River Water Quality Model no. 1 (RWQM1): Case study I. Compartmentalisation approach applied to oxygen balances in the River Lahn (Germany)

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Abstract A case study on the application of the River Water Quality Model No. 1 (RWQM1) is presented in order to illustrate the importance of modelling a sediment compartment for an ecologically meaningful assessment of the impact of wastewater effluents and combined sewer overflows. The focus of this case study is on the compartmentalisation approach of the RWQM1 that makes such a description possible. In contrast to this, a strongly simplified biochemical submodel is used that considers only oxygen and dissolved substrate. The object of the case study is the River Lahn, a moderately polluted 5th order stream in Germany, for which the connectivity of surface/subsurface flows and mass fluxes within river sediments have been intensively investigated. The hyporheic flow between a downwelling and upwelling zone of a riffle-pool sequence has been studied with the aid of tracer experiments and continuous records of water constituents. High diurnal fluctuations of oxygen travelled to considerable depth of the sediment and oxygen in the interstitial water decreased considerably while travelling through the riffle. Starting with the implementation of a strongly simplified version of the biochemical part of the RWQM1, but with the consideration of a sediment pore water compartment in addition to the water column compartment, a calibration procedure is performed using tracer data from the water column and the sediment. The calibrated model is then used to study the system response to wastewater treatment plant effluent and combined sewer overflow emissions. The modelling approach makes it possible to quantify the sediment oxygen demand and the spatial and temporal extent of sediment zones with oxygen depletion. However, the spatially averaged approach does not account for inhomogeneities in the sediment. It is shown that for this river with its alluvial coarse sediments even moderate emissions from sewerage systems may be high enough to drop sediment oxygen concentrations to low levels while those in the surface flow remain close to saturation. Similarly, it is demonstrated that combined sewer overflows may cause anoxic sediment oxygen conditions for extended time periods. The implications for ecologically sound river water quality modelling and for specific quality objectives are discussed.

Keywords Water quality models; rivers; hyporheic zones; dissolved oxygen; eutrophication; sediment oxygen demand; impact assessment

Introduction

The River Water Quality Model No. 1 (Shanahan *et al.*, 2001; Reichert *et al.*, 2001, Vanrolleghem *et al.*, 2001) was developed in order to create standardised and consistent river water quality models. Besides the basic formulation of biochemical conversion processes a focus is the compartment structure of running water ecosystems including their longitudinal, vertical and lateral zonation patterns (Shanahan *et al.*, 2000). This aspect of the river has not gained much attention in river water quality modelling so far. Nevertheless, this may be an important aspect to be considered in order to achieve an ecologically appropriate choice of model compartments and state variables.

Running waters are linked elements within the hydrological continuum. As a consequence, the hydrological interactions between surface and subsurface flows are important for system functions in rivers as they influence the transport and storage of water, chemical compounds and nutrients. Furthermore, the hyporheic zone of running waters has been recognized as an ecologically essential compartment of running waters. Especially the upper layers act both as important habitat for the benthic community (at least every lotic species

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has life stages being linked to the hyporheic zone) and as reactor with intense metabolism. As a consequence, water quality constituents may not only be related to the surface flow but have to include the upper layers of the river sediment. This is especially important for impact assessments of point and diffusive pollution on benthic macroinvertebrates and gravel spawning fish and for an ecologically meaningful application of water quality standards.

Quantifying the significance of exchange processes is complicated due to the high spatial and temporal variation of the hydrological system, which depends on a set of factors with river morphology, sediment structure and hydraulic gradients being most important. Moreover, metabolic dynamics of rivers are shaped by a complex temporal pattern due to diurnal and seasonal changes in autotrophic and respiration activities. We narrowed this complexity by a systematic procedure and analysed the relevance of temporal dynamics of water constituents in a eutrophic shallow river. The case study considers the River Lahn, Germany, which has been intensively studied over two years. The objectives of our study are:

(i) outline of the compartmentalisation approach of RWQM1;
(ii) analysis of the connectivity between surface and subsurface flows in running waters with emphasis on oxygen fluxes and sediment oxygen demand;
(iii) discussion of implications for future river water quality management.

Study site

The River Lahn is a right-sided tributary in the middle reach of the River Rhine with a total length of 245 km. The study site is located in the upstream part at Sarnau 53 km from the source with a catchment area of 453 km^2 and a medium gradient of 2.36‰. The average discharge amounts to 7.3 m^3/s with a base-flow of 0.567 m^3/s (annual precipitation: 810 mm). We selected a reach 450 m in length with two regular pool-riffle-sequences (10–15 m in width) and seven sampling cross-sections (I – VII in Figure 1). At base flow mean flow velocity approximates 0.32 m/s. A wastewater treatment plant for 15,500 inhabitant equivalents discharges to the river directly downstream of cross-section III. The upstream human population approximates 100,000 inhabitants with their wastewater being discharged from seven additional treatment plants. The proportion of treated sewage from wastewater at river base flow is calculated to be 26% from upstream and 5% from the Sarnau plant.

The temporal and spatial dynamics of flow and physico-chemical parameters was studied by employing 50 stainless steel pipes distributed at seven cross-sections (see Figure 1). The standard length was 50 cm with four sampling depths at 5, 15, 25 and 45 cm in the sediment, respectively. The pipes of each cross-section were simultaneously connected with teflon tubes to a collecting sampler operating at low pressure of maximum 0.2 bar with sampling volumes of 300 ml. Sampling of interstitial water was carried out between 10 and 12 am MET. The volumes were sufficient for the analysis of tracer (uranine with a Turner fluorometer) and

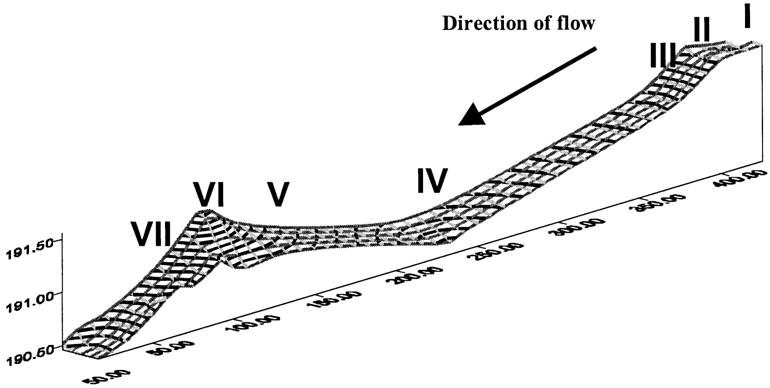

Figure 1 Longitudinal profile of the sediment surface with sampling cross-sections

nutrients (NH_4–N (method: E5 DIN 38406), NO_2–N, NO_3–N (method: D28 EN ISO 13395), phosphorus (method: DIN EN 1189)). Tracer experiments with uranine indicated that the suction pressure was low enough to avoid short-circuits of interstitial flow along the sampling pipes. The surface water body was continuously measured in a monitoring station with a flow-through device, standard electronic equipment for temperature, pH, oxygen, and conductivity and meteorological parameters. Therefore, it was possible to sample both the surface and subsurface flow simultaneously with a high resolution in space and time.

Experimental series were conducted over three to four days in August and October 1997 and considered between 10 and 34 out of the 53 sampling pipes. They were started with water sampling and subsequent addition of uranine for three hours 1 km upstream of the first measurement cross-section in order to avoid interference of tracer in the chemical analysis. The distance has been proved sufficient for almost complete transversal mixing of the tracer.

Modelling approach

The study reach was modelled using measured cross-sectional profiles within the sampling reach and simplified profiles, a constant slope, and an effective friction coefficient upstream of the sampling reach. River hydraulics was calculated with diffusive wave approximation to the full one-dimensional river hydraulics equations according to de St. Venant. The empirical expression

$$S_f = \frac{1}{K_{st}^2} \frac{1}{R^{4/3}} v^2 \tag{1}$$

according to Manning-Strickler was used to calculated the friction slope. In this equation K_{st} is the friction coefficient according to Strickler, R is the hydraulic radius of the river, and v is the cross-sectionally averaged flow velocity. The longitudinal dispersion coefficient was estimated according to Fischer *et al.* (1979)

$$E = c_f \frac{w^2 v^2}{u * d} \tag{2}$$

where c_f is a nondimensional dispersion coefficient, w is the surface width of the river, d is the mean river depth, and

$$u* = \sqrt{g d S_f}$$

is the friction velocity.

In addition to the vertically and laterally mixed water column, a sediment pore water compartment describing a vertically mixed sediment layer of 40 cm depth and a porosity of 0.23 was introduced. Diffusive as well as advective exchange (within in- and exfiltration zones) between these two compartments was considered. The parameters of these exchange processes were derived from tracer experiments, continuous temperature records in different sediment layers and freeze cores (Lenk and Saenger, 1999; Saenger and Lenk, 1999).

All simulations were performed with an extended version of the simulation and data analysis tool AQUASIM (Reichert, 1994; 1995). More information on this program is available at *http://www.aquasim.eawag.ch*.

Calibration of hydraulics and exchange with bed pore water

We started the calibration for tracer transients (uranine) in the water column as well as in the sediment for two experimental series in August and October 1997. Because of the small effect of sediment exchange on the tracer concentrations in the water column, calibration could be done in two steps.

Table 1 Parameter estimates from tracer transients in the water column

Parameter	Unit	Value	Std. err.
η_1		0.2	0.1
η_2		0.76	0.05
$K_{st,eff,1}$	$m^{1/3}s^{-1}$	3.9	1.9
$K_{st,eff,2}$	$m^{1/3}s^{-1}$	8.7	0.6
c_f		0.006	0.009

Table 2 Parameter estimates from tracer transients in the sediment

Parameter	Unit	Value	Std. err.
$Q_{sed,1}$	m^3s^{-1}	0.0031	0.0006
$Q_{sed,2}$	m^3s^{-1}	0.0018	0.0004
v_{ex}	ms^{-1}	0.061	0.018

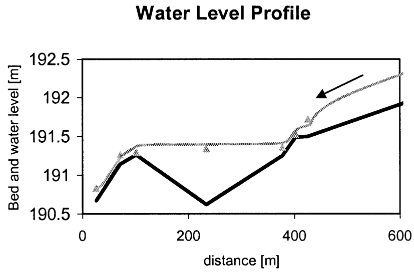

Figure 2 Level of the river bed (black line) and measured (grey markers) and calculated (grey line) water level in the study reach (left) and in part of the upstream, simplified reach (right)

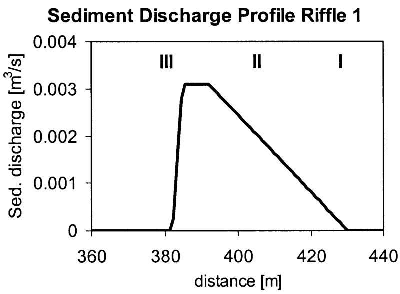

Figure 3 Sediment discharge in riffle 1. The maximum discharge was fitted with the aid of uranine data, the positions of in- and exfiltration zones (linearly in- or decreasing discharge) were fixed. The vertical lines mark the positions of the three measurement cross-section in the riffle

Step 1: Calibration of the tracer mass (reduction factors η_1 and η_2 for experiment 1 and 2, respectively), the effective Strickler friction coefficient in the reach with simplified geometry upstream of the investigation reach ($K_{st,eff,1}$ and $K_{st,eff,2}$ for experiment 1 and 2, respectively), and the non-dimensional dispersion coefficient (c_f; same value for both experiments) based on the tracer transients in the water column (using both tracer experiments). The values of the estimated parameters are given in Table 1. Figure 2 shows the water level profile in the investigation reach and in a part of the simplified upstream reach. Hydraulic height gradients between riffles and pools can be clearly seen with the calculated longitudinal water surface profile being in acceptable agreement with measured data.

Step 2: Calibration of the discharge in the sediment ($Q_{sed,1}$ and $Q_{sed,2}$ for riffle 1 and 2, respectively), and for the diffusive exchange velocity (v_{ex}) based on the transients in the sediment. The positions of in- and exfiltration reaches were chosen based on results from tracer experiments (Figure 3). Measurements were cross-sectionally and depth averaged (averages of measurements taken in 15 cm and 25 cm depth) for comparison with calculated concentrations in the sediment. Both tracer experiments were used simultaneously for the fit. The values of the estimated parameters are given in Table 2.

There is a complex pattern of flow and tracer transport in the riffle and pool (Figure 4). Mass transport in the surface flow is characterised by distinct and symmetric break through curves. For the riffle section significant exchange processes can be identified from the delayed and asymmetric temporal concentration profiles. In contrast, as indicated by the low concentrations of tracer in the sediments of the pool, there are much smaller exchange rates with the surface flow in these river sections.

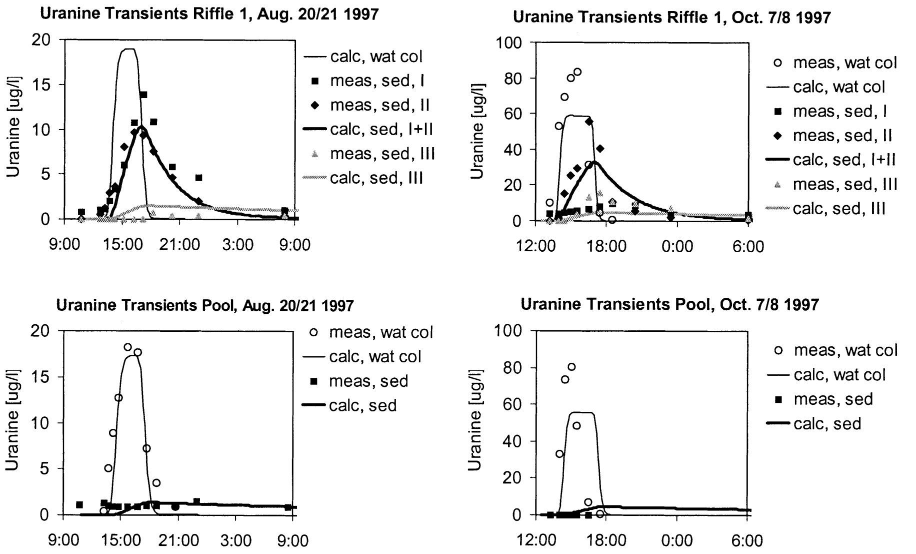

Figure 4 Measured (markers) and calculated (lines) tracer transients in riffle 1 (top) and in the pool (bottom) for the tracer experiment at August 20/21, 1997 (left) and at October 7/8, 1997 (right)

Modelling of oxygen time series in surface flow and in sediment

The oxygen balance of the River Lahn in the surface flow is characterised by high daily and seasonal temporal dynamics triggered from radiation and intense production–respiration processes (Figure 4, top). Despite of enhanced gas exchange with the atmosphere due to low depth and turbulent flow, daily oxygen amplitudes exceeded saturation up to 8 mg l^{-1} in August 1997 (Figure 4, top-left), while oxygen deficits were less pronounced. In October these patterns were still existent but in a more narrow range of oxygen concentrations (Figure 4, top-right).

When considering the oxygen balance in the surface flow of eutrophic rivers with well developed hyporheic zones, one important question concerns the deformation of daily amplitudes in the uppermost sediment layers as one important habitat feature for the benthic community.

In a first step we modelled the oxygen balance with a simple version of RWQM1 using Eq. (4):

$$r = K_2(C_{sat} - C_{O2}) + \frac{PI}{d} - \frac{R}{d} \tag{4}$$

where r is the net oxygen production rate, K_2 is the reaeration rate constant, C_{sat} is the oxygen saturation concentration, C_{O2} is the oxygen concentration in the water column, I is light intensity, d is mean river depth and P and R are production and respiration parameters, respectively. Estimates for physical reaeration were based on empirical assessments (Owens *et al.*, 1964; Wolf, 1974) with consideration of given flow velocities and water depth for the investigation periods. Empirical formulas resulted in K_2 values ranging from 17.0–29 d^{-1}. For model calculations we selected a value for K_2=20 d^{-1}. The fit results shown in Tables 3 and 4 below are conditional on this value.

Based on these boundary conditions, production and respiration rate parameters were estimated from continuously measured oxygen time series (Table 3 and 4). With this approach, a meaningful agreement between modelled and calculated oxygen concentrations could be achieved (Figure 4, top). The model was then used to calculate oxygen time series in the sediment layers in the riffle and pool sections of the investigation site (Figure 4, middle and bottom). A sediment respiration rate coefficient of 2.5 d^{-1} was used to adjust

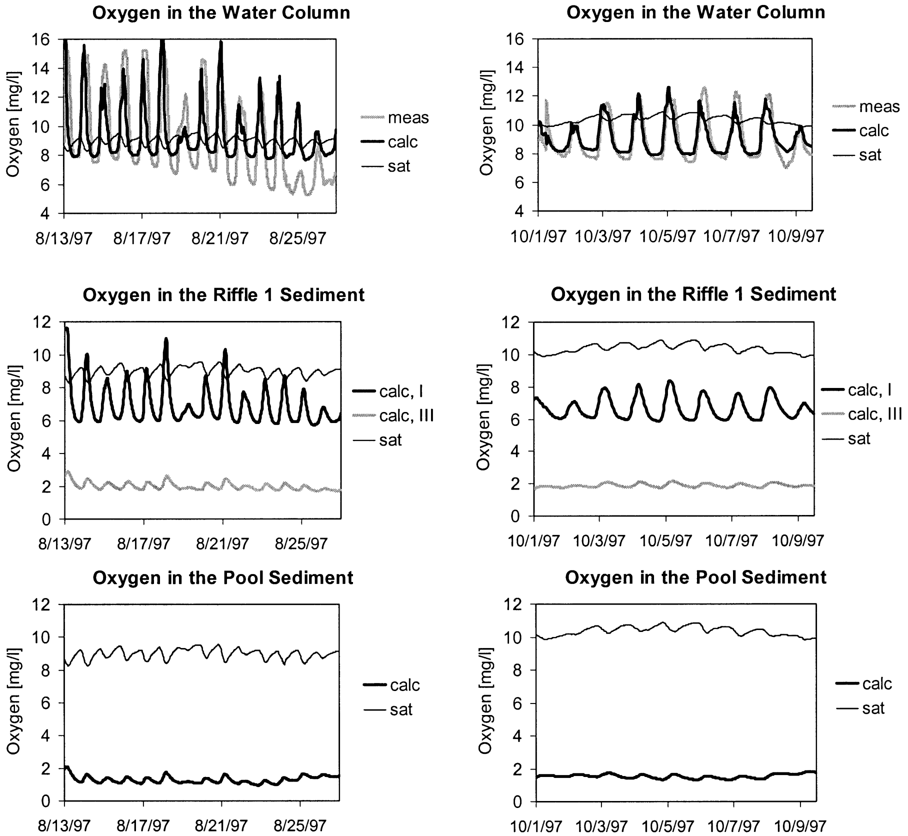

Figure 5 Oxygen time series in the water column (top), in the sediment of the pool (middle) and in the sediment of riffle 1 (bottom) for the August 1997 (left) and the October 1997 (right) measuring campaign. In the legends, "meas" means measured, "calc" means calculated, "sat" means saturation concentration in the water column, and "I" and "III" refer to the measurement cross-sections mentioned in the text (and shown in Figures 1 and 3)

Table 3 Parameter estimates from oxygen time series in the water column; measurement August 1997

Parameter	Unit	Value	Std. err.
PI	g/(Wd)	0.07810	0.0008
R	g/(m^{2}d)	7.1	0.2

Table 4 Parameter estimates from oxygen time series in the water column; measurement October 1997

Parameter	Unit	Value	Std. err.
PI	g/(Wd)	0.1472	0.0008
R	g/(m^{2}d)	16.04	0.06

calculated oxygen concentrations to some measured values available only at specific dates and for specific locations.

This results in a significant drop of the oxygen concentrations down to concentrations of 2 –3 mg/l with an attenuation of the daily amplitude to 0.5 – 1 mg/l O_2 in the pool sediments (Figure 4, bottom). A completely different pattern can be identified for the three measurement cross-sections in the upstream riffle (Figure 4, middle). At the infiltration area and transition zone (cross-section I, see Figure 1 and 3) highly fluctuating oxygen concentrations are present. While infiltrated water travels through the riffle to the exfiltration zone (cross-section III, Figure 1 and 3) a significant depletion of oxygen concentrations occurs to a pattern which is comparable to the pool conditions. The difference of median concentrations in a range of 3.5 – 5 mg/l is close to levels reported for oxygen mass balances from in situ samples (Borchardt and Fischer, 1999). We therefore conclude, that our modelling approach may be sufficient to meaningfully describe surface-subsurface connectivity and oxygen concentration patterns in a eutrophic fluvial system in a spatially averaged way. It is clear, that the approach is insufficient for a description of the spatial inhomogeneity being documented in the actual river by Borchardt and Fischer (1999).

System response to inputs of organic matter from a wastewater treatment plant and combined sewer overflow

In a third step we applied our modelling approach to questions of system analysis and impact assessment of external inputs of organic matter from sewerage systems. In case of the River Lahn and the boundary conditions of wastewater load (see section "study site" above) an important aspect is the relevance of biologically treated wastewater and combined sewer overflows infiltrating the riffles on sediment oxygen concentrations and on sediment oxygen demand.

A sewage treatment plant located at x = 350 m has a mean dry weather discharge of 0.04 m^3s^{-1} and a mean COD of 40 mg/l. In order to compare oxygen concentrations calculated with this actual load with a situation with stronger pollution, we calculated oxygen concentrations in riffle 2 below the sewage treatment plant effluent under the assumption of a constant COD concentration of 90 mg/l (upper legislation limit) and for a combined sewer overflow with a duration of 2.4 h, a discharge of 2 m^3/s and a COD concentration of 100 mg/l (approximately yearly average event). The effect of these effluents on oxygen concentrations in the river are based on a degradation rate coefficient of 1 d^{-1} in the water column and 10 d^{-1} in the sediment pore water.

Figure 5 shows that the first case of an increased dry weather COD effluent concentration leads to a significant decrease in dissolved oxygen concentrations in the sediment. The decrease is between 1 and 2 mg/l while diurnal fluctuations do not significantly change.

The effect of the second case of a combined sewer overflow is seen in the last day of the simulation shown in the right-hand plot of Figure 5 and in more detail in Figure 6. The simulation is in agreement with documented effects of immediate and delayed oxygen depletion in the surface flow of running waters (Harremoes, 1982). Krejci *et al.* (1994) showed that combined sewer overflows may result in very low oxygen concentrations in the hyporheic zone (<1 mg/l O_2) of a small urban running water while the surface flow was almost saturated at the same time. As a consequence, an important question for receiving water protection has to be addressed to the identification of critical boundary conditions for those effects.

The results in Figure 6 show the time series for COD and oxygen in Riffle 2. The combined sewer overflow increased the COD concentrations in the sediment at cross–section V significantly for a time period of more than 6 hours. Almost parallel to this increase in COD the oxygen concentrations decreased to very low oxygen levels close to zero for several

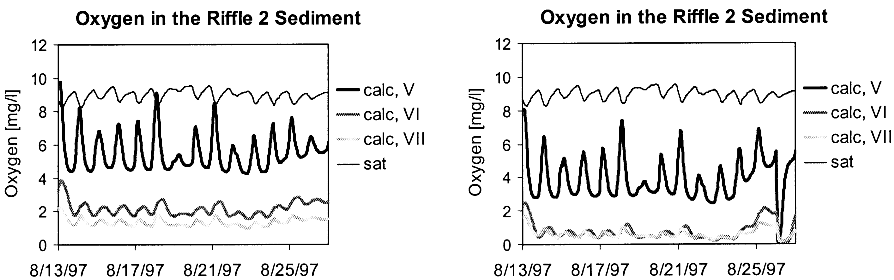

Figure 6 Sediment oxygen time series in riffle 2 (below the wastewater treatment plant effluent) for the August 1997 measuring campaign (left) and for a hypothetical situation with a wastewater treatment plant effluent with a COD of 90 mg/l instead of 40 mg/l (right)

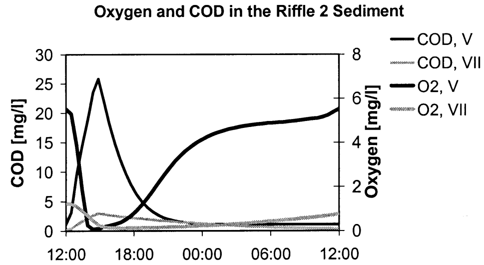

Figure 7 Sediment time series for COD and oxygen in riffle 2 for a hypothetical situation with a combined sewer overflow effluent (discharge of 2 m^3/s with a duration of 2.4 h and a COD of 100 mg/l)

hours followed by a slow recovery of oxygen levels. The oxygen depletion is even longer at cross section VII where the exchange processes are slower. At the same time, water column oxygen concentrations do not fall below 4 mg/l. It may be concluded, that for the boundary conditions given for the River Lahn combined sewer overflows have the potential to disrupt sediment oxygen balances in riffle sections for extended time periods. Those single events would mean a substantial endangering for populations of sediment dwelling benthic macroorganisms and gravel spawning fishes.

Conclusions

The River Water Quality No. 1 approach was proved to be sufficient to meaningfully quantify the surface/subsurface connectivity and oxygen balance of a highly eutrophic shallow river for both the surface and sediment flows. This could be achieved with a systematic procedure of river compartmentalisation including identification of flows and a strongly simplified description of biochemical conversion processes.

The modelling approach makes it possible to quantify the temporal dynamic of oxygen in surface flow and sediment zones for spatially averaged scales, but with consideration of distinct patterns in pool and riffle zones. This opens new perspectives to study ecological relevant system responses to anthropogenic impact.

This potential is demonstrated by results showing the effect of emissions from wastewater treatment plants operating according to emissions standards infiltrating the riffles, which may be high enough to drop sediment oxygen concentrations to low levels while those in the surface flow remain elevated at corresponding times. At the same level of specific domestic wastewater pollution, combined sewer overflows may cause anoxic sediment oxygen conditions for extended time periods. Therefore, oxygen concentrations and sediment oxygen demand in the hyporheic flow of rivers with alluvial coarse sediments are a potential limiting factor for benthic macroinvertebrate communities and gravel spawning fish species even under conditions of moderate wastewater loading.

Further research should be directed into these subjects in order to achieve an ecologically meaningful river water quality modelling. In those efforts the RWQM No. 1 modelling approach may be applied to questions of system analysis at different levels of complexity and for different types of human impact. The approach would support our functional understanding of ecological processes in running waters and the identification of ecological effective management strategies.

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