A SIMPLE DYNAMIC MULTISPECIES BIOFILM MODEL WHICH CONSIDERS DIFFUSION AND DEGRADATION OF MULTIPLE SUBSTRATES

W. Rauch[*] and P. Vanrolleghem[**]

[*]Department of Environmental Science and Engineering,
Technical University of Denmark, Bldg. 115, 2800 Lyngby, Denmark
[**]BIOMATH Department, University Gent, Coupure links 653, 9000 Gent, Belgium

ABSTRACT

A new model is presented for fast calculation of the removal of multiple substrates by different bacterial species growing in a biofilm reactor. The model is an extension to the well-known half-order reaction concept that combines a zero order kinetic dependency on substrate concentration with diffusion limitation. In a first step active fractions of the biomass present in the biofilm are calculated and subsequently used in a process matrix which is highly inspired by the IAWQ model nr 1 representation. In a case study a dynamic change in organic loading on a heterotrophic-autotrophic biofilm is evaluated and found to be realistically described by the new model.

INTRODUCTION

Biofilm models have to account for both mass transport by diffusion and kinetic reactions. 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 spatial description allows to determine correct process rates and consequently also an accurate description of species development. However, such detailed mathematical description of transport phenomena, substrate utilization and population dynamics for multiple species in the biofilm has also some shortcomings. Most important among these are the required computational effort for solving the resulting set of partial differential equations and the lack of straightforward implementations in wastewater treatment process simulators. Another point is the high complexity of the model, which makes the estimation of accurate parameter values and initial conditions a tedious task.

Simpler models that allow for faster computation and easier calibration either assume constant biofilm thickness (e.g. Rittmann et al., 1980) or fixed reaction rates (e.g. Harremoes, 1978). In the following we present a simplified model that aims to describe both the dynamics and the competition of bacteria species during growth on multiple substrates. The basic idea of the model is to decouple the consideration of the diffusion process and 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.

GENERAL CONCEPT

Mass transport and 0-order reaction in a biofilm

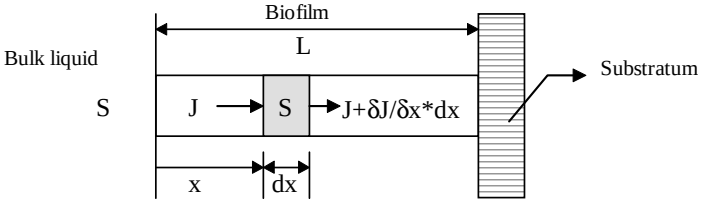

Figure 1: Idealized biofilm system.

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. In case the substrate does not fully penetrate the biofilm the reaction is considered as diffusion limited.

Harremoes (1978) developed analytical solutions for the problem by adopting mass balance equations for biofilms with an idealized geometry (Fig. 1) and under steady state conditions:

$$\frac{\partial^2 S}{\partial x^2} = \frac{r}{D} \qquad (1)$$

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. 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 assumption of zero order kinetics does not hold, is very small and can be conveniently neglected.

Diffusion limitation in a multiple substrate/species system - general theory of active fractions

Applying the theory of diffusion limitation and zero order substrate utilization to biological processes, it needs to be considered that bacteria generally require multiple substances for growth, usually an electron acceptor, an electron donor and nutrients. Moreover, the issue is certainly not simplified by the fact that there are various bacterial species present in the biofilm, which sometimes compete for the same substrate (e.g. both heterotrophic and autotrophic bacteria require oxygen for aerobic growth as well as ammonia). In the following, the basic theory is outlined for a system with i substrates S and j species X. Based on the considerations above, the volumetric (zero order) reaction rate of a species with respect to each substrate is written as:

$$r_{ij} = -\mu_j . X_j . \nu_{ij} \qquad (2)$$

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.
Hence, the biofilm is partitioned in an active (upper) part and an inactive part (close to the substratum). Implying that 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:

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

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 [-]

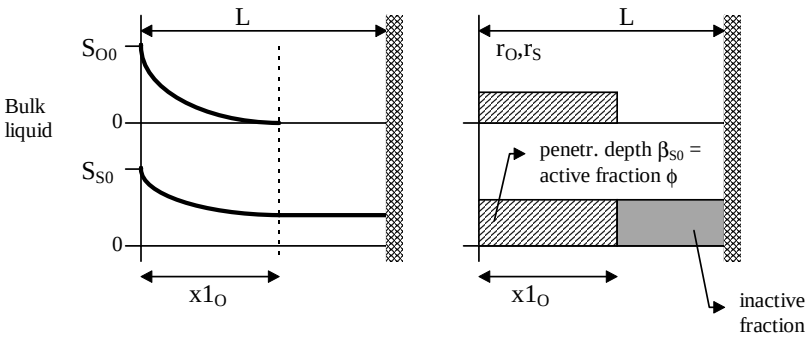

Figure 2: Illustration of a diffusion limited reaction. S_O is the limiting substrate.

Fig. 2 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 a 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.

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. 2) is also equal to the active fraction of the biomass ϕ. The fluxes of substrates into the biofilm are then derived directly from equation 3. However, the straightforward relation $\beta_{i,limiting} = \phi_j$ only holds for very simple systems as 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.

Analytical derivation of the penetration depth of substrates

Fig. 2 outlines, in fact, the simplest case with respect to diffusion limitation: From the point of view of a spatial distribution all processes are stopped when the limiting substrate is exhausted. The actual penetration depth for any substrate, given all other substrates are in excess, can be derived from an analytical solution to equation 1 (for details, see Harremoes, 1978):

$$x1_i = \sqrt{\frac{2 D_i S_{i0}}{r_i}} \qquad \text{and} \qquad \beta_i = \sqrt{\frac{2 D_i S_{i0}}{r_i . L^2}} \qquad (4)$$

where β_i = dimensionless penetration depth of substrate i [-], S_{i0} = concentration of substrate i in bulk liquid [$ML^{-3}T^{-1}$] and r_i = total zero order reaction rate with respect to S_i (all species) [$ML^{-3}T^{-1}$]. Note that equation 4 obviously led to calling this type of models half-order.

However, for a multiple substrate / multiple species system the aspect of diffusion limitation might easily become more complex. Generally, sequential diffusion limitation occurs if one substrate S_i is used in two (or more) reactions and one of these reactions is limited earlier by another substrate S_i^*. As a result, the overall conversion rate of the substrate S_i is no longer of 0 order. The total penetration depth $x2_i$ of the substrate is divided in two parts where the total conversion rate in the upper part (r_{ui}) is different (higher) from the one in the lower part close to the substratum (r_{li}).

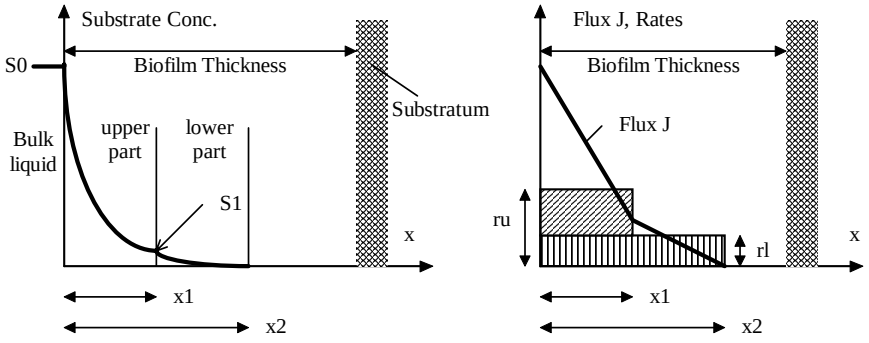

Figure 3: General description of sequential diffusion limitation.

The length of the upper part is determined by the penetration depth $x1_i$ of the substrate S_i^* that is limited first. Consequently, the flux of the substrate S_i into the biofilm is linearly decreasing only within those two fractions but no longer over the whole penetration depth. Still, the penetration depths $x1_i$, $x2_i$ can again be derived analytically (Rauch, 1997):

$$x1_i = \sqrt{\frac{2D_iS_{i0}^*}{r_i^*}} \qquad \text{and} \qquad x2_i = \sqrt{x1_i^2\left(1-\frac{ru_i}{rl_i}\right)+\frac{2D_iS_{i0}}{rl_i}} \qquad (5)$$

where r_i^* = total zero order reaction rate in the upper part with respect to the first limiting substrate S_i^* (all biomass species) [$ML^{-3}T^{-1}$], ru_i = total zero order reaction rate in the upper part with respect to S_i (all biomass species) [$ML^{-3}T^{-1}$], rl_i = total zero order reaction rate in the lower part with respect to S_i (all biomass species not already limited by another substrate) [$ML^{-3}T^{-1}$], Su_i = concentration of substrate i in the upper part [ML^{-3}], Sl_i = concentration of substrate i in the lower part [ML^{-3}], S_{i0}^* = bulk liquid concentration of substrate i* that is limited first [ML^{-3}] and S_{i0} = bulk liquid concentration of substrate i [ML^{-3}].

ACTIVE FRACTIONS IN A MULTIPLE SUBSTRATE - SPECIES SYSTEM

The problem tackled here considers the main carbon/nitrogen cycles in a biofilm, i.e. carbon removal, nitrification and denitrification. Heterotrophic bacteria are growing under two different environmental conditions in the system, i.e. under both aerobic and anoxic conditions. Other than in continuously stirred tank reactors, a spatial distribution of the oxygen concentration exists in biofilms. Consequently, in biofilms simultaneous nitrification and denitrification can occur in full accordance with the basic theory, which is an interesting feature. The spatial distribution is taken into account by means of the anoxic active fraction coefficient ϕ_H^* for heterotrophic bacteria. The anoxic growth rate is denoted as μ^*. However, note that heterotrophic bacteria have a preference for oxygen. As a result nitrate can never be the substrate that is limiting in the first place but only after all oxygen is utilized. Furthermore the biokinetic model assumes that species growth is ammonia limited.

Table 1: Matrix representation of aerobic/anoxic growth of heterotrophic/autotrophic bacteria

Process	S_O ML^{-3}	S_S ML^{-3}	S_{NO} ML^{-3}	S_{NH} ML^{-3}	Process rate $ML^{-3}T^{-1}$
aerobic het. growth	$-(1-Y_H)/Y_H$	$-1/Y_H$		$-i_{xH}$	$\mu_H.X_H$
aerobic aut. growth	$-(4.57-Y_A)/Y_A$		$1/Y_A$	$-1/Y_A-i_{xA}$	$\mu_A.X_A$
anoxic het. growth		$-1/Y_H$	$-(1-Y_H)/2.86Y_H$	$-i_{xH}$	$\mu_H^*.X_H$

For the calculation of the fate of nitrate in the system an additional simplifying assumption needs to be made: Any product created within the biofilm is instantaneously transported to the bulk liquid and does not accumulate in the biofilm. Hence, the production of nitrogen inside the biofilm is considered only by means of the flux transport through the biofilm surface. Consequently, when more nitrate is produced via nitrification than utilized due to denitrification a flux in the opposite direction occurs, actually a substrate transport back into the bulk liquid. The effect to the diffusion limitation is taken into account directly in equation 4 and 5.

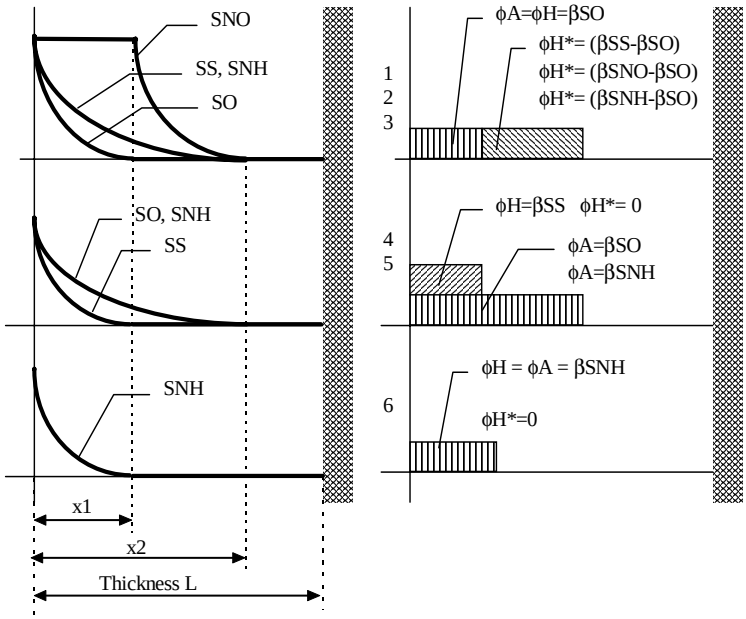

Figure 4: Six possible situations for substrate limitation in the competition of heterotrophic and autotrophic growth in a biofilm. Left: Substrate profiles and Right: active biomass fraction. Case 1,2,3 = first oxygen limited and then either organic matter, nitrate or ammonia limited, Case 4,5 = first organic matter and then either oxygen or ammonia limited and Case 6 = ammonia limited .

The procedure to derive for each specific situation the active fractions of the species in the biofilm can be outlined as follows:

(1) For each of the substrates S_O, S_S, and S_{NH} the dimension-less penetration depth β_i is calculated from equation 4. If none of the substrates is limiting the biofilm is fully penetrated and all active fractions ϕ are equal to one. If not, the substrate with the smallest value β_i is limiting first.

(2) The actual case of substrate limitation is derived from Fig. 4 where the order of limitation is listed together with the active fractions of the relevant species. Unless S_{NH} is limiting another substrate might cause a sequential diffusion limitation that has to be taken into account.

(3) Based on the possible order of limitations the penetration depth of the substrates are calculated from equation 5. Note the special situation in case No 2: Oxygen is the first limiting substrate. However nitrate is not utilized in the upper zone as S_S and S_{NH}. Hence, the principle of sequential diffusion limitation does not apply here. In a first approximation nitrate can be assumed to diffuse that fast to this upper zone that the nitrate concentration at the location x1 is equal to the one in the bulk liquid, i.e. $S_{NO(0)} = S_{NO(x1)}$. More detailed approaches developed for describing the diffusion phenomena in the stagnant layer on the biofilm could be applied here for increased accuracy.

(4) If any of these dimensionless penetration depths is smaller than one, the corresponding reaction is limited and the active fraction is obtained from Fig. 4.

MODEL DESCRIPTION

Concept for describing water phase - biofilm interaction

The procedure outlined above is only the first step for deriving a mathematical description of the biokinetic processes within the biofilm and of the mass exchange between bulk liquid and biofilm. The result of the analysis with respect to diffusion limitation is a quantification of the active mass of each species present in the whole biofilm with respect to the processes. 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.

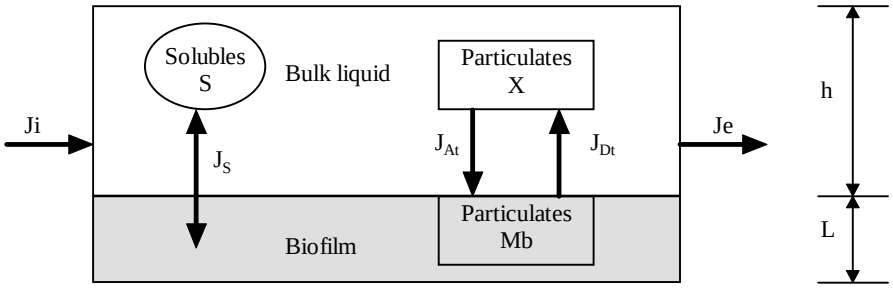

Figure 5: Interaction processes between biofilm and bulk liquid components due to mass fluxes J_i.

The 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. 5). 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].

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

$$L = \frac{\sum M_{bi}}{\rho^* . A_0} \qquad (6)$$

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

$$rVi = \sum_j -\mu j . \nu ij . \phi j . \frac{Mbj}{V} = \sum_j -\mu j . \nu ij . \phi j . Xbj \qquad (7)$$

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 f rom 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 conservationprinciples. 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 6: Process matrix for biokinetic processes in the biofilm and corresponding effect to the concentration of soluble components in the bulk liquid.

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				$\mu_H.X_{bH}.\phi_H$
anoxic het. growth		$-1/Y_H$	$-(1-Y_H)/2.86Y_H$	$-i_x$	1				$\mu_{HH}.X_{bH}.\phi_H$*
aerobic aut. growth	$1-4.57/Y_A$		$1/Y_A$	$-1/Y_A-i_x$		1			$\mu_A.X_{bA}.\phi_A$
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		$kh.X_{bS}$

CASE STUDY

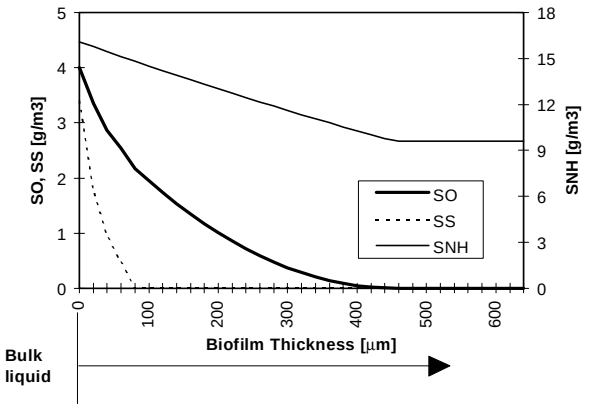

Figure 5: Concentration profiles (analytical solution).

The applicability and realism of the new model was tested for an experimental setup used to study degradation of pretreated municipal wastewater in a submerged filter (Horn, 1992). The filter has a specific surface of 460 m^2/m^3 and a nominal filter velocity of 0.63 m/h. The aerial loading is 7.5 $gCOD/(m^2.d)$ and 1.1 $gNH_4/(m^2.d)$ with COD being fractionated according to default values (Henze et al., 1995). The oxygen in the bulk liquid is 4 g/m^3 and the biofilm thickness is constant with 1500 μm.

In Fig. 5 the simulated concentration profiles in the biofilm are plotted as derived from the analytical solution. Bacterial growth in the biofilm is here limited by the absence of, first, organic matter (S_S) and then oxygen (S_O). From the procedure described earlier the active fractions could be computed as ϕ_H=0.04 and ϕ_A=0.30 respectively.

The predicted dynamics in the biofilm are outlined for an increase of the COD loading in Fig. 6. As a result the heterotrophic bacteria are growing fast in the biofilm thus competing for oxygen and space with the autotrophs. The fraction of the nitrifiers is decreasing and nitrification is, hence, significantly

reduced. After the end of the temporarily increased COD loading the thickness of the biofilm is decreasing again. As the mass of nitrifiers is changing only slowly compared to the mass of heterotrophs (growth and death rate is small) the fraction of autotrophic bacteria is increasing again and nitrification starts up slowly.

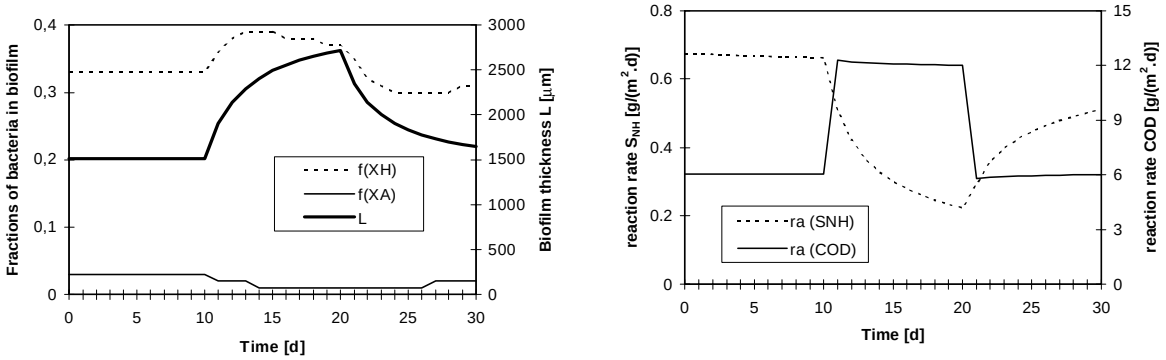

Figure 6: Competition of bacteria in biofilm under dynamic COD loading in the period day 11 to 20 where the aerial loading is increased from 7.5 to 15 gCOD/(m2.d). Left: Temporal development of biofilm thickness and bacteria species (XH and XA) and Right: biofilm reaction rates for S_{NH} and COD.

CONCLUSIONS

In this paper a conceptually simple numerical model for the simulation of multispecies biofilm dynamics is developed. The mathematical description of biochemical processes is largely based on the background given in the IAWQ activated sludge model No. 1 in order to ensure 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 for uncertainty analysis and optimization.

ACKNOWLEDGEMENT

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