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Modelling COD and N removal in the water and in the benthic biofilm for the River Wupper in Germany

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Abstract The River Wupper, a tributary of the River Rhine, is at several locations influenced by anthropogenous nitrogen input, hydraulic structures, and influents from other tributaries. These influences have an impact both on the water quality and on the hydrodynamic conditions. The model approaches used for this article are based on work of Rauch *et al.* and the River Water Quality Model No. 1; they allow the simulation of the nitrogen conversion in the River Wupper. They are compatible with the activated sludge models and can thus be used also for integrated approaches. The calibration and validation of the model was realized using actual data of the River Wupper over a length of 60 km with one dam, 10 weirs, three wastewater treatment plants and 11 tributaries. The model considers the nitrogen conversion and COD removal and has a strong focus on biofilm processes in the benthic zone. Additional information is given about the sedimentation processes, the physical oxygen input processes, biofilm detachment processes, molecular diffusion, the influence of the laminar border layer and the changing of COD fractions and biofilm densities.

Keywords Benthic biofilm; mathematical modelling; nitrogen conversion; River Wupper; RWQM No.1

Introduction

Even though the modelling of waterway quality already has a long history, and although the high importance of the biofilm impact on the water quality has been known, there are only relatively few models available in the reference literature that use the fundamental concepts of biofilm modelling for the simulation of the dynamics in the riverbed (Rauch and Vanrolleghem, 1998). Many models are still based on the nitrogen conversion in the water phase, although there are more and more hints that this process is influenced by the sediment (Pauer and Auer, 2000). The mathematical model for the River Wupper presented here assumes a conversion of the nitrogen compounds within the benthic biofilm, and can thus be regarded as belonging to a relatively new generation of river water quality models.

Description of the modelled river

The river section selected for the modelling was provided by an approx. 60 km long part of the River Wupper which is situated completely within the lower Wupper that starts at the storage lake at Beyenburg and eventually flows into the River Rhine. The catchment area of the River Wupper comprises rural areas to the east, but also the large cities of Wuppertal, Solingen, Remscheid and Leverkusen; it provides living space for about 900,000 inhabitants, 835,000 of whom live in the area of the lower Wupper. The average annual discharge of the River Wupper amounts to 14.2 m^3/s. The flow of the river is in the simulation section impaired at several locations by storage lakes and other water engineering structures. Important anabranches in the simulated area are the Schwelme,

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Morsbach and Eschbach. In the simulation area, one dam, ten weirs, three wastewater treatment plants, and eleven tributaries need to be considered.

Mathematical modelling

The developed model consists of three mathematical sub-models which are interconnected: one "hydrodynamic sub-model" describing the hydrodynamic of the effluent; one "water phase sub-model" describing the conversion and transport processes in the water body; and a "river bottom sub-model" describing the conversion and transport processes within the benthic biofilm. The realisation of the entire model concept was achieved with the software tool AQUASIM (Reichert, 1998) by the sequencing of 35 inter-connected river segments.

Biofilm model

It is assumed that the nitrogen conversion happens mainly within the sediment or in the biofilm at the bottom of the river. This corresponds to the results of practical experiments (Horn and Wulkow, 1996; Pauer and Auer, 2000; Reichert, 2001; Horn, 2003). Although this assumption is valid mainly for flat rivers with a high ratio between water surface and water volume, the dominance of the biofilm for the nitrogen conversion has already been confirmed for relatively big rivers.

Biofilm model 1 is based on an approach according to Rauch *et al.* (1999); it considers not only substance conversion processes, but also contains a mathematical description of the diffusion processes within the biofilm. Different from the original model, here easily degradable organic material is produced by lysis of heterotrophic biomass and autotrophic biomass in the biofilm. The idea behind the modelling concept is the separation of the two main processes in the biofilm: substance diffusion and bio-chemical conversion. The biofilm model is based on the assumption that the characteristic times of the diffusion processes are much shorter than the times of the transformation processes within the biofilm (Gujer and Wanner, 1990; Rauch *et al.*, 1999).

For the incorporation of the benthic biofilm activity into the River Water Quality Model No. 1 (RWQM No. 1), the IWA Task Group on River Water Quality Modelling (Biofilm model 2) proposes a modelling approach which basically differs from the concept sketched above (Reichert *et al.*, 2001). Limiting effects are considered by an empirical limitation factor which is multiplied by the kinetic expressions for the growth rates in the biofilm. Thus, there is no direct description of the transport processes. The description of the nitrification in the IWA based model is done different from the one-step process in the Rauch model. Nitrification was modelled as two separate steps (nitritation and nitratation), furthermore heterotrophic growth and lysis were considered, as well as autotrophic decay.

Processes in the water phase

As in the present model lateral influents and effluents are regarded as point sources at the beginning of the different river segments, and as a one-dimensional model approach is used, the basic equation for the entire water body or for the entire model is given in a one-dimensional dispersion–advection equation without consideration of lateral tributaries. The transformation processes in the water phase described in the model differ from those in the biofilm. Sedimentation of particle substances, oxygen input into the river, different COD fractions as well as growth and lysis of heterotrophic biomass were examined. Hydrolysis is described under the assumption that hardly degradable organic material is adsorbed at the surface of the microorganisms and degraded through extra-cellular enzymes (Morgenroth *et al.*, 2002).

Simulation results

The simulation with the two biofilm models yielded good results, despite the long simulation section and the numerous influences along the river. As the graphs show, deviations from the measuring data exist in the first place directly at or shortly after the wastewater treatment plants or the discharges of the tributaries. Especially the wastewater treatment plant at Buchenhofen (first WWTP) had a strong impact on the simulation results. Reasons for the deviations between measuring data and simulation results are inexact measurements, a inappropriately averaged data set, unknown external diffusive or point sources (Reuter *et al.*, 2003) or additional influences from the sediment. Figure 1 shows the simulation results after calibration with the parameter set given in Tables 1 and 2. Arrows are indicating locations with wastewater treatment plant discharges.

Sedimentation

The sedimentation of hardly degradable organic substances in particle form and of heterotrophic organisms was modelled. Sedimentation processes are considered by a first-order term. This means that the influence of parameters such as particle and fluid properties as

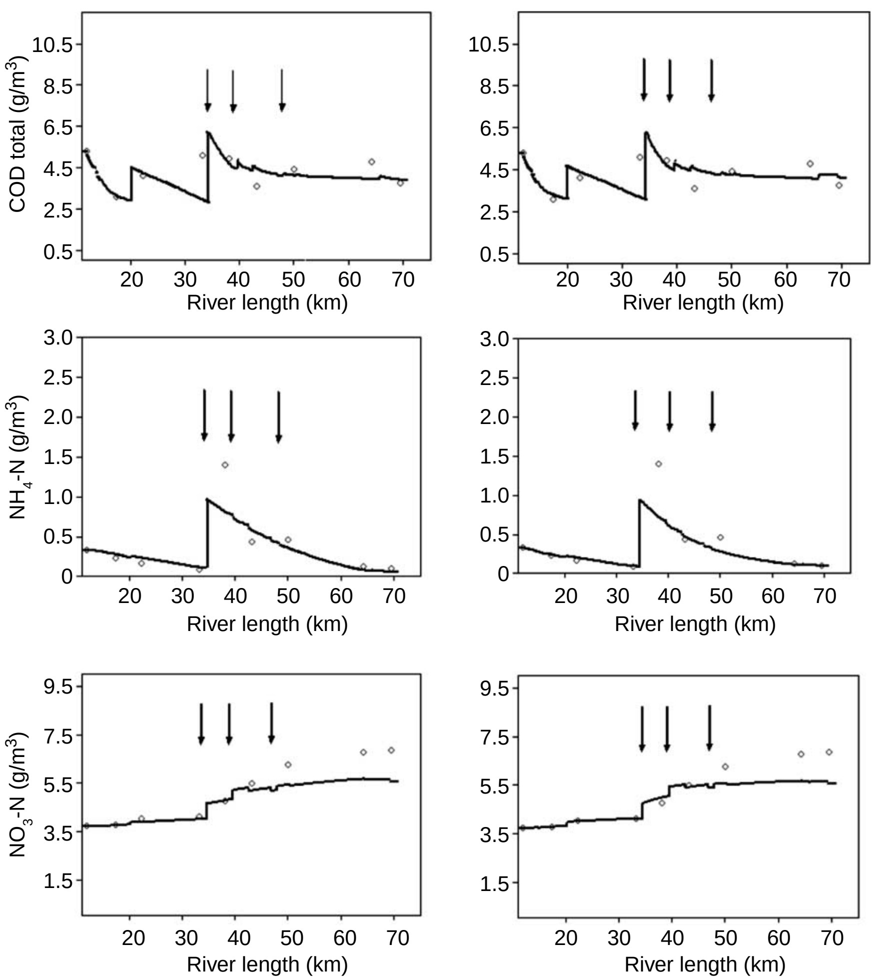

Figure 1 Simulation results, left Biofilm model 1, right Biofilm model 2, simulation: solid line, measured data: dots. Row 1: COD total row 2: NH_4-N row 3: NO_3-N. The arrows indicate discharges from wastewater treatment plants

Table 1 Model parameter of the transformation processes

Parameter	Unit	Rauch *et al.*	IWA	Param.	Unit	Rauch *et al.*	IWA	Param.	Unit	Rauch *et al.*	IWA
Physical oxygen input				$\mu_{Water/H}$	1/d	4	4.5	Y_N	–	0.115	/
p	Pa	101325	101325	$r_{max/H}$	g/m^{2}d	/	3.5	Y_{N1}	–	/	0.13
α	–	$3 + 40/K_{st}$	$3 + 40/K_{st}$	$\beta_{T/H}$	1/°C	0.07	0.07	Y_{N2}	–	/	0.03
β	–	1.0	1.0	Y_H	–	0.1	0.1				
γ	–	2.0	2.0	*Autotrophic organisms*							
δ		0.5/h	0.5/h	K_{O_2}/N_1	g/m^3	/	0.5	*Biofilm detachment*			
θ	–	1	1	K_{O_2}/N_2	g/m^3	/	0.4				
Diffusion				K_{NH_4}/N_1	g/m^3	/	0.42	k_{dt}	1/d	0.008	0.016
D_S	m^2/d	$4*10^{-5}$	/	K_{NO_2}/N_2	g/m^3	/	0.35	*Nitrogen incorporation*			
D_{NH_4}	m^2/d	$3*10^{-5}$	/	$b_{Lysis/N2}$	1/d	/	0.24	I_B	–	0.08	0.08
D_{O_2}	m^2/d	$5*10^{-5}$	/	$b_{Lysis/N1}$	1/d	/	0.12	*Hydrolysis*			
Heterotrophic organisms				$b_{Lysis/N}$	1/d	0.02	/	K_{Hyd}	g/m^3	0.1	0.1
K_{NH_4}/H	g/m^3	0.1	0.05	μ_{N1}	1/d	/	1.5	k_{Hyd}	1/d	8	8
$K_{S/H}$	g/m^3	2.5	1.7	μ_N	1/d	0.045	/	$\beta_{T/Hyd}$	1/°C	0.07	0.07
K_{O_2}/H	g/m^3	0.5	0.5	μ_{N2}	1/d	/	1.8	Y_{Hyd}	–	1	1
$b_{Lysis/Biof.1/H}$	1/d	0.08	/	$r_{max/N2}$	g/m^{2}d	/	1.6	*Inert material*			
$b_{Lysis/Biof.2/H}$	1/d	/	0.4	$r_{max/N1}$	g/m^{2}d	/	0.27	f_I	–	0.1	0.1
$b_{Lysis/Water/H}$	1/d	0.2	0.4	$\beta_{T/N}$	1/°C	0.098	/				
$\mu_{Biof1/H}$	1/d	1.2		$\beta_{T/N1}$	1/°C	/	0.098	*Biofilms density*			
$\mu_{Biof2/H}$	1/d	/	4.5	$\beta_{T/N2}$	1/°C	/	0.069	ρ	g/m^3	70000	70000

Table 2 Nomenclature of the model parameters

Parameter	Description
$\alpha,\beta,\gamma,\delta$	Parameters used for the modelling approaches from ATV (2001)
β_T	Temperature coefficient
μ	Maximum growth rate
ρ	Biofilm density
Biof 1,2	Referring to Biofilm model 1 (Rauch *et al.*, 1999) and Biofilm model 2 (Reichert *et al.*, 2001)
b_{Lysis}	Maximum lysis rate
D	Diffusion coefficient
f_I	Inert ratio of autotrophic and heterotrophic biomass
H	Referring to heterotrophic biomass
Hyd	Referring to hydrolysis
I_B	Incorporated nitrogen
K	Half saturation coefficient
k_{dt}	Biofilm detachment coefficient
k_{Hyd}	Maximum hydrolysis rate
N	Nitrification or nitrifying biomass
N1	Ammonium oxidizing biomass
N2	Nitrite oxidizing biomass
NH_4	Ammonium nitrogen
NO_2	Nitrite nitrogen
O_2	Oxygen
P	Atmospheric pressure
r_{max}	Maximum rates for the calculation of the limitation factor in the IWA model
S	Carbon (COD)
Y	Biomass yield
Water	Referring to the water phase

well as of turbulence and flowing speed on the sedimentation are considered in the model through the sedimentation speed v_{Sed} of the settling substance X_I:

$$r_{Xi} = \nu \cdot \frac{v_{Sed}}{h} \cdot X_I \qquad (1)$$

where r_{Xi} is the sedimentation rate of the sedimentated substance X_I, ν the stochiometric coefficient, h the depth of the river and v_{Sed} the sedimentation velocity.

The results show that a strong decrease of heterotrophic organisms in the waterway occurred already at relatively low sedimentation speeds ($v_{Sed} = 2\,\mathrm{md}^{-1}$), leading also to a low COD in the waterways.

In the calibrated standard case, the fractioning in the influent to the simulated section of the River Wupper was ($X_H = 50\% * COD_{degr}$; $X_S = 20\% * COD_{degr}$), at the Schwelme as the biggest tributary it was ($X_H = 20\% * COD_{degr}$; $X_S = 30\% * COD_{degr}$). In cases of increased sedimentation speeds and a reduction of the heterotrophic biomass in the influent to the River Wupper to $5\% * COD_{degr}$, the hydrolysis was inhibited in those segments where there were not sufficient amounts of heterotrophic organisms for hydrolysis. Thus, from kilometre 40 onwards the concentration of hardly degradable particular substances was influenced almost only by the following discharges, they varied from 2.9 mg/l to 3 mg/l.

Diffusion through laminar border layers

The consideration of the laminar border layer during the calibration was done using a combination of the model concept according to Rauch *et al.* (1999) and an empirically determined approach for the description of the substance conversion at the border area between water and biofilm according to Horn and Wulkow (1996), which considers the dynamic viscosity, the diffusion coefficient, and the average flowing speed of the waterway. The diffusion coefficient within the border layer was assumed as $1.13 * 10^{-4}\,m^2/d$ for NH_4-N, as $4 * 10^{-5}\,m^2/d$ for the dissolved COD, and as $1.2 * 10^{-4}\,m^2/d$ for O_2. The incorporation of the transport-limiting border layer via the biofilm surface did not have any influence on the results with the given parameter combination and the mathematical model approach used for the simulation.

Physical oxygen input and photosynthesis processes

The physical oxygen input into the water phase is of particular importance. The mathematical formulation at the interface water phase/atmosphere can be done with a first-order approach, with the absorption rate being directly proportionate to the oxygen deficit:

$$\frac{\delta S_{O_2}}{\delta t} = \left(\alpha \frac{\nu^{\beta}}{h^{\chi}} + \delta\right) \cdot \left(C_{Sat} - S_{O_2}\right) \qquad (2)$$

where α, β, χ and δ are the reaeration coefficients proposed by ATV (2001), ν is the flow velocity, h is the depth of the River Wupper, C_{Sat} is the oxygen saturation concentration and S_{O_2} is the actual oxygen concentration in the river.

The six analyzed approaches differ in the parameter combination α to δ respectively, yet the differences in the simulation results were relatively low. At the beginning of the river section, photosynthesis processes seem to be the reason why the measured oxygen concentrations lay above the saturation values in the river. As can be seen in Figure 2, the lowest oxygen values were approx. 6.5 mg/l. Thus, the oxygen concentrations in the river and in the biofilm are so high that photosynthesis processes can be neglected in the model.

Detachment processes

The detachment rates in mathematical models published in the reference literature vary; they are given as function of several different parameters (biofilm thickness, shear force, growth rate, density; see Morgenroth and Wilderer, 2000, Horn, 2003). None of the examined models sports a direct consideration of the flowing speed, which according to Lau (1995) is a simplification. The following detachment models were considered: Chang and Rittmann (1987), Kreikenbohm and Stephan (1985). The relation for the detachment rate is here given through $k_{dt} * \rho_F * LF$, where k_{dt} is the detachment rate, ρ_F the density of the biofilm and LF the thickness of the biofilm; Trulear and Characklis (1982), Bryers (1984) with a detachment rate of $k_{dt} * X_f^2$, where k_{dt} is the detachment rate and X_f

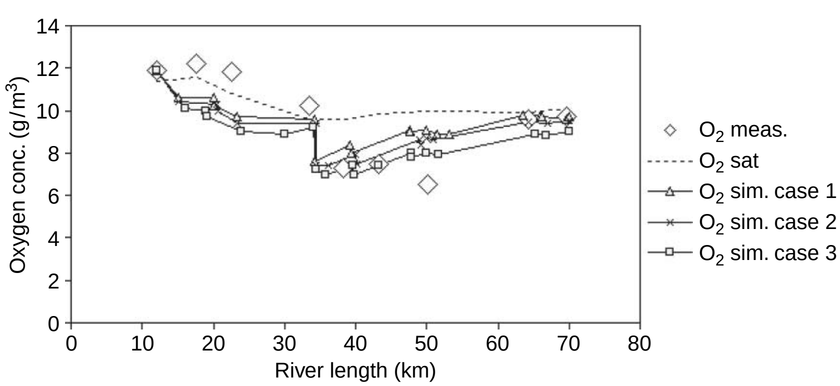

Figure 2 Simulation of O_2: O_2 saturation concentration (dotted line) and O_2 measured (lozenges), exemplary cases 1 to 3 taken from ATV (2001)

the biofilm concentration; Wanner and Reichert (1996), Horn and Hempel (1997). Horn (2003) uses the relation $k_d * \rho_F$, where k_d is the detachment rate and ρ_F is the density of the biofilm. In contrast to the other two models, this model relates the detachment rate to the vertical growth rate of the biofilm.

In the final model, the description of the detachment rate according to Chang and Rittmann (1987) and Kreikenbohm and Stephan (1985) is used (Model 1). Figure 3 shows the simulated thicknesses at a biofilm density of 70000 g/m^3. By using a detachment rate according to Trulear and Characklis (1982) and an identical value for k_{dt}, however, there appeared a considerably lower biofilm thickness (Model 2). It becomes obvious that the square dependence of the detachment rate had the effect that the biofilm thickness became more homogenous along the river section. The concentrations of COD and oxygen showed hardly any changes, whereas the ammonium degradation decreased in the model according to Rauch *et al.* (1999) due to the detachment of autotrophic bacteria. The model according to the IWA reacted much less sensitively in this respect, and the substance degradation stayed mainly unchanged. Using the detachment rate according to Wanner and Reichert (1996) (resp. Horn and Hempel, 1997; Horn 2003) had the effect that no stationary biofilm could emerge within the benthic zone.

Biofilm density

The biofilm density is initially assumed as temporally constant over the entire length of the river (70000 g/m^3). For the variations of the biofilm densities, the variation was based on a reference literature range for small rivers between 60000 g_{TSS}/m^3 and 120000 g_{TSS}/m^3 (Horn and Wulkow, 1996). Increasing the density of the biofilm to 80000 g_{TSS}/m^3 led to increased ammonium degradation, increased biomass, and lower biofilm thickness.

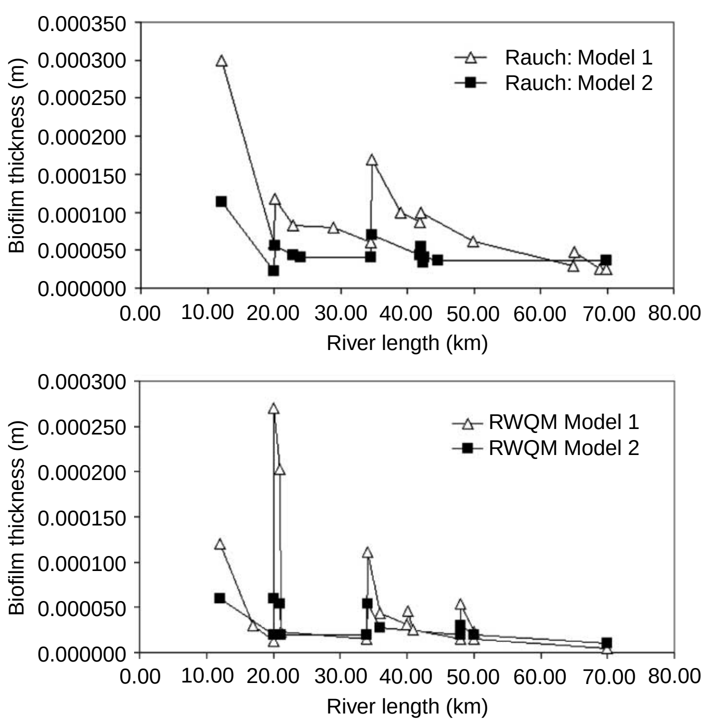

Figure 3 Simulation of the biofilm thickness: Model 1 according to Kreikenbohm and Stephan (1985), Model 2 according to Trulear and Characklis (1982)

Diffusion coefficients

During the calibration phase, the diffusion coefficients within the biofilm were examined as well. Lowering the diffusion coefficient for ammonium from $1.8 * 10^{-4}$ to $3 * 10^{-5}\,m^2\,d^{-1}$ led to a decreased autotrophic biomass and thus to decreased ammonium degradation at lower absolute infiltration depths. A decrease of the diffusion coefficient for easily degradable dissolved COD from $0.58 * 10^{-4}$ to $0.3 * 10^{-5}\,m^2\,d^{-1}$ achieved only a relatively low influence on the total COD in the river. The biofilm thickness and the concentration of heterotrophic biomass in the biofilm, however, were considerably lower, particularly at locations of COD input. At these locations, the heterotrophic biomass was now up to 80% lower than in the simulation prior to the changing of the coefficient.

Biomass growth and decay

The changing of the maximum growth rate of the nitrifiers from 0.075 to $0.055\,d^{-1}$ in the model according to Rauch *et al.* (1999) had the effect that the penetration of the biofilm with ammonium and oxygen amounts to 100% at almost all locations. The degradation of NH4-N reached too low values in areas where autotrophic biomass could emerge only insufficiently. The reduction of the lysis rates for the autotrophics from $0.04\,d^{-1}$ to $0.015\,d^{-1}$ made for a reduction of the relative penetration for oxygen and ammonium, which now lay in a range $>50\%$ diffusion for ammonium and $>60\%$ diffusion for oxygen. The diffusion profiles showed that denitrification processes were not possible in the biofilm, because oxygen-limited zones did not coincide with zones where COD had been available.

Conclusions

In this analysis, two models based on the RWQM No. 1 (Reichert *et al.*, 2001) and the model according to Rauch *et al.* (1999) were examined. Both models could excellently simulate the COD and the nitrogen degradation in a 60 km long stretch of the lower part of the River Wupper. The analysis comprised examinations of growth and decay processes, the substance conversion processes of autotrophic and heterotrophic microorganisms in the biofilm and water phase, the sedimentation processes of substances in particle form, the physical oxygen input, biofilm detachment, molecular diffusion, the influence of the laminar border layer, the changing of COD fractions and biofilm densities. Eventually, the question as to which model is the most suitable can only be decided for the individual application scenario. If detailed information about the biofilm transport processes is needed the Rauch model is more suitable. The IWA model can be more easily integrated into software, so this model is a good choice when detailed information about the benthic biofilm is not available or when nitrite needs to be considered as part of a two-step nitrification process.

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