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Phase-Field Models for Biofilms II. 2-D Numerical Simulations of Biofilm-Flow Interaction

Tianyu Zhang[1], Nick Cogan[1] and Qi Wang[1,2,*]

[1] *Department of Mathematics, Florida State University, Tallahassee, FL 32306-4510, USA.*
[2] *School of Mathematics, Nankai University, Tianjin 300071, China.*

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Abstract. We study the biofilm-flow interaction resulting in biofilm growth, deformation and detachment phenomena in a cavity and shear flow using the phase field model developed recently [28]. The growth of the biofilm and the biofilm-flow interaction in various flow and geometries are simulated using an extended Newtonian constitutive model for the biofilm mixture in 2-D. The model predicts growth patterns consistent with experimental findings with randomly distributed initial biofilm colonies. Shear induced deformation, and detachment in biofilms is simulated in a shear cell. Rippling, streaming, and ultimate detachment phenomena in biofilms are demonstrated in the simulations, respectively, in a shear cell. Possible merging of detached biofilm blobs in oscillatory shear is observed in simulations as well. Detachment due to the density variation is also investigated shedding light on the possible bacteria induced detachment.

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Key words: Biofilm, Cahn-Hilliard equation, phase filed, finite difference method, multiphase flow.

1 Introduction

Biofilms are ubiquitous in nature and manmade materials. Biofilms form when bacteria adhere to surfaces in moist environments by excreting a slimy, glue-like substance. Sites for biofilm formation include all kinds of surfaces: natural materials above and below ground, metals, plastics, medical implant materials, plants and body tissues. Wherever you find a combination of moisture, nutrients and a surface, you are likely to find biofilms [8,14,16,20].

A biofilm community can be formed by a single bacterial species, but in nature biofilms almost always consist of rich mixtures of many species of bacteria, as well as fungi, algae,

*Corresponding author. *Email addresses:* `zhang@math.fsu.edu` (T. Zhang), `cogan@math.fsu.edu` (N. Cogan), `wang@math.fsu.edu` (Q. Wang)

yeasts, protozoa, other microorganisms, debris and corrosion products. Biofilms are held together by sugary molecular strands, collectively termed "extracellular polymeric substances" or "EPS". The cells produce EPS and are held together by these strands, allowing them to develop complex, three-dimensional, resilient, attached communities. Biofilms cost the U.S. literally billions of dollars every year in energy losses, equipment damage, product contamination and medical infections. But biofilms also offer huge potential for bio-remediating hazardous waste sites, bio-filtering municipal and industrial water and waste water, forming bio-barriers to protect soil and ground water from contamination, as well as heap leaching.

It is a challenge to model the live microorganism in biofilms and their transient growth and transport behavior. There have been various multi-fluid models proposed to predict growth behavior of biofilms [1,7,19,27] and models to simulate biofilm growth and transport phenomena [9,17,18,22–25]. However, it becomes tricky when one uses the multi-fluid models to study biofilm dynamics in another fluid since the velocity boundary conditions for the multi-fluid model are often hard to define. When constitutive equations are also present for viscoelastic components, there could also be boundary conditions for the extra elastic stress tensor corresponding to the components, creating another layer of complications for the use of the models. Hence, for flow-biofilm interaction, a single fluid model would be more appropriate and efficient, in which a single mass average velocity serves as the measurable macroscopic velocity.

Recently, we developed a phase-field based hydrodynamic theory for mixtures of biofilm and solvent using the one fluid multi-component formulation [2,28]. The model captures the long wave growth phenomenon exhibited in the biofilm growth. The preliminary study on 1-D biofilm growth shows promising results for the theory to be used in studying dynamics of the biofilm and the interaction with the ambient solvent. In this paper, we continue our investigation of the biofilm dynamics in 2 space dimensions using the phase field theory with an extended Newtonian constitutive equation for the EPS polymer network in the biofilm.

2 Mathematical model

We first recall the mathematical model developed for the mixture of biofilms and solvent in [28]. Let $\mathbf{v}$ be the average velocity, p the pressure, ϕ_n and ϕ_s the volume fraction of the polymer network and solvent respectively, and c the nutrient concentration. The phase field theory for biofilms consists of four sets of equations of multiple variations.

2.1 Momentum and continuity equation

Consider

$$\begin{aligned} &\nabla\cdot\mathbf{v}=0,\\ &\rho\frac{d\mathbf{v}}{dt}=\nabla\cdot(\phi_n\tau_n+\phi_s\tau_s)-[\nabla p+\gamma_1 kT\nabla\cdot(\nabla\phi_n\nabla\phi_n)], \end{aligned} \tag{2.1}$$