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A FLUID-STRUCTURE INTERACTION STUDY OF BIOFILM DETACHMENT

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ABSTRACT

During the biofilm development process, bacterial cells may detach from the biofilm into the surrounding fluid. The key question in relation to detachment from bacterial biofilm is the mechanical response to hydrodynamic forces. In this study, a Finite Volume Method (FVM) based Fluid-Structure Interaction (FSI) solver in OpenFOAM package has been developed to model the biofilm response to flow [1]. Dynamic interaction was simulated between an incompressible Newtonian fluid and a bacterial biofilm described as a linear viscoelastic solid. Viscoelastic response of the biofilm was represented by the hereditary integral form of constitutive relation [2] while tensile relaxation modulus was expressed by the Generalised Maxwell Model (GMM) in the form of Prony series (a discrete retardation spectrum). GMM was obtained from the rheometry creep experimental data using a three-step method proposed by Dooling et al. [3]. The creep curves were all viscoelastic in nature and approximated by a linear viscoelastic model represented by Generalised Voigt Model (GVM). Elastic shear modulus (G), obtained from the three-step method, ranged from 583Pa to 1368Pa which were similar to the previous rheometry studies. In this two-dimensional model, biofilm was considered as semi-hemispherical shape (thickness of 100μm and width of 346μm) attached to the center of the bottom boundary of the square cross-section flow cell. Fluid flow through the flow cell was in laminar regime. Simulation results predicted the potential site for biofilm detachment subjected to increasing fluid flow rate through the flow cell.

Key Words: Biofilm, Viscoelasticity, Fluid-Structure Interaction, Finite Volume Method.

1. INTRODUCTION

Biofilms are formed when bacterial cells attach to submerged solid surfaces and accumulate to form a multilayered cellular structure. Biofilm structure may change in numerous ways such as detaching, streaming, rolling and rippling subjected to fluid stresses in a flowing system. Biofilm detachment is a term which is used for the cell cluster detachment from a biofilm and/or detachment of biofilm from the substrate. The phenomenon of detachment from biofilm is now recognised as a serious concern in public health and clinical fields. Growth of biofilm on medical devices and human organs may result in persistent infections, which may spread to other sites via detachment processes [4]. There is currently a wholly inadequate mechanistic understanding of biofilm deformation/failure in a biofilm-fluid interaction description. The nature of biofilm response is greatly influenced by material properties. Shear deformation of biofilm was modeled as a viscoelastic material using 4-elements Burger model in rheometry experiments [5] and a 2D Finite Element model of biofilm-fluid interaction was developed based on this model [6]. The aim of this study was to model a dynamic interaction between an incompressible Newtonian fluid and a
bacterial biofilm described by a linear viscoelastic solid. FVM based FSI modeling has been previously
developed to model fluid-structure systems [7, 8 & 9]. In this work, OpenFOAM package, which is a C++
library of FVM, was used to model the fluid-biofilm interaction problem.

2. EXPERIMENTAL

Creep analysis was carried out on mixed culture biofilms using the concentric cylinders rheometer (TA
INSTRUMENTS, CSL2 100 Carimed Rheometer). Biofilm samples were cultivated using methods
described previously [10]. The creep analysis was performed for 3min loading and 3min unloading
subjected to constant shear stresses of 0.5 & 1Pa to monitor creep and recovery phases.

3. MODELING

A linear viscoelastic stress-strain constitutive relation was described by a hereditary integral [2]. The
incremental form of this constitutive relation has been introduced in geometrically nonlinear momentum
equation in an updated Lagrangian formulation to model biofilm deformation. Tensile relaxation modulus
\( E(t) \) was expressed by a discrete relaxation spectrum (Prony series) and it was calculated from
experimental creep data according to a three-step method as follows [3]: 1) Discrete retardation spectrum
\( J_i & \tau_i \) of a GVM (Equation-1) was fitted to experimental creep data, \( J(t) \), using a non-negative least
square method. It should be noted that a Genetic Algorithm (GA) was used to obtain optimal retardation
times. In Equation-1, \( J_0 \) is the equilibrium compliance, \( J_i \) is retardation strength, and \( \tau_i \) is retardation time, 2) GVM was solved numerically to calculate shear relaxation modulus data, \( G(t) \) based on Finite Difference
method [3], and 3) Discrete shear relaxation spectrum \( (G_i, \rho_i) \) of a GMM (Equation-2) was fitted to the
calculated \( G(t) \). In Equation-2, \( G_0 \) is the equilibrium modulus, \( G_i \) is relaxation strength, and \( \rho_i \) is relaxation
time. At the end, tensile relaxation modulus \( E(t) \) was obtained from shear relaxation modulus.

\[
J(t) = J_0 + \sum_i J_i e^{-\frac{t}{\tau_i}} \\
G(t) = G_0 + \sum_i G_i e^{-\frac{t}{\rho_i}}
\]

Equation 1

Equation 2

In fluid-structure interaction model, laminar fluid flow has been modeled by the Navier-Stokes equations in
an Arbitrary Lagrangian-Eulerian (ALE) formulation. Spatial discretisation of both domains was performed
using the second-order accurate unstructured cell-centred FVM. The fluid model was discretised on the
moving mesh, while the viscoelastic model was discretised on the fixed mesh in an updated configuration.
Automatic vertex-based mesh motion solver was used to accommodate the fluid mesh to the fluid-solid
interface deformation. Temporal discretisation of both models was performed using a fully implicit second-
order accurate three-time-levels difference scheme. Coupling between the domains was achieved using a
strong implicit coupling algorithm. The biofilm was considered as semi-hemispherical shape attached to the
center of the bottom boundary of the square cross-section flow cell (Figure-1). Thickness and width of the
biofilm were 100μm and 346μm respectively, and flow cell dimensions were 3mm × 3mm × 50mm. Fluid
flow through the flow cell was assumed to be in laminar regime and a fully developed flow approached the
biofilm structure, therefore, a non-uniform parabolic velocity distribution was applied at inlet boundary.
Water \((\mu=1\times10^{-4}kg/mm.s, \rho=1\times10^{3}kg/mm^3)\) flows from the left to right in X direction at \( V_{max} \) of 0.05m/s
that suddenly increased to 0.1, 0.15 & 0.2m/s at the time interval of 0.0125Sec. In addition to inlet
boundary, the so-called “no slip” condition was applied to the channel walls. The walls were also fixed in
space; the biofilm-fluid interface was not. The normal derivative of pressure was set to zero at all
boundaries, but the pressure value was specified in one point to satisfy solution convergence for pressure
equation.
4. RESULTS

Linear viscoelasticity behavior was observed up to the shear stress of 1 Pa (data are not shown here). The experimental creep response may indicate the existence of instantaneous elastic and retardation phases (Figure 2A). The value of the instantaneous shear modulus, $G$, of the biofilms, obtained by GMM, was in the range of 583-1368 Pa. The agreement between the experimental creep data and the creep response predicted by GVM for a typical biofilm sample is illustrated in Figure 2A. GMM fitted to the numerically calculated shear stress relaxation data is shown in Figure 2B. Table 1 lists tensile relaxation modulus data used in viscoelastic solver. Viscoelastic solver was successfully validated as a good agreement was observed between experimental and numerically predicted creep response in rheometry testing.

Figure 2: A: measured creep compliances fitted by GVM & B: calculated stress relaxation fitted by GMM

<table>
<thead>
<tr>
<th>Table 1 GMM coefficients used in the viscoelastic solver ($*E(t)=2(1+v)G(t)$ &amp; $v=0.45$)</th>
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<td>Tensile relaxation modulus</td>
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<td>-------------------------------</td>
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<tr>
<td>$E(t)$</td>
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<tr>
<td>$\rho(t)$</td>
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<tr>
<td>Relaxation time</td>
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Figure 3 shows magnitude of tangential shear force at point A as well as normal and tangential tractions at point B on biofilm subjected to increasing initial flow velocities at inlet boundary (points A & B are marked in Figure 1). Simulation results showed a sudden increase in all tractions at the moment inlet flow velocity ($V_{max}$) was applied followed by a gradual decrease within the developing boundary layers. Observation of higher magnitude of normal and tangential tractions at point B compared to tangential shear force at point A suggests that point B may be a potential site for biofilm detachment.
5. CONCLUSIONS AND FUTURE WORK

The results have demonstrated that the linear viscoelastic response of biofilm to shear stresses can be approximated by Prony series (GVM). A sophisticated three-step method has been developed to numerically obtain respective stress relaxation response of biofilm. Simulations showed that the FSI approach may illuminate interesting details of biofilm deformation/detachment subjected to increasing flow velocities. In the next stage of this work the Cohesive Zone Model (CZM) will be implemented in such a way to allow numerical modeling of the biofilm detachment paths via Traction-Separation (TS) law. The TS law can be obtained by force-distance curve analysis in conjunction with Atomic Force Microscopy (AFM). Experimental measurement of the shear induced detachment characteristics will be conducted for FSI model validation.

REFERENCES