Biofilm growth: a multi-scale and coupled fluid-structure interaction and scalar transport model

Mirella Coroneo, Lena Yoshihara, Wolfgang A. Wall

Institute for Computational Mechanics, Technische Universität München, Germany

{coroneo, yoshihara, wall}@lnm.mw.tum.de

Motivation

- Biofilm growth and development are influenced by hydrodynamic conditions and nutrient availability [1]

- The mutual interaction of all the involved phenomena is not well understood and results to be difficult to be investigated experimentally

- A modeling approach taking in account the effect of local structure deformation and fluid flow on mass transfer and growth can help the understanding of biofilm macro-scale dynamics

- While constituted of micro-scale objects, biofilm structures interact with the surrounding fluid as macro-scale materials and can be studied as flexible structures located in a moving liquid flow

Objective

- Development of a multi-scale and coupled fluid-structure interaction (FSI) and mass transfer model for modelling biofilm growth

- Study of the fluid-structure interaction and of the substrate transport and reaction of big growing biofilm aggregates, for which continuum models can be applied, at the purpose to develop successful strategy for biofilm control

Modeling approach

- A novel growth model for the multi-scale simulation of biofilm structures development [2]

- Based on a finite-element approach, developed in our in-house research code BACI, for the numerical simulation of a sequential one-way coupling of FSI and scalar transport [3]

MULTI-SCALE ALGORITHM

- The different involved phenomena happen at different time-scales

- A multi-scale algorithm was applied, consisting of:
  - an inner time loop solving FSI and scalar transport at fluid-dynamic time-scale
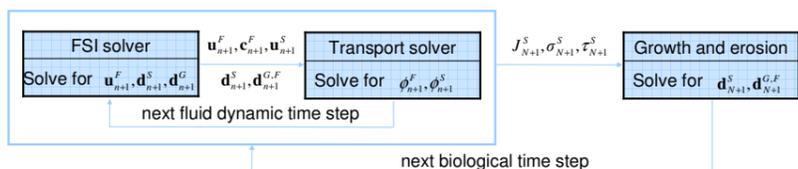 - an outer time loop solving only the biofilm growth at biological time-scale

Figure 1: Algorithm of the multi-scale and coupled fluid-structure interaction and scalar transport model for biofilm growth simulations

FLUID-STRUCTURE INTERACTION

- Arbitrary Lagrangian-Eulerian (ALE) approach

- Non-linear equations governing the fluid flow and the biofilm displacements solved monolithically

- Fluid dynamics
$$\rho^F \frac{\partial \mathbf{u}^F}{\partial t} + \rho^F (\mathbf{c}^F \cdot \nabla)\mathbf{u}^F - 2\mu\nabla \cdot \varepsilon(\mathbf{u}^F) + \nabla p^F = \rho^F \mathbf{b}^F \qquad \forall(\mathbf{x},t) \in \Omega^F \times (0,T)$$
$$\nabla \cdot \mathbf{u}^F = 0$$

- Structural dynamics
$$\rho^S \frac{d^2 \mathbf{d}^S}{dt^2} = \nabla \cdot (\mathbf{F} \cdot \mathbf{S}) + \rho^S \mathbf{b}^S \qquad \forall(\mathbf{x},t) \in \Omega^S \times (0,T)$$

- ALE dynamics
$$\nabla \cdot \sigma^{G,F} = 0 \qquad \forall(\mathbf{x},t) \in \Omega^{G,F} \times (0,T)$$

- FSI coupling conditions
$$\mathbf{h}_\Gamma^S = -\mathbf{h}_\Gamma^F; \quad \mathbf{u}_\Gamma^F = \mathbf{u}_\Gamma^{G,F}; \quad \frac{\partial \mathbf{d}_\Gamma^S}{\partial t} = \mathbf{u}_\Gamma^F \qquad \forall(\mathbf{x},t) \in \Gamma_{FSI} \times (0,T)$$

SCALAR TRANSPORT

- Dynamic convection-diffusion-reaction equation for the scalar transport solved using the calculated local velocities and deformations

- The substrate reaction is expressed by the non-linear Monod kinetic

- Convection-Diffusion in the fluid
$$\frac{\partial \phi^F}{\partial t} + c^F \cdot \nabla \phi^F - \nabla \cdot (D^F \nabla \phi^F) = 0 \qquad \forall(\mathbf{x},t) \in \Omega^F \times (0,T)$$

- Diffusion-Reaction in the solid
$$\frac{\partial \phi^S}{\partial t} + \phi^S (\nabla \cdot \mathbf{u}^S) - \nabla \cdot (D^S \nabla \phi^S) + k \frac{\phi^S}{K + \phi^S} = 0 \qquad \forall(\mathbf{x},t) \in \Omega^S \times (0,T)$$

- Coupling conditions
$$\phi^F = \phi^S \qquad \forall(\mathbf{x},t) \in \Gamma_{mass} \times (0,T)$$
$$\nabla \phi^F \cdot \mathbf{n} = \nabla \phi^S \cdot \mathbf{n}$$

GROWTH & EROSION

- Stress and mass flux at the interface resulting from the FSI and scalar transport step used to calculate the local amount of growth or erosion

- The local growth is calculated in term of displacement perpendicular to the biofilm surface

$$\tilde{\mathbf{d}}^F = -\tilde{\mathbf{d}}^S = K_1 J^S - K_2 \sigma^S - K_3 \tau^S \qquad \forall(\mathbf{x},t) \in \Gamma_g \times (0,T_{bio})$$

- An ALE approach is then applied both to the fluid and structure domains in order to appropriately deform the mesh (the calculated displacement due to growth is applied as a Dirichlet condition)

$$\nabla \cdot \sigma^{G,F} = 0 \quad \forall(\mathbf{x},t) \in \Omega^{G,F} \times (0,T) \qquad \text{with} \qquad \mathbf{d}^{G,S} = \tilde{\mathbf{d}}^S \quad \forall(\mathbf{x},t) \in \Gamma_g \times (0,T_{bio})$$
$$\nabla \cdot \sigma^{G,S} = 0 \quad \forall(\mathbf{x},t) \in \Omega^{G,S} \times (0,T) \qquad \text{with} \qquad \mathbf{d}^{G,F} = \tilde{\mathbf{d}}^F \quad \forall(\mathbf{x},t) \in \Gamma_g \times (0,T_{bio})$$

- At the end of the growth and erosion step, nodes reference position are changed for all fields and all state vectors are reset

Results

MASS BALANCE

- Growth of a simple flat biofilm, with initial linear profile of concentration and prescribed concentration at top and bottom surfaces

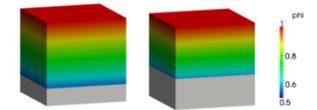- Results proves the mass conservation of the substrate inside the overall domain

Figure 2: Distribution of concentration in the fluid domain and biofilm structure at the initial (left) and at the final step (right).
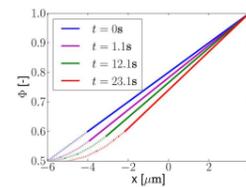

Figure 3: Simulated concentration profiles in time along the vertical axis in the fluid (solid lines) and in the solid domains (dashed lines).
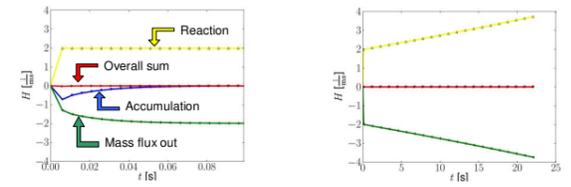
Figure 4: Time-dependent progress in the first time loop (left) and in the overall simulation (right) of the change in the overall mass within the fluid and the structure domain (blue), of the mass flux out of the domain (green), of the change of mass due to reaction (yellow) and of the sum of all the previous terms (red).

EFFECT OF DIFFERENT BOUNDARY CONDITIONS

- The growth model is suitable to model simple growing biofilm structures under different operating conditions

- The model is able to predict the expected behaviour not only when the structure is exposed to uniform fluxes but also when different concentration gradients are present
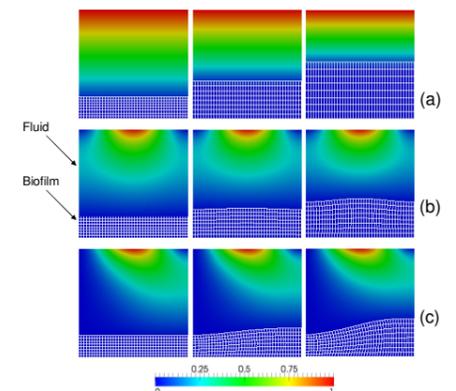

Figure 5: Concentration distribution and structure shape at different time steps. Uniform mass flux at the top boundary, zero velociy (a). Non-uniform mass flux at the top boundary, zero velociy (b). Non-uniform mass flux at the top boundary, velociy inlet from the left boundary (c).

REALISTIC BIOFILM STRUCTURE

- Growth of a finger-like biofilm structure under real operating conditions, material and geometrical characteristics
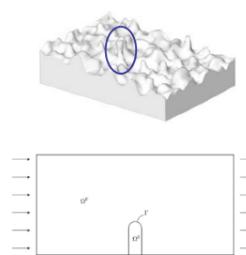

Figure 6: Reconstructed biofilm structure from CLSM images [4] (top) and computational domain under investigation (bottom).

Table 1: Material parameters and operating conditions.

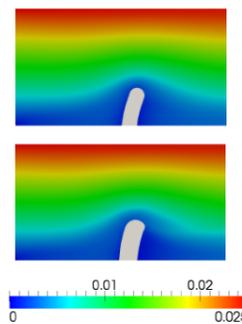| Parameter	Symbol	Value	Unit
Liquid			
Dynamic viscosity	μ^F	10^{-3}	kg m^{-1} s^{-1}
Density	ρ^F	10^3	kg m^{-3}
Inlet velocity	u^F_{IN}	$2 * 10^{-2}$	m s^{-1}
Biofilm			
Density	ρ^S	$3*10^3$	kg m^{-3}
Youngs modulus	E^S	10^2	kg m^{-1} s^{-2}
Poissons ratio	ν^S	$4 *10^{-1}$	-
Substrate			
Diffusion coefficient	D	$2.5 *10^{-9}$	m^2 s^{-1}
Uptake rate coefficient	k	$3 *10^{-2}$	mol m^{-3} s^{-1}
Saturation coefficient	K	$3 *10^{-3}$	mol m^{-3}
Inlet concentration	ϕ^F_{IN}	$2.5 *10^{-2}$	mol m^{-3}

Figure 7: Concentration distribution in the initial (top) and final (bottom) deformed domain.

Conclusions

- Development of a novel and advanced multi-scale computational model for the numerical simulation of fluid-structure interaction and mass transfer of growing biofilm structures

- The model was proven to conserve mass and to be able to predict the effect of different boundary conditions on biofilm final shape

- The applicability of the novel approach to a realistic structure and at realistic operating conditions and material parameters

Outlook

- Calibration of the proposed growth model based on experimental data

- Application of the presented coupled and multi-scale approach to reproduce experimental biofilm development at different operating conditions

- Utilization of the developed approach as a prediction tool also in conditions difficult to investigate experimentally

References

[1] P. Stoodley, I. Dodds, J. Boyle, H. Lappin-Scott, Influence of hydrodynamics and nutrients on biofilm structure. Journal of Applied Microbiology, 85 (1999),19S–28S.

[2] M. Coroneo, L. Yoshihara, W.A. Wall., Biofilm growth: a multi-scale and coupled fluid-structure interaction and mass transfer approach, In preparation (2013)

[3] L. Yoshihara, M. Coroneo, A. Comerford, G. Bauer, T. Klöppel, W. A. Wall, A combined fluid-structure interaction and multi-field scalar transport model for simulating mass transport in biomechanics, In preparation, (2013).

[4] M. Böl, R.B. Möhle, M. Haesner, T.R. Neu, H. Horn, R. Krull: 3D finite element model of biofilm detachment using real biofilm structures from CLSM data . Biotechnology and Bioengineering, 103 (2009), 177–186.