MODELLING BENTHIC ACTIVITY IN SHALLOW EUTROPHIC RIVERS

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ABSTRACT

In this paper a simple modelling approach is presented that allows fast computation of benthic activity in rivers. The approach extends the half-order reaction concept used in biofilm models for use in a multiple substrate/multiple bacterial species system. Moreover, it is compatible with the IAWQ Activated Sludge Model no. 1 format and has closed mass balances. The conversion of carbonaceous organic matter under aerobic and anoxic conditions and nitrification are represented in the model. The case study to which it was applied revealed that benthic activity is highly influenced by the eutrophic state of the river (presence/absence of algae) leading to diurnal oxygen fluctuations. More specifically the spatial distribution of species along the river was significantly different, resulting in postponed (downstream) nitrification in the eutrophied river. Also, oxygen depletion is found to be more severe and its spatial extension is larger. © 1998 IAWQ. Published by Elsevier Science Ltd

KEYWORDS

Benthic activity; biofilm; eutrophication; half-order kinetics; modeling; river water quality.

INTRODUCTION

In river beds often a stable layer of organic material is found consisting of sediments, attached bacteria, algae etc. The conversion processes within this benthic biomass can have a considerable effect on the concentration of soluble compounds in the overlying water column, such as oxygen, organic matter and nutrients. Hence, benthic activity as the exchange of material between the water column and the benthos, is an important component of the processes responsible for water quality in the river, especially in shallow waters. Sediment oxygen demand, for example, may consume a significant amount of the available oxygen in the water phase (see Boyle and Scott, 1984; Rutherford *et al.*, 1991; Horn and Wulkow, 1996). Furthermore, sediments can act both as a source and a sink for nutrients depending on the environmental conditions (aerobic, anoxic or anaerobic).

While the importance of benthic activity to the water quality is undoubted, the actual relations implemented in models to describe the phenomena are usually quite simple. Most often user specified fluxes such as the sediment oxygen demand are applied to predict the removal rate for the dissolved components in the bulk liquid above the benthos (see e.g. Bowie *et al.*, 1985). Another simplified approach is to neglect the problem of mass transport inside the benthos. As a result, the conversions by the heterotrophic and autotrophic bacteria species inside the benthos can be calculated in the same way as being suspended, the only

difference being that the biomass is attached and the substrates (oxygen, organic matter and nutrients) are utilized from the water phase (see e.g. Reichert, 1994).

In the literature only very few models are found that apply the fundamentals of biofilm modeling to simulate the dynamics of the river benthos. This is mainly due to the complexity of the biofilm modeling approaches. Klapwijk and Snowgrass (1982) considered diffusion and zero order kinetics in three zones (aerobic, anoxic and anaerobic) in order to describe oxygen consumption, nitrification and denitrification in the sediments. The model has been applied mainly for large water bodies (case studies Hamilton Harbor and Lake Erie). Lau (1990) applied an analytical model to compute the effect of benthic activity to the removal of organic matter and oxygen consumption in open channel flow. The analytical solution of the second order differential equation describing diffusion and conversion inside the biofilm considers both zero - and first order reaction kinetics. Li and Chen (1996) also used an idealized description of the biofilm system but applied Monod - kinetics for the description of the bacterial metabolism. Hence, the equation had to be solved numerically by a trial and error method. Recently, Horn and Wulkow (1996) presented a model that describes the spatial variation of the conversion processes inside the biofilm in detail. The system of partial differential equations was solved numerically by means of a discrete Galerkin method. However, the model did not account for a dynamic development of the bacteria species in the biofilm and applied a constant fractionation of heterotrophic and autotrophic bacteria as well as a constant biofilm thickness.

In the following a simplified biofilm model is developed that aims at the description of the dynamics of the benthic biofilm and the influence of the conversion processes to the water quality in shallow eutrophic rivers. The model is based on an analytical solution that predicts the exchange of converted material between the bulk liquid and the biofilm, which is known as the half-order kinetic biofilm model (Harremoes, 1978). In this work, this approach was extended for description of the simultaneous or sequential conversion of multiple substrates such as readily biodegradable organic matter, ammonia, nitrate and dissolved oxygen by multiple bacterial species such as heterotrophic, nitrifying and denitrifying organisms. The dynamics of biofilm thickness are predicted on the basis of growth, decay, attachment and detachment and assumes constant biofilm density. One of the main features of this novel modeling concept is the fact that biochemical conversion processes can be described according to the background given in the IAWQ activated sludge model No. 1 (ASM1; Henze et al., 1987). Moreover, being an analytical solution, a substantial gain in computational efficiency can be achieved.

MODEL DEVELOPMENT

Background

The main feature of biofilm modeling is that both mass transport due to diffusion and kinetic reactions have to be considered in one. The usual procedure is to derive a model that describes the system behaviour both in time and in space, the latter over the depth of the biofilm (e.g. Kissel et al., 1984; Wanner and Gujer, 1984). The basic idea of the simplified model presented here is to decouple the consideration of the diffusion process and the spatial distribution of bacteria species from the biokinetic reactions. This is done by means of a two - step procedure where (1) for each conversion process that is influenced by diffusion, the active fraction of the biomass within the biofilm is computed by means of a simple analytical solution to the problem and (2) all processes within the biofilm are then calculated as in a continuously stirred reactor but with only the active fraction of the species. This approach allows to describe biochemical conversion processes according to the background given in the IAWQ activated sludge model No. 1 (Henze et al., 1987) The concept requires the assumption of

· -   idealized spatial distribution of species
   -       ideal biofilm with homogeneous structure and density
   -       instantaneous steady state substrate profile
   -       absence of a stagnant liquid layer and
   -       absence of a temporal development of soluble components inside the biofilm.

Mass transport and 0-order reaction in a biofilm

Assuming an ideal situation, soluble substrate from the bulk liquid is transferred inside the biofilm and then transported further by means of molecular diffusion. The substrate is simultaneously utilized in the film by the bacterial species for growth. Harremoes (1978) developed the analytical solution for a steady state description of the problem:

$$\frac{\partial^2 S}{\partial x^2} = \frac{r}{D} \tag{1}$$

where S = concentration of substrate at location x in the biofilm $[ML^{-3}]$, D = diffusion coefficient for the substrate $[L^2T^{-1}]$ and r = volumetric reaction rate in the biofilm $[ML^{-3}T^{-1}]$. To derive a solution to this second order differential equation the reaction rate needs to be defined. Harremoes (1978) pointed out that the specific growth rates of bacteria can be assumed zero order with respect to the concentration of the substrate S in the biofilm.

Table 1. Default values for diffusion coefficients

	Substrate	cm^2/d
D_{SO}	oxygen	2.1
D_{SNH}	ammonia	1.8
D_{SNO}	nitrate	1.6
D_{SS}	COD / BOD	0.6

The reason is that the intrinsic saturation coefficients (assuming Monod type kinetics) are very small for the substrates at hand (dissolved oxygen, soluble organic matter, ammonia and nitrate). Hence, the biofilm volume where the 0 order kinetics assumption does not hold, is very small and can be conveniently neglected. On the basis of these considerations analytical solutions can be derived which are well known as half order kinetic models (Harremoes, 1978). Table 1 outlines default values for the diffusion coefficients.

General theory of active fractions

Applying a more refined concept (introduced by the IAWQ activated sludge model No 1 report; Henze et al., 1987) the reaction rate for the removal of soluble compounds from the water phase can be expressed also from the point of view of bacterial growth inside the biofilm. Equation 2 is a basic expression for a removal rate in a system with i substrates S and j species X. It specifies the volumetric reaction rate of a species with respect to each substrate:

$$r_{ij} = - \mu_j.X_j.\nu_{ij} \tag{2}$$

where r_{ij} = zero order reaction rate for X_j with respect to S_i $[ML^{-3}T^{-1}]$, μ_j = specific (max.) growth rate of species X_j $[T^{-1}]$, X_j = bacterial species $[ML^{-3}]$, ν_{ij} = stoichiometric coefficient $[-]$, i = suffix denoting the substrates and j = suffix denoting the species.

The basic consideration which has to be made is whether the biofilm is fully penetrated by all substrates or not. In case the biofilm is fully penetrated (no substrate limitation) the solution to the problem is obvious, as all reactions take place over the full depth of the biofilm L with a constant (zero order) maximum rate. However, in case any substrate limitation occurs the reaction is taking place only over a certain depth of the biofilm and a partition occurs into (1) an active (upper) part and (2) an inactive part (close to the substratum). Since each reaction is governed by only one particular species, the limitation effect can be expressed by assuming only a certain fraction of this species to be active. Hence, a general solution can be given for the flux of each substrate into the biofilm:

$$J_i = \sum_j -\mu_j . X_j . v_{ij} . \phi_j . L \qquad\qquad \text{and} \qquad \phi_j \ [0,1] \qquad\qquad\qquad (3)$$

where J_i = total transport of substrate i through surface of biofilm $[ML^{-2}T^{-1}]$, L = biofilm thickness [L] and ϕ_j = active fraction of species X_j [-]

Figure 1 outlines the general idea of the theory to the simple example of a 2 substrate/1 species system: For growth of heterotrophic bacteria in the biofilm two substrates are required, that is an electron acceptor (S_O dissolved oxygen) and an electron donor (S_S soluble organic matter). Both substrates are essential for bacterial growth and, consequently, the whole process stops when one of them is not fully available.
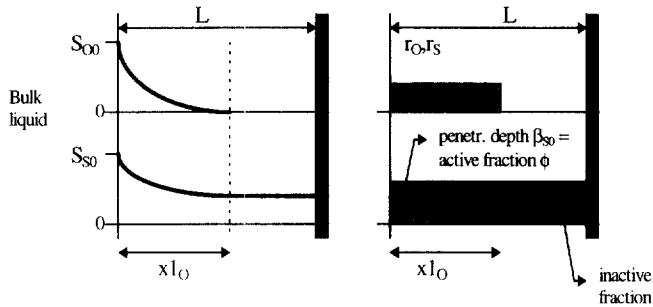

Figure 1. Illustration of a diffusion limited reaction. S_O is the limiting substrate.

In this simple system the limitation of bacterial growth and the total conversion rate with respect to the substrate concentration in the liquid phase can be derived very easily. The underlying idea is that the dimensionless penetration depth of the limiting substrate β_{SO} ($x1_O/L$ in Fig. 1) is also equal to the active fraction of the biomass ϕ. As the dimensionless penetration depth can be calculated analytically (Harremoes, 1978; Rauch, 1997) the fluxes of substrates into the biofilm are then derived directly from equation 3. However, note that the straightforward relation $\beta_{i,limiting} = \phi_j$ holds only for very simple systems as discussed in Fig. 2.

Indeed, a problem arises when this simple active fraction concept is applied to more complex problems due to the fact that, on the one hand, equations are given for the dimensionless penetration depth β_i that relate to the exhaustion of substrates, while, on the other hand, the active fraction ϕ_j for each biomass species is needed for further calculation. Although there exists a relationship between these two types of variables it is easily seen that this relation is case specific and requires a thorough analysis of the specific problem at hand, as illustrated below. A full description of the procedure is found in Rauch (1997). An application to wastewater treatment biofilm systems can be found in Rauch and Vanrolleghem (1997).

Concept for describing water phase - biofilm interaction

The procedure outlined above is actually only the first step for deriving a mathematical description of the biological conversion processes within the biofilm and of the mass exchange between bulk liquid and biofilm. The result of the analysis of the situation with respect to diffusion limitation is a quantification of the active mass of each bacterial species present in the whole biofilm. It is clear that also the dynamic changes in the bulk liquid need to be considered and the mass transfer between those two phases. The fact is that biofilm kinetics are directly connected with transport phenomena and, hence, it is not possible to put up a stringent separation of biokinetic and physical processes.

The whole system is seen in the following as two connected continuously stirred tank reactors where one is representing the water phase and the other the biofilm (Fig. 2). The components in both tanks are expressed

differently, in the water phase in terms of concentrations $[ML^{-3}]$,as usual, and in the biofilm as mass M_b $[M]$.
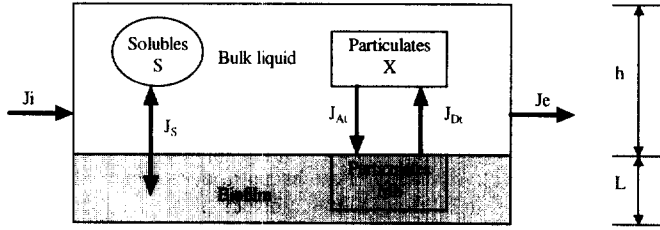

Figure 2. Interaction processes between biofilm and bulk liquid components due to mass fluxes J_i.

The reason is that the thickness of the biofilm compartment is constantly changing, which can be taken into account more easily by balancing masses than by concentrations. Neglecting the dynamic changes in biofilm density the thickness of the biofilm is computed at each time instant from

$$L = \frac{\sum M_{bi}}{\rho^*.A_0}$$ (4)

where ρ^* = constant mass of dry biomass per wet biofilm volume $[ML^{-3}]$, A_0 = surface of biofilm $[L^2]$ and M_{bi} = mass of particulate component i in the biofilm $[M]$.

The different dimensions of the particulate components in both reactors (concentrations in the bulk liquid and mass in the biofilm) do not allow a direct conversion of components in both compartments. The formulation of the mass transfer between the phases has to account for that. However the volumetric reaction rate r_{Vi} with respect to the substrate concentration in the bulk liquid can also be expressed as

$$r_{Vi} = \sum_j - \mu_j.v_{ij}.\phi_j.\frac{M_{bj}}{V} = \sum_j - \mu_j.v_{ij}.\phi_j.X_{bj}$$ (5)

where V = volume of bulk liquid compartment $[L^3]$, $X_{bj} = M_{bj}/V$ concentration of particulate matter j in the biofilm per unit of volume of the bulk liquid compartment $[ML^{-3}]$. Hence, the problem of the different dimensions of the particulate components in both phases is taken care of directly and must no longer be considered for description of the mass transfer between bulk liquid and biofilm.

Physical interaction between biofilm and bulk liquid

Attachment (flux J_{AT}) is addressing a number of physical processes where suspended matter is transported from the water phase to the biofilm compartment. The most important phenomenon is sedimentation which is generally described as a first order process with respect to the concentration of the particulate matter in the water phase. The reverse process of displacement is addressed as detachment (flux J_{dt}). Detachment describes the material loss from the biofilm matrix and is usually categorized into the phenomena erosion, sloughing and abrasion. In the following no distinction is made between these three phenomena as it is felt that the detailed processes significantly lack understanding. Detachment is assumed to be proportional to the friction forces onto the surface of the biofilm as well as to the material mass. Hence, the process is described as being proportional to the product of mass of particulate matter in the biofilm and flow in the water phase.

Description of biokinetic processes in the biofilm - Process matrix

The biokinetic process description is straightforward once the fractions of the active biomass have been computed as previously outlined. Expressing the components in the biofilm as above in terms of concentrations with respect to the volume of the bulk liquid compartment (X_{bj}) does not violate mass conservation principles. In the following aerobic and anoxic growth of heterotrophs and autotrophs is simulated, as well as hydrolysis and decay. Although the description of the biokinetic processes in the biofilm follows as closely as possible the concept of ASM1 some simplifications had to be implemented. First of all bacterial growth is not expressed as a Monod type reaction as done in ASM1 but instead as a first order process with respect to the active fraction of the bacterial mass alone. This is due to the requirements for zero order in substrate kinetics and diffusion limitation. In ASM1 also the limitation of reactions with respect to oxygen and ammonia is expressed by Monod type switching functions. Conveniently these functions can be dropped as all limitations are already considered in the active fractions.

It is postulated that hydrolysis is a first order process with respect to the substrate concentration. Furthermore, it is assumed that readily biodegradable organic matter from hydrolysis is instantaneously transferred into the bulk liquid. This assumption might be a rather crude simplification of reality, however, the fact is that we still do not know enough about this process in order to make a better funded statement.

Table 2. Process matrix for biokinetic processes in the biofilm and corresponding effect to the concentration of soluble components in the bulk liquid. Below: default values used in the case study (for nomenclature, see Henze *et al.*, 1987).

Process	S_O ML^{-3}	S_S ML^{-3}	S_{NO} ML^{-3}	S_{NH} ML^{-3}	X_{bH} ML^{-3}	X_{bA} ML^{-3}	X_{bS} ML^{-3}	X_{bI} ML^{-3}	Process rate $ML^{-3}T^{-1}$
aerobic het. growth	$1-1/Y_H$	$-1/Y_H$		$-i_x$	1				$\mu_H.X_{bH}.f_H$
anoxic het. growth		$-1/Y_H$	$-(1-Y_H)/2.86Y_H$	$-i_x$	1				$\mu_{HH}.X_{bH}.f_H{}^*$
aerobic aut. growth	$1-4.57/Y_A$		$1/Y_A$	$-1/Y_A-i_x$		1			$\mu_A.X_{bA}.f_A$
decay het.					-1		1-fp	fp	$b_H.X_{bH}$
decay aut.						-1	1-fp	fp	$b_A.X_{bA}$
hydrol.		1		i_x			-1		$kh.X_{bS}$

Stoichiometric Parameters		Kinetic Parameters	
Y_H	= 0.20	m_H	= 3.00 (d^{-1})
Y_A	= 0.06	m_{HH}	= 1.50 (d^{-1})
ix	= 0.08 (gN/gCOD)	m_A	= 0.15 (d^{-1})
fp	= 0.08	b_H	= 0.20 (d^{-1})
		b_A	= 0.03 (d^{-1})
		kh	= 1.00 (d^{-1})

CASE STUDY

The applicability and realism of the model was tested in a virtual case study where the temporal and spatial impacts of a constant discharge of municipal wastewater is evaluated in a shallow eutrophic river. The system is a steady state system (Table 3 outlines the physical properties) with only the eutrophication being dynamic and following a diurnal pattern. It is assumed that (in this case) the benthic activity in the river has an overwhelming effect to the degradation of soluble compounds in the water phase and, hence, the influence of suspended bacteria is negligible. Consequently, also the bacterial biomass discharged in the treatment plant effluent has been considered here as being slowly biodegradable organic matter, which is subject to degradation, and not as a pelagic bacteria compound (see also Rauch and Harremoes, 1996).

Table 3. Constant system properties

	Natural River	WWTP Effluent
Flow (m³/s)	0.04	0.01
Velocity (m/s)	0.25	
Width (m)	2.0	
S_S (gCOD/m³)	0.0	1.0
X_S (gCOD/m³)	0.0	20.0
S_{NH} (gN/m³)	0.0	10.0
S_{NO} (gN/m³)	0.0	10.0
Temperature (°)	15	15

Algae and rooted macrophytes cause a significant diurnal variation in the oxygen concentration due to photosynthesis and respiration. This eutrophication effect was here taken into account by means of dynamic forcing functions as described in Harremoes (1990). Expressed in aerial units the maximum photosynthesis is 10.0 $gO_2m^{-2}d^{-1}$, the respiration rate 5.0 $gO_2m^{-2}d^{-1}$ and the reaeration coefficient k_2 is 10.0 d^{-1}. Reaeration is modeled according to the literature as a first order process (Bowie et al., 1985). The longitudinal transport processes of soluble compounds in the water phase is described by a box model, i.e. by interlinked mixed reactors (Rauch et al., 1997).

In Fig. 3 predicted oxygen and ammonia concentrations are plotted for a dynamic steady state of the system, meaning that the system shows a recurring photosynthesis induced diurnal variation. Profiles are given at different times of the day for the eutrophic system described above and for a reference non-eutrophied situation, where photosynthesis/respiration are absent. The interesting aspect is that the DO in the water phase downstream of the discharge significantly differs. Although photosynthesis and respiration only cause a sinusoidal variation of oxygen (ΔDO= 4.0 gO/m^3) around the mean value of DO_{mean} = 10.0 gO/m^3 the effect of a presence of photosynthesis/respiration on the oxygen consumption by the benthic activity is stunning: The minimum DO concentration in the river is significantly lower and also the spatial extension of the depletion is larger as compared to the reference situation. A similar difference can be observed in the higher ammonia concentrations observed over longer distances along the river stretch (Fig. 3 right).
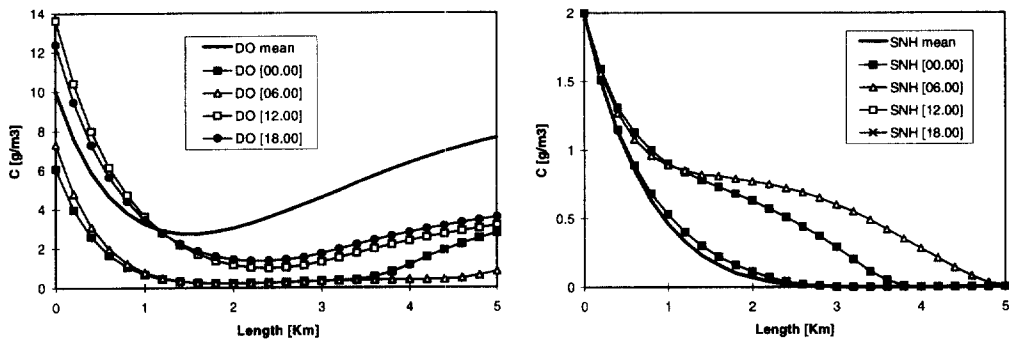

Figure 3. Steady state oxygen (DO) and ammonia (SNH) profiles in the eutrophic river at different times of the day and for a reference situation, i.e. for a constant mean oxygen concentration (DO mean) in the river upstream of the discharge point.

To explain this difference, Figure 4 (right) outlines the situation: Both the heterotrophic and the autotrophic bacterial species compete for substrate (DO) and space inside the biofilm. The slowly biodegradable organic matter (X_S) in the municipal wastewater discharge has to settle first and is only then converted to easily biodegradable organic matter (S_S) by hydrolysis. Consequently, immediately downstream of the discharge point more substrate is found for nitrifiers (S_{NH}) than for heterotrophs (S_S). Hence, there is a larger fraction of nitrifying bacteria in this part of the river. More substrate is available for the growth of heterotrophic biomass further downstream of the discharge point. Accordingly, the fraction of nitrifiers in the benthic

biomass rapidly declines in this river stretch to the favor of the heterotrophic bacteria. Note that the fraction of inert solids in the biofilm (1-f(MH)-f(MA)) increases downstream as the substrate loading decreases.
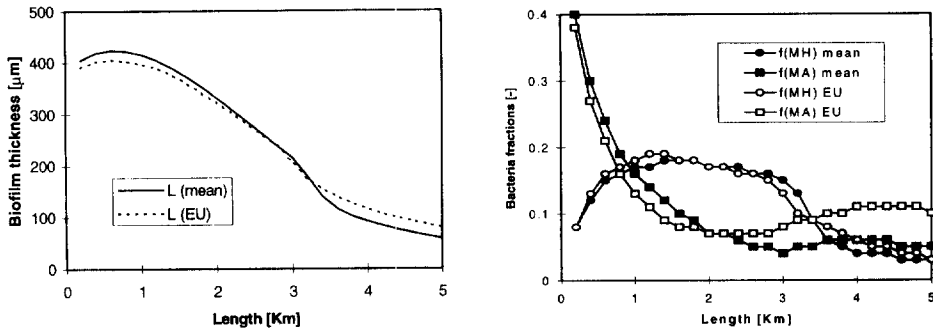

Figure 4. Steady state profiles for the situation with DO fluctuations (EU) and without (mean). Left: Biofilm thickness in mm and Right: fractions of heterotrophic (MH) and autotrophic (MA) biomass in the benthos.

Moreover, this competition of the bacterial species is also the reason for the large differences found in the systems' behaviour between the eutrophic and non-eutrophic situation: as the heterotrophic bacteria can adapt much easier to changing environmental conditions they have an advantage in the competition for substrate (DO) and space under natural DO fluctuations. Hence, the fraction of nitrifiers is slightly reduced in the first 2 km after the municipal wastewater discharge as compared to the non-eutrophic situation.

Between km 2 and 5 downstream of the discharge the amount of substrate available for the heterotrophs gets sparse (both S_S and X_S are removed from the bulk liquid) and nitrifying bacteria grow more abundant. Here the situation with respect to the nitrifying bacteria is reverse as the fraction is higher in case of eutrophication as in the reference situation. The reason is clear from Fig. 3 right: in case of DO fluctuations less ammonia is degraded in the first 2 km and, therefore, substrate for growth is still available. This behaviour is also reflected in the differences in the biofilm thickness profile (Fig 4 left) calculated with a biofilm density ρ^* being 60 kg COD/m^3. Concluding, in the presence of photosynthesis and respiration activity nitrification occurs further downstream from the point of discharge as compared to the non-eutrophic reference situation.

CONCLUSIONS

In this paper a conceptually simple numerical model for the description of the dynamics of the benthic activity is developed. The model builds on the concepts of biofilm modeling and relies also on the background given in the IAWQ activated sludge model No. 1. This approach ensures compatibility with the state of the art in describing biochemical conversion processes. Substrate utilization of carbonaceous matter, nitrification and denitrification is taken into account as well as hydrolysis of attached organic material. The main advantage of this new approach is seen in the reduced complexity of the model compared to classical biofilm modeling, which allows fast computation and, therefore, the application of the model for simulating the impact of benthic activity on water quality in rivers. The case study reveals that the development of bacterial species is very sensitive to eutrophication. A significant fluctuation of the dissolved oxygen concentration in shallow rivers due to photosynthesis and respiration is likely to yield a competition of the different bacteria species in the benthos. In this case, the result was a severe detrimental impact to the oxygen profile downstream of the discharge of municipal wastewater as compared to a non-eutrophic situation.

ACKNOWLEDGEMENT

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