

River Water Quality Model no. 1 (RWQM1): I. Modelling approach

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Abstract Successful river water quality modelling requires the specification of an appropriate model structure and process formulation. Both must be related to the compartment structure of running water ecosystems including their longitudinal, vertical, and lateral zonation patterns. Furthermore, the temporal variability of abiotic boundary conditions may be important and must be incorporated by an appropriate choice of model parameters. A six-step decision procedure is proposed to achieve these objectives. The steps address the determination of the following model features: (1) temporal representation (dynamic or steady-state); (2) model dimensionality; (3) mixing; (4) advection; (5) reaction terms; and (6) boundary conditions. Numerical criteria based on process time constants and length scales provide a basis for these decisions.

Keywords Activated sludge models; eutrophication; dissolved oxygen; rivers; water quality models

Introduction

The IWA (formerly IAWQ) Task 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 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.

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 first of a three-part series that outlines a decision process for model formulation. This paper addresses selecting the appropriate model structure and hydraulic formulation for a specific application. The second paper (Reichert *et al.*, 2001), gives equations for the formulation of biochemical conversion processes for a basic river water quality model. The third paper (Vanrolleghem *et al.*, 2001) provides recommendations for selecting and representing biochemical processes in the model. In addition to these three theoretical papers, model applications to actual data sets demonstrate the usefulness of the proposed approach (Reichert, 2001; Borchardt and Reichert, 2001).

Types of rivers

Figure 1 presents a conceptual model of running water ecosystems consisting of abiotic and biotic elements linked within a hydrological continuum. Processes within and between elements are complex and can be described by a series of physico-chemical, hydro-morphological, and biological parameters.

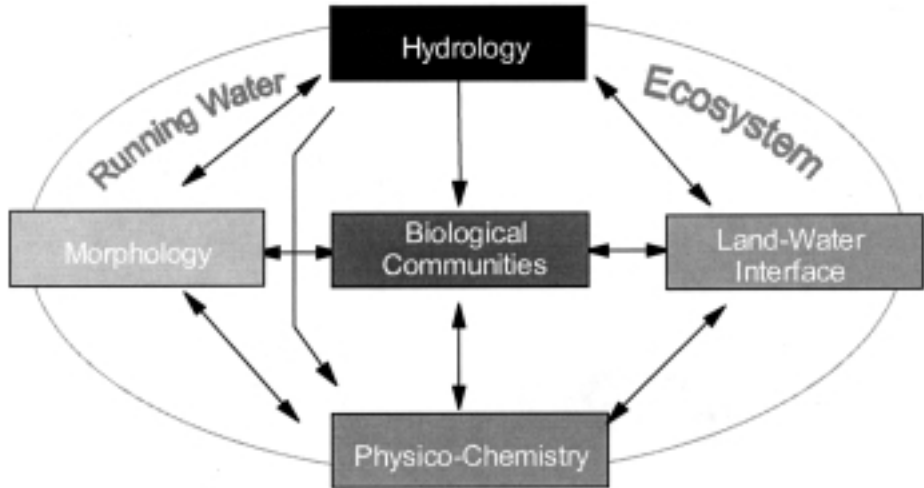


Figure 1 Structure of running water ecosystems

The abiotic and biotic structures of running waters are characterised by longitudinal, vertical, lateral, and temporal gradients (Table 1). This is especially important for the connectivity between surface and subsurface compartments, particularly the hyporheic zone (the zone in fluvial sediments in which the chemistry of the pore fluids is influenced by both ground water and surface water). The upper layers of the hyporheic zone act both as an important habitat for the benthic community (Schwoerbel, 1961) and as a reactor with intense metabolism (Fisher and Likens, 1973). River water quality modelling approaches must address these ecological characteristics by appropriate consideration of compartments and processes on representative spatial and temporal scales (steps 1 through 4 below). For example, for headwater streams and mid-stream regions with coarse substrates, it is necessary to consider both suspended and benthic processes including the hyporheic zone. In contrast, large rivers are more likely to be dominated by transport and conversion processes in the surface flow. Furthermore, there are basic ecological relations of autotrophic and heterotrophic processes with characteristic ratios of Production/Respiration (P/R). This might influence the consideration of processes and conversion rates in step 5 (Vanrolleghem *et al.*, 2001).

Model formulation

The decision process may be thought of as defining terms in the water-quality mass balance equations and averaging these equations over space. The basic set of equations is given as:

$$\frac{\partial \mathbf{c}}{\partial t} = -u \frac{\partial \mathbf{c}}{\partial x} - v \frac{\partial \mathbf{c}}{\partial y} - w \frac{\partial \mathbf{c}}{\partial z} + \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial \mathbf{c}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial \mathbf{c}}{\partial y} \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial \mathbf{c}}{\partial z} \right) \mathbf{r}(\mathbf{c}, \mathbf{p}) \quad (1)$$

where \mathbf{c} is the n -dimensional vector for mass concentration of the n state variables in the water phase in both the water column and the sediment pore water; t is time; x , y , and z are spatial coordinates; u , v , and w are the corresponding velocity components; ϵ_x , ϵ_y , and ϵ_z are turbulent and/or molecular diffusion coefficients for the directions x , y and z , respectively; and \mathbf{r} is an n -dimensional vector of conversion rates of state variables due to biological, chemical, and other conversion processes as a function of concentration, \mathbf{c} , and model parameters, \mathbf{p} (subject to calibration). The variables \mathbf{c} , u , v , w , ϵ_x , ϵ_y , ϵ_z , and \mathbf{r} may all vary with time t and location x , y , z . Eq. 1 is subject to various initial and boundary conditions whose formulation varies depending upon the application. The variables u , v , and w and ϵ_x , ϵ_y , and ϵ_z are independent of \mathbf{c} and thus may be determined externally to the water-quality model. This process is further discussed below.

Table 1 Conceptual description of physico-chemical characteristics and important system compartments of unpolluted running waters (modified from River Continuum Concept; Vannote *et al.*, 1980)

Zone	Processes and physico-chemical characteristics	Important compartments
Headwater stream (Krenal, Epirhithral)	Temperature regime dependent on spring type Temperature fluctuations low Nutrient import from geogenous sources and bank/riparian vegetation Ratio of Production (P) versus Respiration (R) $P/R < 1$ (without allochthonous sources) Most important nutrient source for aquatic communities is allochthonous detritus; carbon import from ground water	Pelagial River bed Hyporheic compartment (Groundwater)
Mid-reach stream Metarhithral; Hyporhithral; Epipotamal	Elevated temperature amplitudes. Primary production (PP) from sessile algae, beginning PP in surface flow/channel water Primary production from submersed macrophytes ($P/R > 1$) Elevated nutrient concentrations. Increased variation of oxygen concentrations. Most important nutrient source: allochthonous and autochthonous detritus	Pelagial River bed Hyporheic compartment
Downstream regions Meta-/Hypopotamal	Temperature amplitudes balanced. Primary production dominated by phytoplankton with limitation by turbidity/suspended solids. Growth of herbivorous zooplankton. $P/R < 1$. Oxygen variations smaller. Increased nutrient concentrations. Most important nutrient source: autochthonous detritus	Pelagial Riparian compartment Floodplain

Definitions: allochthonous – originating from external sources
 autochthonous – originating from internal sources
 epipotamal – ecological term (based on zoological criteria) for the upstream zones of rivers
 epirhithral – ecological term (based on zoological criteria) for the upstream zones of streams
 geogenous – originating from geological sources
 hypopotamal – ecological term (based on zoological criteria) for the downstream zones of rivers
 hyporheic – ecological term for the transition zone between surface water and ground water
 hyporhithral – ecological term (based on zoological criteria) for downstream zones of streams
 krenal – ecological term (based on zoological criteria) for the spring zones of running waters (creeks)
 metapotamal – ecological term (based on zoological criteria) for the midstream zones of rivers
 metarhithral – ecological term (based on zoological criteria) for the midstream zones of streams
 pelagial – ecological term for the open water compartment of surface waters
 riparian – ecological term (based on botanical criteria) for the bank compartment of running waters with vegetation dependent from fluctuating water tables

Decision procedure

The decision process is provided here as a series of six steps in which specific aspects of the model are determined.

Step 1. Define temporal representation

Different water-quality processes are exerted and manifested over different length scales, and with proportionally different time constants (i.e., the time frame within which changes are expected to occur). The length scale, l , is related to the time constant, τ , as:

$$\tau = l / \bar{u}$$

where \bar{u} is the average velocity over the length scale l . In nearly stagnant water bodies, such as lakes, l is often large while \bar{u} is small, thus leading to long time constants. Water bodies with long time constants typically require a much less detailed representation than those

that respond quickly. For example, lake eutrophication is a response to annual nutrient loading and advances over many years and many short-duration phenomena may be overlooked. In contrast, combined sewer overflows affect a river's water quality within minutes or hours and must be modelled in considerable detail. Such disparate time constants necessitate different water-quality model formulations and, accordingly, the length scale and time constant are key factors in the model decision process. For this reason, we make it Step 1 of the decision process.

Step 1 requires defining τ_1 and τ_2 , the lower and upper bounds of the characteristic time constant based on l_1 and l_2 , the corresponding length scales. These bounds depend upon the problem being modelled and the processes that dominate that problem. As such, they depend upon both Eq. 1 and its boundary conditions. Examples of time constants potentially involved include: rainstorm duration and watershed time of concentration for nonpoint source pollution problems, a day for photosynthesis, a day or week for variations in domestic wastewater flow, travel time for pollutant advection, operational periods for reservoirs, seasons for population dynamics, and longer periods for accumulative pollutants.

Once τ_1 and τ_2 have been defined, the representation of processes over time – either dynamic or steady-state – can be selected. If the process of interest proceeds at some rate constant k (in units of inverse time), then a process time constant of $\tau_c = 1/k$ may be defined. If $\tau_1 < \tau_c < \tau_2$, then a dynamic model is required. If $\tau_c \gg \tau_2$ then the process may be omitted. If $\tau_c \ll \tau_1$ then a steady-state model will suffice.

Still another factor to be considered is the influence of sediment processes. A sediment time constant can be defined as τ_s which may be defined as the time between floods that precipitate sediment resuspension and sedimentation or between similar relevant events, where typically, $\tau_s \gg \tau_2$. Processes in the sediment can be neglected only if $\tau_c \gg \tau_s$. Processes in the sediment should be described dynamically if $\tau_1 < \tau_s < \tau_c$. This is typically the case in shallow rivers where benthic activity contributes significantly to conversion processes within the stream. In the typical case that sediment processes occur slowly, $\tau_s \gg \tau_c$, then sediment processes can be captured as a time-invariant parameter, such as the sediment oxygen demand (SOD) term in traditional stream dissolved oxygen models.

Step 2. Determine model spatial dimensions

Choosing the spatial dimensions to be represented in the water-quality model has significant implications for the model formulation. Particularly, the choice of dimensionality alters the representation of boundary conditions and model parameters. In this decision step, we consider the choices regarding the vertical resolution of the model as well as model dimensionality per se.

Selection of model dimension is associated with the spatial resolution of the water body. A fully continuous three-dimensional description of the water column and sediment can often be reasonably approximated by a vertically mixed water column and one or two sediment zones. Such a compartmentalization of the water body leads to a formal reduction in dimensionality of the differential equations without the loss of all of the spatial resolution. This reduction is associated with a change of flux terms (across the new compartment boundaries) to source terms in the differential equations. Similarly, the boundary condition for gas exchange with the atmosphere changes to a source term. Deep soil can be captured simply as a "burial" flux, which represents matter lost from the active sediment to deeper layers in which transformation rates are much slower. There can also be an opposite flux due to diffusion from deeper layers to the active layer. In traditional stream dissolved oxygen modelling, even the active sediment is not represented, but is instead captured through a SOD term.

The choice of vertical resolution ultimately depends upon the problem being considered. The sediment is almost universally included in models of toxic substances, which

adsorb to sediment particles, but only rarely in dissolved oxygen models. In Shanahan *et al.* (1999) we indicated the importance of representing sediment oxygen demand and how it may change over time; thus, we recommend that sediment be represented in river dissolved oxygen problems in which sediment demands are significant. How specifically to treat the sediment must also be decided. In the activated sludge models, there is no formal distinction between the water column and the sediment (sludge). The sediment (sludge fractions like heterotrophic bacteria, X_{H} , and others) is considered mixed into the water column. In that type of formulation, vertical movement of particulates is represented by a vertical velocity that is the net of water advection, particulate settling, and particle buoyancy. Transport between the water column and sediment is determined by this continuous velocity function. Such a formulation is also possible for river water-quality models, however a more practical alternative is to model physically distinct vertical zones, e.g. for the water column and sediment. In this case, transport between the sediment and the water column is represented through explicit transfer terms, such as a settling flux and resuspension flux. These terms capture both advective and diffusive transport. An excellent example of this approach is the sediment oxygen demand model by DiToro *et al.* (1990).

Vertical resolution also needs to be determined for the water column. In shallow waters, no differentiation within the water column may be needed. In deeper waters, such as the metapotomal or hypopotomal zones listed in Table 1, there may be significant differences in water quality with depth, requiring greater vertical resolution to properly represent the deeper water column.

Once the resolution of the model is decided, its dimensionality can be chosen. Models can be three-dimensional, two-dimensional horizontally (xy -plane), two-dimensional vertically (xz -plane), one-dimensional in the x -direction, and finally zero-dimensional. A zero-dimensional formulation is a so-called “box model” in which the water body is represented as one or more fully mixed tanks.

Dimensionality may be selected by consideration of length scales. The length scales for lateral and vertical mixing, l_l and l_v , in a river may be estimated as:

$$l_l \approx \frac{W^2}{2K_y} \bar{u} \quad l_v \approx \frac{h^2}{2K_z} \bar{u}$$

where W and h are the river width and depth, $K_y \approx 0.6 u^* h$ is the lateral dispersion coefficient, $K_z \approx 0.067 u^* h$ is the vertical dispersion coefficient,

$$u^* = \sqrt{ghS_0}$$

is the friction velocity, g is gravitational acceleration, and S_0 is the stream bottom slope. (Formulae for K_y and K_z are taken from Fischer *et al.* (1979), pp. 112 and 106, respectively.) Criteria for dimensionality based on length scales are: if $l_l \gg l_v$, then a one-dimensional model will suffice; if $l_l \gg l_v$, but not $l_l \gg l_l$, then a two-dimensional model is needed; and if not $l_l \gg l_v$, then a three-dimensional model is needed.

Step 3. Determine representation of mixing

The representation of mixing is also dependent on the choice made in Step 2 as to dimensionality. If three dimensions are modelled, then turbulent diffusion is the operative mixing mechanism in the water column. However, if fewer dimensions are represented, then the resulting averaging of advection gives rise to the artificial mixing represented as dispersion.

Whether modelled as dispersion or diffusion, the need to represent mixing processes varies from problem to problem. In traditional one-dimensional dissolved oxygen models, dispersion is often considered negligible when flow and sources are all steady. Dispersion

may be neglected if:

$$\tau_c \gg 2K_x / \bar{u}^2 \quad \text{and} \quad \tau_c \gg \sqrt{2K_x l_2 / \bar{u}^3}$$

where $K_x \approx 0.011 W^2 \bar{u}^2 / u_*^* h$ is the longitudinal dispersion coefficient (Fischer *et al.*, 1979) and τ_c is the time constant associated with variations in concentrations induced by external processes or boundary conditions.

Step 4. Determine representation of advection

Advection concerns the movement of water, sediment, dissolved substances, or particulates. The advection of the water phase can in almost all instances be calculated independently of the water-quality model. The exceptions are pollutants that alter hydrodynamics, such as high-concentration solids or high-volume thermal discharges, each of which may create a significantly nonuniform density distribution within the water column. These exceptions aside, a wide variety of methods to calculate flow are available based on the degree to which the St. Venant equations are or are not simplified. In many instances, hydrodynamic calculations are dispensed with in preference to simple measures of stream velocity such as time-of-travel studies (Kirkpatrick and Wilson, 1989). In situations in which stream flow varies significantly over time, such as nonpoint source pollution problems or where reservoir operations control flow, more complex hydrodynamics need to be considered. In terms of the time period of interest discussed above, this may be stated as a requirement to consider hydrodynamics when $\tau_1 < \tau_{\text{flow}} < \tau_2$, where τ_{flow} is a representative time constant for flow variation.

In those instances when field data are inadequate to define advection, it is necessary to employ a modelling approach. Consistent with the typical geometry of rivers, this review considers only one-dimensional models of stream hydraulics. Two- and three-dimensional representations are also possible, but carry considerable computational complexity. A comprehensive review is provided by Bedford *et al.* (1988). Mahmood and Yevjevich (1975) and Cunge *et al.* (1980) provide lengthy treatises on the one-dimensional solution for unsteady flow in open channels including discussions of the various degrees to which the St. Venant equations may be simplified. The St. Venant equations represent the conservation of mass and momentum, as shown in Eqs. 2 and 3 for one dimension:

$$\frac{\partial h}{\partial t} = -\frac{1}{W} \frac{\partial Q}{\partial x} + \frac{q}{W} \quad (2)$$

$$\frac{\partial Q}{\partial t} = -\frac{\partial}{\partial x} \left(\frac{Q^2}{A} \right) - gA \frac{\partial h}{\partial x} + gA(S_o - S_f) \quad (3)$$

where, Q is the streamflow, q is the lateral inflow per unit length of the river, S_f is the friction slope, and all other variables are as defined above. The full St. Venant equations are only rarely solved for water quality problems – the computational burden of the full solution is substantial – and simplifications are typically employed. One particularly effective simplification, the kinematic wave model, recognises that the slope terms, S_o and S_f , dominate Eq. 3. Thus, in the kinematic approach, Eq. 2 is fully represented, but the differential terms of Eq. 3 are neglected, resulting in the approximation that $S_o = S_f$. The resulting equations are considerably simpler to solve, but result in a reasonable representation of advection affected by an increase in stream flow (“flood wave”).

In some systems, storage zones along the river or a mild channel slope tend to disperse a flood wave or dams create backwater effects, none of which are processes well represented by the kinematic approach. For these situations, Eq. 3 may be solved along with Eq. 2, but with only the S_o , S_f , and $gA \partial h / \partial x$ terms retained in Eq. 3. This results in the diffusive wave approximation, so-named because the resulting equation takes the form of the diffusion equation

(Eq. 1) with a “diffusion” coefficient that captures the dispersion of the flood wave. In practice, this coefficient is empirically increased in order to represent the storage effects caused by channel irregularities and off-channel storage. The diffusive wave approach represents a good compromise between computational complexity and accuracy for most rivers.

There may also be advection of solid phases either through water-column sediment transport or via bed movement. Generally, the predominant movement of particulates in the water column is vertically downwards as represented through the settling velocity. However, during periods of high flow, or in some parts of the river system where streamflow velocities are high, resuspension and/or horizontal sediment and bedload transport may be significant (Vanoni, 1975). These episodic events and other advective fluxes across the water-sediment boundary are not included in Eq. 1b above but are considered boundary conditions.

The time constant for solid-phase advection may be represented as $\tau_s = h/w_s$, where w_s is the settling velocity, which is a function of particle size and density (Thomann and Mueller, 1987, pg. 545). If $\tau_s \ll \tau_1$ then sedimentation is effectively instantaneous and the water-column sediment phase need not be modelled. If $\tau_s \gg \tau_2$ then sedimentation occurs sufficiently slowly that the settling process may be neglected. In the situation that $\tau_1 < \tau_s < \tau_2$, then the sediment phase and sedimentation process must be considered. A similar analysis can be applied to the resuspension process by considering a resuspension velocity (i.e., $w_s < 0$) that is a function of the bottom shear stress exerted by the stream velocity (Chapra, 1997, p. 312). The potentially episodic character of this process needs also to be considered in developing a modelling approach.

Step 5. Determine reaction terms

Step 5 is a fundamental part of the decision process: the determination of which constituents and processes to include in the model and which to omit. In terms of Eq. 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 Reichert *et al.* (2001). Vanrolleghem *et al.* (2001) address this step, and the several decisions concerning specific model constituents and processes that it entails.

Step 6. Determine boundary conditions

Once the model variables and reactions have been determined, it is possible to complete the final decision, the determination of model boundary conditions. The specification of boundary conditions is intrinsically related to the choice of model dimensionality. Boundary conditions of the fully three-dimensional model (Eq. 1) become source terms in equations in which the corresponding dimension is integrated or averaged over. For example, in a three-dimensional representation of stream dissolved oxygen, oxygen transfer across the water surface is a boundary condition at $z = z_0$:

$$\varepsilon_z \left. \frac{\partial h}{\partial t} \right|_{z=z_0} = K_L \left(\frac{c_{\text{air}}}{H} - c \right) = K_L (c_s - c)$$

where K_L is the interfacial transfer velocity, c_{air} is the concentration of oxygen in the air, H is the Henry’s Law constant, c is the concentration of oxygen in the water, and c_s is the saturation concentration of dissolved oxygen.

In contrast, in a traditional one-dimensional model of stream dissolved oxygen the vertical dimension is integrated out, and oxygen transfer across the water surface becomes the familiar source term based on a reaeration rate (Thomann and Mueller, 1987):

$$r_{\text{reaeration}} = K_a (c_s - c)$$

where $r_{\text{reaeration}}$ is the reaeration component of the $r(c, p)$ term in Eq. 1, c is the concentration of dissolved oxygen, and K_a is the reaeration coefficient $= K_L/h$, h is the water depth.

Other fluxes at the vertical boundaries include oxygen and COD flux across the bottom boundary (corresponding to SOD in a traditional one-dimensional model), water flux at the bottom due to seepage loss or ground-water inflow, and other gas transfers at the surface. Similarly, boundary conditions for the flux of pollutants at lateral inflows become sources (pollutant loads) in models in which lateral distance (the y -coordinate) is averaged out.

In this step of the model decision process, the modeller must identify these and other boundary conditions that affect the processes of interest and, depending upon the model dimensionality, formulate these as true boundary conditions or equivalent source terms. An example of rigorous treatment of model boundary conditions is the sediment oxygen demand model by DiToro *et al.* (1990). In addition, at the boundaries of the primary directional coordinate (usually the longitudinal distance x in a river model), the modeller must assign appropriate boundary conditions. In a typical river model, these will be a specified inflow concentration at the model headwater ($c = c_0$ at $x = 0$, or flux $f = Qc - K_x A \partial c / \partial x$), and zero change in concentration at the model terminus ($\partial c / \partial x = 0$ at $x = L$).

Conclusion

Construction of a river water quality model must be based on a logical development of the elements in the model. The model will vary, due to local conditions and the model's purpose. The six-step procedure presented in this paper is a framework for developing the model structure and its supporting hydraulic model.

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