

Modeling of Biofilm Systems: A Review

Harald Horn and Susanne Lackner

Abstract The modeling of biochemical processes in biofilms is more complex compared to those in suspended biomass due to the existence of substrate gradients. The diffusion and reaction of substrates within the biofilms were simulated in 1D models in the 1970s. The quality of these simulation results was later improved by consideration of mass transfer at the bulk/biofilm interface and detachment of biomass from the surface. Furthermore, modeling of species distribution along the axis perpendicular to the substratum helped to simulate productivity and long-term behavior in multispecies biofilms. Multidimensional models that were able to give a realistic prediction of the surface structure of biofilms were published in the 1990s. The 2D or 3D representation of the distribution of the species in a matrix of extracellular polymeric substances (EPS) helped predict the behavior of multispecies biofilm systems. The influence of shear forces on such 2D or 3D biofilm structures was included by solving the Navier–Stokes equation for the liquid phase above the biofilm. More recently, the interaction between the fluid and biofilm structures was addressed more seriously by no longer considering the biofilm structures as being rigid. The latter approach opened a new door, enabling one to describe biofilms as viscoelastic systems that are not only able to grow and produce but also be deformed or even dislodged if external forces are applied.

Keywords Biofilm model • Detachment • Fluid structure interaction • Mass transfer • Multidimensional

Abbreviations

AOB	Ammonium oxidizing bacteria
BbM	Biomass-based model
C	Constant in Eq. (14)
c	Concentration (g/m^3)

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CA	Cellular automata
c_{Fi}	Concentration of dissolved substance i at the biofilm surface (g/m^3)
c_{Bi}	Concentration of dissolved substance i in the completely mixed liquid phase (bulk phase) (g/m^3)
CBL	Concentration boundary layer
D	Diffusion coefficient (m^2/s)
d	Diameter (m)
IbM	Individual-based model
j	Mass flux ($\text{g/m}^2 \text{ d}$)
k_d	Detachment coefficient ($1/d$)
$k_{d,\text{random}}$	Detachment coefficient for random detachment events ($1/d$)
k_L	Mass transfer coefficient (m/s)
K_S	Monod constant (g/m^3)
L	Number of grid cells in height/Length (m)
L_C	Thickness of the concentration boundary layer (m)
L_F	Biofilm thickness (m)
$L_{F,\text{base}}$	Base biofilm thickness (m)
m_X	Mass of biomass (g)
N	Number grid cells in length
NOB	Nitrite oxidizing bacteria
Pe	Peclet number
p	Pressure (N/m^2)
Re	Reynolds number
RS	High rate strategist
r	Conversion rate ($\text{g/m}^3 \text{ d}$)
Sc	Schmidt number
Sh	Sherwood number
t	Time (d)
u	Flow velocity (m/s)
u_F	Relative velocity of a particulate component in the biofilm perpendicular to the substratum (m/d)
V	Volume (m^3)
X	Biomass concentration (g/m^3)
Y	Yield coefficient (g/g)
YS	High yield strategist
Z_f	Position of an occupied grid cell above the substratum within the grid (N,L)
$Z_{f\text{max}}$	Highest occupied grid cell above the substratum within the grid (N,L)
z	Space coordinate perpendicular to the substratum

Greek Letters

α	Biofilm surface enlargement
ε	Porosity
ε_S	Fraction of the solid phase in the biofilm volume

ε_{Fl}	Fraction of the liquid phase in the biofilm volume
κ	Parameter in Eq. (9)
δ	Parameter in Eq. (9)
μ	Growth rate (1/d)
$\mu_{\max}$	Maximum growth rate (1/d)
Ω	Parameter in Eq. (12)
σ	Biofilm surface roughness
ν	Kinematic viscosity (m ² /s)
ρ	Biofilm density (gX/m ³) or
ρ	Density of fluid (kg/m ³)
τ	Shear stress (N/m ²)

Subscripts

EPS	Extracellular polymeric substances
F	Biofilm
i	Component i
O ₂	Oxygen
P	Particle
S	Substrate
X	Biomass

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1 Introduction

The wish for a better understanding of the organization and function of microorganisms in biofilms has led to the development of a variety of models that capture the knowledge of biofilm systems which has accumulated over the last three decades. Such models are more than just an assembly of the biochemical processes that occur in biofilm systems. To represent a biofilm system adequately by mathematical

simulations, physical aspects such as transport mechanisms, shear forces, and mechanical strength have to be addressed in addition to the microbiological and/or ecological aspects of the “micro” organisms involved in biofilms. The modeling of biofilm systems thus quickly becomes a multidisciplinary effort combining microbiology, biogeochemistry, and fluid mechanics. Although biofilms do not yet play an important role in chemical production, the interest in modeling biofilm systems has been steadily increasing within the last 30 years [1]. One main reason has been an increasing acceptance that microorganisms in the real world like to organize themselves in biofilms and not as suspended individuals [2]. By opening this door a broad research field has emerged, and dozens of research groups worldwide have taken on the challenge of identifying the main factors influencing the structure and function of biofilms [3]. In recent years, specific aspects such as communication or quorum sensing between bacteria [4] have been implemented into a mathematical framework for biofilm modeling [5].

Very often the published manuscripts on biofilm models picked up new insights that have been generated with new experimental tools. The first significant contributions that led to a better understanding of mass transfer and mass transport in biofilm systems have been made with microelectrode studies [6–9] (see contribution of Beyenal in this volume). In the 1990s imaging of biofilm structures with confocal laser scanning microscopy (CLSM) became popular [10] and was then a driving force for multidimensional biofilm models [11] (see contribution of Neu and Lawrence in this volume). In the same decade molecular methods including DGGE, FISH, and PCR increased knowledge of microbiological composition and spatial distribution of biofilms [12]. Such methods are capable of showing the high diversity of microorganisms in mixed cultures. Nevertheless, the contribution of every single strain to the structure and function of mixed culture biofilm systems has seldom been addressed in biofilm models [13, 14].

In general, two main aspects can be found in the literature that led to the development and/or application of biofilm models.

Biofilm reactor models The first wave of model concepts for biofilms were all presented around the same time and were mainly designed to describe phenomena in fixed-bed reactors for wastewater treatment. All of these authors recognized that established mathematical models for suspended biomass were inadequate for fixed-bed reactors as they did not take the limiting diffusion in the biofilm matrix into account, and tried to remedy this by including reaction–diffusion mass balances. In the following three decades many models were developed and published that described mass transport and substrate conversion in biofilm reactors for wastewater treatment or other technical systems [15–18]. Most of these models can typically be linked to environmental engineering. A very good review on this topic was published in Ref. [19]. The authors provide an excellent overview of the existing tools for modeling biofilm reactors in wastewater treatment. Models aimed at consultants and engineers specific for the design of biofilm reactors are still scarce compared to those of activated sludges, although more and more commercially available software packages also include sections for the modeling of biofilms.

General biofilm models The second group of models was developed to describe processes and structures in biofilms, and was not aimed at specific applications. These models addressed issues such as detachment and attachment of particles at the biofilm surface, incorporation of EPS within the biofilm structure, population dynamics, and biofilm structure development. The latter can only be done with 2D or 3D models. These models form the majority of the publications in the last two decades [11, 20–26]. Recent developments deal with incorporation of physical biofilm properties into biofilm modeling [27, 28].

The number of reviews dealing with modeling of biofilm systems is limited. Reference [29] presented an early review of biofilm models. In 2006 an IWA task group produced a publication describing the state of the art of the mathematical modeling of biofilms [30]. In several benchmark problems the capability and limitations of both analytical and numerical solutions were discussed. The main focus of this report was on the comparison of 1D and 2D, respectively, 3D models. Advances in biofilm modeling with special focus on multidimensional aspects are presented in Ref. [31]. Klapper and Dockery [32] presented another review linking modeling and microbial ecology. A special focus in that review is on antimicrobial tolerance of microorganisms, biofilm mechanics, and quorum sensing. Medical biofilms and their tolerance against antibiotics has been a popular topic in biofilm research in the last decade. The review in Ref. [33] presents the main topics in this research area.

The review presented here discusses traditional biofilm models, coupling reaction/diffusion with population dynamics and biofilm structure. Both one-dimensional and multidimensional approaches are discussed. The focus is on the coupling of structure and function of biofilms. The often underestimated effect of mass transfer is also discussed as well as the impact of detachment. These processes form part of most one- and multidimensional biofilm models. Finally, the latest developments incorporating biofilm mechanics are shown.

2 1D Biofilm Models

2.1 Mass Transfer at the Bulk/Biofilm Interface

In many existing biofilm models the bulk/biofilm interface is not handled properly. Mass transfer at this interface is decisive for the supply of the active biomass with all types of soluble substrates. Assuming that the biofilm surface is separated from the bulk by a laminar layer, classical film theory can be applied. In several models the thickness of this layer has been set to values around 100 μm [34–37]. In film theory the mass transport within this layer is assumed to be diffusive. Therefore the layer is often called the diffusion boundary layer (DBL) [38, 39]. The mass transfer coefficient k_L can then be calculated by dividing the diffusion coefficient D_i by the thickness of the boundary layer L_C :

$$k_L \cong \frac{D_i}{L_C} \quad (1)$$

Nevertheless, numerous microelectrode measurements indicate that both diffusive and advective transport drive the transport within the boundary layer [40–44]. Therefore, a linear approach as shown in Eq. (1) is not close to reality, as, for example, can be seen in Fig. 2 for an oxygen profile measured with a microelectrode in a hetero-/autotrophic biofilm. Consequently, the boundary layer should be addressed as the concentration boundary layer (CBL). The mass transfer at the bulk/biofilm interface is a result of flow conditions in the bulk phase and can be calculated if an empirically derived relation between flow and mass transfer is available. The Sherwood number Sh is the dimensionless number for mass transfer. It is used to determine the ratio of the total mass transfer flux to the diffusion flux:

$$Sh = \frac{k_L \cdot d}{D_i} \quad (2)$$

The characteristic length d depends on reactor geometry; in the case of a tube it is the tube diameter. The Sherwood number can be expressed as a function of the Reynolds number Re and the Schmidt number Sc :

$$Sh = f(Re, Sc) \quad \text{with} \quad Sc = \frac{\nu}{D_i}, \quad Re = \frac{u \cdot d}{\nu} \quad \text{and} \quad Pe = Re \cdot Sc \quad (3)$$

where u is the average flow velocity, ν the kinematic viscosity, and Pe is the Peclet number as the product of Re and Sc . An overview of variations of the Sherwood number in biofilm systems is given in Table 1. Only a few of these equations were adapted specifically to biofilm systems by the authors. In fact, most of the equations were taken from process engineering where they were mainly used in connection with biofilm-free surfaces.

Equation (11) is based on microelectrode measurements [52]. The steepness of the oxygen concentration profiles has been combined with the measured mass flux j_{O_2} . Thereby, averaged mass transfer coefficients k_L could be calculated based on the Neumann boundary condition at the bulk/biofilm interface:

$$j_i = k_L \cdot (c_{Bi} - c_{Fi}) \quad (4)$$

Picioreanu et al. [54] extended the equation for the Sherwood number for biofilms by including the enlargement of the surface area α [Eq. (14)]. A comparable approach was published in Ref. [53] both for laminar and turbulent flow in tubes [Eqs. (12) and (13)]. The structure factor $\mathcal{Q}$ is a function of growth rate μ and flow conditions during growth. Such approaches attempting to incorporate the effect of biofilm structure into 1D models have not been fully successful. The possibility of generating the required “real” surface structures is better provided with 2D or 3D models (see Chap. 3).

Table 1 Equations for the sherwood number in biofilm systems (adapted from Ref. [45])

Sherwood number Sh	Reactor type	References	Equation
Laminar: $88 + (1.11 \times 10^{-11}/d_p) Re^{4.33} \times Sc^{1/3}$	Gravel in a flow channel	[46]	(5)
$2 + f_K (Re Sc)^{1.7}/(1 + (Re Sc)^{1.2*})$ with $f_K = 0.66/[1 + (0.84 Sc^{1.6})^3]^{1/3}$	Immobilized biocatalyst	[47, 48]	(6)
Laminar: $1.615 (Re d/L)^{1/3} Sc^{0.27*}$ Turbulent: $0.037 (Re^{0.75} - 180) Sc^{0.27} [1 + (d/L)]^{2/3*}$	Membrane tube reactor	[49]	(7) (8)
Turbulent: $0.0153 Re^{0.833} Sc^{0.32*}$	Open flow channel	[50]	(9)
Laminar: $2 + 0.51 (\kappa Re_p \delta)^{0.6} Sc^{1/3*}$ ($\kappa, \delta = f(Re_p)$ with $Re_p \equiv u d_p/\nu$)	Biofilter with particle-fixed biofilms	[51]	(10)
Laminar: $2 Re^{1/2} Sc^{1/2} (d/L)^{1/2} (1 + 0.0021 Re)$ $2 Re^{1/2} Sc^{1/2} (d/L)^{1/2} (0.24 \Omega)^{-1}$ Turbulent: $0.037 Re^{0.75} Sc^{1/2} (0.24 \Omega)^{-1}$	Biofilm tube reactor	[52, 53]	(11) (12) (13)
Laminar: $C \alpha^{-n} Re^{1/3} Sc^{1/3}$	Particle-fixed biofilms	[54]	(14)

*Not specifically adapted to biofilms

2.2 Reaction/Diffusion Models

Knowledge of the substrate concentration at the biofilm surface [Eq. (14)] is essential for solving models of reaction/diffusion processes in the biofilm. As mentioned above, the first model approaches were published around 1976 [55–58]. The authors tried to describe mass transport and conversion in fixed-bed reactors used for wastewater treatment. Substrate conversion in the biofilm was coupled to diffusion and a steady-state approach ($dc/dt = 0$) based on Fick's second law was used:

$$D_S \frac{\partial^2 c_S}{\partial z^2} = r_S \quad (15)$$

with

$$r_S = \mu_{\max} * \frac{1}{Y_{X/S}} \frac{c_S}{(c_S + K_S)} X$$

This reaction/diffusion model is still used. The biggest challenge is still how to describe the distribution of biomass along the axis perpendicular to the substratum. As long as one species or one group of microorganisms (i.e., biomass X) has to be modeled, the biomass can be handled easily and more or less evenly distributed

based on the availability of substrate S . As soon as two or more species with different growth rates μ and yield coefficients Y are involved, the outcome of the model strongly depends on where the different species can be found at which concentration along the z -axis.

Kissel et al. [20] made one of the first significant contributions to overcome this problem. The biofilm was divided into segments. Both the biomass growth and the proportion of the involved species as well as their distribution in the biofilm were then calculated. Another approach [22] discretized both biofilm and water layer perpendicular to the substratum. The authors identified the important influence of biofilm density ρ_X , which is formulated as follows:

$$\rho_X = m_X/V_F \quad (16)$$

ρ_X determines the amount of biomass X of a certain species that is available in a volume element. Depending on cultivation conditions and specific growth rate of the species ρ_X can vary between 10,000 g/m³ [53] and 110,000 g/m³ [59]. The general assumption is that the lower the growth rate, the higher the density, and the lower the flow velocity (or shear rate) above the biofilm the lower the density [60, 61].

One of the most used 1D models was published in 1986 by Wanner and Gujer with further developments over the following 10 years [23, 62]. The particulate components (i.e., biomass and particulate inert material) were treated in a continuum approach. Wanner and Gujer used a differential equation to describe the mass balance of particulate components in biofilms:

$$\frac{\partial X_i}{\partial t} = -\frac{u_F}{\partial z} \frac{\partial X_i}{\partial z} + r_{Xi} \quad (17)$$

Inclusion of this made it possible to synchronize substrate transport and utilization [Eq. (15)] along the z -axis with the change of particulate component concentration X_i . In Eq. (15) r_S describes the substrate conversion whereas the rate for conversion of particulate components X_i is symbolized in Eq. (17) by r_{Xi} .

The key parameter u_F represents the velocity of particulate components i moving perpendicular to the sub-stratum (see Fig. 1). The velocity can be positive if the component X_i is produced by growth and can be negative if the component undergoes, for example, lysis.

$$u_F = u_{F(z=0)} + \int_0^{L_F} \sum_{i=1}^n \frac{r_{Xi}}{\rho_i} dz \quad (18)$$

The value of ρ_i will have a strong impact. If the biofilm density ρ_i is set to a low value the biofilm thickness L_F will grow with a higher velocity. Most published 1D simulation studies do not try to predict the biofilm density but rely on experience or measured values [63–66]. An advanced approach of the model shown above, which

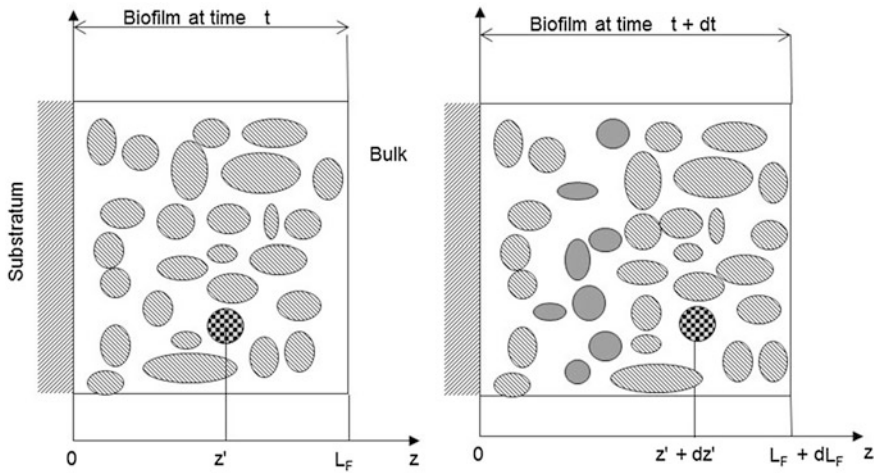


Fig. 1 Transport of a particulate component (*crossed sphere*) after growth of new components (*dark grey*) in the underlying layer (adapted from Ref. [62])

was published in 1989 by Gujer and Wanner, separated the biofilm into a liquid phase ε_{FI} and a solid phase ε_S [62]. Microorganisms and other particulate material are part of the solid phase and the dissolved components such as substrate and oxygen are transported in the liquid phase.

$$\varepsilon_{FI} + \sum \varepsilon_{Si} = 1 \quad (19)$$

Figure 2 shows a typical example for an application of the Wanner–Gujer model, a competition between ammonium oxidizing autotrophic bacteria and organic carbon utilizing heterotrophic bacteria, which is often used as the classic case for 1D biofilm models [34, 67, 68] in wastewater treatment. In the latter case micro-electrode measurements are used to optimize the kinetic parameters. Similar simulation studies have been conducted for biofilms growing on permeable membranes [69]. In this case the biofilm is membrane bound and supplied with oxygen from the membrane side. The setup allows for simultaneous nitrification and denitrification in one biofilm. Membrane bound biofilm reactors also offer different selection mechanisms, for example, to select for ammonium or nitrite oxidizing bacteria (AOB and NOB) [70, 71].

The outcome of such simulation studies is mainly driven by the underlying kinetics of the involved species. In this case ammonium oxidizing bacteria AOB, nitrite oxidizing bacteria NOB, heterotrophic bacteria HB, and inert material are competing for space and oxygen. For wastewater treatment the activated sludge model ASM is typically applied to describe the kinetics [72]. Nevertheless, as the competition of AOB and NOB is not explicitly described in the ASM, most modelers use the kinetic parameters accumulated for these two types of organisms by [65] from different sources.

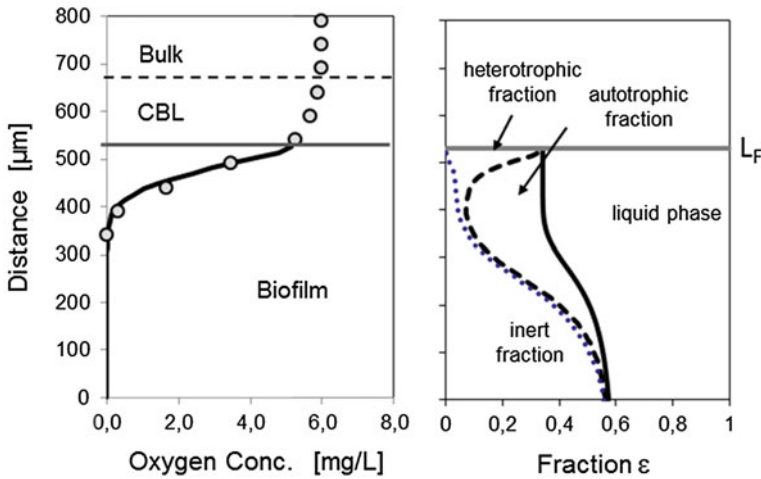


Fig. 2 Simulation results for a heterotrophic/autotrophic biofilm system. *Right graph* species distribution; *left image* measured (grey circle) oxygen profile with concentration boundary layer (CBL) and the simulated profile within the biofilm for the same day (data and permission from Ref. [68])

If there are large differences between the growth rates μ of the bacteria involved, the species will be stratified as shown in Fig. 2. Physical parameters, such as the mass transfer coefficient k_L and diffusion coefficient D , will not have a high impact, as the diffusion coefficients of the different substrate molecules involved are rather similar [73–75].

A successful tool for the above-described 1D simulations of biofilm systems is AQUASIM, which has been available for 20 years and is still widely used [76] (<http://www.eawag.ch/forschung/siam/software/aquasim/index>). Various types of active or inactive particulate biological or inorganic components within the biofilm can be included in the simulations including:

- Bacteria (AOB, NOB, AnAOB, heterotrophic bacteria) [69, 70, 77–81]
- Extracellular polymeric substances (EPS) produced by bacteria [82, 83]
- Phototrophic microorganisms [84–86]
- Fungi [87, 88]
- Inorganic materials [89]

The results of such simulation studies might be partly predictable, as most of the dynamic processes behave quite linearly. More or less unexpected results are achieved if instationary detachment processes are applied to allow slower growing microorganisms to appear at the biofilm surface because of detachment of the faster ones [90].

2.3 Detachment

The prediction of detachment is still an unsolved problem. Like transport processes, it is driven more by physics and less so by the microbiology. Already in the 1980s simple models were proposed on how the process of biomass detachment should be described. Several approaches have been published aiming to model the loss of biomass by detachment. These biofilm models mainly focus on erosion and sloughing. Erosion is characterized by the detachment of smaller particles in the range of 10 μm , whereas sloughing involves the removal of large parts up to several mm from the biofilm. Two other mechanisms that may also cause biofilm to be removed have not really been addressed by modelers, that is, abrasion and grazing by higher organisms.

Detachment occurs when external forces (e.g., through shear) are larger than the internal strength of the biofilm matrix. In principle there are two mechanisms that can lead to detachment: (i) increase of the external shear forces (e.g., during backwashing), or (ii) decrease of the internal strength (e.g., through hydrolysis of the polymeric biofilm matrix) [91]. Generally the detachment process can be formulated as

$$\frac{dL_F}{dt} = f(\rho_F, L_F, \mu, \tau, \dots) \quad (20)$$

Detachment is caused by a combination of biological, chemical, and physical processes [92] and detachment has been linked to different parameters [see Eq. (20)]. Little is known about the biological mechanisms of the bacterial species involved. As a result detachment is often incorporated into biofilm models on the basis of simplified assumptions [68, 93]. Sometimes a constant biofilm thickness is assumed to focus on the microbial processes inside the biofilm [21, 94]. Table 2 provides several approaches by which detachment can be incorporated into biofilm modeling. Typically a detachment coefficient k_d is used as the lumped parameter. Early models often used biofilm thickness [34, 95–98]. A more physical approach is the use of shear stress τ [26, 99, 100] or the change of shear stress τ [101]. The rate of increase of shear stress delivers an especially significant contribution to detachment [91].

Other authors identified the influence of growth rate μ of the microorganisms as a significant factor in the detachment process [101, 103, 105, 106, 107]. Detachment processes can be a function of time, for example, during back washing [64, 108]. A dimensionless analysis of the detachment rate is provided by Nicolella [109]. One-dimensional models with shear and nonshear detachment are compared in Ref. [110].

Table 2 Detachment models for one-dimensional biofilm models (adapted from Ref. [102])

Biofilm growth under constant substrate load	Formulation of the detachment rate (g/m ² d)	References	Equation
Constant	Constant biofilm thickness	[21]	
Constant	$k_d X_f^2$	[98, 95]	(21)
Constant	$k_d \rho_F L_F \tau^{0.58}$	[100]	(22)
Constant	$k_d \rho_F L_F^2$	[34]	(23)
Constant	$L_F (k_d' + k_d'' \mu)$	[103]	(24)
Constant	$k_d \rho_F L_F$	[96, 97, 104]	(25)
Constant	$k_d \rho_F \tau$	[99]	(26)
Constant	$k_d \rho_F u_F$	[23]	(27)
Time dependent detachment differentiating between normal operation and backwashing*	No detachment ... In operation $k_d (L_F - L_{F,base})$... During backwash	[102]	(28)
Random	$k_{d,random}(L_F - L_{F,base})$	[91]	(29)

The dimensions of k_d , k_d' and k_d'' are different for different models

*Model of a sequencing batch reactor (SBR)

3 Advanced Multidimensional Biofilm Models: Biofilm Structure

3.1 Cellular Automata (CA)

At the end of the 1990s the first multidimensional biofilm models were published on cellular automata (CA). The authors used a discrete formulation, which was able to describe the spatial heterogeneity of biofilms produced by growth and decay of microorganisms [24, 111, 112]. Two-dimensional approaches used a uniform rectangular grid, whereas 3D models used cubical elements. The available squares (2D) or cuboids (3D) were filled with biomass based on growth driven by the turnover of available substrate. The state of a system was determined based on the substrate concentration S and biomass density C (in dimensionless form). A third matrix element described whether a space was filled with bacteria, inert material, or liquid [113].

Figure 3 shows an example for a 2D grid. The substrate concentration is calculated based on the reaction diffusion Eq. (5). The biomass density is a key parameter as it drives the turnover of the reaction/diffusion model. The modeler has to decide how much biomass is allowed for one square. If the biomass density reaches its maximum level the excess biomass will be transferred to one of the

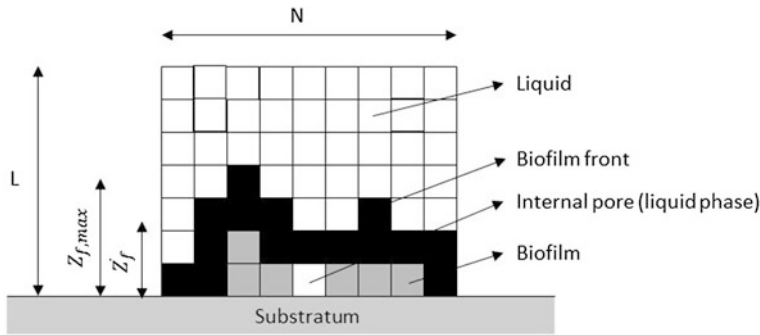


Fig. 3 Grid (N,L) for CA with cells filled with biomass or liquid phase (adapted from Ref. [11])

adjacent cells. If all adjacent cells are occupied one randomly chosen cell is displaced following the same rule.

When run, these 2D or 3D structures develop a structural heterogeneity of biofilms similar to those seen with CLSM techniques in the 1990s (see review on imaging by Neu and Lawrence in this volume). Picioreanu et al. further specified the CA approach with respect to the different states of the cells within their model [11]. Figure 3 shows the different states of the cells within a grid that are defined as with liquid phase, biomass at the biofilm front, biomass within the biofilm, and internal pores. The work shows how biofilm roughness σ developed based on substrate availability. The roughness was calculated based on the state of matrix c and the deviation of the local biofilm thickness Z_f (see Fig. 3).

Figure 4 shows a biofilm structure generated with the CA approach [11]. The example is based on slow-growing bacteria with a growth rate $\mu_{\max}$ of 1.2 d^{-1} . Different biofilm structures can develop based on inoculation strategy, substrate availability, and flow field [24, 114]. In general the surface roughness σ increases with decreasing substrate availability. Fingerlike structures as can be seen in Fig. 4 have also been generated with continuum approaches using pressure (generated within the biofilm by growth) as the driver for biofilm growth [115]. Other continuum approaches tried to describe the spreading of biomass with diffusion [116].

Detachment has been included in biofilm models based on CA. For example, in Ref. [117] detachment of biomass was assumed to be caused by the internal stress generated by a liquid phase moving above the biofilm. The biofilm was assumed to be a homogeneous and isotropic elastic material. The biofilm would detach if the external forces driven by the flow field exceeded the internal strength. A more conservative CA approach for describing detachment that included detachment coefficients and maximum biofilm height was presented by Chambless and Stewart [118].

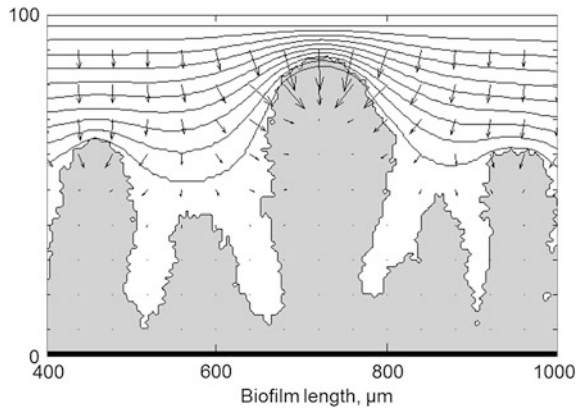


Fig. 4 Application of the CA-based biofilm model, shown with permission from Ref. [11]. The model shows a biofilm structure after 31 days at an average substrate concentration. The lines above the biofilm structure show the substrate concentration field; the *arrows* indicate the flux

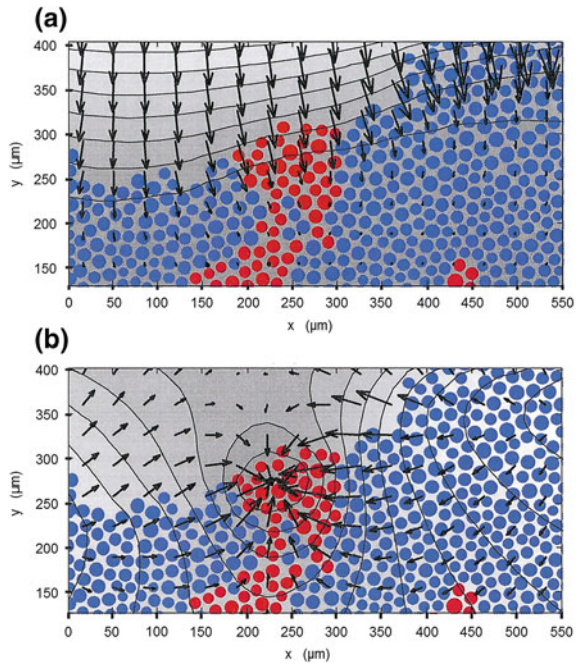
3.2 Individual-Based and Particle-Based Biofilm Models

A main trigger for the development of 3D model approaches other than CA was the question of how single cells really behave in terms of spreading. Kreft et al. were the first to develop an individual-based model that focused on single cells as individual particulate units [93]. The idea was to generate biofilm structures that give a more realistic distribution of bacteria in a biofilm matrix. The model, BacSim, was organized similar to the CA models described above. Cells were represented by shapes, typically spheres. A minimum distance was maintained between the neighboring cells [119]. Growth was again based on the reaction/diffusion equation for the soluble substrates [see Eq. (5)] The biomass accumulation was simulated by the insertion of new cells. After insertion the new position of cells within the matrix was determined based on the calculated overlap with neighboring cells.

In general CA biomass-based models (BbM) and individual-based models (IbM) show no major differences except in biofilm shape and distribution of so-called minority species [119]. The behavior of competing egoistic and altruistic bacteria has been studied with IbM [120]. The author compared two bacteria with different strategies but growing on the same substrate: a high yield (YS) and a high rate strategist (RS). Compared to suspended cultures, where the RS are better off, YS can dominate biofilms. YS do have a chance to maintain within the system if they form clusters, which have to be broken up in single cells occasionally to colonize new surfaces. The simulation shows a possible benefit of multidimensional models compared to the 1D approach. The behavior of different strategies or species in terms of dispersal can be studied easily.

To reduce the resources needed for computing an extension of the IbM has been proposed in which the particles are clumped together to form units with a larger diameter (up to 20 μm compared to 1 μm in the standard IbM) [121]. The particles

Fig. 5 Particle-based biofilm model with AOB (*blue*) and NOB (*red*). Particle size is around 20 μm . Fluxes of oxygen (**a**) and nitrite (**b**) indicated by the length of the *arrows*. The two images nicely show the concentration fields for the two substrates of which one (nitrite) is produced within the biofilm and the other (oxygen) comes with the liquid phase from outside the biofilm (reproduced with permission from Ref. [121])



consist of one type of bacteria and inert biomass. Redistribution of the clumps is organized in the same way as in the standard IbM. The spread of biomass is again the result of biomass growth, and occurs by spheres pushing each other out of the way when they get too close to each other [121].

Figure 5 shows one advantage of 2D models over the traditional 1D simulation. A cluster of NOB is embedded in AOBs, receiving their substrates from different sources (nitrite from AOB activity and oxygen from the bulk). The necessary resolution of AOB and NOB in two dimensions to demonstrate the impact on local substrate distribution is not possible with 1D models.

Most of the early individual-based models did not address hydrodynamics. The main problem was the time scale. There were several magnitudes of difference in the time scales between processes such as advective flow and the growth of new bacteria:

- Advection (10^{-2} – 10^{-1} s)
- Biochemical substrate conversion (10^{-1} – 10^2 s)
- Diffusion (10^3 s)
- Biomass growth (10^5 s)
- Detachment, erosion (10 s), and sloughing (10^5 s)

Xavier et al. published a particle-based model that included a realistic liquid flow above the biofilm structure [122] by calculating the laminar flow field above the biofilm structure using the Navier–Stokes equation:

$$\frac{\partial u}{\partial t} = \nu \nabla^2 u - u \cdot \nabla u - \frac{1}{\rho} \nabla p \quad \nabla \cdot u = 0 \quad (30)$$

By solving this equation the mass transfer at the bulk/biofilm interface could be solved in parallel and the Sherwood number no longer had to be calculated based on empirical equations (see Table 1). Furthermore, the detachment was addressed in the particle-based biofilm models by the use of a level-set method to identify the bulk/biofilm interface [123]. The model incorporates the production of heterotrophic biomass, EPS, and inert material. Detachment processes including erosion and sloughing are coupled, with higher erosion less sloughing can be observed.

In the last decade multidimensional biofilm models have been used to simulate processes in technical aquatic systems mainly by the biofilm modeling group at TU Delft:

- Anaerobic ammonium oxidation [121]
- Microbial fuel cells [124]
- Porous media [125]
- Biofouling in membrane technology [126]

Recently Lardon et al. formulated a general IbM (IDYNOMICS) with an open-source code [127]. The biofilm pressure field introduced by Alpkvist and Klapper [27] was also implemented. These approaches directly lead to the fluid–structure interaction, which is discussed in the next chapter.

4 Coupling Fluid Dynamics with Biofilm Structure

Although the multidimensional structure and function of biofilms can be simulated with the models described before, the incorporation of physical processes such as deformation by shear forces is not addressed by these models. This can be difficult. The problem begins with the identification of required parameters [128]. Methods to measure physical biofilm characteristics are challenging and do not easily provide the necessary parameters (Young’s modulus, shear modulus, adhesive or tensile strength) that are needed to feed such models [129, 130]. It is, however, worthwhile. Biofilms typically behave as viscoelastic structures if shear forces are applied. The deformation that follows the application of shear will have an impact on mass transfer, compactness of biomass, and detachment. A moving structure will also back-couple on the flow field.

A ball-spring model for biofilms was proposed by Alpkvist and Klapper (2007), which applied an immersed boundary method to describe the mechanical response and in the end detachment of biomass from biofilms in a flow field [27]. This contribution was a significant step forward in biofilm modeling because the biofilm structure was no longer assumed to be rigid. The role of biofilm cohesion with respect to growth-induced pressure stress within the biofilm was described by Dockery and Klapper [131]. Another example of a two-dimensional biofilm

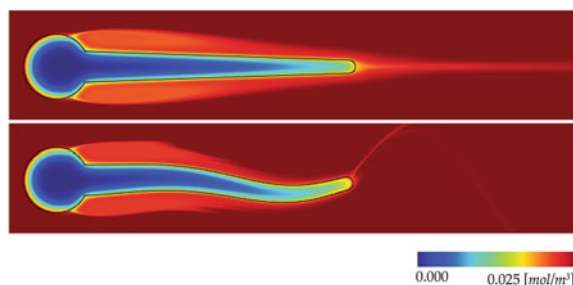


Fig. 6 Substrate concentration around a rigid (*upper image*) and an oscillating (*lower image*) biofilm streamer (reproduced with permission from Ref. [137])

structure deformed due to applied shear forces was presented by Cogan (2008). The author assumed the biofilm as viscoelastic fluid surrounded by another fluid with a lower viscosity [132].

Recently, finite element methods (FEM) or extended finite element methods (XFEM) found their way into the modeling of fluid–structure interaction in biofilm systems [133]. One example is provided by Duddu et al. [134], who presented a model that included mass transfer, growth, and detachment of biomass based on XFEM and a level-set interface tracking method. Another development is the use of images from CLSM to study detachment of biomass in combination with FEM [28]. Real biofilm structures are used to simulate the detachment. Such a combination of imaging with CLSM and simulation with FEM was also applied for a surgical suture covered with colonies of *Staphylococcus aureus* [135]. The aim was to predict the detachment of bacterial cells as a result of the deformation of the suture.

The influence of flow velocity on the oscillation of a biofilm streamer and the back coupling on the surrounding flow field was studied by Taherzadeh et al. [136]. The formation of a Kármán vortex street behind the biofilm streamer was shown to create eddies that influenced the streamers growing downstream. The oscillation of the streamer reduced the forces that were induced by the moving fluid. Furthermore, the movement clearly led to improved mass transfer at the tip of the streamer. Comparison of a rigid structure and an oscillating streamer (Fig. 6) showed a significantly better substrate supply for the latter [137].

5 Conclusions and Future Perspectives

The last three decades have seen huge developments in biofilm modeling. Simple reaction/diffusion models for biofilms have been further developed into multidimensional, multispecies models that are used in biofilm research today. However, compared to the activated sludge models (ASM) [72] that are intensively used for the design and operation of wastewater treatment plants, the available biofilm models have not had much success [30, 138–140]. It seems that isolated questions

about mass transfer, species distribution, and detachment can be answered with the available modeling tools but the entire situation in a full-scale biofilm reactor cannot easily be predicted. This is because, on top of the biofilm, the geometry of the reactor and carrier material has to be considered. This makes it difficult to make accurate predictions as the necessary data for the reactor model are seldom available.

It is evident that the dilemma described above cannot be solved by more complex multidimensional or multiphysics biofilm models. The development of multidimensional biofilm models (CA, IBM, and particle-based models) has, however, a positive impact on the understanding of the underlying processes in biofilms. One good example is the development of biofouling in reverse osmosis (RO) spiral-wound modules. As this is a very local problem the simulation results of 2D studies with a fully resolved flow field provide a very good insight into the development of biofilms on the feed spacer material in RO [141].

The perspective of having more models that are able to couple the above-described biochemical part (substrate transport/consumption and biomass growth/distribution) with mechanical characteristics and behavior is very promising. Computing time remains an issue; however, it has become a minor one. Measurement of the necessary parameters continues to be challenging and needs further improvement. Forty years ago microelectrode studies pushed the first reaction/diffusion models [40]. Twenty years ago the multidimensional models were inspired by imaging techniques such as CLSM [10]. Perhaps current biofilm models can take a step forward by the characterization of mechanical properties of biofilms [129, 130].

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