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Numerical modeling of the mechanical response of bacterial biofilm to flow by using an SPH poroviscoelastic model

Dianlei Feng[1,*], **Insa Neuweiler**[1], **Moubin Liu**[2], and **Udo Nackenhorst**[3]

[1] Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, Leibniz Universität Hannover, Hannover, Germany

[2] BIC-ESAT, College of Engineering, Peking University, China

[3] Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover, Germany

We present a weakly-compressible two-phase poroviscoelastic biofilm model based on Smoothed Particle Hydrodynamics (SPH) method. The biofilm is modeled as a mixture of solid and fluid phases interacting via drag forces. Benefiting from the Lagrangian feature of the SPH method, large deformations of the solid structure can be modeled straightforwardly.

1 Introduction

Understanding the mechanical response of bacterial biofilms is important for designing types of wastewater treatment reactors. Numerical modeling of the fluid-structure interaction (FSI) process of the biofilm systems helps to reduce the investigation expense compared to carrying out experiments. Many studies have shown that a biofilm behaves as a viscoelastic material in the fluid. This is mostly due to the extracellular polymeric substances (EPSs), which are natural polymers secreted by the bacteria. Moreover, The network structure of the EPSs makes the biofilm a porous medium which can be heterogeneous and undergo large deformation in the fluid. In this paper, we present our recent results on the development of the SPH poroviscoelastic biofilm model, which can be applied to simulate the FSI process in a microfluid channel.

2 Mathematical model

We model the biofilm, based on the mixture theory, as a fully saturated porous medium which consists of a fluid and a solid phase. The summation of the volume fractions of both phases yields

$$\theta_f + \theta_s = 1, \tag{1}$$

where, θ refers to the volume fraction, indexes f and s denote the fluid and solid phases, respectively. The mass balance equation of each phase within a representative elementary volume (REV) of the porous medium can be written as

$$\frac{\mathrm{d}\rho_\alpha}{\mathrm{d}t} + \rho_\alpha \nabla \cdot \boldsymbol{v}_\alpha = 0, \quad (\alpha = s, f)\,. \tag{2}$$

In equation (2), $\rho_\alpha = \rho_\alpha^0 \theta_\alpha$ refers to the averaged density of the αth phase, and ρ^0 is the material density. The velocity of each phase in the RVE is denoted as $\boldsymbol{v}_\alpha$.

We neglect the gravity effect on the microfluid system. The momentum balance equation of each phase reads

$$\rho_\alpha \frac{\mathrm{d}\boldsymbol{v}_\alpha}{\mathrm{d}t} - \nabla \cdot \boldsymbol{\sigma}_\alpha + \boldsymbol{\Pi}_\alpha = 0, \quad (\alpha = s, f)\,. \tag{3}$$

The viscosity of the fluid is only considered outside the porous medium. We apply the Maxwell viscoelastic model for describing the solid material behaviors. The momentum exchange between the solid and fluid phases is modeled by a drag force $\boldsymbol{\Pi}$ [1]. Obviously, $\boldsymbol{\Pi}_f + \boldsymbol{\Pi}_s = 0$. In this paper, we model the drag force by $\boldsymbol{\Pi}_f = \xi \theta_s \theta_f \left(\boldsymbol{v}_f - \boldsymbol{v}_s\right) - p \nabla \theta_f$. The drag force $\boldsymbol{\Pi}$ is parametrized by employing a drag coefficient ξ, which depends on the material properties of the phases. In the drag force model, p denotes the pressure in the pore-space.

3 Numerical treatment

Smoothed Particle Hydrodynamics (SPH) method is used to solve the model. The fluid and solid phases are discretized separately by using the Lagrangian SPH particles as shown in Figure 1 a). A scalar function at the ith particle $F\left(\boldsymbol{x}_i\right)$ and

* Corresponding author: e-mail feng@hydromech.uni-hannover.de, phone +49 511 762 4294, fax +49 511 762 3777

its first derivative $\nabla F(\boldsymbol{x}_i)$ can be approximated by interpolating the quantities of its neighbouring N particles within the corresponding supporting domain of the kernel function W

$$\langle F(\boldsymbol{x}_i)\rangle = \sum_j^N \frac{m_j}{\rho_j} F(\boldsymbol{x}_j) W(\boldsymbol{x}_i - \boldsymbol{x}_j, h), \quad \langle \nabla F(\boldsymbol{x}_i)\rangle = \sum_j^N \frac{m_j}{\rho_j} F(\boldsymbol{x}_j) \nabla W(\boldsymbol{x}_i - \boldsymbol{x}_j, h) \tag{4}$$

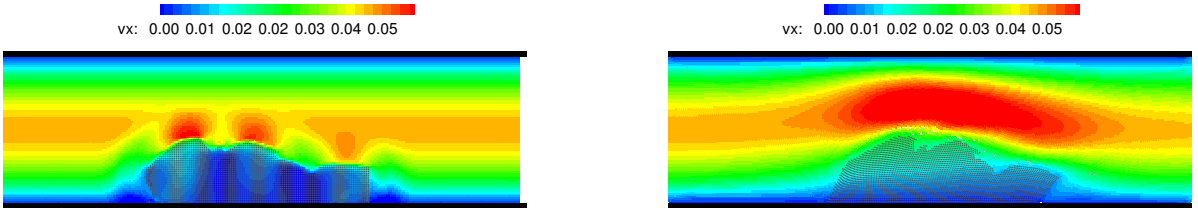
where, the notation $\langle\cdot\rangle$ is used for representing the numerical approximation of a function, and m_j and ρ_j denote the mass and density of the jth particle. The variable h is the so-called smoothing length, which defines the local supporting domain's volume at the location of $\boldsymbol{x}_i$. We apply the wall boundary conditions following [2] in this study, and an inflow domain with pre-defined velocity profiles is used for modeling the inlet boundary condition (see Figure 1 b)). A parabolic inflow velocity profile as $v_x(y) = v_{max}\left[1 - \left(\frac{y-R}{R}\right)^2\right]$ is applied here. The y- axis parallels to the dimension of the height of the flow channel, which has a radius of R. The δ-SPH method [3] is also employed in numerical discretization for stabilization purpose.

a) b)

Fig. 1: Illustrations of the numerical setups of the two-phase SPH biofilm model. **a**: Two-phase SPH particle discretization. **b**: Numerical setup of the microfluid channel with a biofilm.

4 Results and discussions

Simulation results of the FSI process at an early and later time are shown in Figure 2. In total, 49,175 SPH particles are employed in the simulation. The biofilm material parameters are taken from the Microbead Force Spectroscopy measurements [4]. The presented SPH poroviscoelastic biofilm model captures the large structure deformations well. The model also shows



a) b)

Fig. 2: Simulation results of the biofilm-water interaction in a micro-fluid channel. The color map corresponds to the horizontal fluid velocity magnitude. **a**: at $t = 5 \times 10^{-5}$ s **b**: at $t = 1.25 \times 10^{-2}$ s.

excellent potential for future investigations of heterogeneous biofilm problems. In the above simulations, a constant porosity of $\theta_f = 0.47$ has been used as an initial value. Since the volume fraction of each phase is solved directly from the model, a heterogeneous development of the porosity during the FSI process can be modeled. In nature, biofilms are, in general heterogeneous in terms of most of the physical properties. The presented SPH poroviscoelastic biofilm model can be a powerful numerical tool for such problems. However, developing a stable and accurate SPH scheme for solving the presented model is nontrivial. Small pressure fluctuations can easily lead to numerical instability when solving the two-phase model with SPH. The SPH inflow boundary usually has a drawback of resulting in such fluctuations. In this study, we found stable solutions by using the δ-SPH method.

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