



A novel model for biofilm growth and its resolution by using the hybrid immersed interface-level set method



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ABSTRACT

In this work we propose a new model to simulate biofilm structures (“finger-like”, as well as, compact structures) as a result of microbial growth in different environmental conditions. At the same time, the numerical method that we use in order to carry out the computational simulations is new to the biological community, as far as we know. The use of our model sheds light on the biological process of biofilm formation since it simulates some central issues of biofilm growth: the *pattern formation of heterogeneous structures, such as finger-like structures*, in a substrate-transport-limited regime, and the formation of more compact structures, in a growth-limited-regime. The main advantage of our approach is that we consider several of the most relevant aspects of biofilm modeling, particularly, the existence and evolution of a biofilm–liquid interface. At the same time, in order to perform numerical simulations, we have used sophisticated numerical techniques based on mixing the immersed interface method and the level-set method, which are well described in the present work.

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1. Introduction

Biofilm processes are of interest to researchers in a wide variety of fields including purposes of filtration, bioremediation, or barrier formation. A biofilm is a complex and heterogeneous matrix of microorganisms attached to and growing on a surface. Biofilms are most often found on solid substrates that are exposed to an aqueous solution [1]. The liquid usually supplies nutrients (substrates) utilized by the microorganisms in the biofilm, while pieces of biofilm solids detach from the biofilm compartment and move to the bulk-liquid compartment. The exchange between the biofilm and the liquid may lead to spatially heterogeneous architectures that can induce complex flow patterns and affect mass transport. Thus, mass transport due to diffusion and advection in the fluid compartment should be explicitly considered. The latter implies that the hydrodynamic flow field should be taken into account as well [2–6]. The accumulation of biofilm depends on hydrodynamic processes that bring cells to the biofilm surface, physical–chemical properties that determine the propensity of microbes to attach to the biofilm, and environmental characteristics such as substrate concentrations that determine biofilm growth. Cells may also be removed from the biofilm by biological processes or flow properties that lead to desorption and detachment [1].

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In this paper, we study a model that considers most of the key aspects mentioned in the previous paragraph. The only feature that we do not consider is the attachment/detachment of cells to the biofilm. Instead, we consider a biofilm already attached to a surface and study the effects of the substrate, the pressure inside of the biofilm, as well as the hydrodynamic flow field in its growth. A model, which considers attachment/detachment, would require discrete representations of microorganisms that may hold them together or, if fluid stress is large, the fluid may yield and release microbes [1]. There is consensus that the most relevant aspects in a biofilm model are, on the one hand, the existence of an interface between the biofilm and the liquid and, on the other hand, the biofilm structure, which is affected by the influence of biomass growth in relation to substrate transport. Porous biofilms, with many channels and voids between the “finger-like” or “mushroom” outgrowth, were obtained in a substrate-transport-limited regime. Conversely, compact and smooth biofilms occurred in systems limited by the biomass growth rate and not by the substrate transfer rate [3].

In this paper we propose a new model for biofilm formation and use the *immersed interface method* (IIM), coupled to the *level set method* for its numerical implementation. The IIM, first introduced by LeVeque and Li [7] to model elliptic problems with discontinuous coefficients and singular source terms, has evolved (coupled with others methods) into a general blended method that can be used to study two-phase flows, among others applications. The name of the method derives from the fact that the interface between both fluids is modeled as a free boundary, which may have a complex structure, immersed in a *unique* fluid. Thus, this interface defines and separates different regions inside the fluid.

Biofilm research is an active area within the microbiology community, as researchers recognize that attached organisms often predominate in a wide range of medical, natural, and industrial environments. Consequently, effective biofilm models could be a fast and cost-effective aid for biologists. The problem of biofilm growth has been studied intensively in the recent years. Here we mention the following papers, which are closely related with the use of partial differential equations based models:

- The paper by Dockery and Klapper [8], in which a biofilm model is considered to be analogous to a fluid flowing in a porous medium. These authors compute the velocity and pressure of the biofilm, modeling it as an incompressible viscous fluid.
- The paper by Eberl and Demaret [9] studies a biofilm model based on a degenerated diffusion–reaction equation, in which the biomass density of the biofilm is the unknown, and assuming a non-linear dependence of the diffusion coefficient on this biomass density.
- The paper by Dillon et al. [1], in which a biofilm model is studied using a variant of the *immersed boundary method*, introduced by Peskin [10] in the modeling of blood flow in the heart. This model incorporates various hydrodynamic coupled effects like reaction, diffusion and convection of a substrate, as well as the chemotactic response of microbes to attachment/detachment (both cell–cell aggregation and cell-wall adhesion). The problem of this model is the fact that it is too difficult to be implemented and requires numerical resolution of Navier–Stokes equations with a singular force term.
- Studies by others authors [3–6] analyze a biofilm model based on a hybrid differential-discrete cellular automaton approach. Picioreanu et al. [3] characterized the complete biofilm structure (surface and volume structure) and found that a key factor affecting biofilm structure is the influence of biomass growth in relation to the substrate transfer. These authors represent soluble components (e.g., substrates) in a continuous field, whereas a discrete mapping is used for the solid components (e.g., biomass). They validate their results with measured data from a well-characterized system: the growth of immobilized cells in a gel matrix. Finally, Picioreanu et al. [6] investigated the effect of convective and diffusive substrate transport on biofilm heterogeneity. They obtained similar results as in their previous work, namely that variations in external mass transfer resistance (due to convection and flow-driving mechanisms) have less effects on biofilm development. Thus, they concluded that the determining factor is still the internal resistance to substrate transport.
- The paper by Alpkvist and Klapper [11] proposes a model for the heterogeneous growth of biofilm systems with multiple species and multiple substrates. This paper is a generalization of the previous 2-D model [8] and of the earlier 1-D model [12], and enabled the authors to perform simulations that may represent biofilm systems for which a one-dimensional model is an inadequate description or, conversely, may under some circumstances, verify adequacy of one dimensional representation.
- The paper by Duddu et al. [13] proposes a hybrid extended Finite Element Method (XFEM)–level set method for the growth of biofilms. This method does not require an explicit representation of the biofilm–fluid interface (as in our method). These authors obtained finger formation and incipient tip splitting, behaviors observed in real biofilms.
- The paper by Cogan [14] proposes a model of biofilm disinfection in two dimensions, where the biofilm is treated as a viscous fluid immersed in a fluid of less viscosity. The motion of the fluid is coupled to the biofilm inducing motion in it. Both the biofilm and the bulk fluid are dominated by viscous forces; hence the Reynolds number is negligible and the appropriate equations are Stokes equations. In our paper, we also model the biofilm as a slow viscous fluid, but we assume that the biofilm as well as the liquid satisfies the Hele–Shaw equations instead of the Stokes equations.
- The paper by Ward et al. [15] proposes mathematical models for the formation, growth and quorum sensing activity of bacterial biofilms in its early development.
- Similarly in others papers [16–18] a hierarchy of mathematical models for antibacterial therapies targeted at the primary quorum-sensing system of a well-mixed, planktonic population and an early-stage (closely packed) biofilm is developed.
- The papers by Zhang et al. [19,20] develop a hierarchy of phase field-based models for biofilms in 1-D and 2-D respectively. In [19] a set of phase field models for biofilms using the one-fluid two-component formulation is derived, in which the combination of extracellular polymeric substances (EPS, or polymer networks) and the bacteria is effectively modeled as one fluid component, while the collective ensemble of nutrient substrates and the solvent are modeled as the

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