



An efficient nonlinear finite-difference approach in the computational modeling of the dynamics of a nonlinear diffusion-reaction equation in microbial ecology



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ARTICLE INFO

Article history:

Received 3 October 2012

Received in revised form 29 May 2013

Accepted 29 May 2013

Keywords:

92B05

92D25

92D40

65M06

MSC:

Computational model

Mathematical ecology

Microbial film

Nonlinear modeling

Finite-difference method

ABSTRACT

In this manuscript, we present a computational model to approximate the solutions of a partial differential equation which describes the growth dynamics of microbial films. The numerical technique reported in this work is an explicit, nonlinear finite-difference methodology which is computationally implemented using Newton's method. Our scheme is compared numerically against an implicit, linear finite-difference discretization of the same partial differential equation, whose computer coding requires an implementation of the stabilized bi-conjugate gradient method. Our numerical results evince that the nonlinear approach results in a more efficient approximation to the solutions of the biofilm model considered, and demands less computer memory. Moreover, the positivity of initial profiles is preserved in the practice by the nonlinear scheme proposed.

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1. Introduction

In the last decade, there has been an increasing interest on the investigation of the growth dynamics of microbial biofilms, both to understand comprehensively the physical and the mathematical principles that govern biofilm growth, and to elucidate possible, relevant biomedical and biotechnological applications. Undoubtedly, biological films entail both an economic and a biological importance. Indeed, nowadays biofilms are considered a common cause of persistent infections; for instance, the Chinese National Institute of Health has estimated that at least 65% of all bacterial infections in humans are related to certain types of biological colonies (Chen et al., 2012). In addition, several nosocomial infections are presumed to be the result of the presence of pathogenic films in a wide range of medical devices, like catheters and probes used in

different hospital services. It is worthwhile to recall that microbial colonies in general are highly organized structures integrated by communities which are surrounded by a protective extracellular matrix. This important feature makes them resistant to both antibiotic treatment and host defense systems.

On the other hand, microbial films can grow in many different natural and no-natural environments, and may be considered benign or detrimental depending upon its place of growth. Biological films may be conformed by a single or by multiple species with different metabolic mechanisms which, in many cases, function as cooperative consortia. Here, it is important to mention that these cooperative consortia have encountered useful practical applications in the treatment of polluted water (Cao et al., 2012; Castillo et al., 2011; Ellwood et al., 2011; Jiao et al., 2011), in the development of microbial fuel cells to produce electricity (Jain et al., 2011; Liu et al., 2008, 2010; Yang et al., 2011), in the design of biosensors (Checa et al., 2012; Velusamy et al., 2010), among other applications of practical relevance. However, there are also scenarios in which the formation of biological films results in the deterioration of surfaces due to the microbial-influenced corrosion (Upadhyayula and Gadhamshetty, 2010; Little et al., 2008). Despite the many efforts to simulate and understand the complex nature of microbial

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aggregates, there still exists the need to explore deeper into the many variables that accompany this mechanism. For instance, the influence of self-generated attractants on *Escherichia coli* clustering has been studied in Kim et al. (2007). In that report, a discrete model was used to investigate the role of parameters such as chemotaxis sensitivity, geometry and initial conditions, in order to describe the joint dynamics of bacteria and attractants.

From a more mathematical point of view, the models which describe the growth dynamics of biological film are mainly provided in the form of systems of partial differential equations with nonlinear diffusion and reaction terms (Efendiev et al., 2002). Some of these mathematical models take into account the most important features of biological films observed in the practice, like

- (a) the presence of a sharp front of biomass at the fluid/solid transition,
- (b) the existence of a threshold of biomass density,
- (c) the fact that the biomass spreading is significant only when the biomass is close to the threshold,
- (d) the application of reaction kinetics mechanisms in the production of biomass,
- (e) the compatibility of the biomass spreading mechanism with hydrodynamics and with nutrient transfer/consumption models,

among other characteristics observed experimentally. Moreover, some mathematical background for these systems of equations is readily available in the literature, in the form of theorems on the existence and uniqueness of positive and bounded solutions. However, in view of the enormous mathematical complexity of these nonlinear partial differential equations, the task of providing analytical expressions of the solutions to meaningful initial conditions is practically impossible to accomplish.

In view of such mathematical limitations, several computational approaches have been taken to simulate the growth dynamics of microbial colonies. For instance, some related techniques are based on stochastic computational modeling (McCollum et al., 2006). For deterministic models, the finite-difference approach has been proposed in works like Eberl et al. (2001), and some differential-discrete cellular automata have been employed with success in the growth of gel beads (Picioreanu et al., 1998, 1999). The finite-element and the finite-volume methodologies have proved fruitful, too, like in Duddu et al. (2008), Böl et al. (2008), Smith et al. (2007) or Gallo and Manzini (2003), Picioreanu et al. (2000), Szego et al. (1993), respectively.

In the present work, we employ a finite-difference approach to approximate solutions of a nonlinear partial differential equation in the investigation of biological films. More concretely, our investigation is partly motivated by the results presented in Eberl et al. (2001), which reports on a successful finite-difference discretization of a nonlinear equation from mathematical ecology, which is capable of preserving the positivity of the approximations among other relevant mathematical characteristics of the solutions. The discretization introduced in that work is an implicit, linear approach whose implementation is provided in terms of a sparse matrix with number of rows equal to the discrete grid size. The preservation of the properties of positivity and boundedness is achieved using the theory of M-matrices, which are non-singular, real matrices for which the entries of their inverses are all positive numbers (Fujimoto and Ranade, 2004). The method works at the expense of large computational memory and lengthy simulation times. In the present work, however, we provide an explicit, nonlinear finite-difference technique to approximate the solutions of the same model investigated in Eberl et al. (2001) but, as the numerical simulations show, our approach is computationally faster and absorbs less computational resources.

The present manuscript is divided as follows. In Section 2, we introduce the mathematical model of interest in this work. We present therein some relevant results on the existence and uniqueness of positive and bounded solutions of the biofilm equation under investigation. In Section 3, we introduce the finite-difference discretization of our model. The method is an explicit, nonlinear technique whose computational realization requires a convenient implementation of Newton's method for solving nonlinear equations. Section 4 presents some simulations that evince the fact that the method is capable of preserving the property of positivity in the practice. Finally, we close this manuscript with some discussions and some concluding remarks.

2. Mathematical model

2.1. Simplified model

Let Ω be a closed and connected subset of \mathbb{R}^2 or \mathbb{R}^3 , and let $u : \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}$ be a function. Throughout this work, we suppose that α, β and γ are positive real numbers, such that $\alpha > 1, \beta > 1$ and $\gamma \ll 1$. In this manuscript, we consider the partial differential equation with nonlinear diffusion factor

$$\frac{\partial u}{\partial t}(\mathbf{x}, t) = \nabla \cdot (D(u(\mathbf{x}, t))\nabla u(\mathbf{x}, t)) + G(\mathbf{x}, t)u(\mathbf{x}, t), \quad (1)$$

where $(\mathbf{x}, t) \in \Omega \times \mathbb{R}^+$, and ∇ denotes the gradient operator in the spatial domain. Here, the reaction function $G : \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}$ is continuous, and the diffusion factor $D : [0, 1) \rightarrow \mathbb{R}$ is provided by the expression

$$D(u) = \frac{\delta u^\alpha}{(1-u)^\beta}. \quad (2)$$

Evidently, the variable \mathbf{x} represents spatial position, while t denotes time.

2.2. General model

Eq. (1) is a simplified version of the growth model investigated in Eberl et al. (2001). Indeed, let s_0 and u_0 be real functions defined on Ω , and consider the spatially two- or three-dimensional equation

$$\begin{cases} \frac{\partial s}{\partial t}(\mathbf{x}, t) = d_1 \nabla^2 s(\mathbf{x}, t) - K_1 \frac{s(\mathbf{x}, t)u(\mathbf{x}, t)}{K_4 + s(\mathbf{x}, t)}, \\ \frac{\partial u}{\partial t}(\mathbf{x}, t) = d_2 \nabla \cdot D(u(\mathbf{x}, t))\nabla u(\mathbf{x}, t) - K_2 u + K_3 \frac{s(\mathbf{x}, t)u(\mathbf{x}, t)}{K_4 + s(\mathbf{x}, t)}, \end{cases} \quad (3)$$

for every $(\mathbf{x}, t) \in \Omega \times \mathbb{R}^+$. Appropriate initial-boundary conditions are required, namely,

$$\begin{cases} s(\mathbf{x}, t) = 1, u(\mathbf{x}, t) = 0, & \forall \mathbf{x} \in \partial\Omega, \forall t \geq 0, \\ s(\mathbf{x}, 0) = s_0(\mathbf{x}), u(\mathbf{x}, 0) = u_0(\mathbf{x}), & \forall \mathbf{x} \in \Omega. \end{cases} \quad (4)$$

In this model, s physically represents the substrate concentration and u denotes the biomass density. The non-negative constants d_1, d_2, K_1, K_2, K_3 and K_4 stand for the substrate diffusion coefficient, the biomass diffusion coefficient, the maximum specific consumption rate, the biomass decay rate, the maximum specific growth rate, and the monod half saturation constant.

2.3. Existence and uniqueness

The following theorem guarantees the existence and the uniqueness of positive and bounded solutions of (3) subject to the

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