Introduction to the IWA Task Group on Biofilm Modeling

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Abstract An International Water Association (IWA) Task Group on Biofilm Modeling was created with the purpose of comparatively evaluating different biofilm modeling approaches. The task group developed three benchmark problems for this comparison, and used a diversity of modeling techniques that included analytical, pseudo-analytical, and numerical solutions to the biofilm problems. Models in one, two, and three dimensional domains were also compared. The first benchmark problem (BM1) described a monospecies biofilm growing in a completely mixed reactor environment and had the purpose of comparing the ability of the models to predict substrate fluxes and concentrations for a biofilm system of fixed total biomass and fixed biomass density. The second problem (BM2) represented a situation in which substrate mass transport by convection was influenced by the hydrodynamic conditions of the liquid in contact with the biofilm. The third problem (BM3) was designed to compare the ability of the models to simulate multispecies and multisubstrate biofilms. These three benchmark problems allowed identification of the specific advantages and disadvantages of each modeling approach. A detailed presentation of the comparative analyses for each problem is provided elsewhere in these proceedings.

Keywords Analytical; benchmark problems; biofilm modeling; monospecies; multidimensional; multispecies; pseudo-analytical

Introduction The mathematical representation of microbial biofilms has been widely used as a key tool in biofilm research since the 1970s (Atkinson and Davies, 1974; Harremoës, 1976; Williamson and McCarty, 1976). Initially, mathematical models depicted the biofilm as a homogeneous structure, with uniform composition and thickness, and attached to a flat impermeable surface. Based on this idealization, multiple solutions to the biofilm problem have been proposed for a variety of cases, such as steady-state conditions, transient loadings, first-order degradation kinetics, etc. In addition, analytical and pseudo-analytical solutions have been developed, facilitating the mathematical analysis of biofilm problems, as these solutions often avoid the need for computationally intensive numerical analyses.

The complexity of published biofilm models parallels the steady increase in computing technology. As better computational tools became available to researchers, several of the simplifying assumptions about biofilm systems were relaxed, and models describing the activity of multispecies and multisubstrate biofilms were developed. The initial models of this type maintained the assumption of uniform thickness and simulated biofilm development as stratified microbial communities (Wanner and Gujer, 1986). The more recent discovery that microbial biofilms can be highly heterogeneous in microstructure, without uniform thickness, provides a further challenge to biofilm modelers, as the mathematical representation of these biofilm characteristics demands simulations in two-dimensional (2D) or three-dimensional (3D) domains. This produces a significant leap in the need for computing resources (i.e., memory and speed), which is often met by using supercomputers (Noguera et al., 1999b; Picioreanu et al., 1998). Taking advantage of the latest computing
technology, the most recent biofilm models even consider the effect of fluid motion through the biofilm (Eberl et al., 2000).

The inevitable result of this evolution in biofilm modeling is the existence of a large range of modeling approaches, from simple analytical solutions, which imply a large number of assumptions made about the biofilm system, to complex 3D models that try to minimize restricting assumptions and rely on the self-organization of the biofilm.

From a practical standpoint, the diversity of existing models makes it difficult for a researcher or engineering practitioner interested in using biofilm modeling as a tool for design, monitoring, or analysis, to select the appropriate level of model complexity (Morgenroth et al., 2000b; Noguera et al., 1999a). This issue was discussed in an earlier workshop on biofilm modeling (Noguera et al., 1999a), and following up on the conclusions and recommendations of that workshop, an IWA Task Group on Biofilm Modeling was created with the purpose of performing a comparative analysis of different modeling approaches and providing researchers and practitioners with guidance for selecting appropriate models for the solution of their specific biofilm problems. In the following, the benchmark problems are described together with modeling approaches employed, and a brief discussion of results. Accompanying manuscripts from the Task Group will describe in greater detail the specific modeling tools used and the results of the comparative simulations performed (Morgenroth et al., 2004; Eberl et al., 2004; Rittmann et al., 2004).

Task group on biofilm modeling
Table 1 lists the members of the Task Group, their affiliations, and the type of modeling approach that each individual used to solve the benchmark problems. In addition to these members, the following individuals significantly assisted with solutions to some of the benchmark problems: Gonzalo E. Pizarro, Universidad Católica de Chile, Alex Schwarz, Northwestern University, and Julio Perez, Kluyver Institute for Biotechnology, Delft University of Technology.

Modeling approaches
Four different modeling approaches were evaluated for the solution of three benchmark problems, as follows.

- **Analytical solutions.** The objective of this type of solution was to make appropriate simplifying assumptions and solve the benchmark problems without the need of computationally intensive numerical approaches (Pérez and van Loosdrecht, 2003).

- **Pseudo-analytical solutions.** These solutions were based on the pseudo-analytical approach developed by Sáez and Rittmann (1992), which uses explicit mathematical equations to calculate substrate flux into biofilms at steady state conditions, thus avoiding numerical solutions.

- **One-dimensional numerical solutions.** This approach required the biofilm problem to be simplified to a one-dimensional condition before a numerical solution could be derived. The numerical solutions were based on traditional finite-difference approximations, and solved with the Aquasim software (Reichert, 1994; Wanner and Reichert, 1996).

- **Multidimensional numerical solutions.** These modeling approaches did not require the biofilm to be of uniform thickness and represented biofilm heterogeneity in 2D and 3D domains. One 2D model used solved the biofilm problem using a cellular automaton (CA) approach (Noguera et al., 2003; Pizarro et al., 2001), while the two 3D models used (Eberl et al., 2000; Picioreanu et al., 1998) provided numerical solutions based on finite-difference approximations. Furthermore, a pseudo 2D approach, based on a combination of 1D Aquasim simulations (Morgenroth et al., 2000a), was also used.
Benchmark problems
Three biofilm problems were defined to compare the different modeling approaches.

Benchmark Problem 1 (BM1)
This problem simulated a monospecies biofilm growing on a flat surface, in a completely-mixed reactor, and with a fixed amount of biomass. The influent substrate concentration and flow rate were known. The main goals were to calculate the flux of organic substrate (electron donor) and oxygen into the biofilm and the concentration of these substrates in the bulk liquid. The standard case included influent substrate and oxygen concentrations of 30 gCOD/m³ and 10 gO₂/m³, respectively. The total biomass per unit area and the biomass density were set to 5 gCOD x/m² and 10⁴ gCODx/m³, respectively, resulting in an average biofilm thickness of 500 μm. The problem statement also defined the diffusion coefficients in the biofilm matrix equal to the diffusion coefficients in the bulk liquid, and no external mass transfer limitations. Other special cases were simulated, including oxygen limited conditions, biomass limited conditions, and different levels of internal and external mass transfer limitations. Internal mass transfer limitations were defined by a diffusion coefficient that was significantly smaller than the diffusion coefficient in the bulk liquid, while external mass transfer limitations were simulated by specifying the thickness of a boundary layer located at the surface of the biofilm.

Benchmark Problem 2 (BM2)
This problem was designed to compare the ability of the models to simulate the interconnection between activity within the biofilm, represented by substrate utilization and mass transfer processes, and the movement of the bulk fluid surrounding the biofilm. The problem statement defined the flow velocity profile and the substrate concentrations at the entrance of a rectangular domain, in which the biofilm was growing on a flat surface. Different biofilm geometries were tested to represent different degrees of structural heterogeneity and different hydrodynamic conditions. All the simulations assumed a single limiting substrate, a monospecies biofilm, and a diffusion coefficient in the biofilm matrix equal to the diffusion coefficient in the liquid. Because of the heterogeneous structure of the biofilm, a boundary layer was not defined a priori. Instead, the problem of external mass
transfer limitations was to be solved by either simulating the hydrodynamic conditions of the system or making appropriate simplifying assumptions. Metrics used to compare the different solutions included overall fluxes into the biofilm and predicted substrate concentrations at the base and at the surface of the biofilm. The results from a 3D simulation that included the solution of the Navier-Stokes equations were used as the baseline for comparison of all the models.

**Benchmark Problem 3 (BM3)**

This benchmark problem was set up to compare model predictions for a multispecies and multisubstrate biofilm. The system corresponded to a nitrifying biofilm in which competition for space between heterotrophic, autotrophic, and inactive biomass took place. The simulated domain was identical to the domain in BM1, that is, a completely-mixed reactor with a biofilm of known average thickness (i.e. 500 µm) growing on a flat surface. The limiting substrates were COD, ammonia-N, and oxygen, which had influent concentrations of 30 gCOD/m³, 6 gN/m³, and 10 gO₂/m³, respectively. The simulated cases were restricted to biofilms having a uniform total biomass density of 10⁴ gCODx/m³, diffusion coefficients in the biofilm equal to diffusion coefficients in the liquid, and a thin boundary layer of 0.01 µm. Several special cases were also simulated, including conditions with high N:COD ratio, low N:COD ratio, oxygen limitation, high biomass detachment, and low biomass detachment. The output parameters used to compare the simulations included the fluxes of COD and N, and the bulk concentrations of COD and N.

**Results**

In BM1 (Morgenroth et al., 2004), essentially all the modeling approaches assuming a flat biofilm morphology resulted in equivalent predictions of substrate and oxygen concentrations in the bulk liquid, and comparable predictions of substrate and oxygen flux into the biofilm, demonstrating that, for a biofilm problem consisting of a flat and homogeneous biofilm matrix and a well-defined boundary layer, the simplifications and assumptions used in analytical and pseudo-analytical approaches are adequate, and there is no need for time-consuming and computationally intensive numerical simulations. Reasonable simplifications that proved adequate for the particular conditions of BM1 were the assumption that the electron donor was the only limiting substrate and that oxygen fully penetrated the biofilm.

To test the effect of biofilm heterogeneity, some runs with multidimensional models eliminated the flat biofilm assumption and tested biofilm geometries that preserved the average thickness and the total biomass content. The solution of the problem with these modified conditions required an assumption to be made regarding the mass transfer mechanisms in the water surrounding the biofilm. If it was assumed that the water in pore spaces (i.e., water volume below the maximum biofilm thickness) was completely mixed and had a concentration equal to the bulk substrate, then the calculated flux increased slightly due to the enlargement in the surface area that was in contact with the liquid. On the other hand, with the assumption that mass transfer in the pore spaces was only due to diffusion, then the external mass transfer resistance was increased and the predicted fluxes significantly decreased.

For the solution of BM2 (Eberl et al., 2004), most of the approaches based on 1D models (analytical, pseudo-analytical, and Aquasim) required making a priori assumptions of an equivalent 1D biofilm thickness and of a representative external boundary layer. For some of these models, the inability to find an appropriate boundary layer thickness based solely on the problem description hindered their capacity to predict biofilm performance. Nevertheless, solutions to BM2 were provided by finding a boundary layer thickness that
best-fitted the results of the 3D model used as the baseline for comparisons, demonstrating that the assumption of having a boundary layer, where all external mass transfer limitations occur, is adequate only if the thickness of that layer is appropriately selected. Only two of the 1D modeling approaches were predictive. In one model, the thickness of the external boundary layer was estimated using empirical correlations derived from fixed-bed biofilms, while the other approach considered the hydrodynamics of the problem using a global mass balance of the system (Eberl et al., 2004).

The multi-dimensional models did not specify a boundary layer a priori. Rather, they incorporated fluid motion and mass transport by convection in a simplified manner by either assuming a fixed flow field (i.e., CA model) or solving the Navier-Stokes equations in 2D or 3D domains with simplified boundary conditions. In addition to predicting substrate fluxes and concentration gradients in the biofilm, these models also predicted concentration gradients in the fluid part of the modeled domain. As expected, an inverse correlation between computing time and accuracy of the solution, as compared to the full numerical simulation of hydrodynamics and biofilm activity in 3D, was observed. Therefore, the selection of modeling approaches for biofilm problems in which heterogeneity and hydrodynamics are to be considered will be a compromise between computing time and accuracy of the model predictions.

Benchmark Problem 3 required the solution of a multispecies and multisubstrate problem (Rittmann et al., 2004). In general, all the models that used a full numerical solution provided comparable results for all the cases studied. For the models that required simplifying assumptions (analytical and pseudo-analytical), it was essential to define a priori whether the different species would be layered or mixed within the biofilm, thus producing different results depending on the initial assumptions.

**Conclusions and recommendations**

The comparative analysis of different modeling approaches for the solution of three benchmark problems allowed the Task Group to undertake an objective evaluation of the benefits and limitations of each model. Important insights into the type of simplifications that are appropriate when analyzing complex biofilm systems were derived from the comparison of simplified and fully quantitative models. Specific conclusions about each of the benchmark problems are provided in the corresponding manuscripts (Eberl et al., 2004; Morgenroth et al., 2004; Rittmann et al., 2004). General recommendations, based on the results of this comparative study, follow.

In general, when the biofilm system is known to be homogeneous and the characteristics of the external mass transfer limitations are known (i.e., boundary layer thickness), simplified models based on analytical and pseudo-analytical approaches are sufficient and efficient at providing accurate solutions. If the effect of external mass transfer is not known a priori, but it is estimated to be significant, then the use of more elaborate multidimensional models may be a requirement, unless an adequate correlation between the hydrodynamic conditions and the thickness of a boundary layer can be established. However, with the realization that full numerical solutions of 3D heterogeneous biofilms are computationally expensive, attention should be placed at identifying methodologies for correctly simplifying the problem. Simplifications that were shown to be adequate (although with loss in accuracy compared to the full 3D solution) were the reduction of the problem to 2D and the simplified simulation of fluid motion with the CA model. In 1D, the definition of an external boundary layer according to correlations based on fixed-bed biofilms was also adequate, especially for low flow velocity cases. Finally, for multispecies problems, methods that use numerical solutions are preferred to the simplified analytical and pseudo-analytical procedures when the architecture of the biofilm (e.g., layering) cannot be estimated a
priori. When the architecture is known, analytical and pseudo-analytical solutions can achieve outputs that are consistent with 1D numerical solutions. On the other hand, the simpler 1D methods cannot predict the architecture de novo, while the 1D numerical solutions can. From the point of view of computational requirements, 1D numerical solutions of multispecies problems are most efficient, unless the biofilm system is highly heterogeneous in structure, or the hydrodynamic conditions are not easily simplified by estimating an equivalent boundary layer.

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References