Phase-Field Models for Biofilms. 3-D Numerical Simulations of Biofilm-Flow Interaction

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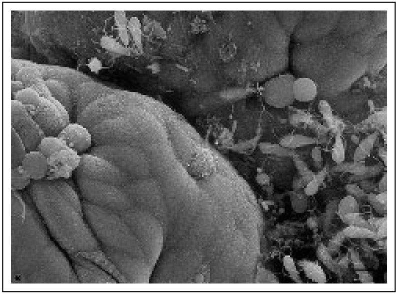
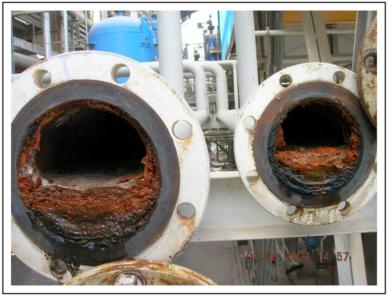
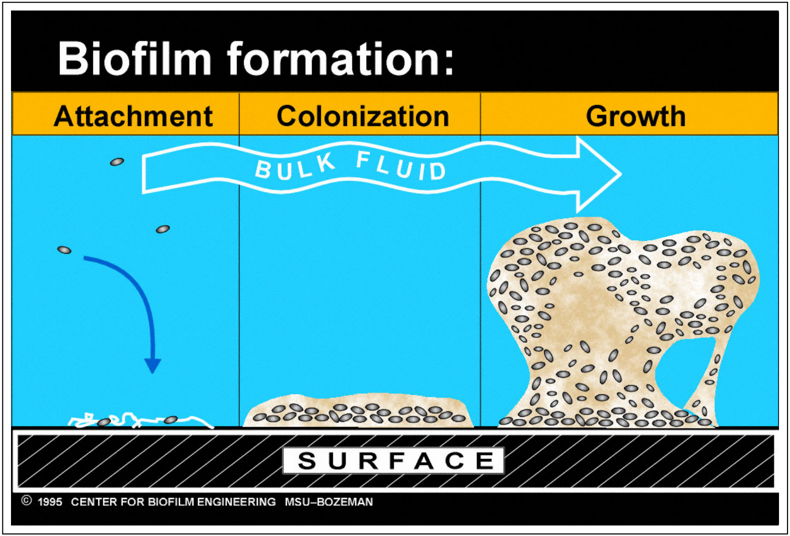
Introduction

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. In nature, biofilms almost always consist of rich mixtures of many species of bacteria. 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.


Biofilm formation:
Attachment
Colonization
Growth
BULK FLUID
SURFACE
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Introduction

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. 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 3-D.

Mathematical model

We derive a set of phase field models for biofilms using two-component formulation in which the combination of extracellular polymeric substances (EPS, or polymer networks) and bacteria is effectively modeled as one fluid component, while the collective ensemble of nutrient substrates and the solvent are modeled as the other.

We denote the following variables:

$\mathbf{v}$ is the average velocity,

ϕ_n is the polymer network volume fraction,

ϕ_s is the effective solvent volume fraction,

p is the pressure.

Flory-Huggin's mixing free energy density is defined by

$$f = \frac{\gamma_1}{2} kT \|\nabla \phi_n\|^2 + \gamma_2 kT \left[\frac{\phi_n}{N} \ln \phi_n + (1 - \phi_n) \ln(1 - \phi_n) + \chi \phi_n (1 - \phi_n) \right]$$

The polymer network velocity is defined by

$$\mathbf{v}_n = \mathbf{v} - \frac{\lambda}{\phi_n} \nabla \frac{\delta f}{\delta \phi_n}.$$

The solvent velocity is given by

$$\mathbf{v}_s = \mathbf{v} + \frac{\lambda}{\phi_s} \nabla \frac{\delta f}{\delta \phi_n}.$$

Constitutive equations

The rate of strain tensor and the vorticity tensor with respect to the average velocity are adopted:

$$\mathbf{D} = \frac{1}{2}[\nabla \mathbf{v} + \nabla \mathbf{v}^T], \quad \mathbf{W} = \frac{1}{2}[\nabla \mathbf{v} - \nabla \mathbf{v}^T].$$

$$\tau_n = 2\eta_n \mathbf{D}, \quad \tau_s = 2\eta_s \mathbf{D}, \qquad \text{VA-model}$$

$$\lambda_1 \left(\frac{\partial \tau_n}{\partial t} + \mathbf{v} \cdot \nabla \tau_n - \mathbf{W} \cdot \tau_n + \tau_n \cdot \mathbf{W} - a[\mathbf{D} \cdot \tau_n + \tau_n \cdot \mathbf{D}] \right) + \tau_n = 2\eta_n \mathbf{D},$$

$$\tau_s = 2\eta_s \mathbf{D}, \qquad \text{JSA-model}$$

Momentum and continuity equation

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot (\phi_n \tau_n + \phi_s \tau_s) - [\nabla p + \gamma_1 kT \nabla \cdot (\nabla \phi_n \nabla \phi_n)]$$

where $\rho = \phi_n \rho_n + \phi_s \rho_s$ is the effective density for the mixture.

Incompressibility implies $\phi_s + \phi_n = 1$.

Transport equation for nutrient substrates

$$\frac{\partial}{\partial t}(\phi_s c) + \nabla \cdot (c\mathbf{v}\phi_s - D_s \phi_s \nabla c) = -g_c$$

where c is the nutrient concentration and the nutrient consumption rate is given by

$$g_c = \frac{\phi_n A c}{K_0 + c}$$

Transport equation for the volume fraction of the polymer network

$$\frac{\partial \phi_n}{\partial t} + \nabla \cdot (\phi_n \mathbf{v}) = \nabla \cdot \left[\lambda \phi_n \nabla \frac{\delta f}{\delta \phi_n} \right] + g_n$$

where λ is the mobility parameter and the polymer production rate is given by

$$g_n = \varepsilon \mu \phi_n \frac{c}{K_c + c}$$

μ is the maximum production rate, K_c is the half-saturation constant and ε is a scaling parameter. The transport equation is a modified or singular Cahn-Hilliard equation with a polymer volume fraction dependent mobility.

Nondimensionalization

The parameters and the system of governing equations for the biofilm in dimensionless variables are given by

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot (\phi_n \tau_n + \phi_s \tau_s) - [\nabla p + \Gamma_1 \nabla \cdot (\nabla \phi_n \nabla \phi_n)]$$

$$\frac{\partial}{\partial t}(\phi_s c) + \nabla \cdot (c\mathbf{v}\phi_s - D_s \phi_s \nabla c) = -g_c$$

$$\frac{\partial \phi_n}{\partial t} + \nabla \cdot (\phi_n \mathbf{v}) = \nabla \cdot \left[\Lambda \phi_n \nabla \frac{\delta f}{\delta \phi_n} \right] + g_n$$

Where

$$\tau_n = \frac{2}{Re_n}\mathbf{D}, \tau_s = \frac{2}{Re_s}\mathbf{D}, g_c = A\phi_n c, g_n = \varepsilon\mu\phi_n \frac{c}{K_c + c}.$$

The dimensionless mixing free energy density is now given by

$$f = \frac{\Gamma_1}{2}\|\nabla\phi_n\|^2 + \Gamma_2\left[\frac{\phi_n}{N}\ln\phi_n + (1-\phi_n)\ln(1-\phi_n) + \chi\phi_n(1-\phi_n)\right]$$

Numerical schemes

We use the finite difference method to solve the coupled flow, phase field equation, and nutrient concentration transport equation. We solve the coupled momentum transport equation and the continuity equation using a velocity corrected projection scheme. We denote

$$\mathbf{R} = -\nabla\cdot(\Gamma_1\nabla\phi_n\nabla\phi_n) + \nabla\cdot(\phi_n\tau_n + \phi_s\tau_s - \frac{2}{Re_a}\mathbf{D}),$$

where Re_a is an averaged Reynolds number. The momentum transport equation is rewriten as

$$\rho(\frac{\partial}{\partial t}\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}) = -\nabla p + \frac{1}{Re_a}\nabla^2\mathbf{v} + \mathbf{R}.$$

For simplicity, the second order extrapolation in time of any function f is denoted by $\overline{f}^{n+1} = 2f^n - f^{n-1}$.

Step 1:

$$\rho^{n+1}\left[\frac{3\mathbf{u}^{n+1} - 4\mathbf{v}^n + \mathbf{v}^{n-1}}{\Delta t}\right] + \rho^{n+1}\overline{\mathbf{v}}^{n+1} \cdot \nabla\overline{\mathbf{v}}^{n+1}$$

$$+ \nabla p^n + \frac{1}{Re_a}[\nabla s^n - \nabla^2\mathbf{u}^{n+1}] = \overline{\mathbf{R}}^{n+1}$$

$$\mathbf{u}^{n+1}|_{y=0} = 0, \mathbf{u}^{n+1}|_{y=H} = \mathbf{v}_0$$

Step 2: We implement the projection step

$$-\nabla \cdot \left(\frac{1}{\rho^{n+1}}\nabla\psi^{n+1}\right) = \nabla \cdot \mathbf{u}^{n+1}$$

$$\frac{\partial\psi^{n+1}}{\partial n}|_{y=0,H} = 0$$

Step 3: We correct the velocity, pressure and the auxiliary variable s.

$$\mathbf{v}^{n+1} = \mathbf{u}^{n+1} + \frac{1}{\rho^{n+1}} \nabla \psi^{n+1}$$
$$s^{n+1} = s^n - \nabla \cdot \mathbf{u}^{n+1}$$
$$p^{n+1} = p^n - \frac{3\psi^{n+1}}{2\Delta t} + \frac{1}{Re_a} s^{n+1}$$

Here $s^0 = 0$ and $\mathbf{v}^1, s^1, p^1, \phi_n^1, c^1$ are computed by a first order scheme.

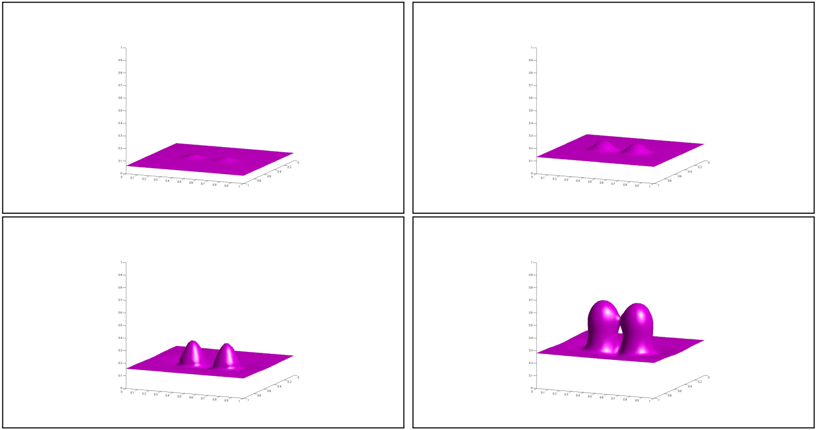
The phase field equation for the polymer volume fraction ϕ_n is discretized by

$$
\frac{3\phi_n^{n+1}-4\phi_n^{n}+\phi_n^{n-1}}{2\Delta t}+\mathbf{v}^{n+1}\cdot\nabla\phi_n^{n+1}
$$
$$
=g_n^{n+1}+\Lambda\nabla\cdot\overline{\phi_n}^{n+1}\nabla(-\Gamma_1\nabla^2\phi_n^{n+1}-2\Gamma_2\chi\phi_n^{n+1}
$$
$$
-\Gamma_2(-\frac{1}{N}\overline{\ln\phi_n}^{n+1}+\overline{\ln(1-\phi_n)}^{n+1}))
$$

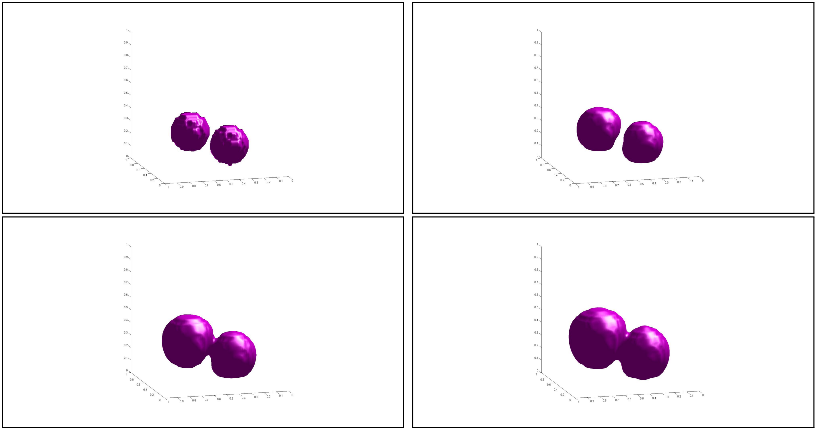
The substrate concentration transport equation is discretized by

$$
\frac{3\phi_s^{n+1}c^{n+1}-4\phi_s^{n}c^{n}+\phi_s^{n-1}c^{n-1}}{2\Delta t}+\mathbf{v}^{n+1}\cdot\nabla(c^{n+1}\phi_s^{n+1})
$$
$$
=-g_c^{n+1}+\nabla\cdot(D_s\phi_s^{n+1}\nabla c^{n+1})
$$

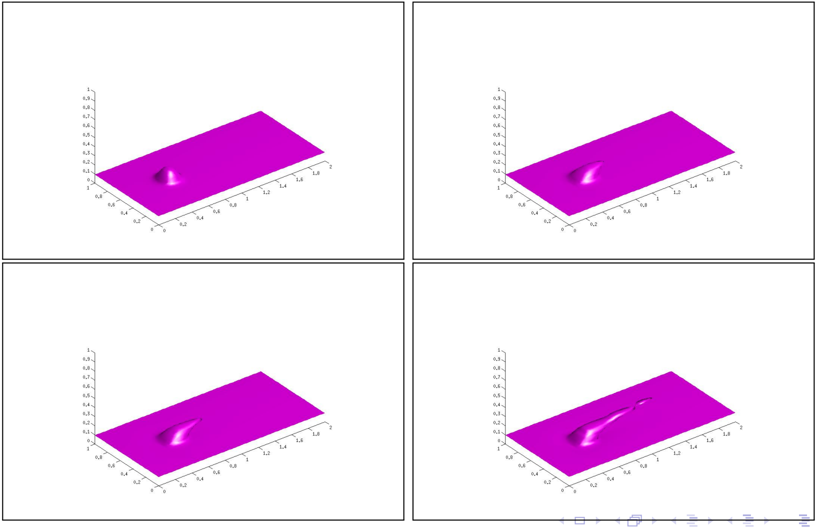
Two humps



Two blobs



Shear flow



Conclusion

We present some numerical simulations of the growth of biofilm colonies, their deformation, and detachment in a cavity and under plane shear using the extended Newtonian model we developed for biofilm and solvent mixtures. We capture some mechanism associated with biofilm in several situations. These studies demonstrate the capability of the model and the numerical simulation tools associated with it.We look forward to seeing simulations of a tri-component model, in which the EPS network, bacteria and effective solvent consisting of the solvent, nutrient, drugs etc. are modeled explicitly.

THANK YOU!