LA SERENA NUMERICA II

Octavo Encuentro de Análisis Numérico de Ecuaciones Diferenciales Parciales Departamento de Matemáticas, Universidad de La Serena, La Serena, Chile, Enero 14 - 16, 2015

Mathematical modeling of bacterial communities: Mechanical behavior of biofilms^{*}

<u>Giordano Tierra</u>[†] Juan P. Pavissich Robert Nerenberg[‡] Zhiliang Xu and Mark S. Alber[§]

Abstract

We present an energetic variational approach to simulate biofilm interaction with fluid flow fields. It is aimed to model biofilm heterogeneity and constitutive behaviour through a formulation that describes multicomponent complex fluids with viscoelastic properties. The biofilm is assumed an incompressible fluid made of a ternary mixture of bacteria, extracellular polymeric substance (EPS), and solvent phases. Biofilm response to mechanical stress is incorporated through cohesion and elastic energy functionals. Our model satisfies an overall dissipative energy law and is solved with an efficient unconditionally energy-stable splitting scheme. Numerical simulations illustrate that the model is able to capture large-scale events of biofilm deformation and detachment under different hydrodynamic conditions in elastic and viscous regimes. The results are qualitatively consistent with laboratory experiments. Simulations show the effect of mechanical parameters and the role of the EPS in the hydrodynamic interaction with flow fields. Higher viscosity provides stronger resistance to deformation, and longer elastic relaxation can lead to the formation of biofilm filaments. This formulation and the numerical algorithm developed provide a robust mathematical and physical framework to study biofilm mechanical behaviour, considering structural heterogeneity and complex rheology.

Key words: biofilm, viscoelasticity, phase-field, energy stability, continuum mechanics, splitting schemes

Mathematics subject classifications (1991): 65M60, 76D05, 76T30, 92B05

^{*}This research was partially supported by NIH 1 R01 GM095959-01A1 and ERC-CZ project LL1202 (Ministry of Education, Youth and Sports of the Czech Republic)

[†]Mathematical Institute, Faculty of Mathematics and Physics, Charles University, 186 75 Prague 8, Czech Republic, email: gtierra@karlin.mff.cuni.cz

[‡]Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, IN 46556, USA, e-mail: {jpavissi,nerenberg.1}@nd.edu

[§]Department of Applied and Computational Mathematics and Statistics, University of Notre Dame, Notre Dame, IN 46556, USA, e-mail: {zxu2,malber}@nd.edu

References

- ALPKVIST, E. & KLAPPER, I. A multidimensional multispecies continuum model for heterogeneous biofilm development. *Bull. Math. Biol.* 69, 765-789, (2007).
- [2] AYATI, B.P. & KLAPPER, I. A Multiscale Model of Biofilm as a Senescence-Structured Fluid. SIAM Multi. Model. Sim. 6, 347-365, (2007).
- [3] COGAN, N. G. & KEENER, J. P. The role of the biofilm matrix in structural development. Math. Med. Biol. 21, 147-166, (2004).
- [4] FRIEDMAN, A., HU, B. & XUE, C. On a Multiphase Multicomponent Model of Biofilm Growth. Arch. Rational Mech. Anal. 211, 257-300, (2014).
- [5] HYON, Y., KWAK, Y. & LIU, C. Energetic variational approach in complex fluids: Maximum dissipation principle. *Discrete Cont. Dyn-A.* 26, 1291-1304, (2010).
- [6] KLAPPER, I. & DOCKERY, J. Role of cohesion in the material description of biofilms. *Phys. Rev. E* 74, 031902, (2006).
- [7] KLAPPER, I. & DOCKERY, J. Mathematical description of microbial biofilms. SIAM Rev. 52, 221-265, (2010).
- [8] LIN, F. H., LIU, C. & ZHANG, P. On hydrodynamics of viscoelastic fluids. Commun. Pur. Appl. Math. 58, 1437-1471, (2005).
- [9] LINDLEY, B., WANG, Q. & ZHANG, T. Multicomponent hydrodynamic model for heterogeneous biofilms: Two-dimensional numerical simulations of growth and interaction with flows. *Phys. Rev. E* 85, 031908, (2012).
- [10] MONDS, R.D. & O'TOOLE, G.A. The developmental model of microbial biofilms: ten years of a paradigm up for review. *Trends Microbiol.* 17(2), 73-87, (2009).
- [11] WANG, Q. & ZHANG, T. Review of mathematical models for biofilms. Sol. State Commun. 150, 1009-1022, (2010).
- [12] WILKING, J. N., ANGELINI, T. E., SEMINARA, A., BRENNER, M. P. & WEITZ, D. A. Biofilms as complex fluids. *MRS Bull.* 36, 385-391, (2011).
- [13] XAVIER, J., PICIOREANU, C. & VAN LOOSDRECHT, M. C. M.A general description of detachment for multidimensional modelling of biofilms. *Biotech. Bioeng.* 91, 651-669, (2005).
- [14] YUE, P., FENG, J. J., LIU, C. & SHEN, J. A diffuse-interface method for simulating two-phase flows of complex fluids. J. Fluid Mech. 515, 293-317, (2004).
- [15] ZHANG, T., COGAN, N. G. & WANG, Q. Phase field models for biofilms. I. Theory and one-dimensional simulations. SIAM J. Appl. Math. 69, 641-669, (2008).
- [16] ZHANG, T., COGAN, N. G. & WANG, Q. Phase-field models for biofilms II. 2-D Numerical simulations of biofilm-flow interaction. *Commun. Comput. Phys.* 4, 72-101, (2008).