabla v_{\delta} + h_{0}(v_{\delta})(1-2u_{\delta})1_{\{0 < u_{\delta} < 1\}}\nabla u_{\delta}$$

is a function in $L^2(\Omega_T)$, so that $[u_{\delta}]_+[1-u_{\delta}]_+h_0(v_{\delta}) \in L^2(0,T;H^1(\Omega)).$

Let h_1 be the weak^{*} limit of $(h_0(v_{\delta}))$ in $L^{\infty}(0,T; L^{\infty}(\Omega))$ and h_2 be the weak limit of $([u_{\delta}]_+[1-u_{\delta}]_+h_0(v_{\delta}))$ in $L^2(\Omega_T)$. We claim that $h_2 = u(1-u)h_1$. Indeed, since (u_{δ}) converges strongly in $L^2(0,T; H^1(\Omega)), [u_{\delta}]_+[1-u_{\delta}]_+h_0(v_{\delta}) \rightharpoonup u(1-u)h_1$ weakly in $L^2(\Omega_T)$

(here, we use $0 \le u \le 1$ in Ω_T); see Lemma 9), and we deduce from the uniqueness of the limit that $u(1-u)h_1 = h_2$.

We can now pass to the limit $\delta \to 0$ in (29) to find that

$$0 \le \int_0^T \left\langle v - y, u(1 - u)(h_1 - h_0(y)) \right\rangle dt = \int_0^T \int_\Omega u(1 - u)(h_1 - h_0(y))(v - y) dx dt.$$

By density, this inequality holds for all $y \in L^2(\Omega_T)$. Let $w \in L^2(\Omega_T)$ and choose $y = v - \eta w$ for $\eta \in \mathbb{R}$. Then

$$0 \le \eta \int_0^T \int_\Omega u(1-u)(h_1 - h_0(v - \eta w))w dx dt.$$

Choosing $\eta > 0$ and performing the limit $\eta \to 0$ yields $\int_0^T \int_\Omega u(1-u)(h_1-h_0(v))wdxdt \ge 0$. On the other hand, if $\eta < 0$ and $\eta \to 0$, we have $\int_0^T \int_\Omega u(1-u)(h_1-h_0(v))wdxdt \le 0$. Since w is arbitrary, $u(1-u)h_1 = u(1-u)h_0(v)$. Thus,

$$h_+(u_{\delta}, v_{\delta}) = [u_{\delta}]_+ [1 - u_{\delta}]_+ h_0(v_{\delta}) \rightharpoonup u(1 - u)h_0(v) \quad \text{weakly in } L^2(\Omega_T).$$

This ends the proof.

Remark 13 (Generalizations). It is possible to generalize the relations (6) and (8) for the mobility and the reaction rates. For instance, we may choose $M(u) = u^m(1-u)^m M_0(u)$ for $m \ge 1$ and $0 < m_* \le M(u) \le m^*$ for $u \in [0,1]$, where $m^* \ge m_* > 0$; see [13]. In fact, we just need M(0) = M(1) = 0 and $M(u)f''(u) \in C^0([0,1])$; see [21]. The latter condition is needed to identify the weak limit J. The reaction terms may be generalized to $g(u, v) = g_0(v)g_1(u)$ and $h(u, v) = h_0(v)h_1(u)$, for instance, where we assume that g_1 is bounded in [0,1]; g_0 grows at most linearly; h_1 satisfies $h_1(u)f'(u) \le C$ for all u[0,1] to cancel the singularities of f'; and $|h_1(u)| \le C(1-u)$ for $u \in [0,1]$ to estimate in Step 1 of the proof of Lemma 7 the integral

$$\int_{\Omega} h_1(u) h_0'(v) \nabla v \cdot \nabla u dx \le \int_{\Omega} |\nabla u|^2 dx + C \int_{\Omega} (1-u) |\nabla v|^2 dx.$$

Clearly, also the free energy f(u) may be generalized if the factors in the diffusion and reaction terms are adapted in such a way that the singularities from f'(u) are canceled.

5. Numerical experiments

5.1. Scaling of the equations. The biofilm model with physical units reads as follows:

$$\partial_t v - \operatorname{div}(D(1-u)\nabla v) = -R_c uv,$$

$$\partial_t u - \operatorname{div}(M'u(1-u)\nabla \mu) = u(1-u)\frac{R_p v}{K_v + v},$$

$$\mu = -\Gamma_1 \Delta u + \Gamma_2 f'(u),$$

and f'(u) is given by (7), observing that the parameters N and λ and the volume fraction u are dimensionless. Here, D > 0 is the diffusivity, M' > 0 the mobility constant, $R_c > 0$ the consumption rate, $R_p > 0$ the production rate, $\Gamma_1 > 0$ the parameter of the distortional energy, and $\Gamma_2 > 0$ the parameter of the mixing free energy.

Choosing the characteristic length x_0 , the characteristic time t_0 , the characteristic concentration v_0 , and the characteristic chemical potential μ_0 , the scaled equations read as follows:

(30)
$$\partial_t v - \operatorname{div}(D_0(1-u)\nabla v) = -R_c^0 u v,$$

(31)
$$\partial_t u - \operatorname{div}(M_0 u(1-u)\nabla\mu) = u(1-u)\frac{R_p^0 v}{K+v},$$

(32)
$$\mu = -\Gamma_1^0 \Delta u + \Gamma_2^0 f'(u),$$

where the dimensionless parameters are

$$D_0 = \frac{Dt_0}{x_0^2}, \quad M_0 = \frac{M't_0\mu_0}{x_0^2}, \quad R_c^0 = R_c t_0, \quad R_p^0 = R_p t_0,$$
$$K = \frac{K_v}{v_0}, \quad \Gamma_1^0 = \frac{\Gamma_1}{\mu_0 x_0^2}, \quad \Gamma_2^0 = \frac{\Gamma_2}{\mu_0}.$$

The model of [24] (without elastic energy contributions) reads as

$$\partial_t ((1-u)v) - \operatorname{div}(D_0(1-1)\nabla v) = -u \frac{R_c v}{\widetilde{K} + v},$$

$$\partial_t u - \operatorname{div}(M_0(1-u)\nabla \mu) = u \frac{R_p v}{K_v + v},$$

$$\mu = -\Gamma_1 \Delta u + \Gamma_2 f'(u).$$

Symbol	Parameter	Value	Unit
D	Diffusivity	10^{-10}	${\rm m}^2{\rm s}^{-1}$
M'	Mobility	$2.5\cdot10^{-8}$	S
R_c	Consumption rate	10^{-2}	s^{-1}
R_p	Production rate	10^{-2}	${\rm kg}{\rm m}^{-3}{\rm s}^{-1}$
K_v	Half-saturation constant	10^{-4}	${ m kg}{ m m}^{-3}$
Γ_1	Distortional energy	$4 \cdot 10^{-15}$	${ m m}^4{ m s}^{-2}$
Γ_2	Mixing free energy	$4 \cdot 10^{-6}$	$\mathrm{m}^2\mathrm{s}^{-2}$
N	Polymerization parameter	10^{3}	
λ	Flory–Huggins parameter	0.55	
x_0	Characteristic length	10^{-4}	m
t_0	Characteristic time	10^{2}	S
v_0	Characteristic concentration	10^{-3}	${ m kg}{ m m}^{-3}$
$k_B T$	Thermal energy at $T = 300 \mathrm{K}$	$4\cdot 10^{-21}$	$\mathrm{kg}\mathrm{m}^2\mathrm{s}^{-2}$
\widetilde{K}	Half-saturation constant for model of [24]	$5\cdot 10^{-4}$	

TABLE 1. Parameters used in the numerical simulations.

The characteristic chemical potential μ_0 is determined by the thermal energy and the characteristic concentration and length (see Table 1) as $\mu_0 = k_B T / (v_0 x_0^3) = 4 \cdot 10^{-6} \,\mathrm{m}^2 \mathrm{s}^{-2}$.

The values of the physical parameters in Table 1 differ from those in [24] but are of a similar order. With our values, the scaled parameters are of order one (except K and Γ_1^0):

$$D_0 = R_c^0 = R_p^0 = 1, \quad K = 10^{-1}, \quad M_0 = 10^{-3}, \quad \Gamma_1^0 = 10^{-1}, \quad \Gamma_2^0 = 1$$

5.2. Numerical discretization. As in [29], we approximate equations (30)–(32) in the one-dimensional domain $\Omega = (0,1)$ by a BDF2 (second-order Backward Differentiation Formula) discretization in time. The spatial discretization is performed by finite volumes. The scheme is explicit for the mobility and potential, using the second-order approximation $\bar{u}^k := 2u^{k-1} - u^{k-2}$, but implicit in the reactions and semi-implicit in the diffusion. Let $\Delta t > 0$ be the time step size, $\Delta x > 0$ the space grid size, and $x_i = i\Delta x$, $x_{i\pm 1/2} = (i\pm 1/2)\Delta x$. We introduce finite-volume cells $K_i = (x_{i-1/2}, x_{i+1/2})$ for $i = 1, \ldots, N_x$. Then the values u_i^k , v_i^k , and μ_i^k approximate $u(x_i, k\Delta t)$, $v(x_i, k\Delta t)$, and $\mu(x_i, k\Delta t)$ respectively for $i = 1, \ldots, N_x$. We introduce for $k \ge 2$ as follows:

$$\begin{aligned} \frac{\Delta x}{2\Delta t} (3v_i^k - 4v_i^{k-1} + v_i^{k-2}) + \mathcal{G}_{i+1/2}^k - \mathcal{G}_{i-1/2}^k &= -\Delta x R_c^0 u_i^k v_i^k, \\ \frac{\Delta x}{2\Delta t} (3u_i^k - 4u_i^{k-1} + u_i^{k-2}) + \mathcal{F}_{i+1/2}^k - \mathcal{F}_{i-1/2}^k &= \Delta x u_i^k (1 - u_i^k) \frac{R_p^0 v_i^k}{K + v_i^k} \\ \mathcal{H}_{i+1/2}^k - \mathcal{H}_{i-1/2}^k + \Delta x f'(\bar{u}_i^k) &= \Delta x \mu_i^k, \end{aligned}$$

where the numerical fluxes are given by

$$\mathcal{G}_{i+1/2}^{k} = -D_0(1 - u_{i+1/2}^{k}) \frac{v_{i+1}^k - v_i^k}{\Delta x},$$

$$\mathcal{F}_{i+1/2}^{k} = -M_0 u_{i+1/2}^k (1 - u_{i+1/2}^{k}) \frac{\mu_{i+1}^k - \mu_i^k}{\Delta x}, \quad \mathcal{H}_{i+1/2}^k = -\frac{u_{i+1}^k - u_i^k}{\Delta x}$$

and $u_{i+1/2}^k = \frac{1}{2}(u_{i+1}^k + u_i^k)$. The approximation (u_i^1, v_i^1, μ_i^1) at the first time step is computed from the implicit Euler method.

In the same way, we discretized a simplified version of [24] which reads in its dimensionless form for $k \ge 2$ as

$$\begin{split} &\frac{\Delta x}{2\Delta t}(3w_i^k - 4w_i^{k-1} + w_i^{k-2}) + \mathcal{G}_{i+1/2}^k - \mathcal{G}_{i-1/2}^k = -\Delta x u_i^k \frac{\widetilde{R}_c^0 v_i^k}{\widetilde{K} + v}, \\ &\frac{\Delta x}{2\Delta t}(3u_i^k - 4u_i^{k-1} + u_i^{k-2}) + \widetilde{\mathcal{F}}_{i+1/2}^k - \widetilde{\mathcal{F}}_{i-1/2}^k = \Delta x u_i^k \frac{R_p^0 v_i^k}{K + v_i^k}, \\ &\mathcal{H}_{i+1/2}^k - \mathcal{H}_{i-1/2}^k + \Delta x f'(\bar{u}_i^k) = \Delta x \mu_i^k, \end{split}$$

where we abbreviated $w_i^k = (1 - u_i^k)v_i^k$, \mathcal{G} and \mathcal{H} are as above, $\widetilde{\mathcal{F}} = -M_0 u_{i+1/2}^k (\mu_{i+1}^k - \mu_i^k)/\Delta x$, and $\widetilde{R}_c^0 = 1$, $R_p^0 = 1$ are scaled rates. We use the Newton method to solve the resulting system of nonlinear equations. For the first three test cases, we used a mesh of 128 cells and the time step size $\Delta t = 10^{-3}$.

5.3. Numerical results.

Test case 1: We consider the initial conditions

$$u^{0}(x) = \frac{1}{2}\sin(2\pi x)^{2} + 2 \cdot 10^{-2}, \quad v^{0}(x) \equiv 0.75.$$

The numerical solutions u and v are presented in Figure 1. The substrate concentration converges uniformly to zero as $t \to \infty$ because of the consumption term, while the volume fraction of the biomass is increasing in time. The increase becomes slower and stops after some time since the production term is proportional to the substrate concentration which almost vanishes for large times and hence the production term vanishes too. In our model, both the biomass fraction and the substrate concentration change at a slower rate compared to the model of [24], which is caused by the additional factor 1 - u in the source term. Accordingly, the convergence to the steady state is smaller in our model than in the model of [24]. Note that, without the additional factor 1 - u, an initial value u^0 smaller but close to one may lead to a volume fraction exceeding its maximal value and consequently break down the numerical scheme.



FIGURE 1. Biomass fraction u (top) and substrate concentration v (bottom) in test case 1 for our system (left) and the system of [24] (right).

Test case 2: We consider the initial conditions

$$u^{0}(x) = \begin{cases} 0.2, & \text{if } 0 \le x \le 0.2, \\ 1 \cdot 10^{-2}, & \text{if } 0.2 < x \le 1, \end{cases} \quad v^{0}(x) \equiv 0.1.$$

In both models, the volume fraction of biomass growths rather fast until the substrate concentration vanishes; see Figure 2. Due to the additional factor 1 - u in our mobility, we can observe a slower diffusion in areas of larger volume fraction compared to [24]. In areas of low volume fractions, we observe a larger growth than for [24], which can be explained by the larger nutrient consumption compared to our model, causing a lack of nutrient supply for further growth.



FIGURE 2. Biomass u in test case 2 for our system (left) and the system of [24] (right).

Test case 3: We choose the initial conditions

(33)
$$u^0(x) = -(x - 1/2)^2 + 1/3, \quad v^0(x) \equiv 0.3$$

As in the previous test cases, we observe in Figure 3 a faster growth of biomass volume fraction in the model of [24]. Moreover, the growth process dominates before the diffusion process flattens the maximal volume fraction towards the steady state. Due to the absence of the factor 1 - u, this effect is stronger than in the model of [24].

Test case 4: We analyze the order of convergence in space with the initial conditions (33). Since there does not exist an explicit solution, we compute a reference solution $(u_{\rm ref}, v_{\rm ref})$ at time T = 1 on a mesh with 2048 cells with time step size $\Delta t = 10^{-5}$. The approximate solutions $u^{(j)}$ are determined on meshes of 2^j cells for $j = 4, \ldots, 10$. We choose a rather small value for T to compute the order of convergence in space before a steady state is reached. Figure 4 (left) illustrates the discrete L^2 norm of the difference $u_{\rm ref} - u^{(j)}$ for $j = 4, \ldots, 10$. As expected, we observe a second-order convergence in space.



FIGURE 3. Biomass u in test case 3 for our system (left) and the system of [24] (right).



FIGURE 4. Convergence in space (left) and convergence in time (right) at time T = 1.

Test case 5: We analyze the order of convergence in time by using as before the initial conditions (33) and by choosing L = 128 cells in space. We compute a reference solution $(u_{\rm ref}, v_{\rm ref})$ at time T = 1 with time step size $\Delta t = 1/(2^{14}L) \approx 5 \cdot 10^{-7}$. The approximate solutions $u^{(j)}$ are determined with time step sizes $\Delta t = 1/(2^{2j}L)$ for $j = 1, \ldots, 6$. Figure 4 (right) illustrates the discrete L^2 norm of the difference $u_{\rm ref} - u^{(j)}$ for $j = 1, \ldots, 6$. We observe a convergence in time of order 1.73 for u and 2 for v, respectively.

References

- M. Jurak, I. Radišić, and A. Žgaljić Keko. Two-phase two-component flow in porous media in low solubility regime. SIAM J. Math. Anal. 51 (2019), 2019–2052.
- [2] D. Antonopoulou, G. Karali, and G. Kossioris. Asymptotics for a generalized Cahn-Hilliard equation with forcing terms. *Discrete Cont. Dyn. Sys.* 30 (2011), 1037–1054.

C. HELMER AND A. JÜNGEL

- [3] J. Cahn and J. Hilliard. Free energy of a nonuniform system. I. Interfacial free energy. J. Chem. Phys. 28 (1958), 258–267.
- [4] L. Cherfils, A. Miranville, and S. Zelik. On a generalized Cahn-Hilliard equation with biological applications. *Discrete Cont. Dyn. Sys. B* 19 (2014), 2013–2026.
- [5] N. Cogan and J. Keener. The role of the biofilm matrix in structural development. Math. Med. Biol. 21 (2004), 147–166.
- [6] B. D'Acunto and L. Frunzo. Qualitative analysis and simulations of a free boundary problem for multispecies biofilm models. *Math. Computer Model.* 53 (2011), 1596–1606.
- [7] B. D'Acunto, L. Frunzo, V. Luongo, and M. Mattei. Free boundary approach for the attachment in the initial phase of multispecies biofilm growth. Z. Angew. Math. Phys. 70 (2019), no. 91, 16 pages.
- [8] E. Daus, A. Jüngel, and A. Zurek. Convergence of a finite-volume scheme for a degenerate-singular cross-diffusion system for biofilms. *IMA J. Numer. Anal.* 41 (2021), 935–973.
- [9] H. Eberl, M. Efendiev, D. Wrzosek, and A. Zhigun. Analysis of a degenerate biofilm model with a nutrient taxis term. *Discrete Cont. Dyn. Sys.* 34 (2014), 99–119.
- [10] H. Eberl, D. Parker, and M. van Loosdrecht. A new deterministic spatio-temporal continuum model for biofilm development. J. Theor. Medicine 3 (2001), 161–175.
- [11] M. Efendiev, H. Eberl, and S. Zelik. Existence and longtime behavior of solutions of the nonlinear reaction-diffusion system arising in the modelling of biofilms. In: *Nonlinear diffusive systems and related topics*, Surikaisekikenkyusho Kokyuroku, vol. 1258 (2002), 49–71.
- [12] B. Emerenini, S. Sonner, and H. Eberl. Mathematical analysis of a quorum sensing induced biofilm dispersal model and numerical simulation of hollowing effects. *Math. Biosci. Eng.* 14 (2017) 625–653.
- [13] C. Elliott and H. Garcke. On the Cahn–Hilliard equation with degenerate mobility. SIAM J. Math. Anal. 27 (1996), 404–423.
- [14] P. Flory. Thermodynamics of high polymer solutions. J. Chem. Phys. 10 (1942), 51–61.
- [15] A. Friedman, B. Hu, and C. Xue. On a multiphase multicomponent model of biofilm growth. Arch. Ration. Mech. Anal. 211 (2014), 257–300.
- [16] S. Frigeri. On a nonlocal Cahn-Hilliard/Navier-Stokes system with degenerate mobility and singular potential for incompressible fluids with different densities. Ann. Inst. H. Poincaré – Anal non lin. 38 (2021), 647–687.
- [17] H. Garcke and K. F. Lam. Global weak solutions and asymptotic limits of a Cahn-Hilliard-Darcy system modelling tumour growth. AIMS Mathematics 1 (2016), 318–360.
- [18] C. Helmer, A. Jüngel, and A. Zurek. Analysis of a finite-volume scheme for a single-species biofilm model. Appl. Numer. Math. 185 (2023), 386–405.
- [19] M. Huggins. Solutions of long chain compounds. J. Chem. Phys. 9 (1941), 440.
- [20] A. Iuorio and S. Melchionna. Long-time behavior of a nonlocal Cahn-Hilliard equation with reaction. Discrete Cont. Dyn. Sys. 38 (2018), 3765–3788.
- [21] B. Perthame and A. Poulain. Relaxation of the Cahn-Hilliard equation with singular single-well potential and degenerate mobility. *Europ. J. Appl. Math.* 32 (2021), 89–112.
- [22] J. Simon. Compact sets in the space $L^{p}(0,T;B)$. Ann. Math. Pura. Appl. 146 (1987), 65–96.
- [23] Q. Wang and T. Zhang. Review of mathematical models for biofilms. Solid State Commun. 150 (2010), 1009–1022.
- [24] Q. Wang and T. Zhang. Kinetic theories for biofilms. Discrete Cont. Dyn. Sys. B 17 (2012), 1027–1059.
- [25] O. Wanner and W. Gujer. A multispecies biofilm model. *Biotechnol. Bioengin.* 28 (1986), 314–328.
- [26] J.-X. Yin. On the existence of nonnegative continuous solutions of the Cahn-Hilliard equation. J. Differ. Eqs. 97 (1992), 310–327.
- [27] T. Zhang. Modeling of biocide action against biofilm. Bull. Math. Biol. 74 (2012), 1427–1447.
- [28] T. Zhang, N. Cogan, and Q. Wang. Phase-field models for biofilms. I. Theory and 1-D simulations. SIAM J. Appl. Math. 69 (2008), 641–669.
- [29] T. Zhang, N. Cogan, and Q. Wang. Phase-field models for biofilms. II. 2-D numerical simulations of biofilm-flow interaction. *Commun. Comput. Phys.* 4 (2008), 72–101.

INSTITUTE OF ANALYSIS AND SCIENTIFIC COMPUTING, VIENNA UNIVERSITY OF TECHNOLOGY, WIEDNER HAUPTSTRASSE 8-10, 1040 WIEN, AUSTRIA *Email address*: christoph.helmer@tuwien.ac.at

Institute of Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstrasse 8-10, 1040 Wien, Austria

Email address: juengel@tuwien.ac.at