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TIME-DISCRETIZATION OF A DEGENERATE REACTION-DIFFUSION EQUATION ARISING IN BIOFILM MODELING*

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Abstract. A numerical method for a reaction-diffusion equation arising in biofilm modelling is presented. The equation shows two non-standard effects in the spatial operator, degeneracy like the porous medium equation and a singularity as an *a priori* known upper bound is approached. The equation is transformed and formulated in terms of a new dependent variable. This transformation is chosen such that the resulting spatial operator is the Laplace operator and that the non-linear effects appear now in the time-derivative. The numerical method for the new equation follows Rothe's approach: while a standard discretization for the spatial domain is used, a fully-implicit time-discretization scheme is developed that takes the special properties of the equation into account. This paper presents the formulation of this time-discretization scheme as well as its analysis.

Key words. degenerate parabolic equations, nonlinear diffusion, numerical solution, biofilm model

AMS subject classifications. 35K65, 65M12, 92B05

1. Introduction. The nonlinear reaction-diffusion equation considered in this paper arises in mathematical modelling of biofilm development. Those are microbial communities, in which microorganisms live embedded in a protecting layer of extracellular polymeric substances. Biofilms grow on interfaces in aquatic systems; they play a beneficial role in environmental settings and a harmful role in medical settings. The prototype continuum-mechanistic biofilm model proposed in [3] for one limiting substrate (e.g., oxygen or a nutrient like glucose) with concentration S and one biomass fraction with density M reads

$$
\left\{
\begin{array}{rcl}
\frac{\partial S}{\partial t} & = & d_1 \Delta S - \frac{k_1 S M}{k_2 + S} \\
\frac{\partial M}{\partial t} & = & \nabla (D_2(M) \nabla M) + M \cdot \left(\frac{k_3 S}{k_2 + S} - k_4 \right) \\
D_2(M) & = & d_2 \frac{\varepsilon M^b}{(1-M)^a}
\end{array}
\right.
\tag{1.1}
$$

and is defined in a domain $[0, \infty[\times \Omega$ with $\Omega \subset \mathbf{R}^d$. The model parameters are positive. Kinetic parameter k_3 denotes the maximum specific growth rate, k_4 is the decay rate, k_2 the Monod half-saturation constant. k_1 is the maximum consumption rate, i.e., the maximum specific growth rate divided by a yield factor. In order to allow for growth of new biomass, $\frac{k_3 S}{k_2+S} - k_4$ must be positive for some positive S. Model (1.1) is completed by appropriate initial and boundary conditions.

The second component of this reaction-diffusion system shows two non-standard effects in the spatial operator: degeneracy as in the porous medium equation for $M \to 0$ and a singularity for $M \to 1$. The first one guarantees that spatial spreading of biomass does not take place for small biomass densities and a finite speed of interface propagation; the second one guarantees that the *a priori* known maximum biomass density is obeyed, i.e., $M \le 1$. This was proven in [4] for relevant sets of boundary conditions. In the current paper we will focus on the analysis of this second effect. For this purpose the biomass equation will

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be transformed and expressed in terms of a new dependent variable. The transformation is chosen such that the resulting spatial operator is the Laplace operator. Proceeding this way shifts the singularity and the associated problems into the time-derivative. The numerical method suggested for the new equation follows Rothe's approach. After time-discretization a sequence of elliptic problems, one per time-step, is obtained. For the analysis of the time-discretization scheme, tools from the theory of nonlinear elliptic problems will be used; see, e.g., [1]. We shall focus on the second component of (1.1). The first equation of (1.1) is a semi-linear reaction-diffusion equation which poses no additional problem in the given context.

The paper is organised as follows: Section 2 contains analytical results about the model which are used later in the analysis of the numerical method and a transformation of the dependent variable is introduced. The numerical method will be based on this transformation. Section 3 formulates the semi-discretization in time of the transformed equation and proves its convergence and stability. In Section 4, some numerical tests are presented.

2. The governing equation and some analytical results. We consider the initial-boundary value problem associated with the density-dependent reaction-diffusion problem

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta\Phi(u) = ku, & x \in \Omega, \quad t \in [0,T], \\ u = 0, & x \in \partial\Omega, \quad t \in [0,T], \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases} \tag{2.1}$$

where

$$\Phi(u) = \int_0^u \varphi(s)ds = \int_0^u \frac{s^b}{(1-s)^a} ds,$$

$a, b \geq 1$ and $\Phi : [0,1) \to [0,+\infty)$. The constants T and k are positive, and $\Omega \subset \mathbf{R}^d$, with $d \in \{1,2,3\}$, is a bounded domain with a piecewise smooth boundary.

This is the simplest variant of the biofilm model (1.1); nevertheless it captures the essential features of the spatio-temporal biomass spreading mechanism. In the biofilm setting, u describes the biomass density. Physiologically, equation (2.1) describes the special situation that nutrients and other beneficial substances are nowhere limited but available in abundance. Note that constant k can be understood as a reaction rate subsuming both, first order growth as well as the first order decay of biomass. First order growth would be a consequence of nutrient abundance, $S \gg k_2$ in (1.1). In this case we have $k \approx k_3 - k_4 > 0$. Thus, the first order reaction ku in (2.1) puts an upper bound on the combined Monod-growth/first-order-decay term in (1.1).

For the initial data we postulate that $u_0 \in L^\infty(\Omega)$, $u_0 \geq 0$, $|u_0|_{L^\infty(\Omega)} < 1$ and $\Phi(u_0) \in H_0^1(\Omega)$. Then it is known from Theorem 2.1 of [4] that problem (2.1) has a unique solution u in the class of functions defined by $u \in L^\infty(\mathbf{R}_+ \times \Omega) \cap C([0,\infty), L^2(\Omega))$, $0 \leq u(t,x) \leq 1$, $|u|_{L^\infty(\mathbf{R}_+\times\Omega)} < 1$ and $\Phi(u) \in L^\infty(\mathbf{R}_+, H_0^1(\Omega)) \cap C([0,\infty), L^2(\Omega))$.

Here and subsequently, the spaces H (with indices) denote the usual Sobolev spaces; similarly, L and C have the usual meaning. The subscript 0 denotes the class of those functions which have compact support, while superscripts denote the regularity. The space H^{-1} later on will denote the set of all linear functionals on H_0^1, i.e., the dual space.

2.1. A Lyapunov functional for problem (2.1). We introduce the nonlinear functional J_0

$$J_0(u) = \frac{1}{2}\int_\Omega |\nabla\Phi(u)|^2 dx - k\int_\Omega dx \int_0^u \Phi'(s)sds \tag{2.2}$$

and prove that it is a Lyapunov functional of problem (2.1) as defined, e.g., in [2]; that is, if u is a solution, then the mapping $t \mapsto J_0(u(t))$ is nonincreasing. To this end we need to prove that the formal "energy inequality", which is the formal result of multiplying the equation by $\frac{\partial}{\partial t}\phi(u)$ and integrating by parts, is satisfied. We use arguments and results from [4] which are repeated here for the convenience of the reader.

The solution of the degenerate problem (2.1) can be obtained as the limit of the solutions w_n of the following second order parabolic systems [4]:

$$\left\{ \begin{array}{rcll} \frac{\partial}{\partial t} w_n - \Delta\Phi_n(w_n) &=& k w_n, & (t,x) \in Q_T := (0,T)\times\Omega, \\ w_n &=& 0, & x \in \partial\Omega, \\ w_n(x,0) &=& u_0(x), & x \in \Omega, \end{array} \right. \tag{2.3}$$

where the functions Φ_n are defined by

$$\Phi_n(w) = \int_0^w \varphi_n(s)ds,$$

and φ_n is the following regularization of φ:

$$\varphi_n(w) = \left\{ \begin{array}{ll} (w+1/n)^b/(1-w)^a, & \text{if } w \le 1-1/n \\ n^a, & \text{if } w > 1-1/n. \end{array} \right.$$

Using a comparison principle an a priori estimate in L^∞-norm for the solutions of the problems (2.3) is obtained and

$$w_n \to u \qquad \text{strongly in} \quad C_{loc}(\mathbf{R}_+, L^2(\Omega)), \tag{2.4}$$

where u is a solution of problem (2.1).

LEMMA 2.1. *The solution w_n of problem (2.3) satisfies the following estimate*

$$\begin{aligned} ||\Phi_n(w_n(\tau))||_{H^1(\Omega)} + \int_\tau^{\tau+1}\int_\Omega |\frac{\partial w_n}{\partial t}|^2 \varphi(w_n(t))dxdt \\ \le C(||\Psi_n(w_n(0))||_{H^1(\Omega)} + 1), \end{aligned} \tag{2.5}$$

where the constant C is independent of n.

Proof: Proposition 1.3 in [4] □

LEMMA 2.2. *Let the initial data u_0 satisfy*

$$u_0(x) \le 1-\delta, \quad \delta > 0. \tag{2.6}$$

Then there exists $\gamma = \gamma(\delta) > 0$ such that for a sufficiently large n, the estimate

$$0 \le w_n(t,x) \le 1-\gamma \tag{2.7}$$

is valid for the solution w_n of the problem (2.3).

Hence, in the case where the L^∞-norm of the initial data u_0 is separated from 1, the solution of the problem (2.3) stays separated from 1.

Proof: Proposition 1.6 in [4] □

In order to simplify notation, we introduce in accordance with [8] the functions

$$P(u) = k\int_0^u s\,\Phi'(s)ds, \qquad \Psi(u) = \int_0^u \sqrt{\Phi'(s)}ds. \tag{2.8}$$

and state the following Lemma.

LEMMA 2.3. *Let the initial data u_0 satisfy (2.6). Then the solution u of problem (2.1) satisfies*

$$\int_0^t \int_\Omega \left(\frac{\partial \Psi(u)}{\partial t}\right)^2 dxdt \leq \left[-\frac{1}{2}\int_\Omega |\nabla\Phi(u)|^2 dx + \int_\Omega P(u)dx\right]\Big|_0^t. \tag{2.9}$$

Proof. First we show that $\frac{\partial}{\partial t}\Psi(u) \in L^2(\Omega)$. To this end we introduce the functions $\Psi_n(v) = \int_0^v \sqrt{\Phi_n'(s)}ds$. According to estimate (2.5) the sequence $\frac{\partial}{\partial t}\Psi_n(w_n)$ is uniformly bounded in $L^2(Q_T)$. Consequently there is a subsequence $n_k \to \infty$ and a function $z \in L^2(Q_T)$ such that $\frac{\partial}{\partial t}\Psi_{n_k}(w_{n_k}) \to z$ weakly.

Since $\Psi_n(s) \leq s+\Phi_n(s)$, the L^2-norm of $\Psi_n(w_n)$ is uniformly bounded (due to estimate (2.5)). To see that actually $z = \frac{\partial}{\partial t}\Psi(u)$, it is sufficient to verify that

$$\Psi_n(w_n(t,x)) \to \Psi(u(t,x)) \qquad \text{for almost all } \ (t,x) \in (0,T)\times\Omega. \tag{2.10}$$

Because of (2.4) we may assume without loss of generality that

$$w_n(t,x) \to u(t,x) \qquad \text{for almost all } \ (t,x) \in (0,T)\times\Omega.$$

Then, using the inequality

$$\begin{aligned} |\Psi_n(w_n(t,x)) - \Psi(u(t,x))| \leq & \, |\Psi_n(w_n(t,x)) - \Psi_n(u(t,x))| \\ & + |\Psi_n(u(t,x)) - \Psi(u(t,x))| \end{aligned} \tag{2.11}$$

and taking into account that $0 \leq w_n(t,x) \leq 1-\gamma$ and that the family of functions $\Psi_n(s)$ is uniformly continuous on the interval $[0, 1-\gamma]$, we derive that each term on the right hand side of (2.11) tends to zero almost everywhere. Thus, we have proved (2.10) and, therefore, $z = \frac{\partial}{\partial t}\Psi(u)$.

Due to estimate (2.5), the sequence $\{\nabla\Phi_n(w_n(.,t))\}$ is bounded in $L^2(\Omega)$ and there exist $z \in L^2(\Omega)$ and $n_k \to \infty$ such that

$$\nabla\Phi_{n_k}(w_{n_k}(.,t)) \to z$$

weakly in $L^2(\Omega)$. Since also $\Phi_n(w_n(.,t)) \to \Phi(u(.,t))$ weakly in $L^2(\Omega)$, we must have $z = \nabla\Phi(u(.,t))$. Since the limit is unique, it follows that

$$\nabla\Phi_n(w_n(.,t)) \to \nabla\Phi(u(.,t)) \qquad \text{as} \quad n \to \infty,$$

weakly in $L^2(\Omega)$. After some obvious transformations, we have

$$\int_\Omega kw_n \frac{\partial\Phi_n(w_n)}{\partial t} dx = \frac{\partial}{\partial t}\int_\Omega \int_0^{w_n(t)} v\phi_n(v))dv.$$

Thus,

$$\int_0^t \int_\Omega kw_n \frac{\partial\Phi_n(w_n)}{\partial t} dx = \int_\Omega dx \int_0^{w_n(t)} v\phi_n(v)dv - \int_\Omega dx \int_0^{u_0} v\phi_n(v)dv.$$

Taking into account that $0 \leq w_n(t,x) \leq 1-\gamma$ and that the family of functions $\xi_n(v) = \int_0^v s\phi_n(s)ds$ is uniformly continuous on the interval $[0, 1-\gamma]$, we derive that

$$\xi_n(w_n(t,x)) \to \xi(u(t,x)) \qquad \text{for almost all } \ (t,x) \in (0,T)\times\Omega,$$

where $\xi(v) = \int_0^v s\,\phi(s)ds$. Since the sequence $\{\xi_n(w_n)\}$ is bounded in $L^1((0,T)\times\Omega)$ independently of n, we derive that

$$\int_\Omega dx \int_0^{w_n(t)} v\phi_n(v)dv \to \int_\Omega dx \int_0^{u(t)} v\phi(v)dv.$$

Similarly, we have that

$$\int_\Omega dx \int_0^{u_0} v\phi_n(v)dv \to \int_\Omega dx \int_0^{u_0} v\phi(v)dv.$$

For the proof of (2.9) we may multiply (2.3) by $\frac{\partial}{\partial t}\Psi_n(w_n)$ and integrate over Q_T to obtain

$$\int_0^t \int_\Omega \left(\frac{\partial \Psi_n(w_n)}{\partial t}\right)^2 dxds + \frac{1}{2}\int_\Omega |\nabla \Phi_n(w_n(.,t))|^2 dx$$
$$= \frac{1}{2}\int_\Omega |\nabla \Phi_n(u_0))|^2 dx + \int_0^t \int_\Omega k w_n \left(\frac{\partial \Phi_n(w_n)}{\partial t}\right) dxds.$$

Passing to the limit as $n \to \infty$ and taking into account the lower semi-continuity of the norm with respect to weak convergence we obtain

$$\int_0^t \int_\Omega \left(\frac{\partial \Psi(u)}{\partial t}\right)^2 dxds + \frac{1}{2}\int_\Omega |\nabla \Phi(u(.,t))|^2 dx$$
$$\leq \frac{1}{2}\int_\Omega |\nabla \Phi_n(u_0))|^2 dx + \int_0^t \int_\Omega \left(\frac{\partial P(u)}{\partial t}\right) dxds.$$

which is equivalent to (2.9). This completes the proof. $\square$

As a direct consequence of Lemma 2.3, we conclude that in the case where the L^∞-norm of the initial data u_0 is separated from 1, the functional $J_0(u)$ as defined by (2.2) is a Lyapunov functional for the problem (2.1).

2.2. Transformation of equation (2.1). In order to remove both non-standard diffusion effects from the spatial operator, we introduce the new dependent variable $v = \Phi(u)$ and define its inverse as $\beta = \Phi^{-1}$. Then v satisfies

$$\begin{cases} \frac{\partial}{\partial t}\beta(v) - \Delta v = k\beta(v), & x \in \Omega,\quad t > 0, \\ v = 0, & x \in \partial\Omega,\quad t > 0, \\ v(x,0) = v_0(x) = \Phi(u_0(x)), & x \in \partial\Omega. \end{cases} \tag{2.12}$$

It is easy to verify that $\beta : [0,+\infty) \to [0,1)$ is a strictly increasing function and behaves like $Cx^{\frac{1}{b+1}}$ $(C > 0)$ in a neighborhood of 0. Moreover, β satisfies the inequalities

$$\int_0^v \beta(s)ds \leq \beta(v)v \leq v.$$

By combining this transformation and (2.2), we define a functional J on $H_0^1(\Omega)$ as

$$J(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 dx - k\int_\Omega dx \int_0^v \beta(s)ds, \quad \forall v \in H_0^1(\Omega). \tag{2.13}$$

This is a Lyapunov functional for problem (2.12), as shown by the following Lemma

LEMMA 2.4. *Let v be a solution of the problem (2.12). Then the mapping $t \mapsto J(v(t))$ is decreasing.*

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Proof. Since the functional J_0 defined in (2.2) is a Lyapunov functional for problem (2.1), the result follows by a change of variables. □

For the convenience of the notation we denote by A the operator $-\Delta$ of domain $D(A) = H_0^1(\Omega) \cap H^2(\Omega)$. Then the problem (2.12) can be re-written as

$$\begin{cases} \frac{\partial}{\partial t}\beta(v) + Av = k\beta(v), \\ v(0) = v_0. \end{cases} \tag{2.14}$$

We try to find an *a priori* upper estimate for the solution of the problem (2.1) and respectively of the problem (2.14). Suppose we can find a function $w_0 > 0$, $w_0 \in L^\infty(\Omega)$ satisfying

$$\begin{cases} -\Delta(\Phi(w_0)) & \geq & kw_0, & x \in \Omega, \\ w_0 & = & 0, & x \in \partial\Omega. \end{cases} \tag{2.15}$$

Then the function $w(x,t) = w_0$, which is constant in time, is a supersolution of the time dependent problem

$$\frac{\partial w}{\partial t} = \Delta(\Phi(w)) + kw, \quad x \in \Omega,$$

i.e, it satisfies the differential inequality

$$\frac{\partial w}{\partial t} - \Delta(\Phi(w)) \geq kw, \quad x \in \Omega. \tag{2.16}$$

Hence, if $|u_0| \leq w_0$ then we have the a priori estimate $|u(x,t)| \leq w_0(x)$ for any solution u of (2.1).

In order to verify that there indeed exists such a function w_0 satisfying (2.15), we consider the corresponding stationary problem of (2.14). We pick a function u_0 such that $\Phi(u_0) = v_0 \in H_0^1(\Omega)$ and define the set

$$\mathbf{K} := \{w \in H_0^1(\Omega) : w \geq v_0 \quad \text{a.e. in} \quad \Omega\}$$

The associated obstacle problem

$$\text{Find } w \in \mathbf{K} : \ \langle Av, v - w\rangle \geq \langle k, v - w\rangle \quad \text{for all } v \in \mathbf{K}. \tag{2.17}$$

has a unique solution w, which is also the solution of the minimization problem

$$\min_{v\in\mathbf{K}}\{\langle Av, v\rangle - 2\langle k, v\rangle\}.$$

Furthermore, in [11] it is shown (in Theorem 6.9) that the solution w of the obstacle problem (2.17) satisfies the inequality

$$\begin{cases} Aw & \geq & k, & x \in \Omega, \\ w & \geq & 0, & x \in \partial\Omega. \end{cases}$$

Since $k \geq k\beta(w)$, we have also

$$\begin{cases} Aw & \geq & k\beta(w), & x \in \Omega, \\ w & = & 0, & x \in \partial\Omega, \end{cases} \tag{2.18}$$

Moreover, since $w \in H_0^1(\Omega)$, in the case $d = 1$ we derive immediately that $w \in L^\infty(\Omega)$ and then also $\beta(w) \in L^\infty(\Omega)$. If $d \neq 1$, an additional assumption is required. For this purpose, we suppose that $-\Delta v_0 \leq 0$ (as an element from $\mathcal{D}'(\Omega)$ and thereby as a measure on Ω) or that $-\Delta v_0$ is a measure on Ω with the property $\sup\{-\Delta v_0, 0\} \in L^p(\Omega)$, $p > d$. With the standard regularity theory for variational inequalities (see for example [9], Theorem 8.8., or [11], Chapter 4.2) we obtain that $w \in H^{2,p}(\Omega)$. This implies that $w \in L^\infty(\Omega)$.

Thus, we have the a priori estimate $|u(x,t)| \leq \beta(w(x))$ for the solution u of (2.1) and the a priori estimate $|v(x,t)| \leq w(x)$ for the solution v of (2.14).

3. Time-discretization.

3.1. Definition of the numerical scheme. Following Rothe's method we propose a semi-discretization in time of the nonlinear parabolic problem (2.14). If the function v_n is the solution at the time level $t_n = n\Delta t$, then the solution v_{n+1} at the time level t_{n+1} is the solution of the elliptic problem

$$\beta(v_n) - \beta(v_{n+1}) + k\Delta t\beta(v_{n+1}) = \Delta t A v_{n+1} \tag{3.1}$$

This is the implicit Euler discretization of the evolution equation (2.14). It can be re-written as

$$A v_{n+1} = f(v_{n+1}), \tag{3.2}$$

where the function f is defined by

$$f(v) = \frac{1}{\Delta t}(\beta(v_n) - \beta(v)) + k\beta(v). \tag{3.3}$$

The choice of the implicit Euler method, despite its low order convergence, was motivated by a special property that will greatly simplify the analysis of the numerical scheme later on. Since the time-discretization (3.1) of the evolution equation (2.14) leads to a sequence of elliptic problems, one per time-step, it will be studied with the tools of the nonlinear elliptic theory that was established in [1].

3.2. Existence of the numerical solution. We prove that (3.1) has a unique non-negative solution if v_n is non-negative in Ω for $n \leq N$, where N is a positive integer such that $N\Delta t = T$. If we are looking for a classical solution of the problem (3.1), we suppose also that the initial condition v_0 is in $H_0^1(\Omega) \cap C(\overline{\Omega}) \cap C^\alpha(\Omega)$, $0 < \alpha < 1$, where $C^\alpha(\Omega)$ is the space of Hölder continuous functions with exponent α.

LEMMA 3.1. *If the function v_n is non-negative in Ω and continuous in $\overline{\Omega}$, and if the condition*

$$||v_n||_\infty < \Phi(1 - k\Delta t) \tag{3.4}$$

is satisfied, then (3.1) has a maximal non-negative solution $\hat{v}$; moreover if v is a solution, then $v \in C(\overline{\Omega}) \cap C^2(\Omega)$ and it satisfies $0 \leq v \leq \hat{v}$.

Proof. Since $f(0) = \beta(v_n)/\Delta t \geq 0$, the constant function $\overline{v} = 0$ is a minimal non-negative solution of the boundary value problem (3.1). In addition, if (3.4) is satisfied, (3.1) has a constant positive supersolution. In fact, if C_n is a supersolution, it must satisfy

$$f(C_n) = \frac{1}{\Delta t}(\beta(v_n) - \beta(C_n)) + k\beta(C_n) \leq 0.$$

Thus the constant

$$C_n = \Phi\left(\frac{1}{1 - k\Delta t}\beta(||v_n||_\infty)\right)$$

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is such a supersolution. Hence, (3.1) has a maximal solution $\hat{v}$, and any non-negative solution v satisfies $v \in C(\overline{\Omega}) \cap C^2(\Omega)$ and $0 \leq v \leq \hat{v}$ as was shown in [1, Theorem A]. □

LEMMA 3.2. *If (3.4) is satisfied, then problem (3.1) has a unique nonnegative solution in the class* $C(\overline{\Omega}) \cap C^2(\Omega)$.

Proof. Theorem A of [1] gives the existence of a non-negative solution of the problem (3.1). Since for every ξ,η with $\overline{v} \leq \xi \leq \eta \leq \hat{v}$,

$$f(\xi) \geq f(\eta),$$

Theorem 2 of [1] gives the uniqueness of this non-negative solution. □

REMARK 3.3. *The theorems A and 2 in [1] use the hypotheses that* Ω *is a smooth domain and that* f *belongs to class* $C^\alpha(\overline{\Omega})$. *According to [5], it is sufficient for our purpose to have a bounded domain, which satisfies an exterior sphere condition at each point of the boundary* $\partial\Omega$ *and* $f \in C^\alpha(\Omega)$, $0 < \alpha < 1$.

REMARK 3.4. *For* $k\Delta t < 1$, *the operator* $B : H_0^1(\Omega) \to H^{-1}(\Omega)$, $B(v) = Av + (1/\Delta t - k)\beta(v)$ *is bounded, semi-continuous, strictly monotone and satisfies*

$$\frac{(B(v), v)}{||v||} \to +\infty \quad \textit{when} \ ||v|| \to +\infty.$$

Therefore, the problem (3.1) has a unique non-negative solution $v \in H_0^1(\Omega)$ *for non-negative* $v_n \in H_0^1(\Omega)$. *(See, e.g., [9].)*

3.3. Properties of the numerical solution. In preparation of a proof of convergence of the numerical method that will be given in the next paragraph, we describe some properties of the numerical solution. In particular these are results on the boundedness of the sequences (v_n) and (∇v_n).

LEMMA 3.5. *Let* $w \in L^\infty(\Omega)$ *be a solution of the obstacle problem (2.17). For* $n \geq 0$, *it holds*

$$v_n \leq w.$$

Proof. From the definition of w, we have $v_0 \leq w$, and we prove recurrently that $v_{n+1} \leq w$.

$$\begin{aligned} f(w) &= \frac{1}{\Delta t}(\beta(v_n) - \beta(w)) + k\beta(w) \leq \frac{1}{\Delta t}(\beta(w) - \beta(w)) + k\beta(w) \\ &= k\beta(w) \leq Aw. \end{aligned}$$

Thus, w is a supersolution of (3.1), which proves the Lemma. □

Since

$$\int_0^v \beta(s)ds \leq \beta(v)v \leq v,$$

finding the solution v_{n+1} of (3.1) is equivalent to finding a v_{n+1} that minimizes the functional

$$I(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 dx + \left(\frac{1}{\Delta t} - k\right) \cdot \int_\Omega \int_0^v \beta(s)dsdx - \frac{1}{\Delta t}\int_\Omega \beta(v_n)vdx,$$

where the lower bound is taken over the closed convex set K,

$$K = \{v \mid v \in H_0^1(\Omega),\ v \geq 0\}.$$

Therefore, we have the following inequality

$$I(v_n) \geq I(v_{n+1}),$$

and thus,

$$\begin{aligned}&\frac{1}{2}\int_\Omega |\nabla v_n|^2 dx + \left(\frac{1}{\Delta t} - k\right) \cdot \int_\Omega \int_0^{v_n} \beta(s) ds dx - \frac{1}{\Delta t}\int_\Omega \beta(v_n) v_n dx \\ &\quad\geq \frac{1}{2}\int_\Omega |\nabla v_{n+1}|^2 dx + \left(\frac{1}{\Delta t} - k\right) \cdot \int_\Omega \int_0^{v_{n+1}} \beta(s) ds dx - \frac{1}{\Delta t}\int_\Omega \beta(v_n) v_{n+1} dx.\end{aligned}$$

We can write the integral over Ω as integral over $\{x \in \Omega \,|\, v_{n+1}(x) \geq v_n(x)\} \cup \{x \in \Omega \,|\, v_{n+1}(x) < v_n(x)\}$ and obtain

$$\begin{aligned}&\int_\Omega \left(\int_0^{v_{n+1}} - \int_0^{v_n}\right) \beta(s) ds dx \\ &\quad = \int_{v_{n+1} \geq v_n} \int_{v_n}^{v_{n+1}} \beta(s) ds dx + \int_{v_{n+1} < v_n} \int_{v_{n+1}}^{v_n} -\beta(s) ds dx \\ &\quad \geq \int_{v_{n+1} \geq v_n} \beta(v_n)(v_{n+1} - v_n) dx + \int_{v_{n+1} < v_n} -\beta(v_n)(v_n - v_{n+1}) dx \\ &\quad = \int_\Omega \beta(v_n)(v_{n+1} - v_n) dx.\end{aligned}$$

Combining both inequalities yields

$$\frac{1}{2}\int_\Omega |\nabla v_n|^2 dx - k\int_\Omega \int_0^{v_n} \beta(s) ds dx \geq \frac{1}{2}\int_\Omega |\nabla v_{n+1}|^2 dx - k\int_\Omega \int_0^{v_{n+1}} \beta(s) ds dx.$$

Thus, we have proved the following Lemma:

LEMMA 3.6. *The sequence $(J(v_n))_{n\geq 0}$ is non-increasing, where J is defined by (2.13).*

From both previous Lemmas we can now derive that also $(\nabla v_n)_{n \geq 0}$ is uniformly bounded:

LEMMA 3.7. *The sequence $(\nabla v_n)_{n\geq 0}$ is uniformly bounded in $\mathbf{L}^2(\Omega)$.*

Proof. Since the sequence $(J(v_n))_{n\geq 0}$ is non-increasing, we get

$$\begin{aligned}||\nabla v_n||_2^2 &\leq k\int_\Omega \int_0^{v_n} \beta(s) ds dx + 2J(v_0) \leq k\int_\Omega \beta(v_n) v_n dx + 2J(v_0) \\ &\leq k\int_\Omega v_n dx + 2J(v_0) \leq \frac{k}{2}||v_n||_2^2 + \frac{|\Omega|}{2} + 2J(v_0).\end{aligned}$$

Since the sequence (v_n) is uniformly bounded in $L^2(\Omega)$, the Lemma is proved. ∎

LEMMA 3.8. *The sequence $(v_n)_{n\in\mathbf{N}}$ satisfies*

$$\sum_{n=0}^{N-1} \int_\Omega (\beta(v_{n+1}) - \beta(v_n))(v_{n+1} - v_n) dx \leq \frac{\Delta t}{1 - k\Delta t}(J(v_0) - J(v_N)) \tag{3.5}$$

Proof. Multiplying equality (3.1) by $v_{n+1} - v_n$ and integrating over Ω we obtain

$$\int_\Omega (\beta(v_n) - \beta(v_{n+1}))(v_{n+1} - v_n)dx + k\Delta t \int_\Omega \beta(v_{n+1})(v_{n+1} - v_n)dx$$
$$= \Delta t \int_\Omega \nabla v_{n+1} \nabla(v_{n+1} - v_n)dx = \frac{\Delta t}{2} \int_\Omega (|\nabla v_{n+1}|^2 - |\nabla v_n|^2 + |\nabla(v_{n+1} - v_n)|^2),$$

and thus

$$\int_\Omega (\beta(v_{n+1}) - \beta(v_n))(v_{n+1} - v_n)dx + \frac{\Delta t}{2} \int_\Omega (|\nabla v_{n+1}|^2 - |\nabla v_n|^2 + |\nabla(v_{n+1} - v_n)|^2)$$
$$= k\Delta t \int_\Omega \beta(v_{n+1})(v_{n+1} - v_n)dx.$$

From which we derive the inequality

$$\begin{aligned}
&\int_\Omega (\beta(v_{n+1}) - \beta(v_n))(v_{n+1} - v_n)dx \\
&\quad\le \frac{\Delta t}{2} \int_\Omega (-|\nabla v_{n+1}|^2 + |\nabla v_n|^2) + k\Delta t \int_\Omega \beta(v_{n+1})(v_{n+1} - v_n)dx \\
&\quad= \Delta t(J(v_n) - J(v_{n+1})) + \\
&\qquad\quad + k\Delta t \left(\int_\Omega \int_0^{v_n} \beta(s)dsdx - \int_\Omega \int_0^{v_{n+1}} \beta(s)dsdx + \int_\Omega \beta(v_{n+1})(v_{n+1} - v_n)dx \right) \\
&\quad\le \Delta t(J(v_n) - J(v_{n+1})) + \\
&\qquad\quad + k\Delta t \left(\int_\Omega -\beta(v_n)(v_{n+1} - v_n)dx) + \int_\Omega \beta(v_{n+1})(v_{n+1} - v_n)dx \right) \\
&\quad\le \Delta t(J(v_n) - J(v_{n+1})) + k\Delta t \int_\Omega (\beta(v_{n+1}) - \beta(v_n))(v_{n+1} - v_n)dx.
\end{aligned}$$

Therefore,

$$\int_\Omega (\beta(v_{n+1}) - \beta(v_n))(v_{n+1} - v_n)dx \le \frac{\Delta t}{1 - k\Delta t}(J(v_n) - J(v_{n+1})).$$

Adding this expression for n from 0 through $N - 1$, we obtain (3.5). ◻

3.4. Convergence of the method (3.1). We prove now that the solution of the backward Euler method (3.1) converges to the weak solution of (2.1) on the interval $[0, T]$. Furthermore, we obtain estimates on the numerical solution that allow us to extract by compactness a subsequence that converges to a function v.

First we define a piecewise linear approximation $u_{\Delta t}$ of u by

$$u_{\Delta t} := \beta(v_n) + \frac{t - t_n}{\Delta t}(\beta(v_{n+1}) - \beta(v_n)), \quad t_n \le t \le t_{n+1}. \tag{3.6}$$

and by $v_{\Delta t}$ we denote a corresponding approximation of v, which is defined by

$$v_{\Delta t} := \Phi(u_{\Delta t}). \tag{3.7}$$

THEOREM 3.9. *The sequence $(v_{\Delta t})$ is uniformly bounded in $C(0, T; H_0^1(\Omega))$ and its derivative in time is uniformly bounded in $L^2(0, T; L^2(\Omega))$.*

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Proof. Since the function Φ is convex and the sequence (v_n) is uniformly bounded in $H_0^1(\Omega)$, we can conclude that the sequence $(v_{\Delta t})$ is uniformly bounded in $C(0,T;H_0^1(\Omega))$. It remains to show that the sequence $dv_{\Delta t}/dt$ is uniformly bounded in $L^2(0,T;L^2(\Omega))$. From (3.6) and (3.7) we obtain with $T = N\Delta t$

$$\begin{aligned}\left\|\frac{d}{dt}v_{\Delta t}\right\|^2_{L^2(0,T;L^2(\Omega))} &= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega \Phi'(u_{\Delta t})^2\left(\frac{\beta(v_{n+1})-\beta(v_n)}{\Delta t}\right)^2 dxdt\\ &= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega \varphi(u_{\Delta t})^2\left(\frac{\beta(v_{n+1})-\beta(v_n)}{\Delta t}\right)^2 dxdt\\ &= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega \varphi\left(\beta(v_n)+\frac{t-t_n}{\Delta t}(\beta(v_{n+1})-\beta(v_n))\right)^2\left(\frac{\beta(v_{n+1})-\beta(v_n)}{\Delta t}\right)^2 dxdt\\ &= \frac{1}{\Delta t}\sum_{n=0}^{N-1}\int_\Omega(\beta(v_{n+1})-\beta(v_n))\int_{\beta(v_n)}^{\beta(v_{n+1})}\varphi(s)^2 dsdx\end{aligned}$$

Let us consider the integral $\int_{\beta(v_n)}^{\beta(v_{n+1})}\varphi(s)^2 ds$. By a change of variable $s = \beta(v)$ we can simplify this to

$$\int_{\beta(v_n)}^{\beta(v_{n+1})}\varphi(s)^2 ds = \int_{v_n}^{v_{n+1}}\varphi(\beta(v))^2\frac{dv}{\varphi(\beta(v))} = \int_{v_n}^{v_{n+1}}\varphi(\beta(v))dv.$$

Since the sequence $(v_n)_{n\geq 0}$ is uniformly bounded in $L^\infty(\Omega)$ this gives us

$$\int_{\beta(v_n)}^{\beta(v_{n+1})}\varphi(s)^2 ds \leq C(v_{n+1}-v_n).$$

With Lemma 3.8, we obtain thus

$$\begin{aligned}\left\|\frac{d}{dt}v_{\Delta t}\right\|^2_{L^2(0,T;L^2(\Omega))} &\leq \frac{C}{\Delta t}\sum_{n=0}^{N-1}\int_\Omega(\beta(v_{n+1})-\beta(v_n))(v_{n+1}-v_n)dx\\ &\leq \frac{C}{1-k\Delta t}(J(v_0)-J(v_N)) = \frac{C}{1-k\Delta t}\left(J(v_0)+k\frac{|\Omega|}{2}-\left(J(v_N)+k\frac{|\Omega|}{2}\right)\right).\end{aligned}$$

We want $J(v_N)+k\frac{|\Omega|}{2}$ to be bounded from below,

$$\begin{aligned}J(v_N) &= \frac{1}{2}\int_\Omega|\nabla v_N|^2dx - k\int_\Omega\int_0^{v_N}\beta(s)dsdx\\ &\geq \frac{1}{2}\int_\Omega|\nabla v_N|^2dx - k\int_\Omega v_N dx \geq \frac{1}{2}\int_\Omega|\nabla v_N|^2dx - \frac{k}{2}\int_\Omega v_N^2dx - k\frac{|\Omega|}{2}.\end{aligned}$$

Let λ_1 be the first eigenvalue of the Dirichlet problem, $-\Delta u = \lambda u,\ x\in\Omega;\ u = 0,\ x\in\partial\Omega$. If $k\leq\lambda_1$, we have $J(v)+k\frac{|\Omega|}{2}\geq 0$ for any $v\in H_0^1(\Omega)$; hence we get

$$\left\|\frac{d}{dt}v_{\Delta t}\right\|^2_{L^2(0,T;L^2(\Omega))} \leq \frac{C}{1-k\Delta t}\left(J(v_0)+k\frac{|\Omega|}{2}\right).$$

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If $k > \lambda_1$, we have

$$J(v_N) + k\frac{|\Omega|}{2} \geq \frac{1}{2}(\lambda_1 - k)||v_N||_2^2$$

and

$$\left\|\frac{d}{dt}v_{\Delta t}\right\|^2_{L^2(0,T;L^2(\Omega))} \leq \frac{C}{1-k\Delta t}\left(J(v_0) + k\frac{|\Omega|}{2} + \frac{1}{2}(k-\lambda_1)||v_N||_2^2\right).$$

This concludes the proof. □

THEOREM 3.10. *The sequence $(v_{\Delta t})_{\Delta t \geq 0}$ converges for $\Delta t \to 0$ to a weak solution v of (2.12) in $C(0,T;L^r(\Omega))$ ($r < \infty$ if $d = 2$, $r < 2/(d-2)$ if $d > 2$) and in $C(0,T;\Omega)$ (if $d = 1$).*

Proof. The sequence $(v_{\Delta t})_{\Delta t \geq 0}$ is uniformly bounded in $C(0,T;H_0^1(\Omega))$ and its derivative in time is uniformly bounded in $L^2(0,T;L^2(\Omega))$. According to [12], [9] we can extract a subsequence which converges to a function v in $C(0,T;\Omega)$ if $d = 1$ and in $C(0,T;L^r(\Omega))$ ($r < \infty$ if $d = 2$, $r < 2/(d-2)$ if $d > 2$).

It remains to show that this limit is a solution of (2.12). We again denote by $(v_{\Delta t})$ the extracted subsequence. Let φ be a test function in $C^2(\Omega \times (0,T)) \cap C^1(\overline{\Omega} \times [0,T])$, $\varphi(x,t) = 0$ for $x \in \partial\Omega$.

Multiplying the equality (3.1) by φ and integrating over Ω, we get

$$\frac{1}{\Delta t}\int_\Omega (\beta(v_{n+1}) - \beta(v_n))\varphi dx + \int_\Omega v_{n+1}A\varphi dx - k\int_\Omega \beta(v_{n+1})\varphi dx = 0.$$

Hence for $T = N\Delta t$, we have

$$\begin{aligned}\sum_{n=0}^{N-1}\frac{1}{\Delta t}\int_{t_n}^{t_{n+1}}\int_\Omega (\beta(v_{n+1}) - \beta(v_n))\varphi dxdt + \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega v_{n+1}A\varphi dxdt \\ - \sum_{n=0}^{N-1} k\int_{t_n}^{t_{n+1}}\int_\Omega \beta(v_{n+1})\varphi dxdt = 0.\end{aligned} \tag{3.8}$$

The second term in this equality may be written

$$\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega v_{\Delta t}(t)A\varphi dxdt + \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega (v_{n+1} - v_{\Delta t}(t))A\varphi dxdt. \tag{3.9}$$

If $\Delta t \to 0$, then the first part of this term converges to

$$\int_0^T\int_\Omega v(t)A\varphi dxdt.$$

Since

$$|v_{n+1} - v_{\Delta t}(t)| \leq |v_{n+1} - v_n|,$$

we estimate the second term of (3.9) by

$$\left|\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_\Omega (v_{n+1} - v_{\Delta t}(t))A\varphi dxdt\right|$$

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$$\leq \sum_{n=0}^{N-1} \Delta t \left(\int_\Omega |v_{n+1} - v_n| dx \right) ||A\varphi||_{C(0,T;\,\Omega)}$$
$$\leq \Delta t \left\| \frac{d}{dt} v_{\Delta t} \right\|_{L^1(0,T;L^1(\Omega))} ||A\varphi||_{C(0,T;\,\Omega)}.$$

This term tends to 0 and we have

$$\lim_{\Delta t \to 0} \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_\Omega v_{n+1} A\varphi dx dt = \int_0^T \int_\Omega v(t) A\varphi dx dt.$$

We study now the first term of (3.8). It can be written as

$$\sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_\Omega \frac{d}{dt}\beta(v_{\Delta t}(t))\varphi dx dt + \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_\Omega \left(\frac{\beta(v_{n+1}) - \beta(v_n)}{\Delta t} - \frac{d}{dt}\beta(v_{\Delta t}(t)) \right) \varphi dx dt. \tag{3.10}$$

The first part is equal to

$$\sum_{n=0}^{N-1} \int_\Omega (\beta(v_{n+1})\varphi(t_{n+1}) - \beta(v_n)\varphi(t_n)) dx - \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_\Omega \beta(v_{\Delta t}(t)) \frac{d\varphi}{dt} dx dt,$$

and this term converges to

$$\int_\Omega (\beta(v(x,T))\varphi(x,T) - \beta(v(x,0))\varphi(x,0)) dx - \int_0^T \int_\Omega \beta(v(t)) \frac{d\varphi}{dt} dx dt.$$

Since

$$\frac{d}{dt}\beta(v_{\Delta t}(t)) = \frac{\beta(v_{n+1}) - \beta(v_n)}{\Delta t},$$

the second term in (3.10) is equal to zero. We turn now to the estimate of the quantity

$$\sum_{n=0}^{N-1} k \int_{t_n}^{t_{n+1}} \int_\Omega \beta(v_{n+1})\varphi dx dt.$$

which can be re-written as

$$\sum_{n=0}^{N-1} k \int_{t_n}^{t_{n+1}} \int_\Omega (\beta(v_{n+1}) - \beta(v_{\Delta t}(t)))\varphi dx dt + \sum_{n=0}^{N-1} k \int_{t_n}^{t_{n+1}} \int_\Omega \beta(v_{\Delta t}(t))\varphi dx dt. \tag{3.11}$$

The second part of this term converges to

$$\int_0^T \int_\Omega \beta(v(t))\varphi dx dt.$$

The first part of (3.11) is equal to

$$\sum_{n=0}^{N-1} k \int_{t_n}^{t_{n+1}} \int_{\Omega} \left(1 - \frac{t-t_n}{\Delta t}\right) (\beta(v_{n+1}) - \beta(v_n))\varphi dx dt.$$

and is bounded by

$$\begin{aligned}
&\Delta t \sum_{n=0}^{N-1} k \left(\int_{\Omega} |\beta(v_{n+1}) - \beta(v_n)| dx\right) ||\varphi||_{C(0,T;\,\Omega)} \\
&\quad \leq C\Delta t \sum_{n=0}^{N-1} k||\beta(v_{n+1}) - \beta(v_n)||_2 ||\varphi||_{C(0,T;\,\Omega)} \\
&\quad = C\Delta t \sum_{n=0}^{N-1} k\Delta t||Av_{n+1} - k\beta(v_{n+1})||_2 ||\varphi||_{C(0,T;\,\Omega)} \\
&\quad \leq C\Delta t ||\varphi||_{C(0,T;\,\Omega)}
\end{aligned}$$

It follows that for every $\varphi \in C^2(\overline{\Omega} \times [0,T])$, v satisfies

$$\begin{aligned}
&\int_{\Omega} (\beta(v(x,T))\varphi(x,T) - \beta(v(x,0))\varphi(x,0))dx - \int_0^T \int_{\Omega} \beta(v(t)) \frac{d\varphi}{dt} dx dt \\
&\quad + \int_0^T \int_{\Omega} v(t) A\varphi dx dt - \int_0^T \int_{\Omega} \beta(v(t))\varphi dx dt.
\end{aligned}$$

Hence, v is a weak solution. Since this solution is unique, the sequence $(v_{\Delta t})_{\Delta t \geq 0}$ converges to v. This concludes the proof. ☐

REMARK 3.11. *The fact that for our method* $\frac{d}{dt}\beta(v_{\Delta t}(t)) - \frac{\beta(v_{n+1}) - \beta(v_n)}{\Delta t} = 0$ *simplifies the proof of Theorem 3.10. For other time-discretization scheme we should prove that the difference between the time derivative of the approximation* $u_{\Delta t}$ *and the approximation of the time derivative of* u *is small enough.*

REMARK 3.12. *In the case where the constant* k *is smaller than zero, the proof of the convergence for the numerical method is the same. It is easy to see that the null function is a subsolution and* $||v_n||_\infty$ *is a supersolution of problem (3.1).*

4. Application of the numerical method. In order to illustrate the proposed numerical method, we apply it to the prototype biofilm model (1.1) with initial and boundary conditions

$$\begin{cases} S|_{\partial\Omega} = S_1, & M|_{\partial\Omega} = 0, \\ S|_{t=0} = S_0, & M|_{t=0} = M_0 \end{cases}$$

describing a single-species/single-substrate biofilm. It is known that under these boundary conditions a unique solution with $M < 1$ exists for all $t > 0$ [4]. Although our method was derived independent of the space dimension we restrict ourselves to the one-dimensional case here, because this allows a simple visual representation of the numerical solution as a surface over the x-t-plane.

We carry out the transformation of the dependent variable M as described in section 2.2 above. Accordingly, by v we denote $\Phi(M)$ and instead of system (1.1) we solve the system

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for S and $v = \Phi(M)$

$$\left\{\begin{array}{l} \frac{\partial S}{\partial t} = d_1 \Delta S - \frac{k_1 S \beta(v)}{k_2 + S} \\ \frac{\partial \beta(v)}{\partial t} = d_2 \varepsilon \Delta v + \beta(v) \cdot \left(\frac{k_3 S}{k_2 + S} - k_4 \right) \\ S|_{\partial\Omega} = S_1, \quad v|_{\partial\Omega} = 0, \\ S|_{t=0} = S_0, \quad v|_{t=0} = \Phi(M_0). \end{array}\right. \tag{4.1}$$

The equation for S is a semi-linear reaction-diffusion equation, which does not pose any additional difficulties in the present context. For the sake of simplicity we use an implicit Euler method for its time-discretization. Thus, our semi-discretization in time leads to the following problem:

Let $N \in \mathbf{N}$ and $\Delta t = \frac{T}{N}$. For $n = 1, ..., N$ we look for functions S_n and v_n such that

$$\left\{\begin{array}{lcl} S_{n+1} - S_n & = & \Delta t d_1 \Delta S_{n+1} - \Delta t \frac{k_1 S_{n+1} \beta(v_{n+1})}{k_2 + S_{n+1}}, \\ \beta(v_{n+1}) - \beta(v_n) & = & \Delta t \epsilon d_2 \Delta v_{n+1} + \Delta t \beta(v_{n+1}) \left(\frac{k_3 S_{n+1}}{k_2 + S_{n+1}} - k_4 \right). \end{array}\right. \tag{4.2}$$

It is easy to see that the sequences (S_n) and (∇S_n) are bounded in L^∞ and L^2 respectively and the convergence result can be established in the same manner as it was done for the method (3.1).

The elliptic boundary value problem that has to be solved in every time-step is discretised by the standard finite element method.

$$\beta(u) \approx \sum_{j=1}^{N} \beta(u_j) \phi_j(x),$$

where ϕ_j are interpolation functions, $u_j \approx u(x^j)$ and $x^j \in \Omega$ are nodal points. As a results of this space discretization, we obtain a system of nonlinear equations in every time-step, which we solve using the one-step SOR-Newton method.

The diffusion coefficient $D_2(M)$ in the equation $(1.1)_2$ vanishes where $M = 0$ and the parabolic equation degenerates there. The set of such points where $M \to 0^+$ is the interface (between the biofilm and the surrounding aqueous phase). This interface defines also a set of points where $\beta(v)$ vanishes. It is known that in the neighborhood of such an interface the finite element method (and similarly other standard discretization schemes like finite differences and finte volumes) can yield oscillatory solutions, that are slightly negative beyond theoretical interfaces. These interface oscillations pose a numerical problem in their own right, which are beyond the scope of our study focusing on time integration. For the time being, we cut the solution and in each time step we use the "modified algebraic correction"

$$v_i := [v_i]_+.$$

A space-discretization scheme that adequately describes the interfaces shall be discussed in a forthcoming study.

4.1. Numerical results. We restrict ourselves to the interval $\Omega = (0, 1)$. The discrete system (4.2) is applied to solve the problem (1.1) with the following model parameters: $a = b = 1$, $d_1 = 60.0$, $d_2\varepsilon = 0.0025$, $k_1 = 3.27$, $k_2 = 0.00875$, $k_3 = 0.19$, $k_4 = 0.00001$. The initial substrate concentration is a given constant $S_0 = 1.5$ and we choose $S_1 = 1.5$. Several variants of initial biomass density M_0 are tested, in particular, a sine function, a sum of sines and a cap function. All simulations are carried out on an equidistant spatial grid.

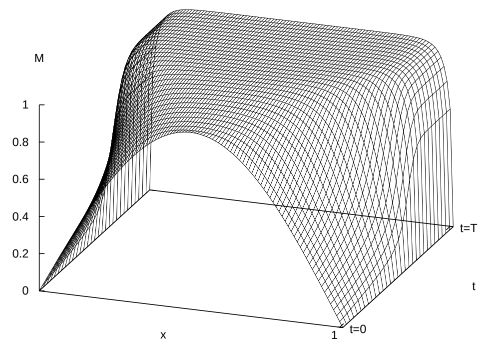

FIG. 4.1. *Evolution of the biomass density $M(t,x)$ for a single-bump initial function. The symmetry around the center of Ω is preserved. As t increases, the biofilm compresses, i.e., $M \to 1$.*

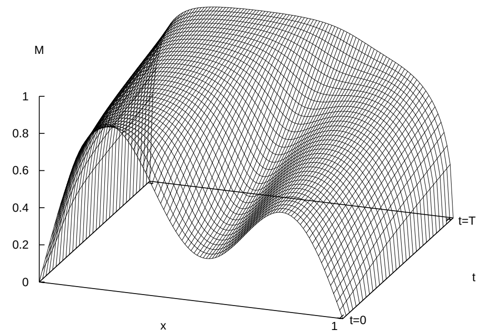

FIG. 4.2. *Evolution of the biomass density $M(t,x)$ for double-bump initial data; as t increases, the initially denser region grows faster, eventually both regions merge into one big colony.*

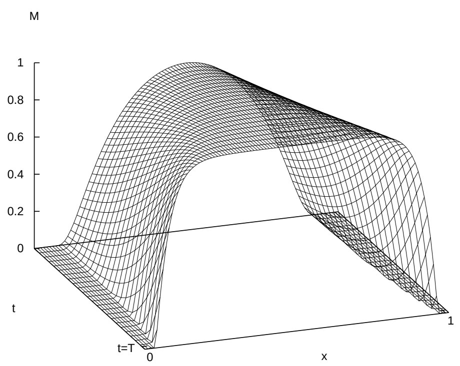

FIG. 4.3. *Evolution of the biomass density $M(t,x)$ for initial data that were positive only over a subset of Ω. The biofilm simultaneously compresses ($M \to 1$) and expands with a moving biofilm/water interface.*

The results for M are plotted in Figures 4.1-4.3. In all simulations S is such that it decreases inside the biofilm, i.e., inside the region where $M > 1$, due to decay as expressed by the negative sign of the reaction term.

Figure 4.1 shows the time evolution of the initial biomass defined by the function

$$M_0(x) = 0.95\sin(\pi x), \quad x \in (0,1).$$

In this example we have $T = 4.0$. In Figure 4.2 we illustrate the evolution of the initial biomass given by

$$M_0(x) = \frac{2}{5}\left(\sin(c\pi x) + \sin(c2\pi x) + \sin(c4\pi x)\right), \quad x \in (0,1),$$

where $c = 0.730445$ and, again, $T = 4.0$. In Figure 4.3 we plot the evolution of the initial biomass

$$M_0(x) = \begin{cases} 0.9\exp(-\frac{0.45^2}{0.45^2-x^2}), & 0.15 \le x \le 0.85, \\ 0, & \text{otherwise}, \end{cases} \tag{4.3}$$

until $T = 3.0$.

The behavior of the system is essentially determined by the value of the coefficients a,b and ε in the non-linear diffusion function. For example for $a = b = 3$ the term $\frac{M^b}{(1-M)^a}$ in the diffusion coefficient $D_2(M)$ is for $M < 10^{-4}$ smaller than $1.1 \cdot 10^{-12}$ and in numerical computation the interface is shifted. The function Φ grows very fast away from 0 and $\Phi(x) < 2.6 \cdot 10^{-13}$ for $x < 10^{-3}$. This implies that the biomass density inside the biofilm increases very slowly, while it grows quickly close to the interface, towards the nutrient source, i.e., the boundaries of the domain. This is due to both, higher nutrient availability at the interface than inside the biofilm, as well as due to pushing of biomass from inside the biofilm towards the interface as new biomass is produced in the biofilm (*squeezing property*). As a consequence, we get very large space derivatives of M at the interface (i.e., $\frac{dM}{dx}$). In case (4.3), where $t = 0$ the biomass density was not everywhere positive, this leads simultaneously to a compression of the biofilm (i.e., $M \to 1$) and to spatial expansion of the biofilm, i.e., to a moving interface.

Since $M = \beta(v)$, as a result of small perturbations in v we have big perturbations in M. In order to avoid these perturbations and consequently errors, we have to refine the mesh in a region where the derivative of $\beta(v)$ is large.

Let us consider the case $a = b = 3$ and pick the remaining parameters as in the previous examples. Starting computation from the initial cap function M_0 given by (4.3) after $t = 0.199$, the uniform spatial mesh was refined by six moving points in the interval (x_{i-1}, x_{i+1}) where the function $\beta(v)$ took a large jump; consequently, the timestep was refined as well. Figure 4.4 shows the evolution of the $\beta(v)$ after the time $T = 0.799$.

Data oscillation is intrinsic information missed by the averaging process associated with FEM. In our model that happened for some model parameters when the biomass grows fast or if the two initial colonies merge. The next step is to construct an efficient adaptive FEM method for the non linear stationary problems which we solve in each time step in order to ensure a reduction rate of data oscillations; this will be dealt with in a forthcoming study.

4.2. Comparison with alternative approaches. Since no non-trivial solution of equation (1.1) is explicitly known, we compare the numerical solution obtained with the proposed method with a solution that was computed by a relaxation method suggested in [10] for a similar problem. In this relaxation method, for a $u_0 \in (0,1)$ the functions $\tilde{b}$ and $\tilde{\beta}$ are defined by linearization as

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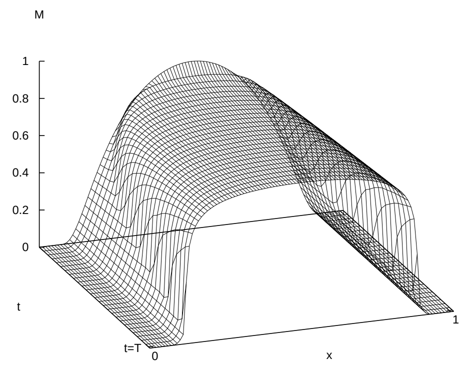

FIG. 4.4. *Solution surface $M(t,x)$ for initial data (4.3) with refined spatial grid at the biofilm/water interface.*

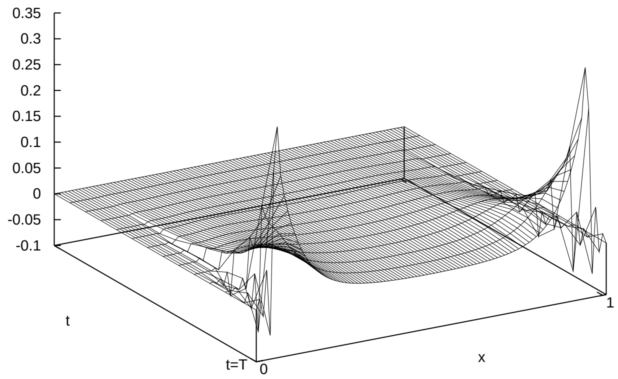

FIG. 4.5. *Comparison of the proposed transformation method (3.1) with the linearization approach (4.6) for the choice of parameter $d = 0.5$; the plotted surface shows the difference between both numerical solutions.*

$$\tilde{\beta}(x) = \begin{cases} \Phi(x), & x \le u_0, \\ \Phi'(u_0)(x - u_0) + \Phi(u_0), & x > u_0, \end{cases}$$

$$\tilde{b}(x) = \begin{cases} x, & x \le u_0, \\ b(\tilde{\Phi}(x)) = \beta(\Phi'(u_0)(x - u_0) + \Phi(u_0)), & x > u_0, \end{cases}$$

Thus, the equation

$$\frac{\partial}{\partial t}\beta(v) - d_2 \Delta v = k\beta(v), \quad x \in \Omega, \quad t > 0, \tag{4.4}$$

can be re-written as

$$\frac{\partial}{\partial t}\tilde{b}(w) - d_2 \Delta \tilde{\beta}(w) = k\tilde{b}(w), \quad x \in \Omega, \quad t > 0, \tag{4.5}$$

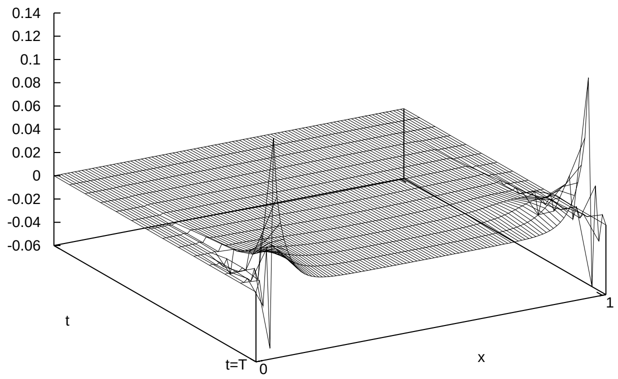

FIG. 4.6. *Comparison of the proposed transformation method (3.1) with the linearization approach (4.6) in section 4.2 for the choice of parameter* $d = 0.99$*; the plotted surface shows the difference between both numerical solutions.*

where $v = \tilde{\beta}(w)$. It is easy to see that the functions $\tilde{b}$ and $\tilde{\beta}$ are strictly monotone and Lipschitz-continuous:

$$0 \le \tilde{b}' \le 1, \qquad 0 \le \tilde{\beta}' \le \Phi'(u_0).$$

The relaxation approximation scheme of [10] applied to the equation (4.5) works as follows: On the time level $t_n = n\Delta t$, Θ_n is determined from the linear elliptic equation

$$\begin{aligned} &\lambda_n(\Theta_n - \tilde{\beta}(w_{n-1})) - \Delta t d_2 \Delta\Theta_n = k\Delta t \tilde{b}(w_{n-1}), \\ &\Theta_n = 0 \qquad \text{on} \quad \partial\Omega, \end{aligned} \tag{4.6}$$

where $\lambda_n \in L^\infty(\Omega)$ is a relaxation function. Function w_n is determined from

$$\tilde{b}_N(w_n) := \tilde{b}_N(w_{n-1}) + \lambda_n(\Theta_n - \tilde{\beta}(w_{n-1})),$$

where $\tilde{b}_N$ is the regularization of the function $\tilde{b}$,

$$\tilde{b}_N(s) := \tilde{b}(s) + \Delta t^d s.$$

The relaxation function λ_n is sought recusively in a finite number of steps. The following iteration scheme is used:

$$\begin{aligned} &\lambda_{n,k-1}(\Theta_{n,k} - \tilde{\beta}(w_{n-1})) - \Delta t d_2 \Delta\Theta_{n,k} = k\Delta t \tilde{b}(w_{n-1}), \\ &\Theta_n = 0 \qquad \text{on} \quad \partial\Omega, \end{aligned} \tag{4.7}$$

where

$$\bar{\lambda}_{n,k} := \frac{\tilde{b}(w_{n-1} + \mu_{n,k}(\Theta_{n,k} - \tilde{\beta}(w_{n-1})) - \tilde{b}(w_{n-1})}{\Theta_{n,k} - \tilde{\beta}(w_{n-1})} + \frac{2}{3}\Delta t^d, \tag{4.8}$$

$$\begin{aligned} &\lambda_{n,k} := \min\{\bar{\lambda}_{n,k}, \lambda_{n,k-1}\} && \text{for} \quad k = L, L+1, ... \qquad \text{and} \\ &\lambda_{n,k} := \bar{\lambda}_{n,k}, && \text{for} \quad k = 1, ..., L \end{aligned} \tag{4.9}$$

with

$$(4.10)\qquad \bar{\mu}_{n,k} := \min\left\{K, \frac{\tilde{\beta}^{-1}(\tilde{\beta}(w_{n-1}) + \alpha(\Theta_{n,k} - \tilde{\beta}(w_{n-1})) - w_{n-1}}{\Theta_{n,k} - \tilde{\beta}(w_{n-1})}\right\},$$

$$(4.11)\qquad \begin{array}{lll} \mu_{n,k} := \min\{\bar{\mu}_{n,k}, \mu_{n,k-1}\} & \text{for} \quad k = L, L+1, \ldots & \text{and} \\ \mu_{n,k} := \bar{\mu}_{n,k}, & \text{for} \quad k = 1, \ldots, L. & \end{array}$$

The constants d, α, L and K are parameters of the numerical method that must be chosen appropriately and case dependent. This is in contrast to method (3.1) introduced above, which does not require this kind of user interaction. More specific, $d \in (0,1)$, $\alpha \in (0,1)$ is close to 1, $\infty > L \geq 1$ is an integer, and $K \geq 0$ is a large constant. Since the difference quotient in (4.10) needs not be bounded, it is truncated by K. In the points $x \in \Omega$ where $\Theta_{n,k} - \tilde{\beta}(w_{n-1})$, the difference quotients in (4.8), (4.10) are defined by $\tilde{b}'(w_{n-1}) \min\{K, \frac{\alpha}{\tilde{\beta}'(w_{n-1}))}\}$, $\min\{K, \frac{\alpha}{\tilde{\beta}'(w_{n-1}))}\}$, respectively.

The iterations start with

$$(4.12)\qquad \mu_{n,0} := \min\{K, \frac{\alpha}{\tilde{\beta}'(w_{n-1})}\}, \qquad \lambda_{n,0} := \tilde{b}'(w_{n-1})\mu_{n,0} + \Delta t^d.$$

The choice $\lambda_{n,k} := \bar{\lambda}_{n,k}$, $\mu_{n,k} := \bar{\mu}_{n,k}$ is not convergent for $k \to \infty$, especially in the neighborhood of interfaces ($\tilde{b}'(x) = 0$, $\tilde{\beta}'(x) = 0$). By means of the construction (4.9), (4.11), the sequences $\lambda_{n,k}$,$\mu_{n,k}$ are forced to be monotone and hence convergent. In each time step a linear reaction-diffusion equation (4.6) is solved using the same finite element method for space discretization that was used above. The arising system of linear equations is solved directly (while the corresponding non-linear system of (3.1) is solved by the one-step SOR-Newton method).

In order to compare the relaxation method (4.6) with our method (3.1) in an example, we consider the initial boundary problem for equation (4.4) on interval $\Omega = (0,1)$. Picking $a = b = 1$, $v = 0$ on $\partial\Omega$ and the initial function $v_0 = \Phi(M_0)$, where M_0 is the cap function given by (4.3). To be able to observe the characteristic behavior of our system in a short time, we choose $d_1 = 0.05$ and $k = 5$. Again, equidistant spacing in x-direction is used. Figure 4.7 shows the evolution of the initial function until $t = 1.34$ calculated by method (3.1).

We operate (4.6) with parameters $K = 10^{10}$, $L = 100$ and $a = 0.99999$. The computations show hat for our example this method is greatly influenced by the choice of the methods parameters. The sequences $\bar{\lambda}_{n,k}$ and $\bar{\mu}_{n,k}$ do not converge with respect to k in the neighborhood of interfaces. It is not clear, however, how the choice of L influences the result of the computation. Greater L implies longer computing time (CPU), which makes direct comparison of both methods difficult in this regard; e.g., with chosen parameters, the relaxation method (4.6) needs five times more CPU time than the method (3.1). Figure 4.5 shows the difference between our solution and the solution computed by the method (4.6) with $d = 0.5$, while Figure 4.6 show this difference for $d = 0.99$.

The experiment was repeated with a smaller time step, keeping the remaining parameters unchanged. The difference between the solutions of the method (3.1) and method (4.6) is illustrated in Figure 4.8 for $d = 0.5$ and in Figure 4.9 for $d = 0.99$.

The results obtained by relaxation method (4.6) can be improved by a variant, in which for the iteration scheme for λ_n we use

$$(4.13)\qquad \bar{\lambda}_{n,k} := \frac{\tilde{b}(w_{n-1} + \mu_{n,k}(\Theta_{n,k} - \tilde{\beta}(w_{n-1})) - \tilde{b}(w_{n-1})}{\Theta_{n,k} - \tilde{\beta}(w_{n-1})},$$

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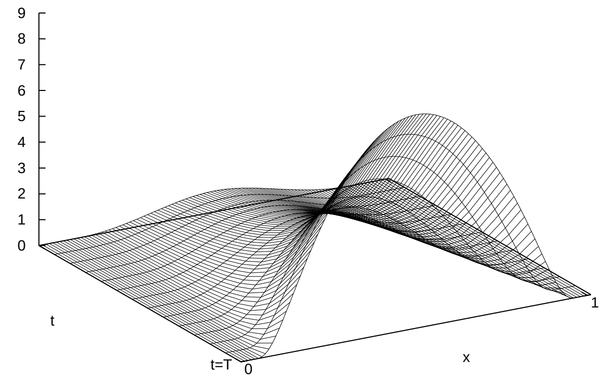

FIG. 4.7. *Solution of the test problem in section 4.2; plotted is the solution surface as computed by the proposed methods (3.1).*

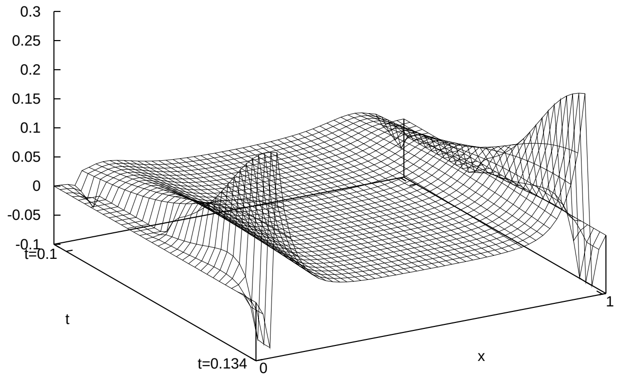

FIG. 4.8. *Comparison of the proposed transformation method (3.1) with the linearization approach (4.6) and the choice of parameter $d = 0.5$ with a smaller time-step than in Figure 4.5; the plotted surface shows the difference between both numerical solutions.*

instead of (4.8) and in which the iteration for λ_n is started with

$$\lambda_{n,0} := \tilde{b}'(w_{n-1})\mu_{n,0}, \tag{4.14}$$

This is illustrated in Figure 4.10 for the difference between the solution of the method (3.1) and the modified relaxation method for $t \leq T = 0.134$; Figure 4.11 shows this comparison for a decreased time-step (by one order of magnitude) for $t \in [0.1, T]$. This method, however, requires additional analysis.

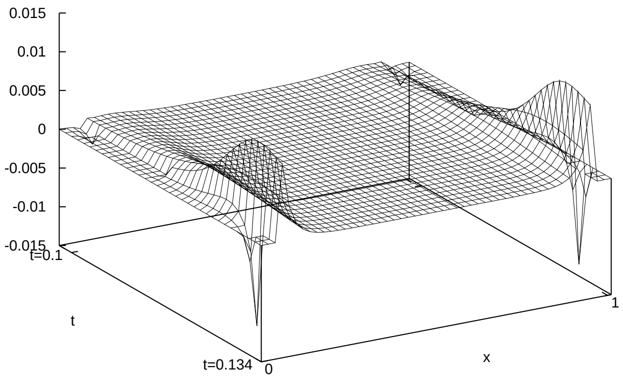

FIG. 4.9. *Comparison of proposed transformation method (3.1) with the linearization approach (4.6) and the choice of parameter $d = 0.55$ with a smaller time-step than in Figure 4.6; the plotted surface shows the difference between both numerical solutions.*

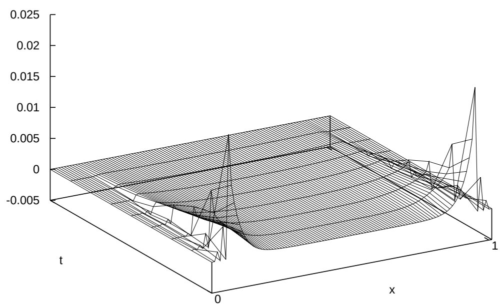

FIG. 4.10. *Comparison of the proposed transformation method (3.1) with the linearization approach (4.6), modified by (4.13), (4.14) with a smaller time-step than in Figure 4.5; the plotted surface shows the difference between both numerical solutions*

5. Conclusion. A numerical method for time-integration of a highly nonlinear reaction-diffusion equation arising in biofilm modeling was presented. This equation shows two non-standard effects: degeneracy as in the porous medium equation and a singularity as the dependent variable approaches its *a priori* known upper bound. The proposed discretization scheme focuses on the latter effect. It is based on a transformation of the dependent variable. The analysis of the method demonstrated its convergence and stability. By examples we illustrated that this method compares well with a previously published scheme for similar problems and a modification thereof. Compared to these alternatives, the scheme proposed here has the advantage of not requiring any additional *a priori* information on parameters that control the behavior of the method. Although the method is perfectly capable of treating the

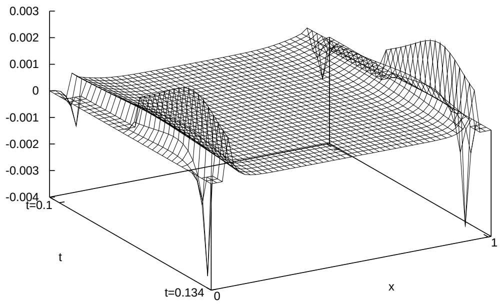

FIG. 4.11. *Comparison of the proposed transformation method (3.1) with the linearization approach (4.6), modified by (4.13), (4.14) with a smaller time-step than in Figure 4.10.*

singularity in the diffusion coefficient, the numerical simulations show that further attention must be brought now to space discretization around interfaces, e.g., where the solution has compact support or when two biofilm colonies merge.

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