Mathematical Modeling of Mixed-Culture Biofilms

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About 10 years ago a set of mass balance equations for mathematical modeling of mixed-culture biofilms (MCBs) was presented. That model was able to describe the progression of the biofilm thickness and the spatial distribution and development in time of particulate and dissolved components in the biofilm as a function of transport and transformation processes. Experimental observations made in the past years have shown that some of the assumptions made in that MCB model were too simple. Therefore, an extended MCB model with additional processes has been developed. This model includes a more flexible description of transport of dissolved components in the biofilm and considers diffusive transport of particulate components in the biofilm solid matrix, changes of the biofilm liquid phase volume fraction (porosity), and simultaneous detachment and attachment of cells and particles at the biofilm surface. The extended MCB model is implemented in AQUASIM, a new computer program designed for the analysis of aquatic systems, which is used here to illustrate and discuss the effect of the additional processes on MCB behavior. © 1996 John Wiley & Sons, Inc.
Key words: Biofilm • diffusion • model • mixed-culture • simulation

INTRODUCTION

About 10 years ago a mathematical mixed-culture biofilm (MCB) model was presented.[14] In subsequent years the formalism of this model was refined.[6,16] Basically, the MCB model consists of a set of one-dimensional mass balance equations by which the progression of the biofilm thickness and the spatial distribution and development in time of various dissolved components (nutrients, electron donors, and electron acceptors) and particulate components (microbial cells, extracellular polymeric substances, organic and inorganic particles) in a biofilm can be modeled as a function of transport and transformation processes. These mass balance equations are generally valid and can be applied to almost any microbial system if the appropriate stoichiometry and kinetics can be provided.

Despite the fact that the proposed MCB model already was relatively complex, experimental observations in recent years have revealed that some of the assumptions made were too simple.[17] It seems that dissolved components in the biofilm are not always transported by molecular diffusion only and that displacement of particulate components is not exclusively related to volume changes of the biofilm solid matrix.[1] Attachment and detachment of cells and particles at the interface between biofilm and bulk fluid can occur simultaneously.[2] The biofilm liquid phase volume fraction (porosity) was found to vary with time and space.[18]

These experimental findings could not be reproduced by the proposed MCB model. Therefore, an extended MCB model has been developed. The philosophy is that the MCB model is refined according to the gain of new experimental information. The extended MCB model includes several additional processes which are able to reproduce the new experimental observations. Furthermore the equations of the extended MCB model offer more flexibility with regard to biofilm geometry, which can be described, e.g., by cylindrical or spherical coordinates. The equations are still based on the continuum approach[15] and are one dimensional in space. All properties of the biofilm are expressed as averages over planes parallel to the substratum. Thus, the MCB model is not suited to describe biofilm phenomena which occur at the scale of single cells.

In this article the equations of the extended MCB model are presented and examples of the effects of the additional processes on biofilm behavior are discussed. The equations consist of a set of partial and ordinary integro-differential equations, which together with their boundary conditions, the equations for a completely mixed bulk fluid and a liquid boundary layer, have been implemented in AQUASIM, a new computer program for the identification and simulation of aquatic systems.[9,10] AQUASIM is used for the calculation of the examples discussed in this article.

MODEL EQUATIONS

One-Dimensional Conservation Laws

One-dimensional conservation laws are formulated as balances of conserved properties (mass, volume, momentum, energy, etc.). If differentiability of the solutions is given, the differential form of the one-dimensional conservation laws can be used. This form is

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$$\frac{\partial \mathbb{D}}{\partial t} + \frac{\partial \mathbb{J}}{\partial z} = \mathbb{R} \quad (1)$$

where $\mathbb{D}$ is the array of one-dimensional property densities (amount of property per unit length), $\mathbb{J}$ is the array of property fluxes (amount transported per unit time), $\mathbb{R}$ is the array of net one-dimensional property production rates (amount produced per unit length and unit time), t is time, and z is the space coordinate.

MCB modeling is based on conservation laws for the mass of particulate components, for the mass of dissolved components, and for the volume of the liquid phase between the particulate components in the biofilm and requires that expressions for $\mathbb{D}$, $\mathbb{J}$, and $\mathbb{R}$ are given.

One-Dimensional Densities in the Biofilm

The product of the biofilm area parallel to the substratum, A, and of the spatial densities averaged over that area yields the array of one-dimensional densities

$$\mathbb{D} = \begin{pmatrix} AX_{F,i} \\ AS_{F,i} \\ A\varepsilon_{\ell_F} \end{pmatrix} \quad (2)$$

where $X_{F,i}$ is the concentration of a particulate component in the biofilm (average over A of mass per unit biofilm volume), $S_{F,i}$ is the concentration of a dissolved component in the biofilm (average over A of mass in the biofilm liquid phase per unit biofilm volume), and ε_{ℓ_F} is the volume fraction of the liquid phase between the particulate components in the biofilm (average over A of liquid volume per unit biofilm volume). In the original MCB model ε_{ℓ_F} was assumed to be constant. In the extended MCB model ε_{ℓ_F} is a state variable; i.e., it can vary with time and space. Sometimes ε_{ℓ_F} also is referred to as *porosity*.

It is convenient to introduce volume fractions,[15] because for all compartments, which in this article are biofilm and bulk fluid, the equation holds

$$\varepsilon_\ell + \sum_{i=1}^{n_X} \varepsilon_{s_i} = 1 \quad (3)$$

where ε_ℓ is the liquid phase volume fraction, ε_{s_i} is the volume fraction of the solid phase i (solid phase volume per unit compartment volume), and n_x is the number of particulate components considered in the model. Each particulate component forms its own solid phase. In the case of a pure-culture biofilm $n_x = 1$ and there is only one solid phase in the biofilm. Concentrations and volume fractions are related to each other by the following equations:

$$X_i = \varepsilon_{s_i}\rho_{s_i} \quad (4)$$

$$S_i = \varepsilon_\ell C_i \quad (5)$$

where ρ_{s_i} is the density of a particulate component (particulate component mass per unit solid phase volume) and C_i is the concentration of a dissolved component in the liquid phase (dissolved component mass per unit liquid phase volume). In the biofilm the variables ε_{s_i}, ε_ℓ, and C_i also represent averages over A. The density ρ_{s_i} is assumed to be a specific constant property of a particulate component.

One-Dimensional Mass Fluxes in the Biofilm

Figure 1 shows the transport processes which are considered in the MCB model. In this section mathematical expressions are given for the mass fluxes of those processes, which describe transport in the biofilm interior.

Flux of Particulate Components

The expansion or shrinking of the biofilm solid matrix in the space between the substratum and the location considered causes a displacement of the particulate components.[11,15] This process can be expressed as an advective flux,

$$\mathbb{J}_{F,X_i,1} = Au_F X_{F,i} \quad (6)$$

where u_F is the displacement velocity at the location considered.[6]

In the extended MCB model there is an additional transport process, which is modeled as an effective diffusive flux,

$$\mathbb{J}_{F,X_i,2} = -AD_{F,X_i}\frac{\partial X_{F,i}}{\partial z} \quad (7)$$

where z is the distance from the substratum and D_{F,X_i} is an effective diffusion coefficient, which typically is much smaller than the coefficient of molecular diffusion of cells and particles in pure water. Equation (7) is introduced to account for "mixing" of cells or particles in the biofilm solid matrix as a result of mechanical deformation of the matrix by hydraulic forces or bioturbation. These events can lead to temporary detachment of single cells or particles from the matrix and subsequent reattachment at another location. Since no data are available on detachment, movement, and reattachment, only the net result of these processes is modeled empirically by an effective diffusive flux.

Flux of Dissolved Components

Transport of dissolved components in the liquid phase of the biofilm is described by Fick's first law as a diffusive flux,

$$\mathbb{J}_{F,C_i,1} = -A\varepsilon_{\ell_F}D_{F,C_i}\frac{\partial C_{F,i}}{\partial z} \quad (8)$$

where D_{F,C_i} is the diffusion coefficient of the dissolved component in the liquid phase of the biofilm.

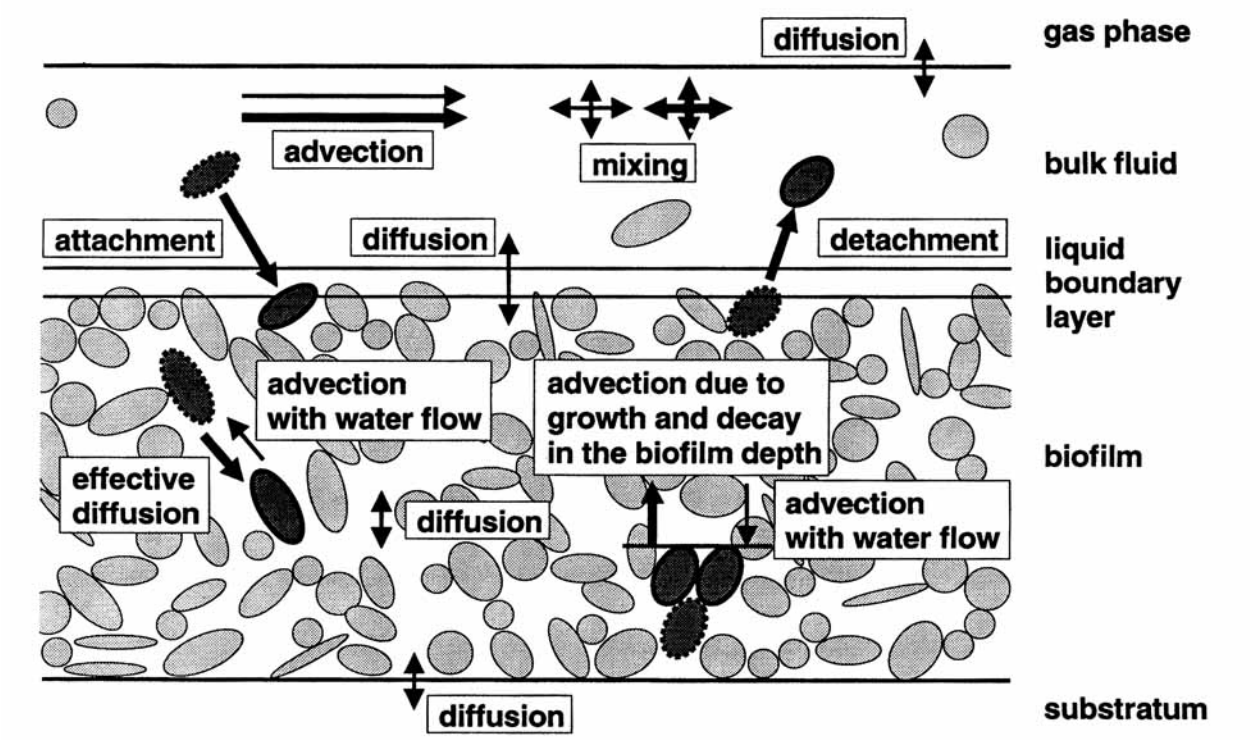

Figure 1. Transport processes considered in the mixed-culture biofilm model. Thick arrows refer to particulate, thin arrows to dissolved components.

It is assumed here that microbial cells primarily consist of water. If the cells grow, they take up water from their environment. If they are displaced, the intracellular water is moved with them. Thus, by the transport of particulate components, as described by Eqs. (6) and (7), a flux of water is induced by which the displaced volume is replaced. This flux in the biofilm liquid phase points in the direction opposite to the motion of the particulate components and leads to an advective transport of dissolved components:

$$\jmath_{F,C_i,2} = -A(1 - \varepsilon_{\ell_F})u_F C_{F,i} + A \sum_{k=1}^{n_X} \frac{D_{F,X_k}}{\rho_{s_k}} \frac{\partial X_{F,k}}{\partial z} C_{F,i}. \quad (9)$$

In most practical applications $\jmath_{F,C_i,2}$ will be negligibly small compared to $\jmath_{F,C_i,1}$; however, in order to make the mass balance equations exact, this flux has to be considered.

Flux of Liquid Phase Volume

In the original MCB model the liquid phase volume fraction ε_{ℓ_F} was assumed to be constant. In the extended MCB model ε_{ℓ_F} is a state variable. Since it is assumed that advective transport of particulate components, as described by Eq. (6), should not change the ratio of liquid phase to solid phases in the biofilm, an advective flux analogous to Eq. (6) has to be introduced, which models the displacement of the liquid phase volume in the biofilm:

$$\jmath_{F,\varepsilon_\ell,1} = Au_F\varepsilon_{\ell_F}. \quad (10)$$

If the particulate components also are displaced by the effective diffusion process as described by Eq. (7), this process has to be compensated by a flux of liquid phase volume in the opposite direction:

$$\jmath_{F,\varepsilon_\ell,2} = A \sum_{k=1}^{n_X} \frac{D_{F,X_k}}{\rho_{s_k}} \frac{\partial X_{F,k}}{\partial z}. \quad (11)$$

Note that Eqs. (10) and (11) describe the transport of the liquid phase volume in the biofilm only and not that of the liquid between the particulate components itself.

Total Flux

Equations (6) to (11) yield the array of mass fluxes as it is used in the conservation laws as given by Eq. (1):

$$\jmath = \begin{pmatrix} Au_F X_{F,i} - AD_{F,X_i} \dfrac{\partial X_{F,i}}{\partial z} \\ -A(1 - \varepsilon_{\ell_F})u_F C_{F,i} + A \displaystyle\sum_{k=1}^{n_X} \dfrac{D_{F,X_k}}{\rho_{s_k}} \dfrac{\partial X_{F,k}}{\partial z} C_{F,i} - A\varepsilon_{\ell_F} D_{F,C_i} \dfrac{\partial C_{F,i}}{\partial z} \\ Au_F\varepsilon_{\ell_F} + A \displaystyle\sum_{k=1}^{n_X} \dfrac{D_{F,X_k}}{\rho_{s_k}} \dfrac{\partial X_{F,k}}{\partial z} \end{pmatrix} \quad (12)$$

One-Dimensional Production Rates

The product of the biofilm area parallel to the substratum and of the spatial production rates averaged over that area yields the one-dimensional production rates

$$\mathcal{R} = \begin{pmatrix} Ar_{X_i} \\ Ar_{C_i} \\ Ar_{\varepsilon_{\ell_F}} \end{pmatrix} \tag{13}$$

where r_{X_i}, r_{C_i}, and $r_{\varepsilon_{\ell_F}}$ are the net production rates of a particulate component (mass per unit compartment volume and unit time), a dissolved component (mass in the liquid phase per unit compartment volume and unit time), and the biofilm liquid phase volume fraction (liquid volume per unit compartment volume and unit time), respectively. The rates r_{X_i} and r_{C_i} are used in all compartments, $r_{\varepsilon_{\ell_F}}$ only in the biofilm compartment. In practice production rates depending on average component concentrations have to be used instead of averaged production rates.

In the extended MCB model a production rate for the liquid phase volume fraction in the biofilm must be given. This rate is formulated as

$$r_{\varepsilon_{\ell_F}} = \frac{\varepsilon_{\ell_F}}{1 - \varepsilon_{\ell_F}} \sum_{k=1}^{nx} \frac{r_{Xk}}{\rho_{sk}} + r'_{\varepsilon_{\ell_F}}. \tag{14}$$

The first term on the right-hand side is chosen such that the production of particulate mass leads to a volume expansion of the biofilm solid matrix only, i.e., ε_{ℓ_F} remains constant. The second term, for which mathematical expressions will be discussed below, can be used to model changes of ε_{ℓ_F} in time and space. This term determines to what extent particulate mass production (microbial growth) leads to a volume expansion or to an increase of the density of the biofilm solid matrix. In conclusion, if $r'_{\varepsilon_F} = 0$, ε_{ℓ_F} remains constant and the situation corresponds to that described in the original MCB model.

Advective Velocity of the Biofilm Solid Matrix

The advective velocity of the biofilm solid matrix at the location z is given as the rate by which the biofilm volume between the substratum and the location z changes divided by the area A at z:

$$u_F = \frac{1}{A} \int_0^z \left(\frac{1}{1 - \varepsilon_{\ell_F}} \sum_{k=1}^{nx} \frac{r_{Xk}}{\rho_{sk}} + r'_{\varepsilon_{\ell_F}} \right) A \, dz'. \tag{15}$$

The space coordinate z is zero at the substratum and is positive in the direction of the biofilm surface.

Progression of the Biofilm Thickness, Detachment, and Attachment

The progression of the biofilm thickness L_F is given by

$$\frac{dL_F}{dt} = u_L \tag{16}$$

where u_L is the velocity of the biofilm surface. This velocity is calculated as

$$u_L = u_F(L_F) - u_{de} + u_{at} \tag{17}$$

where u_{de} is the velocity by which particulate components are detached from the biofilm surface and u_{at} is the velocity by which cells and particles suspended in the bulk fluid are attached to the biofilm surface.

The detachment process usually is specified by the detachment velocity, which can depend on various biofilm and system parameters,

$$u_{de} = u_{de}(L_F, t, u_F(L_F), \tau, \ldots) \tag{18a}$$

where τ is the shear stress at the biofilm surface. In the extended MCB model detachment also can be described by a set of interfacial detachment rates r''_{de,X_k} (mass detached per unit biofilm surface area and unit time). In this case the detachment velocity is calculated as

$$u_{de} = \frac{1}{1 - \varepsilon_{\ell_F}(L_F)} \sum_{k=1}^{nx} \frac{r''_{de,Xk}}{\rho_{sk}}. \tag{18b}$$

Here each particulate component present in the biofilm has its own detachment rate

$$r''_{de,X_i} = k_{de,X_i} X_{F,i} \tag{19}$$

where k_{de,X_i} is the detachment rate coefficient of the particulate component X_i. Note that Eq. (18b) can only be used in the extended MCB model if a diffusive flux of particulate components in the biofilm as described by Eq. (7) is considered, because individual detachment rates of particulate components at the biofilm surface only make sense if these components also can be individually exchanged between biofilm surface and biofilm depth.

The attachment velocity is calculated as

$$u_{at} = \frac{1}{1 - \varepsilon_{\ell_F}(L_F)} \sum_{k=1}^{nx} \frac{r''_{at,Xk}}{\rho_{sk}}. \tag{20}$$

where r''_{at,X_k} is the interfacial attachment rate of a particulate component (mass attached per unit biofilm surface area and unit time). This rate is given by

$$r''_{at,X_i} = k_{at,X_i} X_{L,i} \tag{21}$$

where k_{at,X_i} is the attachment rate coefficient and $X_{L,i}$ is the particulate component concentration in the liquid directly at the biofilm surface. Note that Eq. (20) is derived under the assumption that the liquid phase volume fraction at the biofilm surface, $\varepsilon_{\ell_F}(L_F)$, is not changed by the attachment of cells and particles.

Mass Balance Equations for Mixed-Culture Biofilms

Substituting Eqs. (2), (12), and (13) in Eq. (1) and using Eqs. (14) and (15) leads to a set of mass balance equations which are employed for one-dimensional modeling of MCBs. The mass balance equation which models the development in time and spatial distribution of the

concentration of a particulate component in the biofilm is given by

$$\frac{\partial X_{F,i}}{\partial t} = -u_F \frac{\partial X_{F,i}}{\partial z} + \frac{1}{A}\frac{\partial}{\partial z}\left(AD_{F,X_i}\frac{\partial X_{F,i}}{\partial z}\right) - r'_{\varepsilon\ell_F} X_{F,i} + \left(r_{X_i} - \frac{X_{F,i}}{1-\varepsilon_{\ell_F}}\sum_{k=1}^{nx}\frac{r_{X_k}}{\rho_{s_k}}\right). \quad (22)$$

In this equation the first term on the right-hand side describes the effect on $X_{F,i}$ of the advective transport resulting from the change of the volume of the biofilm solid matrix between the substratum and the location considered. The second term models an effective diffusive transport of the particulate components in the biofilm. The third term considers the effect of changes of the liquid phase volume fraction. The fourth term finally models the effect on $X_{F,i}$ of the differences of the net production rates of the various particulate components present in the biofilm. The development in time and spatial distribution of the concentration of a dissolved component in the biofilm is described by the mass balance equation

$$\frac{\partial C_{F,i}}{\partial t} = \frac{1-\varepsilon_{\ell_F}}{\varepsilon_{\ell_F}} u_F \frac{\partial C_{F,i}}{\partial z} + \frac{1}{\varepsilon_{\ell_F}}\sum_{k=1}^{nx}\frac{r_{X_k}}{\rho_{s_k}} C_{F,i} + \frac{1}{\varepsilon_{\ell_F}}\sum_{k=1}^{nx}\frac{D_{F,X_k}}{\rho_{s_k}}\frac{\partial X_{F,k}}{\partial z}\frac{\partial C_{F,i}}{\partial z} + \frac{1}{\varepsilon_{\ell_F}}\frac{1}{A}\frac{\partial}{\partial z}\left(A\varepsilon_{\ell_F} D_{F,C_i}\frac{\partial C_{F,i}}{\partial z}\right) + \frac{1}{\varepsilon_{\ell_F}} r_{C_i}. \quad (23)$$

In this equation the first term on the right-hand side describes the effect on $C_{F,i}$ of the water flow needed to counterbalance the advective particulate mass transport caused by the volume expansion of the biofilm solid matrix. The second term models the effect of particulate mass production on $C_{F,i}$. The third term considers the effect of the water flow needed to counterbalance the diffusive particulate mass transport in the biofilm. The fourth term models the diffusive transport of dissolved components according to Fick's first law. The fifth term finally describes the net production of mass of the dissolved component. Even if usually only the fourth and fifth terms are significant, the first three terms are included in Eq. (23) in order to make the mass balance exact. The development in time and spatial distribution of the liquid phase volume fraction in the biofilm is described by the mass balance equation

$$\frac{\partial \varepsilon_{\ell_F}}{\partial t} = -u_F \frac{\partial \varepsilon_{\ell_F}}{\partial z} - \frac{1}{A}\frac{\partial}{\partial z}\left(A\sum_{k=1}^{nx}\frac{D_{F,X_k}}{\rho_{s_k}}\frac{\partial X_{F,k}}{\partial z}\right) + (1-\varepsilon_{\ell_F}) r'_{\varepsilon\ell_F}. \quad (24)$$

In this equation the first term on the right-hand side describes the effect on ε_{ℓ_F} of the advective transport resulting from the change of the volume of the biofilm solid matrix between the substratum and the location considered. The second term considers the flow of liquid phase volume necessary to compensate the diffusive particulate mass transport in the biofilm. The third term models the change of the liquid phase volume fraction caused by a rate expression as discussed below.

Together with Eqs. (15) to (21) and the boundary conditions given in the next section, Eqs. (22) to (24) form the basis for one-dimensional MCB modeling. The equations can be solved once the biofilm geometry and the kinetics and stoichiometry of the microbial system to be modeled, i.e., the rate laws and parameter values for r_{X_i} and r_{C_i}, are known and if numerical values for initial conditions, diffusivities, densities, and detachment and attachment coefficients are available.

Boundary Conditions

Substratum–Biofilm Interface

The boundary condition for the particulate components at the substratum–biofilm interface ($z = 0$) is

$$I_{S,X_i} = \jmath_{F,X_i,2}(0) \quad (25)$$

where I_{S,X_i} is the interfacial mass flux of the particulate component X_i. The flux $\jmath_{F,X_i,2}(0)$ is given by Eq. (7); the flux $\jmath_{F,X_i,1}(0)$ is zero since $u_F = 0$ at the substratum. Because it is assumed that no particulate material is exchanged between substratum and biofilm, the interfacial mass flux I_{S,X_i} is zero:

$$I_{S,X_i} = 0. \quad (26)$$

The boundary condition for the dissolved components at the substratum–biofilm interface is

$$I_{S,C_i} = \jmath_{F,C_i,1}(0) \quad (27)$$

where I_{S,C_i} is the interfacial mass flux of the dissolved component C_i. The flux $\jmath_{F,C_i,1}(0)$ is given by Eq. (8); the flux $\jmath_{F,C_i,2}(0)$ is zero since $u_F = 0$ at the substratum. Depending on the properties of the substratum there are different possibilities to calculate I_{S,C_i}:

Impermeable substratum:	$I_{S,C_i} = 0$	(28a)
Diffusion through substratum:	$I_{S,C_i} = A\, k_{S,C_i}(f_i C_{R,i} - C_{F,i})$	(28b)
Sorption at substratum:	$I_{S,C_i} = A\,(k_{ds,C_i} C_{S,i} - k_{as,C_i} C_{F,i})$	(28c)

where $C_{R,i}$ is the concentration at the opposite side of the permeable substratum, f_i is a conversion factor needed if the component solubilities are not equal in the liquids or gases on both sides of the substratum, $C_{S,i}$ is the concentration in the sorptive substratum, and k_{S,C_i}, k_{as,C_i}, and k_{ds,C_i} are the rate coefficients of diffusive mass transfer through the substratum and of adsorption and desorption at the substratum, respectively.

Biofilm Surface

The boundary condition for the particulate components at the biofilm surface requires that the flux I_{F,X_i} of these

components out of the biofilm is equal to the interfacial transfer rate R''_{X_i}:

$$I_{F,X_i} = R''_{X_i} \tag{29}$$

where in the extended MCB model with $D_{F,X_i} \neq 0$ the rate R''_{X_i} is given by

$$R''_{X_i} = A\ (k_{de,X_i} X_{F,i} - k_{at,X_i}\ X_{L,i}) \tag{30a}$$

where $X_{L,i}$ is the concentration of the particulate component directly outside the biofilm. If $D_{F,X_i} = 0$, the rate R''_{X_i} is given by

$$R''_{X_i} = \begin{cases} A(u_{de} - u_{at}) X_{F,i}(z = L_F) \text{ for } u_{de} > u_{at} \\ A(u_{de} - u_{at})\ \dfrac{k_{at,X_i}}{u_{at}}\ X_{L,i} \quad \text{for } u_{de} < u_{at} \end{cases} \tag{30b}$$

as in the original MCB model. For $u_{de} < u_{at}$ the concentration at the surface becomes $X_{F,i}(z = L_F) = k_{at,X_i} X_{L,i} / u_{at}$. The interfacial mass flux I_{F,X_i} of the attached particulate component X_i is given by

$$I_{F,X_i} = \not{J}_{F,X_i,1}(L_F) + \not{J}_{F,X_i,2}(L_F) - A u_L X_{F,i}. \tag{31}$$

The term $A u_L X_{F,i}$ originates from the movement of the biofilm surface in space.

The boundary condition for the dissolved components at the biofilm surface is the continuity condition for the concentration,

$$C_{F,i}(L_F) = C_{L,i} \tag{32}$$

where $C_{L,i}$ is the dissolved component concentration directly outside the biofilm.

A boundary condition for the liquid phase volume fraction ε_{ℓ_F} is necessary only if $u_{at} > u_{de}$. However, Eq. (20) implies that the particles attaching to the biofilm do not change ε_{ℓ_F} at the biofilm surface. With this assumption no additional boundary condition for ε_{ℓ_F} is needed, even if $u_{at} > u_{de}$.

Simple Description of the Liquid Boundary Layer

The equations in this section provide a simple description of a diffusive mass transfer resistance caused by a liquid boundary layer at the biofilm surface. Transformation processes, advective effects, and the volume of the liquid boundary layer are neglected.

For the particulate components of the biofilm such a layer must fulfill the condition that the mass flux I_{L,X_i} through the boundary layer is equal to the interfacial transfer rate of the biofilm, R''_{X_i}, introduced above,

$$I_{L,X_i} = R''_{X_i} \tag{33}$$

where I_{L,X_i} is given by

$$I_{L,X_i} \kappa_{L,X_i} = A(X_{L,i} - X_{B,i}) \tag{34}$$

where κ_{L,X_i} is the mass transfer resistance coefficient in the liquid boundary layer and $X_{B,i}$ is the particulate component concentration in the bulk fluid.

The dissolved components must fulfill the flux continuity equation

$$I_{F,C_i} = I_{L,C_i} \tag{35}$$

where I_{F,C_i} is the flux of the component out of the biofilm and I_{L,C_i} is its flux through the boundary layer given by

$$I_{L,C_i} \kappa_{L,C_i} = A(C_{L,i} - C_{B,i}) \tag{36}$$

where κ_{L,C_i} is the mass transfer resistance coefficient in the liquid boundary layer and $C_{B,i}$ is the dissolved component concentration in the bulk fluid. The mass flux I_{F,C_i} can be calculated as

$$I_{F,C_i} = \not{J}_{F,C_i,1}(L_F) + \not{J}_{F,C_i,2}(L_F) - A u_L \varepsilon_{\ell_F} C_{F,i}. \tag{37}$$

As in Eq. (31) the term $A u_L \varepsilon_{\ell_F} C_{F,i}$ originates from the movement of the biofilm surface in space.

Mass Balance Equations for a Completely Mixed Bulk Fluid

If the bulk fluid compartment is completely mixed, it is modeled by the mass balance equations

$$\frac{d}{dt}(V_B X_{B,i}) = I_{in,X_i} - X_{B,i} Q_{ef} + I_{L,X_i} + V_B r_{X_i} \tag{38}$$

$$\frac{d}{dt}(V_B \varepsilon_{\ell_B} C_{B,i}) = \mathrm{I}_{in,C_i} - \varepsilon_{\ell_B} C_{B,i} Q_{ef} + I_{L,C_i} + V_B r_{C_i} \tag{39}$$

where ε_{ℓ_B} is the liquid phase volume fraction and V_B is the total volume of liquid, cells, and particles in the bulk fluid compartment, Q_{ef} is the effluent volumetric flow rate, and I_{in,X_i} and I_{in,C_i} are the influent mass fluxes of particulate and dissolved components, respectively.

Expressions used to describe influent mass fluxes are, e.g.,

$$I_{in,X_i} = Q_{in} X_{in,i} + k_{R,X_i}(X_{R,i} - X_{B,i}) \tag{40}$$

$$\mathrm{I}_{in,C_i} = Q_{in} \varepsilon_{\ell_{in}} C_{in,i} + k_{R,C_i}(C_{R,i} - C_{B,i}) \tag{41}$$

where Q_{in} is the influent volumetric flow rate, $X_{in,i}$ and $C_{in,i}$ are the influent concentrations of particulate and dissolved components, respectively, $\varepsilon_{\ell_{in}}$ is the influent liquid phase volume fraction, $X_{R,i}$ and $C_{R,i}$ are the concentrations of particulate and dissolved components, respectively, in another reactor, to which the bulk fluid compartment is connected here by a diffusive link, and k_{R,X_i} and k_{R,C_i} are the mass transfer coefficients of particulate and dissolved components, respectively.

Two types of biofilm reactors are distinguished. The first type being a confined reactor of constant volume V_R such as a rototorque. For this type of reactor

$$V_B = V_R - \int_0^{L_F} A\ dz', \qquad Q_{ef} = Q_{in}. \tag{42a}$$

The second type is an unconfined reactor of constant

bulk fluid volume such as a flat-plate reactor. For this type of reactor

$$V_B = \text{constant},$$
$$Q_{ef} = Q_{in} - Au_L. \tag{42b}$$

Numerical Solution of the Model Equations

The equations of the MCB model as presented in this section were implemented as a *biofilm reactor compartment* in AQUASIM, a computer program designed for the identification and simulation of aquatic systems.[9] In this program the partial differential equations are converted by a finite-difference spatial discretization scheme (method of lines) to a system of algebraic and ordinary differential equations. For the time integration of this equation system the fully implicit algorithm of Gear[5] is used, which was extended to differential-algebraic systems and implemented by Petzold.[8] The stiff stability of the Gear algorithm is very important for the solution of the biofilm equation system. More details on the numerical techniques used in AQUASIM and on the implementation concepts are given by Reichert.[10]

DISCUSSION

Comparison between Original and Extended Mixed-Culture Biofilm Model

In the extended MCB model the geometry of the biofilm can be defined as any function $A(z)$, e.g.,

Biofilm on a plane:	$A(z) = \text{constant}$	(43a)
Biofilm outside a cylinder:	$A(z) = 2\pi(z_{cy} + z)\, L_{cy}$	(43b)
Biofilm inside a cylinder:	$A(z) = 2\pi(z_{cy} - z)\, L_{cy}$	(43c)
Biofilm on spheres:	$A(z) = 4\pi n_{sp}\, (z_{sp} + z)^2$	(43d)

where z_{cy} is the radius and L_{cy} is the length of a cylinder, and where z_{sp} is the radius and n_{sp} is the number of spheres.

The equations of the extended MCB model are written in a form that can be readily converted into the equations of the original MCB model. If A and ε_{ℓ_F} are constant and if D_{F,X_i} and $r'_{\varepsilon\ell_F}$ are set equal to zero in Eqs. (14), (15), (22), and (23), the two MCB models become identical, except for Eq. (24), which is not needed in the original MCB model, and for the first term on the right-hand side of Eq. (23), which was neglected in the original MCB model.[6,16]

The extensions of the MCB model originate from experimental observations which were made in the past years and have indicated that some of the simplifications made in the original MCB model were not justified in all situations.[17] The processes concerned are transport of dissolved and particulate components in the biofilm, development of the biofilm liquid phase volume fraction, and detachment and attachment at the biofilm surface.

Development of the Biofilm Liquid Phase Volume Fraction

If the rate by which the biofilm liquid phase volume fraction changes is zero, i.e., if in Eq. (14)

$$r'_{\varepsilon\ell_F} = 0 \tag{44}$$

the void space between the cells and particles in the biofilm remains constant. This is the case which has been implemented in the original MCB model. However, in recent years experiments have been presented which show that the biofilm liquid phase volume fraction, sometimes also referred to as porosity, decreases from the biofilm surface to the substratum.[18] Therefore in the extended MCB model ε_{ℓ_F} is a state variable. Since at present the processes causing the changes of ε_{ℓ_F} are not yet known, one possibility is to just reproduce an experimentally determined spatial profile of ε_{ℓ_F}. This can be achieved by a relaxation process

$$r'_{\varepsilon\ell_F} = \frac{1}{\tau_\varepsilon}\,(\varepsilon_{\ell_{F,\text{given}}} - \varepsilon_{\ell_F}) \tag{45}$$

where τ_ε is a time constant which when chosen in the order of minutes leads to fast convergence of the actual value of ε_{ℓ_F} to the given distribution $\varepsilon_{\ell_{F,\text{given}}}$. An example for $\varepsilon_{\ell_{F,\text{given}}}$ to be discussed below is

$$\varepsilon_{\ell_{F,\text{given}}} = 0.6 + 0.3\frac{\cos(\pi(L_F - z)/L_F) + 1}{2}. \tag{46}$$

An alternative approach to calculate ε_{ℓ_F} is to make the rate $r'_{\varepsilon\ell_F}$ in Eq. (14) a function of processes which take place in the biofilm. However, since the nature of the processes by which this rate is determined still has to be elucidated, this approach is not yet feasible. Thus, a hypothetical example is used here to demonstrate the approach. In this example it is assumed that by heterotrophic growth a biofilm solid matrix is formed, which has a relatively large liquid phase volume fraction ε_H, and that with increasing biofilm age the solid matrix becomes more compact, with a liquid phase volume fraction ε_c. Furthermore it is assumed that by the processes *inactivation* and *endogenous respiration* ε_{ℓ_F} is not changed. In mathematical terms this example is expressed by

$$r'_{\varepsilon\ell_F} = \frac{\varepsilon_H}{1-\varepsilon_H}\frac{r_{H,gro}}{\rho_{s,H}} - \frac{\varepsilon_{\ell_F}}{1-\varepsilon_{\ell_F}}\frac{r_{H,gro}}{\rho_{s,H}} + k_c\,(\varepsilon_c - \varepsilon_{\ell_F}) \tag{47}$$

where $r_{H,gro}$ is the heterotrophic growth rate, $\rho_{s,H}$ is the density of the heterotrophic microorganisms, and k_c is the compaction rate. The first term on the right-hand side of Eq. (47) describes heterotrophic growth with ε_H. The second term is needed to cancel the original term for heterotrophic growth with ε_{ℓ_F} in Eq. (14). The third

term is analogous to Eq. (45); however, here the relaxation occurs much slower.

In order to study the effect of changes of ε_{ℓ_F} on biofilm behavior, three calculations were performed with the MCB model and the computer program AQUASIM.[9] All calculations were based on a heterotrophic biofilm with microbial kinetics as given by the three heterotrophic processes in Table I.[13] The substrate influent concentration and diffusivity in the biofilm was 30 g chemical oxygen demand (COD) m^{-3} and 1.04×10^{-4} m^2 d^{-1}, respectively. The dissolved oxygen (DO) influent concentration and diffusivity in the biofilm was 8 g O_2 m^{-3} and 2.19×10^{-4} m^2 d^{-1}, respectively. The detachment velocity was set equal to the growth velocity of the biofilm, in order to keep the biofilm thickness constant at its initial value of 700 μm.

Figure 2a shows the spatial profiles of ε_{ℓ_F} as measured by Zhang and Bishop[18] and as calculated by Eq. (44) with a constant value of 0.8 (case I), by Eqs. (45) and (46) with $\tau_\varepsilon = 0.001$ d (case II), and by Eq. (47) with $\varepsilon_H = 0.9$, $\varepsilon_c = 0.6$, and $k_c = 5$ d^{-1} (case III). Figure 2b shows the spatial profiles of DO as predicted by the MCB model for the three calculations. Figure 2c shows the spatial profiles of the fraction of viable cells as measured by Zhang and Bishop[18] and as calculated for the three cases by the MCB model as the ratio of heterotrophic to heterotrophic plus inactivated microbial mass.

Figure 2c reveals that the measured spatial profile of the fraction of viable cells in a qualitative sense is correctly reproduced by all calculations. The calculated profiles are very similar. This indicates that the observed spatial gradients of the fraction of viable cells are not directly related to the gradients of the liquid phase volume fraction ε_{ℓ_F} (Fig. 2a). The gradients of ε_{ℓ_F} also do not significantly affect the profiles of DO (Fig. 2b).

Diffusive Transport of Dissolved Components

In most mechanistic biofilm models transport of dissolved components in the biofilm is described by Fick's first law with molecular diffusivities which are assumed to have no gradients. However, in recent experiments it has been demonstrated that spatial gradients of the diffusivity in the biofilm exist,[4] and turbulent and advective transport of dissolved components in biofilms have been observed, too.[1,7] These findings can have a significant influence on biofilm modeling. By the extended MCB model this influence can be investigated. Three alternative calculations were made, which all described transport by Eq. (8) as an effective diffusion process but used different diffusivities,

$$D_{F,C_i} = D_{mo,C_i} \tag{48a}$$

$$D_{F,C_i} = D_{mo,C_i}\varepsilon_{\ell_F}^2 \tag{48b}$$

$$D_{F,C_i} = D_{mo,C_i}\left(1 + (f_D - 1)\exp\left(-\frac{L_F - z}{L_D}\right)\right) \tag{48c}$$

where D_{mo,C_i} is the coefficient of molecular diffusion in water and f_D and L_D are parameters characterizing the shape of the diffusivity profile. In Eq. (48a) the diffusivity is assumed to be equal to D_{mo,C_i}. In Eq. (48b) the diffusivity is reduced due to the tortuosity in the biofilm. It is proportional to the square of the biofilm liquid phase volume fraction.[12] Equation (48b) has been used by Zhang and Bishop[19] to evaluate their experimental data. In Eq. (48c) the diffusivity is described by an exponential function, by which penetration of turbulent diffusion into the biofilm or advection described as an effective diffusion process is modeled.

To assess the effect of the alternative modeling of diffusive transport, three calculations were performed,

Table I. Microbial kinetics and stoichiometry[a]

Process	X_H	X_A	X_I	C_S	C_{NH_4}	C_{O_2}	Process rate
Heterotrophic growth	1	—	—	$-\frac{1}{Y_H}$	—	$-\frac{\alpha_H - Y_H}{Y_H}$	$\mu_{H,max}\frac{C_S}{K_S+C_S}\frac{C_{O_2}}{K_{O_2,H}+C_{O_2}}X_H$
Heterotrophic inactivation	−1	—	1	—	—	—	$k_H X_H$
Heterotropic respiration	−1	—	—	—	—	−1	$b_H\frac{C_{O_2}}{K_{O_2,H}+C_{O_2}}X_H$
Autotrophic growth	—	1	—	—	$-\frac{1}{Y_A}$	$-\frac{\alpha_A - Y_A}{Y_A}$	$\mu_{A,max}\frac{C_{NH_4}}{K_{NH_4}+C_{NH_4}}\frac{C_{O_2}}{K_{O_2,A}+C_{O_2}}X_A$
Autotrophic inactivation	—	−1	1	—	—	—	$k_A X_A$
Autotrophic respiration	—	−1	—	—	—	−1	$b_A\frac{C_{O_2}}{K_{O_2,A}+C_{O_2}}X_A$

α_H	= 1 g O_2/g COD	α_A	= 4.57 g O_2/g COD
Y_H	= 0.4 g COD/g COD	Y_A	= 0.22 g COD/g N
$\mu_{H,max}$	= 4.8 d^{-1}	$\mu_{A,max}$	= 0.95 d^{-1}
K_S	= 5 g COD/m^3	K_{NH_4}	= 1 g N/m^3
$K_{O_2,H}$	= 0.1 g O_2/m^3	$K_{O_2,A}$	= 0.1 g O_2/m^3
k_H	= 0.1 d^{-1}	k_A	= 0.1 d^{-1}
b_H	= 0.2 d^{-1}	b_A	= 0.05 d^{-1}

[a] From ref. 13.

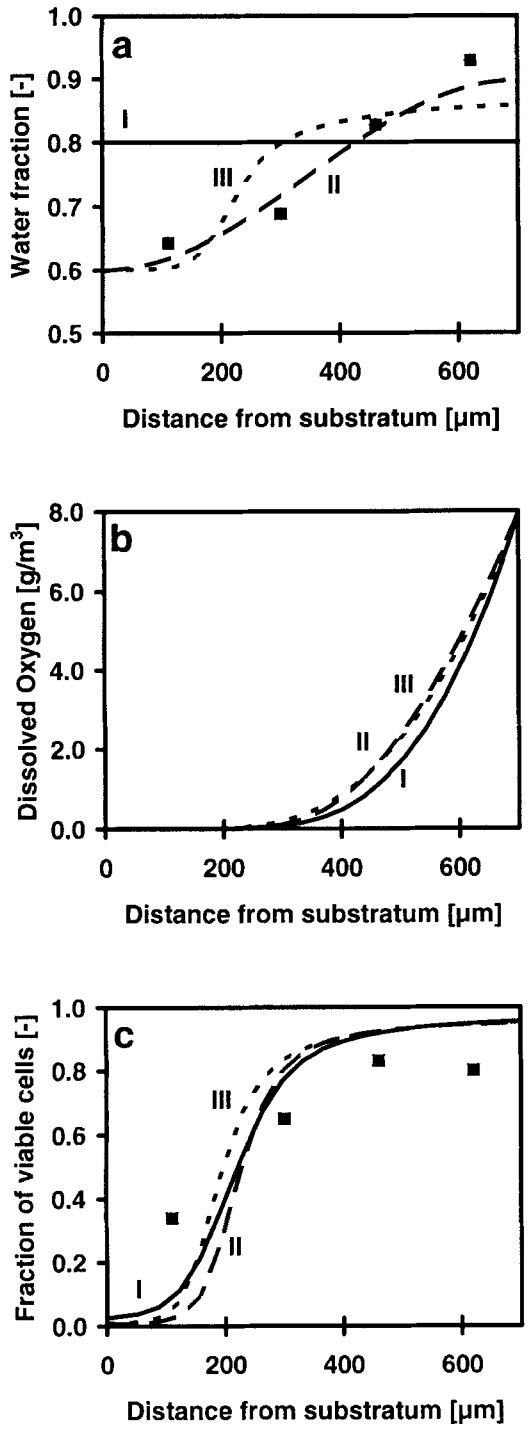

Figure 2. Liquid phase volume fraction (a), dissolved oxygen (b), and fraction of viable cells (c) vs. distance from the substratum. Experimental values (■) originate from Zhang and Bishop.[18] Profiles I, II, and III were calculated by the extended MCB model with Eqs. (44), (45) and (46), and (47), respectively.

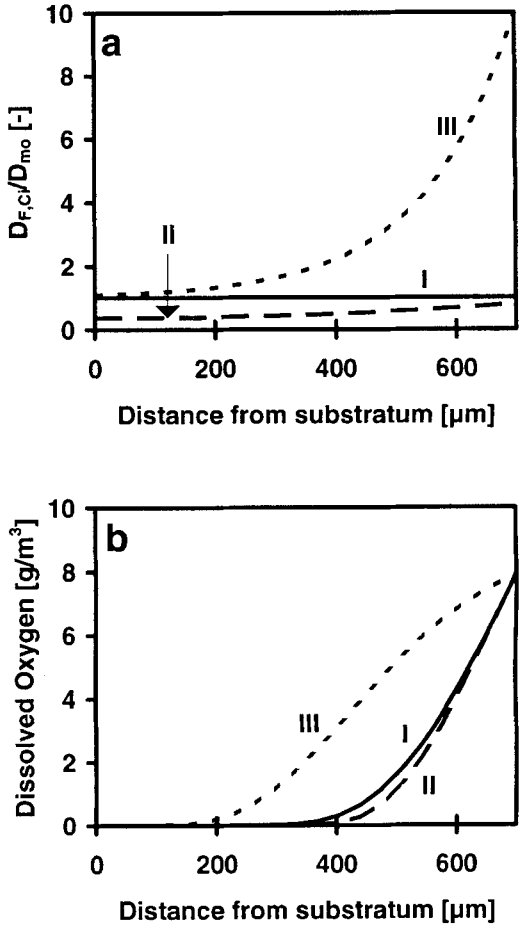

Figure 3. Ratio of diffusivity in the biofilm and in pure water (a) and dissolved oxygen (b) vs. distance from the substratum. Profiles I, II, and III were calculated by the extended MCB model with Eqs. (48a), (48b), and (48c), respectively.

all with the same heterotrophic biofilm as used in the last section and with ε_{ℓ_F} calculated according to Eqs. (45) and (46). Figure 3a shows the spatial profiles of the relative diffusivities. Case I was calculated by Eq. (48a), case II by Eq. (48b), and case III by Eq. (48c), with $f_D = 10$ and $L_D = 150$ μm. Comparison of the spatial profiles of DO as predicted by the MCB model reveals that the profiles of cases I and II are very similar (Fig. 3b). These two cases could not be differentiated by means of measured DO profiles. However, the DO profile of case III differs significantly from the other profiles. Here it was assumed that advective flow or turbulence penetrates about half the biofilm and that the effective diffusivity at the biofilm surface is 10 times higher than the coefficient of molecular diffusion. This results in a profile of DO which near the biofilm surface is concave and only in the biofilm depth exhibits the usual convex shape. In conclusion, the occurrence of turbulent (or advective) transport of dissolved components in the biofilm can be detected by microelectrode measurements. If this phenomenon is found to occur, it should be considered in modeling, since in oxygen-limited biofilms it can have a significant effect on substrate removal rates.

Diffusive Transport of Particulate Components

In the original MCB model, transport of particulate components in the biofilm is described as an advective

process.[6] The concept is that the production of microbial mass in the biofilm depth leads to a volume expansion of the biofilm solid matrix. Since it was assumed that ε_{ℓ_F} is constant, the volume expansion results in a displacement of the cells toward the biofilm surface. The velocity u_F, by which the displacement takes place, formally is an advective velocity. Transport of microbial cells takes place only in the direction of the velocity u_F. If biomass production is positive throughout the biofilm, u_F also is positive everywhere in the film and transport of cells or particles from the biofilm surface to the biofilm depth is impossible. This clearly is contradicting the observation made by Drury et al.[2] that fluorescent microbeads added to a biofilm reactor readily penetrate the biofilm.

In order to account for transport of cells and particles in the direction opposite to that of the velocity u_F, the MCB model was extended by an additional transport process, which is independent of microbial growth and is described as an effective diffusion process [Eq. (7)]. By this process the transport of cells and particles in the biofilm solid matrix is modeled. However, particulate transport in the biofilm liquid phase, as it occurred in Drury's experiments,[3] cannot be modeled by this process. The consequences of this additional transport process for biofilm behavior will be discussed in the next section.

Detachment and Attachment at the Biofilm Surface

The exchange of cells and particles between biofilm and bulk fluid is a very important process in biofilm systems. In the original MCB model detachment as well as attachment was included. However, if both processes occurred simultaneously, only the dominant process could explicitly be modeled. In consequence, if $u_{de} > u_{at}$ only the net detachment was modeled, as detachment minus attachment, and no cells or particles were attached to the biofilm surface. If $u_{at} > u_{de}$ only the net attachment was modeled, as attachment minus detachment, and no cells or particles were detached.

This is an inappropriate limitation, since in several experiments in which a biofilm was steadily growing and cells were continuously eroded from the surface Drury et al.[2] observed that fluorescent microbeads readily penetrated the biofilm when added to a reactor. This observation could undoubtedly also be made if microbial cells instead of microbeads were added to the reactor. Thus, simultaneous detachment and attachment of cells and particles at the biofilm surface is a phenomenon which in some situations can be very significant for MCB modeling.

Thus, the MCB model was extended such that detachment and attachment at the biofilm surface can both be modeled simultaneously and individually for each particulate component. However, modeling of simultaneous attachment and detachment creates a conceptual problem: If a biofilm grows, the velocity u_F of the biofilm solid matrix is positive, i.e., cells and particles are exclusively transported in the direction toward the biofilm surface. In consequence, new attaching particulate material can only adsorb at the biofilm surface but cannot penetrate the biofilm. Therefore, modeling of simultaneous attachment and detachment in the extended MCB model is feasible only in conjunction with the application of diffusive transport of particulate components in the biofilm solid matrix, as described by Eq. (7), which allows for mixing of cells and particles over the biofilm depth.

This problem is illustrated by two calculations performed with the same heterotrophic biofilm as used in the calculations described above. However, here the biofilm was growing in a completely mixed reactor with a detachment velocity $u_{de} = 0.8u_F(L_F)$, and autotrophic cells were added to the reactor influent at a concentration of 2 g m^{-3} until 9.5 days, then at a concentration of 500 g m^{-3}. The diffusivity of the autotrophic species in the biofilm was 1.86×10^{-4} m^2 d^{-1} and the autotrophic kinetics is given in Table I. The progression of u_{de} and of the attachment velocity u_{at}, which was calculated by Eqs. (20) and (21) with an attachment rate coefficient $k_{at,A} = 0.002$ m d^{-1}, is shown in Figure 4a. As can be seen, $u_{de} > u_{at}$ until 9.5 days, then $u_{de} < u_{at}$. The substrate, NH_4, and DO concentrations in the bulk fluid were kept at 3 g COD m^{-3}, 13 g NH_4-N m^{-3} and 8 g O_2 m^{-3}, respectively (Fig. 4b).

The first calculation was performed without an effective diffusion of microbial cells. This situation corresponds to that in the original MCB model. The spatial profiles of the microbial species (Fig. 4c) show that after 9 days there are no autotrophic organisms present in the biofilm, since in this model no microbial cells or particles can attach to the biofilm as long as $u_{de} > u_{at}$. After 9.5 days $u_{at} > u_{de}$. Now the autotrophs can attach to the biofilm surface, but they cannot migrate to the biofilm depth. At 10 days a layer of autotrophic cells has formed at the biofilm surface (Fig. 4d). The slight mixing of heterotrophic and autotrophic organisms is only due to numerical diffusion. Thus, an additional process is required, which allows mixing of the different species at the biofilm surface. This mixing can be achieved by the effective diffusion process of particulate components [Eq. (7)], which has been discussed in the previous section.

To illustrate this, the calculation was repeated with the extended MCB model with conditions that were the same as above, except that the effective diffusion process with $D_{F,H} = D_{F,A} = D_{F,I} = 5 \times 10^{-9}$ m^2 d^{-1} was considered. Now autotrophic cells can penetrate the biofilm right from the beginning of the calculation and start competing with the heterotrophic organisms in the biofilm depth for space and DO (Fig. 4e). Because the biofilm is substrate limited (Fig. 4b), the autotrophic organisms primarily grow in the biofilm depth. The increase of u_{at} at $t = 9.5$ days only enhances the effect of

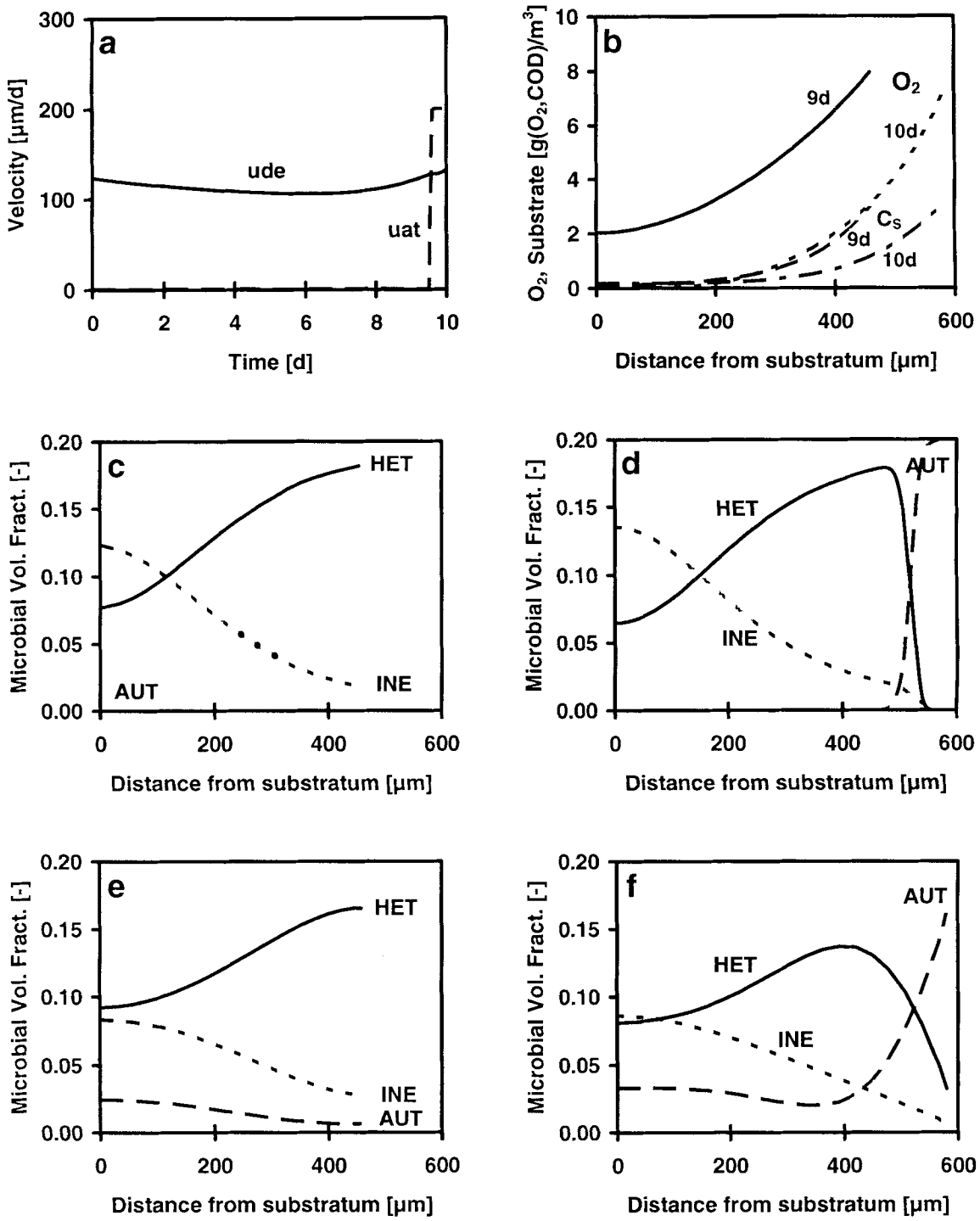

Figure 4. Attachment and detachment velocity vs. time (a) and dissolved oxygen (b) and microbial volume fractions (c–f) vs. distance from the substratum. The profiles in (c) and (d) were calculated by the original MCB model and show the microbial composition at 9 and 10 days, respectively. The profiles in (e) and (f) were calculated by the extended MCB model and also show the microbial composition at 9 and 10 days, respectively.

the attachment of autotrophic cells to the biofilm surface (Fig. 4f).

In conclusion, simultaneous attachment and detachment, combined with diffusive transport of particulate components in the biofilm, allow a permanent exchange of microbial cells and particles between the biofilm and the bulk fluid and between the biofilm surface and the biofilm depth. As has been shown, these processes can have a very significant effect on model predictions of the microbial composition of the biofilm and thus should be considered in MCB modeling.

CONCLUSIONS

By the original mixed-culture biofilm (MCB) model the most important biofilm processes were considered.

However, during the past years new experimental observations were reported which cannot be reproduced by that MCB model. An extended MCB model has been developed, which includes additional processes. By the extended MCB model most of the new experimental data can be reproduced. The additional processes are described by empirical mathematical expressions; i.e., their mechanisms and significance are not yet known. Simulations with the extended MCB model show that changes of the liquid phase volume fraction only have a small effect on the spatial profiles of dissolved oxygen. Transport of dissolved components by turbulent diffusion can have a significant quantitative effect on biofilm behavior, e.g., on substrate removal rates and spatial profiles. Simultaneous detachment and attachment of cells and particles at the biofilm surface, in combination with diffusive transport of particulate components in the biofilm, can significantly affect the microbial composition of the biofilm. It is not yet certain if these findings are generally valid. At present, the extended MCB model primarily is a tool for research on biofilm processes and for the analysis of the new experimental data.

NOMENCLATURE

- A area parallel to the substratum (L^2)
- C dissolved component concentration in the liquid phase, $C = S/\varepsilon_\ell$ (mass per unit phase volume) (ML^{-3})
- D diffusion coefficient (L^2T^{-1})
- $\mathfrak{D}$ array of one-dimensional densities of properties **P** (amount of property per unit length) ($[P]L^{-1}$)
- f conversion factor (dimensionless)
- I interfacial mass flux (MT^{-1})
- $\mathfrak{J}$ array of fluxes of properties **P** (amount of properties per unit time) ($[P]T^{-1}$)
- k mass transfer or rate coefficient (LT^{-1} or T^{-1})
- L length or thickness (L)
- n_x total number of particulate components considered (dimensionless)
- P array of conserved properties (mass, volume, etc.) ($[P]$)
- Q volumetric flow rate (sum of volume of all phases) (L^3T^{-1})
- r production rate of property P (amount of property produced per unit compartment volume and unit time) ($[P]L^{-3}T^{-1}$)
- R'' interfacial transfer rate of property P (amount of property transferred per unit time) ($[P]T^{-1}$)
- r'' interfacial transfer rate of property P (amount of property transferred per unit interface area and unit time) ($[P]L^{-2}T^{-1}$)
- $\mathfrak{R}$ array of net one-dimensional production rates of properties **P** (amount of property produced per unit length and unit time) ($[P]L^{-1}T^{-1}$)
- S dissolved component concentration, $S = \varepsilon_\ell C$ (mass per unit compartment volume) (ML^{-3})
- t time (T)
- u velocity (LT^{-1})
- u_F advective velocity of the biofilm solid matrix (LT^{-1})
- V volume (L^3)
- X particulate component concentration, $X = \varepsilon_s\rho_s$ (mass per unit of compartment volume) (ML^{-3})
- z space coordinate perpendicular to the substratum with origin at the substratum (L)

Greek letters

- ε volume fraction (ratio of phase volume to compartment volume) (dimensionless)
- κ mass-transfer resistance coefficient (TL^{-1})
- ρ particulate component density (particulate mass per unit solid phase volume) (ML^{-3})

Subscripts

- A autotrophic
- as adsorption
- at attachment
- B bulk fluid compartment
- C dissolved component
- cy cylinder
- de detachment
- ds desorption
- ef effluent
- F biofilm compartment
- H heterotrophic
- I inert
- i component
- in influent
- k component (summation index)
- ℓ liquid phase
- L liquid boundary layer
- mo molecular
- R reactor or system
- S substratum
- s solid phase
- sp sphere
- X particulate component

References

1. Costerton, J. W., Lewandowski, Z., DeBeer, D., Caldwell, D., Korber, D., James, G. 1994. Biofilms, the customized microniche. J. Bacteriol. **176**: 2137–2142.
2. Drury, W. J., Characklis, W. G., Stewart, P. S. 1993. Interactions of 1 μm latex particles with *Pseudomonas aeruginosa* biofilms. Water Res. **27**: 1119–1126.
3. Drury, W. J., Stewart, P. S., Characklis, W. G. 1993. Transport of 1-μm latex particles in *Pseudomonas aeruginosa* biofilms. Biotechnol. Bioeng. **42**: 111–117.
4. Fu, Y., Zhang, T. C., Bishop, P. L. 1994. Determination of effective oxygen diffusivity in biofilms grown in a completely mixed biodrum reactor. Water Sci. Tech. **29**: 455–462.
5. Gear, C. W. 1971. The automatic integration of ordinary differential equations. Commun. ACM **14**: 176–179.
6. Gujer, W., Wanner, O. 1990. Modeling mixed population biofilms. pp. 397–443. In: W. G. Characklis and K. C. Marshall (eds.), Biofilms. Wiley, New York.
7. Lewandowski, Z., Stoodley, P., Altobelli, S., Fukushima, E. 1994. Hydrodynamics and kinetics in biofilm systems—recent advances and new problems. Water Sci. Tech. **29**: 223–229.
8. Petzold, L. R. 1983. A description of DASSL: A differential/algebraic system solver. pp. 65–68. In: R. S. Stepleman (ed.), Scientific computing. IMACS, North Holland, Amsterdam.
9. Reichert, P. 1994. AQUASIM—a tool for simulation and data analysis of aquatic systems. Water Sci. Tech. **30**: 21–30.
10. Reichert, P. 1994. Concepts underlying a computer program for the identification and simulation of aquatic systems. Schriftenreihe der EAWAG **7**, Swiss Federal Institute for Environmental Science and Technology, CH-8600 Duebendorf, Switzerland.
11. Rittmann, B. E., McCarty, P. L. 1980. Model of steady-state biofilm kinetics. Biotechnol. Bioeng. **22**: 2343–2357.

12. Tamar, E.-K., Sheintuch, M., Avnir, D. 1991. Steady-state diffusion and reactions in catalytic fractal porous media. Chem. Eng. Sci. **46**: 2787–2798.
13. Wanner, O., Gujer W. 1984. Competition in biofilms. Water Sci. Tech. **17**: 27–44.
14. Wanner, O., Gujer, W. 1986. A multispecies biofilm model. Biotechnol. Bioeng. **28**: 314–328.
15. Wanner, O. 1989. Modeling population dynamics. pp. 91–110. In: W. G. Characklis and P. A. Wilderer (eds.), Structure and function of biofilms. Wiley, New York.
16. Wanner, O. 1994. Modeling of mixed-population biofilm accumulation, pp. 37–62. In: G. G. Geesey, Z. Lewandowski, and H.-C. Flemming (eds.), Biofouling and biocorrosion in industrial water systems. Lewis Publishers, Boca Raton, FL.
17. Wanner, O. New experimental findings and biofilm modeling concepts. Water Sci. Tech. (to appear).
18. Zhang, T. C., Bishop, P. L. 1994. Density, porosity, and pore structure of biofilms. Water Res. **28**: 2267–2277.
19. Zhang, T. C., Bishop, P. L. 1994. Evaluation of tortuosity factors and effective diffusivities in biofilms. Water Res. **28**: 2279–2287.