A mesoscale model for hydrodynamics in biofilms that takes microscopic flow effects into account

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Abstract An extended mathematical mesoscale model for flow effects in a biofilm is developed, allowing flow through the EPS matrix and through microchannels that could not be explicitly resolved in previous mesoscopic simulation studies. The model consists of the usual Navier–Stokes equations in the bulk liquid and a porous medium model in the biofilm itself. The sensitivity with respect to the new model parameter is studied numerically by computer simulations.

Keywords Biofilm; computational fluid dynamics; extracellular polymeric substances; hydrodynamics; mathematical model; porous medium

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Introduction

While the term *biofilm* implies a homogeneous layer, it is well established that biofilms often form in extremely complex spatial structures, as accumulations of bacteria and extracellular polymeric substances (EPS), with water filled pores and channels. These spatial variations are observed on a wide range of length scales, from the individual bacteria scale ($<10\,\mu$m, micro-scale), where biofilms show micro-channels in the EPS matrix, up to the actual biofilm scale ($50\,\mu$m–1 mm, meso-scale), on which they can develop so-called mushroom- or pillar-shaped cluster-and-channel colonies. Without a microscope finally ($\gg 1$ cm, macro-scale), biofilms often appear as a more or less homogeneous layer, e.g. as patches or layers of fouling on surfaces. Thus, biofilms are essentially multi-scale systems.

The aqueous environment and its hydrodynamics play an important role for many biofilm processes and applications, such as biofouling of membranes and stability of biofilm reactors in wastewater treatment. In fact, it was proposed by van Loosdrecht *et al.* (1997), and confirmed in experimental studies (e.g. Ohl *et al.* 2004; Stoodley *et al.* 2001), that hydrodynamics is one of the key factors determining the structure in which a particular biofilm develops. This is due to supply of dissolved substrates but also due to mechanical forces that cause biomass to detach. In previous mesoscopic simulation studies of hydrodynamics in biofilms (*e.g.* Bungartz *et al.* 2000; Eberl *et al.* 2000a, 2004; Picioreanu *et al.* 2000, 2001), the biofilm was always understood as a solid object, impermeable to flow. That is, water flows around the structure but not through it. In computer simulations, the spatial resolution of the biofilm/water interface and the flow field is generally bounded by the available computing resources (Eberl *et al.*, 2000b). Therefore, flow effects smaller than a few μm, *i.e.* the micro-scale, could not be resolved by the computational methods, but only meso-scale flow effects were taken into account. Thus, flow through the EPS matrix and micro-channels is neglected. This can lead to an underestimation of the contribution of convection to the availability of dissolved

substrates like nutrients and oxygen. Furthermore and probably more important, the impermeability of the biofilm interface and the no-slip condition there induce velocity gradients that might overestimate actual detachment forces. We propose here an extended hydrodynamic meso-scale model for biofilms that takes micro-scale flow contribution into account. The key idea is to consider the meso-scopic biofilm as a porous medium in which microscopic objects, such as cells or the EPS network, act as a flow resistor past and through which water can flow. Models for porous medium flow are well established in the literature. Formally, they can be derived by a homogenisation procedure of the heterogeneities on the smaller scale (*e.g.* Hornung, 1997). In our approach, the porous medium model for micro-scale flow in the biofilm is coupled with Navier–Stokes flow around the biofilm, *i.e.* the usual meso-scopic hydrodynamic biofilm model.

The idea of averaging small-scale heterogeneities on the next larger scale has been used in biofilm research before. For example, in imaging of biofilm morphology it was used by Lewandowski (2000) and in mathematical modelling by Reichert and Wanner (1996). In both cases meso-scale heterogeneities are averaged on the macro-scale. We take this principle one length scale lower and apply it to microscopic hydrodynamic effects on the mesoscale.

Mathematical model

The proposed model is based on a distinction of two spatial regions: the biofilm, where all biomass and EPS is concentrated, and the surrounding liquid region. In the liquid region the governing equations are the incompressible Navier–Stokes equations (*e.g.* Bungartz *et al.* 2000; Eberl *et al.* 2000a,b; Picioreanu *et al.*, 2000, 2001). With the usual time scale arguments (*e.g.* Picioreanu *et al.,* 2000) we restrict ourselves to stationary flow, i.e.

$$\nabla U = 0, \quad (U \cdot \nabla)U + \nabla P/\rho = \mu \nabla^2 U \tag{1}$$

where the dependent variables U and P denote the flow velocity vector and the hydrodynamic pressure. In (1) the first equation describes conservation of mass of water, while the second equation describes the conservation of momentum. Previous hydrodynamic models for biofilms on the meso-scale postulated the no-slip boundary condition $U = 0$ for model (1) at the biofilm/liquid interface, and thus made the biofilm region a solid obstacle to the flow of water. We relax this restriction and consider the biofilm region itself as a porous medium, thus allowing flow through the saturated EPS network and through micro-channels. The key idea is that flow can only pass through the fraction of the region that is not occupied by obstacles. These obstacles are too small, numerous and heterogeneous to be accounted for individually. Instead, a volumetric flow rate is introduced. This does not affect the equation of mass conservation but additional sink terms are included in the momentum equation. The modified equations are

$$\nabla U = 0, \quad (U \cdot \nabla)U + \nabla P/\rho = \mu \nabla^2 U - \mu U/\alpha - 0.5C\rho|U|U \tag{2}$$

Across the biofilm/water interface the flow equations (1) and (2) are coupled by continuity conditions for mass and momentum. The new terms in the momentum equation describe flow resistance and determine the pressure drop inside the biofilm. The special form of the sink term $S = -\mu U/\alpha - 0.5C\rho|U|U$ in (2) describes an internally homogeneous biofilm, as depicted in Figure 1. This can easily be modified in order to take spatial effects such as micro-environments or density gradients of the EPS-matrix into account. The new model parameter α describes the permeability and C is an inertial resistance factor.

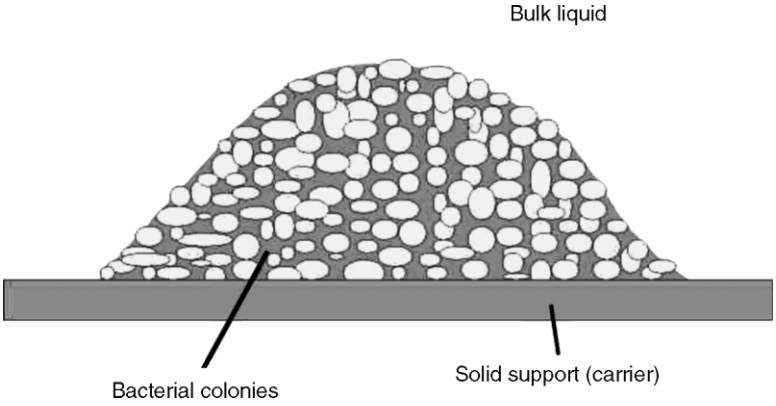

Figure 1 A biofilm as a homogeneous porous medium. It contains cells and EPS (shaded grey)

In typical applications of porous medium flow the domain is formed by a multitude of small, often assumed to be spherical, obstacles around and through which the water can flow. In a biofilm the situation is more complicated. Although we may assume that the cells play a similar role, the spaces between the cells contain EPS, which pose resistance to the flow as well. Thus taking bacteria as the only obstacles into account and estimating the porosity of the biofilm based on this assumption leads to an underestimation of the biofilm's flow resistance. Nevertheless, these well established methods are able to give lower estimates on the parameters. A standard approach is based on Ergun (1952):

$$\alpha = D_P^2/150\varepsilon^3(1-\varepsilon)^{-2}, \quad C = 3.5/D_P(1-\varepsilon)\varepsilon^{-3} \tag{3}$$

In the context of a packed bed, D_P is the mean particle diameter, and ε is the void fraction, *i.e.* the ratio of the volume of voids between the particles and the total volume. The limiting cases $\varepsilon \to 0$ and $\varepsilon \to 1$ imply $S \to \infty$ and $S \to 0$. Thus, they describe the situation of a solid biofilm as in previous biofilm models and no flow resistance at all (*i.e.* absence of a biofilm), respectively. Since (3) is actually derived for a system, which translates into a biofilm that consists only of bacteria and micro-channels but no flow resisting EPS (*i.e.* Figure 1 with the grey shaded region removed), the naive interpretation of D_P and ϵ as bacteria size and void fraction has its limitations and the parameters can only be understood as order of magnitude estimates. The information required in (3), *i.e.* size of bacteria and the void fraction between them, can be determined for particular biofilms from experimental data, *e.g.* by CLSM. For our first simulations we use rule of thumb estimates for bacteria size and void fractions. For the particle size we assume a range between 1 μm and 10 μm. The upper bound of this range exceeds the sizes of most bacteria but tries to compensate for the fact that the EPS network around the cells might also act as a flow obstacle. For the void fraction, we cover the range up to 80%; this includes permeability of the EPS network as well as micro-channels that have the same diameter (order of magnitude) as the cells and that cannot be resolved by the meso-scale description of the biofilm geometry. Under these assumptions we obtain $10^{-14}\,\mathrm{m}^2 < \alpha < 10^{-11}\,\mathrm{m}^2$ (order of magnitude). A similar analysis can be carried out for C. At this point it should be remarked that this new hydrodynamic model is consistent with the density-dependent diffusion-reaction model for growth and spatial spreading of biofilms suggested by Eberl *et al.* (2001) where the term $(1-\varepsilon)^{-2}\varepsilon^3$ of (3) (using biomass fraction $M = 1-\varepsilon$) determines the spatial spreading. Similar as here, $\varepsilon = 1 - M \to 0$ implies a local compression and solidification of biomass.

Numerical computations

The model behaviour and the sensitivity of the model with respect to the permeability parameter α is studied by computer simulations. The parameter C is kept constant at the lower range of its spectrum. This is motivated by the observation that the flow in and around the biofilm is slow and therefore the first-order terms are dominating. The discussion above showed that α can vary over a range of several orders of magnitude. Therefore, we are interested in sensitivity analysis regarding large variations rather than small perturbations. In total we include 13 different values between $10^{-14}\,m^2$ and $10^{-11}\,m^2$. For the sake of simplicity and in order to keep computing time small we restrict ourselves to two-dimensional simulations in this first qualitative study.

The biofilm architecture is formed by two prototype colonies forming a wavy structure, similar to earlier simulation experiments of biofilm hydrodynamics (*e.g.* Picioreanu, 2000, 2001; Eberl *et al.,* 2000a, 2004). It is visualised in Figure 2 together with the computational grid. The flow regime corresponds to Poiseuille flow, perturbed by the biofilm. The size of the simulation domain is $4.5\,mm \times 1\,mm$. The inlet is located at $x = -1\,mm$, sufficiently far upstream of the first colony in order to guarantee a fully developed flow. With a similar argument the outlet is located far enough downstream of the second biofilm colony. The height of the biofilm clusters is $h_1 = 243\,\mu m$ and $h_2 = 278\,\mu m$. The Finite-Volume software Fluent (Lebanon, NH, USA) is used for the simulations. Two free flow velocities are considered, $v = 0.001\,m/s$ and $v = 0.008\,m/s$; the computational mesh consists of 2,730 triangular, and 31,200 non-orthogonal quadrilateral elements.

Results and discussion

Figure 3 shows the pressure distribution along the surface of the first biofilm colony and Figure 4 shows the magnitude of the velocity vector along the line perpendicular to the substratum through the highest points of the first biofilm colony. The numerical results (visualised for $v = 0.001\,m/s$) indicate that the microscopic flow velocity inside the biofilm increases with α. While it is very small compared to the flow around the biofilm, it affects the flow in the liquid region close to the biofilm interface both qualitatively and

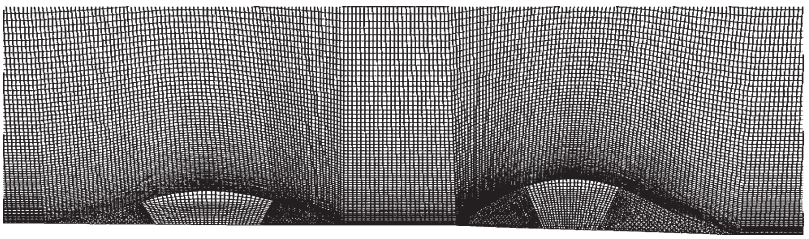

Figure 2 Biofilm domain used in the simulations and its resolution by the computational mesh. The main flow direction x is from left to right. Upstream and downstream regions are cut-off

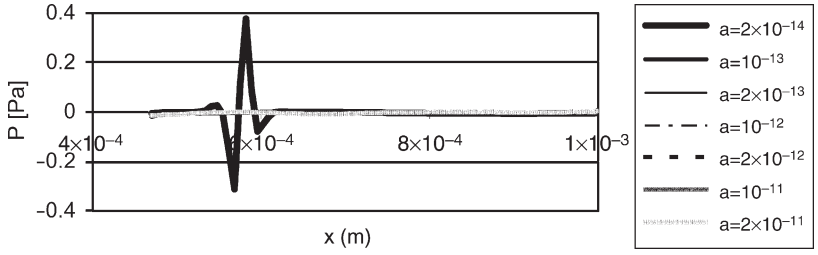

Figure 3 Pressure at the biofilm water interface of the first colony for some values of α

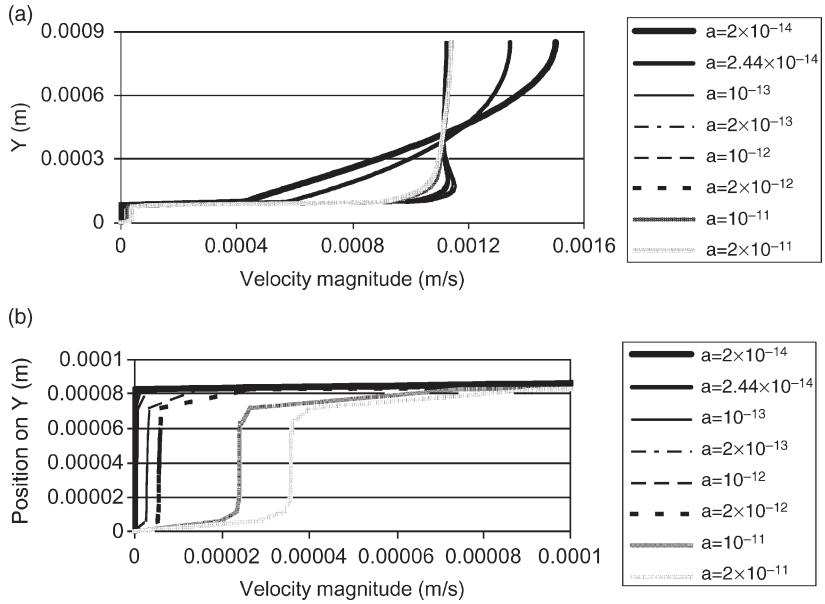

Figure 4 (a) Velocity in the liquid region above the first biofilm colony; (b) velocity inside the first biofilm colony. (selected α, $V = 0.001$ m/s)

quantitatively. In particular it induces a flow slip at the interface, which mimics micro-scale effects that are not reflected by the previous hydrodynamic model. The simulations indicate that there is a critical permeability parameter ($\alpha \approx 2.44 \times 10^{-14}$ for our system) that marks the transition of flow profiles from ones that are qualitatively similar to flow around a solid biofilm to such that are affected by the flow inside the biofilm, i.e. show permeability effects. Moreover, since in our Poiseuille setup the flow rate $Q = udy$ is the same for all α, the maximum flow velocity will become smaller if flow through the biofilm is allowed. This dependency is quantified in Figure 4a. Furthermore, Figure 3 demonstrates how the pressure along the interface is dampened if micro-scale flow is taken into account. The results for the second biofilm colony and the higher flow velocity are qualitatively very similar and omitted here due to space limitations. In particular, the transition value of α seems to the same for both cases. The simulation results imply that the usual model assumption of an impermeable biofilm structure might underestimate convective mass transport in biofilms and overestimate mechanical detachment forces. A quantification of the latter, however, requires a thorough understanding and model formulation of the mechanics of the detachment process, which is yet to be developed (cf. Sudarsan *et al.*, 2005). To which extent it is critical to neglect convective transport in the biofilm cannot be decided based on a hydrodynamic study alone but must be investigated in extended simulation experiments including mass transfer and conversion.

Conclusions

The simulations show that microscopic flow effects in the biofilm matrix affect the local meso-scopic flow field. The proposed hydrodynamic model quantitatively and also qualitatively depends on the new model parameters. Hence more effort must be put into narrowing the range of α to be considered for realistic biofilms. This should be done experimentally and by theoretical and phenomenological considerations. A problem for a theoretical derivation of such an estimate might be the observation that there are indeed three different effects that must be taken into account: the size of the cells, the size of void micro-pores, and the flow resistance of the EPS matrix. On the other hand, an

experimental parameter estimation has to take these effects into account as well and, hence, data determined for one biofilm system might not apply to another one. The simulations show that the average micro-scale flow velocities in the biofilm are small compared to the surrounding flow. This indicates that the experimental study of microscopic flow effects will require measuring techniques that are able to resolve flow velocities varying over several orders of magnitude. On the other hand, in subsequent modelling studies this strong variation in flow velocities will allow us to simplify the model by dropping the nonlinear sink term in the flow model.

Acknowledgements

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