Prediction of biofilm deformation and detachment using shear rheometry, phase-field modeling, and OCT

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In many environmental systems, such as membrane filtration systems, biofilm control is essential, but costly and requiring harsh chemicals. More effective biofilm control may be obtained using a “materials science” approach. Biofilms can be characterized as viscoelastic materials, and biofilm “disruptors” can be characterized for their weakening effect on biofilm mechanical strength. By using a novel mathematical model that incorporates biofilm mechanical properties, fluid flow, and diffusion and reaction of disruptors, better cleaning strategies can be devised.

Phase-field models, where the biofilm is treated like a viscoelastic fluid, are one of the few types of models that can predicting deformation and detachment based on mechanical properties. While several related studies have proposed phase-field models for predicting biofilm deformation, there has not been any validation of these models with experimental data. As a first step towards developing a material science strategy for biofilm control, this study validated the ability of a phase-field model to capture biofilm viscoelastic behavior.

In this study, a two-dimensional continuum biofilm model was implemented with finite element method (FEM) using COMSOL Multiphysics (COMSOL v5.4, Comsol Inc, Burlington, MA). We applied the phase-field model with the Cahn-Hilliard equation to simulate biofilm mechanical behavior under fluid flow. The Oldroyd-B model, the simplest viscoelastic constitutive model, was applied to capture biofilm viscoelasticity. The biofilm was modeled as an incompressible viscoelastic fluid, with EPS and a water solvent. The phase-field physics were adapted from previous studies and applied to biofilm-fluid interactions. Two types of incompressible, immiscible fluids (EPS and water solvent) were studied as two components of a single fluid, with a fluid-fluid interface between the two.

Homogeneous alginate was used as a synthetic biofilm for the experimental validation. The viscoelastic parameters of alginate were obtained by shear rheometry using stress relaxation tests. In experimental tests, the deformation behavior was observed in real time using optical coherence tomography (OCT). By importing the 2-D geometry from OCT and viscoelastic parameters from rheometry, the model was simulated and compared with real deformation in the flow cell.

With the applied constant flow (Re=6), biofilm demonstrated viscoelastic behavior. The same behavior was observed in modeling as well. By tracking the movements of several locations of the
biofilm geometry, it was concluded that the deformation of alginate biofilms was consistent with the computational results of phase-field models. The relative error between experiment and model for this certain location were 12.8%. Heterotrophic counter-diffusional biofilms cultured in membrane-aerated biofilm reactors were also tested in this study, with a relative error of 22.2%.

In conclusion, the phase-field model, coupled with Oldroyd-B equation, could properly capture biofilm viscoelastic behavior. In a complex system, the phase-field model could be used as a tool to characterize the viscoelastic parameters from the observed deformation. With this information, the model can be used to predict the required disruptor dose to achieve high amounts of biofilm removal with a minimal amount of chemical addition. This can reduce operating costs and minimize the use of harsh chemicals.