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3-D Numerical Simulations of Biofilm Flows

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Abstract. We study the biofilm-flow interaction resulting in biofilm growth and deformation in a water channel in a 3-D setting using the phase field model developed recently [28, 29]. In this biofilm model, the biofilm made up of the EPS, bacteria and solvent is tracked using a biofilm volume fraction which vanishes outside the biofilm region. The interface between the biofilm and the solvent is marked by the zero level surface of the volume fraction measured from the biofilm to the solvent. The growth of the biofilm and the solvent-biofilm interaction with the top nutrient feeding condition is simulated in the viscous regime (growth regime) of the biofilm-solvent mixture flow. In quiescent flows, the model predicts growth patterns consistent with experimental findings for single or multiple adjacent biofilm colonies, in which the known mushroom shape growth pattern is obtained. Shear induced deformation in biofilms is simulated in a shear cell, providing a viable numerical evidence for using simulation tool to study biofilm growth and interaction dynamics in aqueous environment.

AMS subject classifications: 65M06, 76D05, 76A05, 76T30, 76Z05, 92C05

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

1. Introduction

Biofilms are ubiquitous in nature, water filtering devices, plumbing pipes, medical implants, and dentistry etc. 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, teeth, plants and body tissues. Wherever you find a combination of moisture, bacteria, nutrients and a surface, you are likely to find biofilms.

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, yeasts, protozoa, other microorganisms, debris and corrosion products. Biofilms are

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held together by sugary molecular strands, collectively termed “extracellular polymeric substances" or “EPS". The bacterial cells produce EPS; and they 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 can 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, and as well as heap leaching [7, 11, 13].

The formation of biofilm colonies is a complex biological and transport phenomenon. The arrival of the EPS producing biological cells react to the environment and communication among themselves to build their biofilm community. In this process, a supporting substrate, sufficient number of EPS producing cells, sufficient delivery and supply of nutrient materials, and cellular communication dictate how the community is built. Experimentally, one notices that the gene expression of the biofilm is quite distinct from the gene expression of a platonic cell and then turn to suspect that the biofilm community not only protect the encased bacterial or other biological cells, but also alter their cellular behavior. The viable explanation is that there exist active cellular communication channels or signaling pathways to alter the cellular response and function in the biofilm community. Quorum sensing is a phenomenon identified with the microorganism like the biofilm in which certain cellular behavior is turned on or off depending on the baseline population in the biofilm community. On the other hand, for the living organisms, supply of nutrients is vital to their survival and development.

Biofilms consist of a large amount of water in addition to bacteria, EPS, and various nutrients. The EPS exists in the form of polymeric networks allowing sustances of small molecules such as water and nutrients to permeate as well as large bacterial cells to migrate. So, the biofilm collectively behave like a gel. It is a challenge to model the live microorganism in biofilms and their transient growth, molecular signaling and transport behavior altogether. There have been various multi-fluid models proposed to predict growth behavior of biofilms, in which the biofilm community is modeled either using hybrid discrete and differential models [20–24] or mechanistically using continuum models as a biological gel [6, 14–19, 27]. However, it becomes tricky when one uses the biogel models to study dynamics of biofilms in another fluid in a geometry where an inflow and outflow boundary condition need to be specified since the velocity boundary conditions for the multi-fluid model are 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 complication for the use of the models.

The fundamental assumption in the multi-fluid models is that the momentum of each fluid component must be conserved so that the individual velocity for each fluid is employed. In practice, it’s the average velocity of the mixture that can be measured in various fluid devices. Often, it is the mass average velocity chosen as the one to be measured. With the notation of the average velocity, each individual velocity is decomposed into a sum of the average one and an excessive one. The hydrodynamical identity of the excessive veloc-