

River Water Quality Model no. 1 (RWQM1): III. Biochemical submodel selection

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Abstract The new River Water Quality Model no.1 introduced in the two accompanying papers by Shanahan *et al.* and Reichert *et al.* is comprehensive. Shanahan *et al.* introduced a six-step decision procedure to select the necessary model features for a certain application. This paper specifically addresses one of these steps, i.e. the selection of submodels of the comprehensive biochemical conversion model introduced in Reichert *et al.* Specific conditions for inclusion of one or the other conversion process or model component are introduced, as are some general rules that can support the selection. Examples of simplified models are presented.

Keywords Activated sludge models; denitrification; dissolved oxygen; eutrophication; model selection; nitrification; rivers; water quality models

Introduction

The IWA (formerly IAWQ) *et al.* Group on River Water Quality Modelling was formed to create a scientific and technical base from which to formulate standardised, consistent river water quality models and guidelines for their use. This effort is intended to lead to the development of (a set of) river water quality models that are compatible with the existing IWA Activated Sludge Models (ASM1, ASM2 and ASM3; Henze *et al.* 1987, Henze *et al.* 1995, Gujer *et al.* 1999) and can be straightforwardly linked to them. Specifically, water quality constituents and model state variables characterising C, O, N and P cycling are to be selected for the basic model.

In a first effort, the task group analysed the state of the art of river water quality modelling, its problems, and possible future directions (Rauch *et al.*, 1998; Shanahan *et al.*, 1998; Somlyódy *et al.*, 1998). This paper is the third of a three-part series series on the development of a model. In the first paper, Shanahan *et al.* (2001) present the general modelling approach and introduce a six-step decision process. Reichert *et al.* (2001) describe in the second paper the equations for the formulation of biochemical conversion processes for a basic river water quality model. This paper gives recommendations for application-specific selection of the biochemical submodel. In addition to these three theoretical papers, two model applications to actual data sets demonstrate the usefulness of the proposed approach (Borchardt and Reichert, 2001; Reichert, 2001).

Situating the biochemical submodel selection step

The Task Group has suggested that the starting point representation of a water quality model consists of the water quality mass balance equations given by Eq. 1:

$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} - v \frac{\partial c}{\partial y} - w \frac{\partial c}{\partial z} + \frac{\partial}{\partial x} \left(\varepsilon_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(\varepsilon_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(\varepsilon_z \frac{\partial c}{\partial z} \right) + r(c, p) \quad (1)$$

explained in more detail in Shanahan *et al.* (2001). Of relevance here is that the changes in concentration c in a river system are influenced by conversion processes whose rates are given by the function $r(c, p)$. The other terms represent the transport of mass.

Shanahan *et al.* (2001) introduce a step-wise procedure based on quantitative measures that helps to decide on the level of detail that is needed to adequately define the transport terms for a particular application of the model. Reichert *et al.* (2001) define a comprehensive set of biochemical process equations making up the term $r(c, p)$. Overall, 23 processes between 24 components are described in this model. This entails a 23×24 stoichiometric matrix describing the relative amounts of components involved in each process and 23 kinetic relationships that allow calculating the dependency of the process rate on the component concentrations. For ease of understanding, the Peterson matrix representation of the model is repeated here (Table 1).

The components are subdivided in soluble and particulate fractions, the latter containing biomass fractions as well, i.e. heterotrophs (X_H), two types of nitrifiers (X_{N1} , X_{N2}), algae (X_{ALG}) and consumers (X_{CON}). Particulate fractions further contain inerts (organic: X_I , phosphate: X_P and inorganic: X_{II}) and biodegradable materials (X_S). In the soluble fraction, organic inerts are also considered (S_I), next to biodegradable organics (S_G), nitrogen fractions (ammonium: S_{NH3} and S_{NH4} , nitrite: S_{NO2} , nitrate: S_{NO3}), phosphate (S_{HPO4} , S_{H2PO4}), oxygen (S_{O2}) and finally the components involved in the bicarbonate equilibrium, i.e. carbon dioxide (S_{CO2}), bicarbonate (S_{HCO3}), carbonate (S_{CO3}), calcium (S_{Ca}) and hydroxyl ions (S_{OH}) and protons (S_H).

The purpose of the current paper is to help users of the River Water Quality Model no. 1 decide on the adequate selection among the multitude of conversion terms, just as Shanahan *et al.* (2001) presented a method for the adequate choice of the transport terms. Unfortunately, the quantitative measures that could be provided in the decision process for the transport equations, are not as abundantly available for the conversion model. Hence, more qualitative reasoning needs to be conducted in the decision process.

The decision on the biochemical process equations is concentrated near the end of the overall decision process introduced by Shanahan *et al.* (2001). We start here by assessing the different steps of this decision process in light of choices concerning biochemical process characteristics. In the next section we then discuss in more detail the actual sub-model selection criteria.

- Step 1: *Definition of the temporal representation* (dynamic versus steady state) of the (sub)models. This step is not only focusing on the transport terms of the model but is also closely linked to the process model. Indeed, this step requires the listing of all characteristic time constants of all relevant processes, including the biochemical processes.
- Step 2: *Selection of the spatial dimensionality*. In this step, a decision is to be made on the inclusion of a sediment/sessile compartment in the representation of the river system. At this stage, it is decided whether this compartment has an important impact on the overall river description. Information is required on the relative importance of conversions happening in the bulk liquid and the sediment.
- Step 3: *Determination of the representation of mixing*.
- Step 4: *Determination of the representation of advection*. Compared to Steps 1 and 2, the decisions in Steps 3 and 4 do not depend on the characteristics of the conversion processes.

Table 1 Qualitative stoichiometric matrix of the complete river water quality model no. 1 (cf. Reichert *et al.*, 2001)

Component → <i>i</i>	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)
<i>J</i> Process ↓	S _S	S _I	S _{NH4}	S _{NH3}	S _{NO2}	S _{NO3}	S _{HPO4}	S _{H2PO4}	S _{O2}	S _{CO2}	S _{HCO3}	S _{CO3}	S _H	S _{OH}	S _{Ca}	X _H	X _{N1}	X _{N2}	X _{ALG}	X _{CON}	X _S	X _I	X _P	X _{II}
(1a) Aerobic growth of heterotrophs with NH4	-	?					?		-	+			?			1								
(1b) Aerobic growth of heterotrophs with NO3	-					-	?		-	+			?			1								
(2) Aerobic resp. of het.		+					+		-	+						-1							+	
(3a) Anoxic growth of heterotrophs with NO3	-			+		-	?			+			?			1								
(3b) Anoxic growth of heterotrophs with NO2	-				-		?			+			?			1								
(4) Anoxic resp. of het.		+			-	+				+						-1							+	
(5) growth of 1st-stage nitrifiers		-		+		-			-	-			+				1							
(6) Aerobic respiration of 1st-stage nitrifiers		+					+		-	+							-1						+	
(7) Growth of 2nd-stage nitrifiers					-	+	-			-								1						
(8) Aerobic respiration of 2nd-stage nitrifiers		+					+		-	+								-1					+	
(9a) Growth of algae with NH4		-					-		+	-									1					
(9b) Growth of algae with NO3						-	-		+	-									1					
(10) Aerobic resp. of algae		+					+		-	+									-1				+	
(11) Death of algae		(+)					(+)		(+)	?			?						-1			+	+	
(12a) Growth cons. on XALG		(+)					(+)		-	?			?						-	1		+		
(12b) Growth of Cons. on XS		(+)					(+)		-	?			?							1		-		
(12c) Growth of Cons. on XH		(+)					(+)		-	?			?							1				
(12d) Growth of Cons. on XN1		(+)					(+)		-	?			?							1				
(12e) Growth of Cons. on XN2		(+)					(+)		-	?			?							1				
(13) Aerobic Resp. of Cons.		+					+		-	+										-1			+	
(14) Death of Consumers		(+)					(+)		(+)	?			?							-1		+	+	
(15) Hydrolysis	+	(+)					(+)		(+)	?			?									-1		
(16) Eq. CO2 ↔ HCO3										-1	1		+											
(17) Eq. HCO3 ↔ CO3											-1	1	+											
(18) Eq. H2O ↔ H+OH													1	1										
(19) Eq. NH4 ↔ NH3													+											
(20) Eq. H2PO4 ↔ HPO4							1	-1					+	+										
(21) Eq. Ca ↔ CO3												+								1				
(22) Ads. of phosphate							-1																1	
(23) Des. of phosphate							1																-1	

Step 5: *Selection of the biochemical submodels* (see below in detail).

Step 6: *Definition of the boundary conditions*. Depending on the model compartmentalization, certain biochemical processes may be represented as boundary conditions (typically boundary fluxes). In these instances, boundary terms may replace one or more biochemical submodels.

Criteria for the selection of the biochemical submodels

In the overall decision process of a water quality modelling exercise summarised above, step 5 forms a fundamental part. Indeed, in this step it is determined which components and processes are to be included in the model and which ones can be omitted. In terms of Equation 1, this step determines the elements in the concentration vector, \mathbf{c} , and the expressions to be included in the reaction vector, $\mathbf{r}(\mathbf{c}, \mathbf{p})$. We propose that this step be completed within the framework of the Peterson stoichiometry matrix as presented by Table 1 in Reichert *et al.* (2001). The step in fact requires several decisions concerning specific model components and processes. These are delineated in the following.

Compartments

One of the most important decisions in terms of submodel selection is of course the decision whether it is necessary to consider one or more compartments in which the reactions summarised in the process matrix are occurring. In case one decides for more compartments, the number of state variables in the models is increased substantially, leading to considerably longer calculation times.

The most complete model would contain all state variables in the water column, particulate state variables attached to the surface of the river bed (interacting with dissolved compounds in the water column), all state variables in the sediment pore volume, and, finally, particulate state variables attached to sediment particles. In case the sediment is modelled as a biofilm then the number of state variables is increased even more. Also in the case of the selection of several compartments, simplifications to such a complicated model will often be appropriate. In the following, we discuss adequate models for typical situations.

- *Large river*. In a very large river, bacteria and algae suspended in the water column may dominate conversion rates. For such a river, a one compartment model, extended by sediment source and sink terms, may be sufficient for the description of nutrient dynamics in the water column (similar to QUAL2E). However, for the investigation of environmental conditions in the sediment, an additional sediment compartment is required.
- *Small river*. The large ratio of wetted surface to volume in a small river makes attached bacteria and algae much more important in comparison to the situation in a large river. In order to calculate nutrient or DO dynamics in such a small river, a one compartment model with dissolved components in the water column, algae and bacteria attached to the river bed, and dead organic particles in the water column and at the river bed is a good modelling option (Reichert, 2001). However, this option requires the consideration of additional processes. Due to the absence of light, nutrient and substrate limitation for sessile algae and bacteria exposed to the water column concentrations and light conditions, the model equations presented in Reichert *et al.* (2001) lead to Lotka-Volterra type oscillations and even to unlimited growth in the absence of consumers. Reichert (2001) shows that this problem can be solved by an empirical saturation factor with respect to algae or bacteria concentration (as a simple measure of biofilm thickness). In addition, deposition and detachment processes must be considered in such a model. Such an extended model can lead to good results in the water column. However, as shown in the case study by Borchardt and Reichert (2001), water column concentrations may not be representative

for the sediment. Then, a sediment compartment is required in order to allow the modeller to estimate the environmental conditions in the pore water of the sediment.

- *River with significant conversion rates in the water column as well as in the sediment.* A combination of the models described above must be applied. However, this leads to a very large number of unknown parameters and, therefore, to a very demanding model calibration.
- *River sediment.* In order to explore environmental conditions in the sediment pore water, in many situations it may be appropriate to decouple the water column and the sediment models. This may be possible due to the small and slowly changing effect of sediment processes on the water column. In this approach, using typical river water concentrations as boundary conditions, the conditions in the sediment and the exchange fluxes between sediment and pore water can be calculated. In a second step, the exchange fluxes can be used as input to a simpler model for the water column of the river.

Replacing concentrations as state variables by constants

A number of decisions (see below) may lead to elimination of the dynamics of certain component concentrations. However, this does not mean that these component concentrations are completely eliminated from the process descriptions. Rather the kinetic expressions in which these component concentrations are present are modified. For instance, in case the dynamics of biomass concentrations are not considered, the X variable is replaced with a constant to be chosen by the user or estimated from data. Similarly, if the concentration of one or the other substrate of a reaction is assumed to be independent of time, the saturation terms involving this variable can be replaced by constants, in this way simplifying the overall model considerably. Such a simplification of the model is of special interest for sessile algae and bacteria, when not enough information for dynamic modelling of their population is available. Such a simplified model at least allows modelling of the short term dynamics of dissolved components using sessile algae and bacteria as model parameters. However, it cannot account for longer term changes in the populations of algae and bacteria (e.g. Reichert, 2001).

Nitrite

Columns 5 and 6 of the matrix (Table 1) show reactions for the nitrite and nitrate species of nitrogen. Nitrite, however, is typically short-lived in rivers and stays low in concentration. For many rivers, it may be omitted from the river water quality model without loss of predictive power. In some rivers, it reaches higher concentrations and can become toxic to aquatic organisms. The decision to include or exclude nitrite thus depends upon observed conditions in the river being modelled, the quality criteria for the river and the goals of the modelling exercise. If there is a significant ammonia input to the river, nitrite should be considered as a state variable, because there can be a significant nitrite build-up due to nitrification, especially during the summer months (Londong *et al.*, 1994). If nitrite is concluded to be unimportant, columns 5 and 6 of the matrix may be consolidated into a single column for oxidised nitrogen species, S_{NO} (as in the Activated Sludge models). Similarly, the first- and second-step nitrifying bacteria, X_{N1} , and X_{N2} , may also be consolidated in a single nitrifying bacteria population, X_N . The corresponding processes 5 and 7, and 6 and 8 can also be consolidated into a single process for nitrifier growth and a single process for aerobic respiration of nitrifiers, respectively. Finally, the growth of consumers on the two nitrifier populations (processes 12d and 12e) can be combined into a single process.

Anoxic conditions

In general, the modeller should assume that anoxic conditions (the absence of oxygen and simultaneous presence of nitrate/nitrite) may occur. However, field data may indicate that

such conditions are virtually impossible. A typical example would be a highly aerated stream with a small organic load. In those cases that the modeller can assume anoxic conditions will not occur, processes 3a/b and 4 for anoxic growth and anoxic respiration can be eliminated from the Peterson matrix.

Algae

In some riverine situations, algal activity may only insignificantly contribute to the dissolved oxygen budget. For instance, if the hydraulic residence time is less than 4 to 7 days, then wash-out will limit the suspended algal population (Kimmel *et al.*, 1991; Thomann and Mueller, 1989). Otherwise, a rule of thumb used in traditional dissolved oxygen modelling is that algal influence can be ignored if the concentration of chlorophyll *a* in the water column is less than 10 µg/l. This rule of thumb is consistent with the approximate formulae given by Thomann and Mueller (1989) that $P = 0.25 \text{ Chl-}a$ and $R = 0.025 \text{ Chl-}a$, where P is the maximum photosynthetic oxygen production rate in mg/l/day; R is the rate of oxygen consumption by algal respiration in mg/l/day; and Chl-*a* is the concentration of chlorophyll *a* in µg/l.

Different considerations govern sessile algae. These algae may influence dissolved oxygen levels under conditions in which planktonic algae are unimportant. However, sessile algae require a rocky substrate and will not be a factor in a river with a mud bottom. They also require good light conditions and small water depth (note that macrophytes can be considered to be equivalent to sessile algal activity and may significantly contribute to the oxygen balance). If algae are not influential, then column 19 may be removed from the table, as well as processes 9 through 11. Predation of algae by consumers is then no longer possible and process 12a can be removed as well.

Consumers

In a great many water quality and aquatic ecosystem models, consumers are not explicitly modelled. Not modelling consumers is tantamount to an implicit assumption that consumers exist at a constant concentration. If this simplification is chosen, the death rate for the different populations must be proportionally adjusted to account for the effects of consumers. If consumers are not modelled, then processes 12 through 14 and column 20 can be eliminated from the process matrix. The effect of consumers is then lumped into expressions for death or respiration of the organisms, leading to apparently higher rates. The decision to model consumers or not is largely driven by data availability: in a great many rivers, there will be insufficient data to evaluate the accuracy of the model of consumers and thus justification will be limited for inclusion of such a model.

Heterotrophs

As with the population of consumers, heterotrophic bacteria need not be explicitly modelled, but may be implicitly treated as a constant concentration in the model (if this is representative for the system under study, of course). In this instance, X_H (column 16) may be eliminated. Model kinetic coefficients would require adjustment to capture the effect of the unmodelled, constant population. The assumption of constant heterotrophic population is, for instance, implicit in the QUAL2E model and other traditional approaches to water quality modelling. In general, we do not recommend this approach with RWQM no.1 inasmuch as a primary goal of the model is to capture heterotrophic population dynamics.

Nitrifiers

Again, only under certain conditions, the size of a nitrifier population will be of such significance that the composition of the river water is influenced by its activity. Such conditions are,

for instance, a sufficient retention time or the possibility to form biofilms that are not overgrown by heterotrophs, i.e. under not too organically polluted conditions. When nitrifiers (and nitrification) can be neglected, columns 17 and 18 can be eliminated, as are the processes 5 to 8. Note that their absence will also allow elimination of processes 12d and 12e from the process matrix.

Another condition for elimination of an equation for the nitrifier concentration occurs when their concentration is not varying significantly over time, e.g. when the load is constant or another constant limitation is affecting their growth. This corresponds to an exact compensation of the processes affecting the nitrifier concentration (and a vanishing of the stoichiometric coefficient when these processes are summed, e.g. for X_{N1} processes 5, 6 and 12d). Under these conditions, the columns 17 and 18 can be eliminated in the process matrix, but one should not forget that the constant value of the biomass concentration must be introduced in the corresponding combined process rate.

Chemical equilibria

The decision of whether or not to model the chemical equilibria involving ammonium (S_{NH3} and S_{NH4}), the carbonate system (S_{H2CO3} , S_{HCO3} , S_{CO3} and S_{Ca}) phosphate (S_{H2PO4} and S_{HPO4}) and hydroxyl and proton concentrations (S_{OH} and S_H) depends upon the river characteristics and the modelling goals. The equilibria can often be eliminated as extraneous to the goals of modelling. Exceptions are those situations where it is important to understand pH dynamics, where field measurements of total inorganic carbon indicate possible limitation of the growth of nitrifiers (X_{N1} and X_{N2}) and algae (X_{ALG}), or where large pH variations have an important effect on the rates of processes included in the model. Such large pH variations can be caused, for instance, by algae growth, nitrification or external disturbances such as acid or alkaline discharges. Other useful application of these equilibria are those riverine situations where it is important to detect potential ammonia (S_{NH3}) toxicity towards fish. If the chemical equilibria are not modelled, columns 4, 8 and 10 through 15 and processes 16 to 21 may be removed from the Peterson matrix.

General rules for submodel selection

Several model components are usually essential. Obviously rapidly biodegradable organic matter, S_S , and dissolved oxygen, S_{O2} , correspond to the fundamental parameters BOD and DO in traditional water quality models and must usually be retained. Ammonium is similarly fundamental.

Slowly biodegradable particulate organic matter (X_S) arises, according to the matrix, from the death of consumers or algae. However, it is commonly introduced into a river by sources (i.e., point- and non-point source loads). Hence, even if algae and consumers are not modelled, X_S and hydrolysis must remain a part of the model. Similarly, S_S , S_{NH4} , and S_{HPO4} commonly derive from source loads.

As indicated in the text above, elimination of some species or process may precipitate the elimination of others. In general, it can be stated that, for any component with a negative relation in a row, the reaction cannot occur if that component is assumed to have a zero concentration, and the row can consequently be eliminated. The same effect could be achieved in the full model by programming a switching function in the process rate equation to yield a zero process rate when the component concentration is zero. However, this causes superfluous calculations to be made, increasing computation time. For example, if there were no X_p , then there could be no phosphorus adsorption, and process 22 could be deleted altogether.

A similar simple rule does not hold for elimination of columns from the process matrix, however. If there are no terms in any particular column (i.e. all boxes in the column are empty), then the column might not necessarily drop out of the process matrix. Indeed, if the

column is dropped out of the Peterson matrix, it means that the component is completely eliminated from the river model (it is no longer in the component vector, c). The component may, however, still be needed in the model, for instance because it is present in one or the other kinetic relation, or it may be necessary to allow calculation of a variable that can be related to measurements, e.g. the total suspended solids. Moreover, the fact that all elements in a column are empty does not necessarily mean that the concentration of the corresponding component is not time-varying because boundary conditions or sources and transport processes may also affect its concentrations.

Some examples above indicated that the net conversion rates for components can become zero if different processes exactly compensate for each other (or are assumed to compensate). Basically, it means that the summation of the different process rates involving the component that could potentially be eliminated should make the stoichiometric coefficient vanish. Only then is the elimination of the column allowed.

Examples of submodel selection

In the following, some examples are presented that illustrate how simplifications of the basic River Water Quality Model no. 1 can be obtained for adequate description of particular situations in rivers.

In Table 2, a simplified model is introduced in which the influences of consumers, pH variations and phosphorus adsorption/desorption on other variables in the system can be assumed to be negligible and their variation itself is of no interest to the model builder. This model may be selected in case pH measurements indicate only slight variations thereof, when phosphate is not the limiting nutrient, and when measurements indicating the activity of consumers are not available or not sufficiently convincing to extend the model with this state variable and the corresponding processes.

Table 2 Simplified river water quality model no. 1 without consumers, pH variation, or phosphorus sorption

Component → i	(1)	(2)	(3)	(5)	(6)	(7)	(9)	(16)	(17)	(18)	(19)	(21)	(22)
j Process ↓	S_S	S_I	S_{NH4}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{O2}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_S	X_I
(1a) Aerobic growth of heterotrophs with NH4	-		?			?	-	1					
(1b) Aerobic growth of heterotrophs with NO3	-				-	?	-	1					
(2) Aerobic respiration of heterotrophs			+			+	-	-1					+
(3a) Anoxic growth of heterotrophs with NO3	-			+	-	?		1					
(3b) Anoxic growth of heterotrophs with NO2	-			-		?		1					
(4) Anoxic respiration of heterotrophs			+		-	+		-1					+
(5) Growth of 1st-stage nitrifiers			-	+		-			1				
(6) Aerobic respiration of 1st-stage nitrifiers			+			+	-		-1				+
(7) Growth of 2nd-stage nitrifiers				-	+	-				1			
(8) Aerobic respiration of 2nd-stage nitrifiers			+			+	-			-1			+
(9a) Growth of algae with NH4			-			-	+				1		
(9b) Growth of algae with NO3					-	-	+				1		
(10) Aerobic respiration of algae			+			+	-				-1		+
(11) Death of algae			(+)			(+)	(+)				-1	+	+
(15) Hydrolysis	+		(+)			(+)	(+)					-1	

Table 3 Simplified river water quality model no. 1 similar to QUAL2E

Component → <i>i</i>	(3)	(5)	(6)	(7)	(9)	(19)	(21)
<i>J</i> Process ↓	S _{NH4}	S _{NO2}	S _{NO3}	S _{HPO4}	S _{O2}	X _{ALG}	X _S
(1+2) Aerobic degradation of organic material	+			+	-	-	-
(3+4) Anoxic degradation of organic material	+		-	+		-	-
(5+6) Growth and respiration of 1st-stage nitrifiers	-	+			-		
(7+8) Growth and respiration of 2nd-stage nitrifiers		-	+		-		
(9b) Growth of algae with NO3			-	-	+	+	

Table 4 Simplified river water quality model no. 1 similar to extended Streeter-Phelps model

Component → <i>i</i>	(3)	(6)	(7)	(9)	(19)	(21)
<i>J</i> Process ↓	S _{NH4}	S _{NO3}	S _{HPO4}	S _{O2}	X _{ALG}	X _S
(1+2) Aerobic degradation of organic material	+		+	-	-	-
(9b) Growth of algae with NO3		-	-	+	+	

Table 5 Minimal river water quality model no. 1 similar to Streeter-Phelps model

Component → <i>i</i>	(7)	(16)
<i>J</i> Process ↓	S _{O2}	X _S
(1+2) Aerobic degradation of organic material	-	-

Table 3 is a model extending the simplifications made in the model of Table 2 with the additional assumptions that

- (i) bacterial growth is compensated by respiration (leading to constant heterotrophic and nitrifying populations),
- (ii) the rate-limiting function of hydrolysis is incorporated into the degradation rate.

This formulation is conceptually similar to the QUAL2E model (Brown and Barnwell, 1987).

As a next example, Table 4 illustrates to what extent the model can eventually be simplified when the additional assumption is made that nitrification is absent (e.g. because the organic load is too high which leads to too strong competition with the heterotrophs) and anoxic degradation can be omitted from the overall description of the riverine situation under study (e.g. because nitrate is absent or because aeration is intensive and no considerable biofilm is present). Here, even in this very simple model, still – and in contrast to many state-of-the-art models – description of biomass accumulation (of algae) is essential to describe the observed oxygen dynamics. This model is essentially the Streeter–Phelps (1925) model extended to include a photosynthesis-respiration term.

Finally, in the very simple model presented in Table 5, the assumption of constant heterotrophic population (hidden in the kinetic coefficient) is sufficient to describe the dissolved oxygen dynamics induced by organic material biodegradation. Additional assumptions here are that algae activity can be neglected and that ammonium and phosphate are not to be modelled, e.g. because they are not limiting the conversion processes. This is the reduction of the River Water Quality Model no. 1 into the classic Streeter–Phelps model.

Conclusion

The River Water Quality Model no.1 presented in Reichert *et al.* (2001) is discussed in this paper. It can under various circumstances be simplified as demonstrated. Guidelines on the choice of different submodels that can be selected from the multitude of biochemical process equations presented in Reichert *et al.* (2001) have been given. There are no clear cut decision criteria for the conversion part of the model, but guidelines have been presented and some general rules for model selection specified

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