Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2017-0165

Vol. **24**, No. 3, pp. 695-741
September 2018

Numerical Solution of a Degenerate, Diffusion Reaction Based Biofilm Growth Model on Structured Non-Orthogonal Grids

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Received 4 August 2017; Accepted (in revised version) 28 December 2017

Abstract. A previously developed semi-implicit method to solve a density dependent diffusion-reaction biofilm growth model on uniform Cartesian grids is extended to accommodate non-orthogonal grids in order to allow simulation on more complicated domains. The model shows two non-linear diffusion effects: it degenerates where the dependent solution vanishes, and a super-diffusion singularity where it approaches its upper bound. The governing equation is transformed to a general non-orthogonal $\xi-\eta$ curvilinear coordinate system and then discretized spatially using a cell centered finite volume method. The nonlinear biomass fluxes at the faces of the control volume cell are split into orthogonal and non-orthogonal components. The orthogonal component is handled in a conventional manner, while the non-orthogonal component is treated as a part of the source term. Extensive tests showed that this treatment of the non-orthogonal flux component on the control volume face works well if the maximum deviation from orthogonality in the region of the grid where the biomass is growing is within 15-20 degrees. This range of validity is smaller than the one obtained with the same method for the simpler porous medium equation which is the standard test problem for degenerate diffusion equation but does not have all of the features of the biofilm model.

AMS subject classifications: 35K57, 35K65, 65N08

Key words: Biofilms, degenerate diffusion, non-orthogonal grids.

1 Introduction

Bacterial biofilms are aggregates of microbes that grow on surfaces in an aqueous environment. They form when bacterial cells attach themselves to the surface and begin

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producing Extracellular Polymeric Substances (EPS) within which the growing bacteria cells remain embedded. Biofilms are ubiquitous, as they can be found growing in all places where sufficient nutrient is available to sustain microbial growth. They are present in both industrial and natural systems; as well as in surface and subsurface waters and soils. In environmental engineering applications like waste-water treatment [36] they play a positive role while in medical context they are the source of many infections [3]. Bacterial biofilms can exhibit complicated morphologies. The morphological features of a growing biofilm depends both on the biological factors like maximum cell density, specific growth rate as well as on the environmental conditions like nutrient availability [10] and hydrodynamic conditions. In nutrient rich environments, individual biofilm colonies grow quickly and form homogeneous compact layers, while in nutrient limited conditions biofilms tend to grow into patchy structures [25].

In combination with the aforementioned factors, the sustainability of biofilms also depends on the surface topography of the substratum on which the biofilms are attached. In the presence of fluid flow, meso-scale surface features like cracks and crevices with size (in the order of 10-100's of microns) greater than that of a single cell have been shown to influence biofilm growth and sustainability through means other than affecting the cell attachment process. For example, studies done in [4] to investigate biofilm accumulation in a model food processing equipment under different flow conditions have observed that increased surface microbial loads was present in the areas around recesses on the surfaces which were characterized by the presence of recirculating flow and low shear stress. Likewise, studies done in [24] to investigate the susceptibility to antibiotics of biofilms growing in glass flow cells with artificial crevices observed that the biofilm growing on the top of the crevices were effectively treated while the biofilm growing in the base of the crevice survived the antibiotic treatment and continued to grow once the antibiotic treatment was discontinued. Biofilms in different applications grow on surfaces with different topographical features, in contrast, biofilm growth experiments conducted in labs as well as biofilm growth modeling studies in simulations are often conducted in simple flow cell geometries which lack these surface features. Therefore to understand the effect of these surface features on biofilm growth, sustainability and removal, experiments and modeling studies need to be conducted in setups which have these specific surface features.

Mathematical modeling and simulation [23,51] provides us an effective way to understand and predict the growth of biofilms under different conditions. The model which is the focus of our current study was proposed as a prototype biofilm growth model in [10] and solved numerically to simulate the growth of a 2D heterogeneous single species biofilm with a single limiting nutrient. Since its introduction in [10], the model has been extended to accommodate a multi-species biofilm, model EPS production, model response to antibiotics, model quorum sensing mode of communication with and without fluid flow, and model internally triggered dispersal (see [8, 11, 14, 16, 17, 22, 27–29, 32, 42]). The model has been derived both from the view point of treating the biofilms as a spatially structured population [12] or as a mechanical object [35, 52], thereby reflecting the