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RIVER WATER QUALITY MODELLING: III. FUTURE OF THE ART

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ABSTRACT

This paper is the third of a three-part series summarizing the background to and objectives of the activity of the IAWQ Task Group on River Water Quality Modelling (RWQM). On the basis of the two other papers and a comparison between the best known state of the art river model, QUAL2E, and the IAWQ Activated Sludge Model (ASM) No. 1, the Task Group proposes to develop improved conversion models for inclusion in a river water quality model. The model should describe the cycling of oxygen, nitrogen, and phosphorus in both water and sediment, and should be compatible with the ASM to support the development of integrated emission reduction strategies. The model should be particularly well suited to handle problems characterized by significant temporal and spatial influences (e.g. CSOs and NPSs). It should serve for research, education, improved communication, knowledge transfer, regulatory applications such as catchment planning, and improved data collection. Anticipated results of the Task Group effort include: (i) standardized conversion sub-models; (ii) a decision support tool to guide model construction and usage; and (iii) case study applications. The model development, which is not intended to result in a software product, is intended to be an open-ended and flexible process to encourage the participation of interested professionals. © 1998 IAWQ Published by Elsevier Science Ltd. All rights reserved

KEYWORDS

Activated sludge model; eutrophication; oxygen household; rivers; software; water quality models.

INTRODUCTION

The IAWQ Task Group on River Water Quality Modelling was formed to create a scientific and technical base from which to formulate standardized, consistent river water quality models and guidelines for their implementation. This effort is intended to lead to the development of river water quality models that are compatible with the existing IAWQ Activated Sludge Models (ASM-1 and ASM-2, Henze *et al.*, 1987, 1995) and can be straightforwardly linked to them (or vice versa). Specifically, water quality constituents and model state variables characterizing O, N and P cycling are to be selected.

This paper is Part III of a three-part series that analyzes water quality modelling with the above aim in mind. As a starting point, Part I (Rauch *et al.*) examines the existing state of the art in river water quality modelling. Part II by Shanahan *et al.* looks at the limitations and problems of the current state of the art. The present paper builds on the first two papers to show possible directions for the future of the art with particular attention to the specifications of standardized river water quality model state variables and process submodels that achieve the aims set out for the Task Group.

OBJECTIVES AND STYLE OF MODEL DEVELOPMENT

Water quality changes in rivers are due to physical transport processes and biological, chemical, biochemical, and physical conversion processes (see Rauch *et al.*, submitted). Physical transport includes advection and turbulent diffusion, which are separately described through hydraulic models of one sort or another. The above processes in the water phase are governed by a set of extended transport equations that can be represented conceptually as:

$$\boxed{\begin{array}{c}\text{Change in}\\\text{concentration}\\\text{with time}\end{array}} = \boxed{\begin{array}{c}\text{Change}\\\text{due to}\\\text{advection}\end{array}} + \boxed{\begin{array}{c}\text{Change due to}\\\text{diffusion or}\\\text{dispersion}\end{array}} + \boxed{\begin{array}{c}\text{Change due to}\\\text{conversion}\\\text{processes}\end{array}} \qquad (1)$$

To this conceptual equation, a similar mass conservation equation for the sediment should be added. Interface terms (sediment-water and water-air) appear as boundary conditions that are completed by specifying in- and outflows and boundary fluxes. Depending on integration, boundary conditions may enter the equation as sink or source terms (as a part of the aggregated conversion processes term).

Here, our goal is to deal solely with the development of conversion sub-models for traditional pollutants (such as included in QUAL2E). This choice of focus is similar to that which led to the activated sludge model. Our choice recognizes that there are well-developed models and tools to address the physical transport components of this problem. Particularly, 1D, 2D, and, increasingly, 3D hydrodynamic models are available to determine the velocity field and are becoming more practical with advancements in computer technology. We therefore see the future in water quality modelling resting on the development of refinements in the description of conversion processes in Eq. (1).

Following the conclusions of Rauch *et al.* and Shanahan *et al.*, our detailed objectives are:

(i) to develop a sequence of standardized and improved conversion submodels from simple to complex;
(ii) to develop a decision support tool to guide the user in field data collection, the selection of hydraulic and physical transport model components, selection of process submodels, and testing of the resulting water quality model; and,
(iii) to apply the submodels to real data from selected case studies.

The first of these objectives entails the following several subtasks:

- to re-evaluate models developed during the past three decades and to eliminate such inherent inconsistencies as the lack of closed mass balances (which mostly arise from an inadequate description of sediment related processes and the use of BOD for characterization of organic matter);
- to guarantee compatibility with the IAWQ Activated Sludge Models to enable integrated analysis of wastewater treatment and receiving water quality impacts; and
- to include and improve process descriptions such as nitrification, denitrification, or those related to sediment, benthic fluxes, attached bacteria and algae, and macrophytes.

We expect these changes in model formulation to improve the predictive power of models to estimate multiple and non-linear effects from emission reduction measures and other artificial alterations (see Shanahan *et al.*).

Water quality models are used for many different problems and purposes. As discussed by Shanahan *et al.* existing models address certain of these problems better than others. Applications that we intend to address through the Task Group effort include:

(i) dynamic problems of combined stormwater overflows and nonpoint source pollution;
(ii) impact of improved wastewater treatment plant operation and control;
(iii) extreme and surprising pollution events;
(iv) improved assessment of artificially influenced rivers (for example, by dams or re-naturalization);
(v) knowledge transfer from other fields such as wastewater biofilm research;
(vi) data collection;
(vii) understanding, research, education and improved communication (e.g. between wastewater engineers and receiving water quality experts); and,
(viii) regulatory applications including catchment planning.

In order to accomplish our intended goal of model refinement, improved data collection is first necessary since the number of state variables, processes, and parameters will be significantly greater than for existing tools. Improved models can in turn lead to advanced design of monitoring programs. Examples are better design of longitudinal water quality profile measurements (e.g. sampling in both space and time), well-defined and controllable laboratory and in situ studies that isolate certain processes for identification purposes, detection of process rates in addition to concentrations, and identification of sensitive variables and processes to be observed in the future.

As stressed by Rauch *et al.* and Shanahan *et al.*, calibration, validation, and model structure identification have become increasingly important and difficult. Thus, although our primary aim is the development of standardized conversion sub-models, this cannot be done without developing a framework for the entire modelling process. The framework should incorporate methods that can and should be employed for the purposes of identification, calibration, validation, and the analysis of uncertainties of differing origins. Moreover, as shown by Eq. (1), the framework should also include hydraulic and transport modules to be able to perform calculations for 'real' systems. There is no unique methodology in this respect: many different but basically equivalent methods are known and frequently it is desired to switch from one approximation to the other (e.g. when moving from the so-called near field to the far field, or from the 2D plume reach to the 'completely' mixed 1D river reach).

We believe that achieving all of the objectives outlined for the Task Group will require about a decade-long process of model development that includes such difficult tasks as improving the description of sediment processes. Our primary goal is only to launch this process, to define the framework, and to provide a first model version that, we hope, can then be extended and further developed by a broad range of professionals dealing with water quality issues.

QUAL2E AND ASM-1: A COMPARISON

Model development process

The development histories of QUAL2E (Brown and Barnwell, 1987), the most current version of QUAL2 which is the best known river water quality model, and ASM-1 (Henze *et al.* 1987a,b), the activated sludge model, are rather different. The roots of QUAL2E go back to the Streeter-Phelps model which was enhanced over the years while retaining the original variables and processes. State variables in QUAL2E can be sorted into three groups reflecting three distinct stages of model development (see Masliev *et al.*, 1995 for details):

Group 1 ('phenomenological' level): traditional Streeter-Phelps state variables;
Group 2 ('biochemical' level): extended Streeter-Phelps and QUAL1 variables; and,
Group 3 ('ecological' level): algae model variables as in QUAL2E.

The three groups represent different concepts. Streeter-Phelps is a purely phenomenological model, where BOD is not the concentration of a chemical substance but the result of a bioassay test. The extended Streeter-Phelps and other models that similarly include nitrogen species share a first-order kinetic structure, in which a group of first-order reactions represent in a cumulative way the complex chain of processes related to electron transfer under aerobic conditions. Finally, the algae model is of the ecosystem dynamics type that accounts for non-linear growth and decay of the living organisms (phytoplankton biomass).

The combination of models of different levels of detail in QUAL2E simply evolved over time: the older 'working and reliable' core models were left operational while the model acquired additional state variables and new process descriptions. Therefore, unlike ASM, these models contain inconsistencies due to the lack of a uniform underlying concept. This in turn leads to problems with substance mass balances. For example, carbonaceous BOD, being a measure of total bioavailable organic carbon, does not include the organic material in algae biomass. Hydrolysis of particulate organic matter is essentially one process, but the rates of hydrolysis of organic nitrogen and phosphorus are different in QUAL2E.

Also unlike ASM-1 (and ASM-2), QUAL2E and similar models lack a clear operational definition of water quality parameters within the model. For example, it is known that there are many forms of organic nitrogen present in natural waters. QUAL2E combines it all under 'organic nitrogen' and does not specify further whether it is total organic nitrogen, Kjeldahl nitrogen, particulate, dissolved, bioavailable, or other.

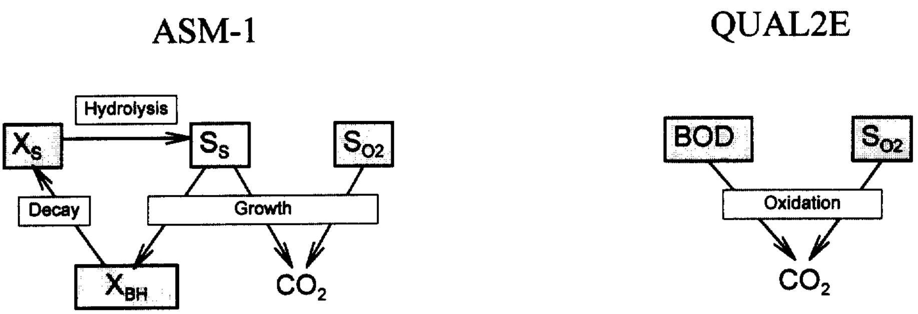
In contrast, the ASM-1 description (Henze *et al.*, 1987a,b) contains a precise specification of the variables and includes methods for their determination. The distinction is that although several models of the activated sludge process predated ASM-1, the ASM-1 developers started by discussing and adopting strict operational definitions for all the state variables and substances included in the model (Grau *et al.*, 1987). Moreover, ASM-1 was developed in 'one piece' by a coordinated effort of professionals sharing this unified conceptual basis. The variables and processes are distinctly specified and material balances are closed by design.

Comparison of state variables

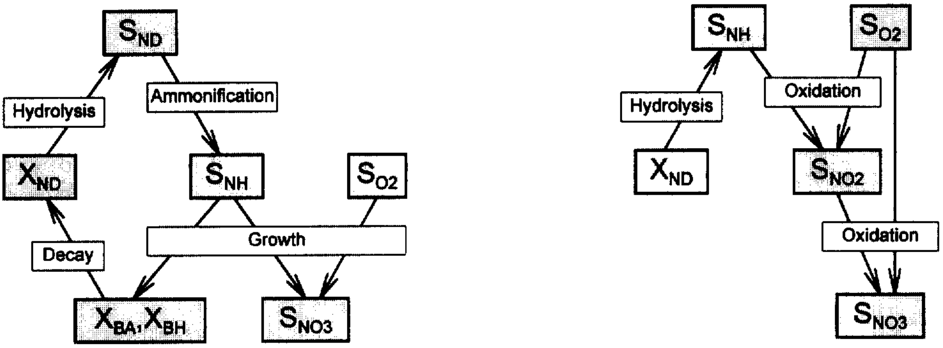
Schematic representations of the O and N cycles of the ASM-1 and QUAL2E models, their state variables, and conversion processes are given in Figure 1 (see Masliev *et al.*, 1995 and Maryns and Bauwens, 1997 for details).

Common principal state variables of QUAL2E and ASM-1 are dissolved oxygen - S_{O2}, particulate organic N (bioavailable) - X_{ND}, nitrate N - S_{NO3}, and ammonia N - S_{NH}. Variables specific to ASM-1 are soluble bioavailable organic matter - S_S, particulate bioavailable organic matter - X_S, autotrophic and heterotrophic biomass - X_{BA} and X_{BH}, respectively, and dissolved organic N (bioavailable) - S_{ND} (inert suspended material X_I, an important sink for organic material, and alkalinity are not included in Figure 1). Variables in only QUAL2E are carbonaceous BOD - CBOD, algae biomass - X_{BP}, nitrite N - S_{NO2}, dissolved reactive P - S_{PO}, and bioavailable particulate P - X_{PD} (sediment oxygen demand, which is a parameter and not a state variable in QUAL2E is not shown in the figure).

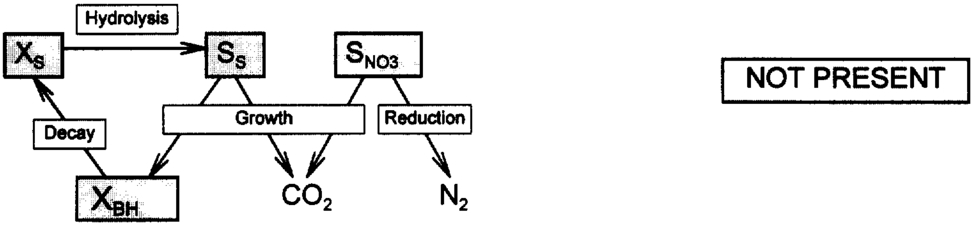
From Figure 1 it is apparent that the state variables in ASM-1 are more numerous and differ from those in QUAL2E. For example, ASM divides both carbonaceous and nitrogenous substrate into readily available and less readily available (which are approximately equivalent to the dissolved and particulate fractions). Substrate utilization during bacterial growth depends on the amount of bacteria. In contrast, in QUAL2E the C substrate is characterized in a lumped way as a BOD test result. The N substrate is expressed as particulate organic N (not bioavailable) and ammonia (readily bioavailable for electron transfer). The process rate in QUAL2E does not consider the amount of bacteria, which is not a state variable.



a. AEROBIC UTILIZATION OF CARBONACEOUS SUBSTRATE



b. AEROBIC UTILIZATION OF NITROGENOUS SUBSTRATE



c. ANAEROBIC UTILIZATION OF CARBONACEOUS SUBSTRATE

Figure 1. Major processes represented in ASM-1 and QUAL2E.

In ASM-1, both DO and nitrate are considered as electron acceptors under aerobic and anaerobic conditions respectively. QUAL2E includes only DO and only aerobic conditions (Figure 1). There are two oxidation agents in ASM-1, autotrophic and heterotrophic bacteria, but none in QUAL2E. Electron acceptors and substrate availability are the limiting factors in ASM-1, while substrate and nutrient limitations are considered in QUAL2E. ASM-1 does not consider nutrients as limiting factors for biomass growth. The reason is the high concentration of all biogenic elements and decomposition products in waste water, which prevents such limitations. Moreover, ASM-1 does not consider phosphorus at all although it was incorporated into the technology-oriented second version, ASM-2, which includes enhanced biological P removal processes that are not relevant for river situations.

Comparison of conversion processes

Conversion processes in activated sludge reactors are essentially non-stationary and non-uniform. Major concentration changes occur within the span of tens of metres (tank dimensions) and hours (retention time); the processes are intensified by artificially maintained high concentrations of the catalyst (bacteria). Stabilization of organic material under such conditions consists of two distinct phases: the primary particulate substrate is removed via hydrolysis and production of a dissolved substrate, and then oxygen is depleted due to biomass growth on the dissolved (secondary) substrate. In the aeration tanks, these processes may or may not be separated both in time and space. In natural waterbodies, the spatial and temporal scales are much larger. The processes usually occur simultaneously and in the same place. Thus lumped models with fewer state variables may be used successfully (see later).

Since ASM-1 contains more processes, it also contains more parameters. In principle, the larger number of parameters in ASM entails more difficulties during model calibration. The authors of ASM-1 reason, however, that since the composition of municipal wastewater is relatively stable (excepting industrial contributions and processes in the sewer system that cause alterations), most parameters remain constant. Only some parameters critically influence model behavior and need case-dependent calibration (Henze *et al.*, 1987a,b). For many applications, the wastewater characteristics have significant impact on treatment processes. Thus the complexity of ASM-1 is to some degree intentional, in order to accommodate a sufficiently detailed description of the incoming wastewater. Also, methods are being developed to handle the problem of identification and wastewater characterization.

In contrast, natural systems such as rivers exhibit large variability and thus parameters are likely to vary over a broader domain than that of ASM-1. Parameters in natural systems also can strongly depend on external climatic and hydrologic conditions and thus one should not anticipate that they can be transferred from the ASMs. For the same reason, the definition of default parameter values as done for the activated sludge models may not be advisable for river models. All in all, both types of models ought to be identified and calibrated to data prior to application particularly in the light of the improved calibration and identification techniques that have become available.

Conclusions from model comparison

Keeping in mind our objective and the comparison above, it seems logical to take a model similar to ASM-1 as the basis of our approach for river water quality modelling. This would allow handling artificial treatment and self purification on common ground. As a first trial, Masliev *et al.* (1995) derived an asymptotic, reduced version of ASM-1 equivalent to an extended Streeter-Phelps model and compared it to the full ASM-1 for a hypothetical riverine situation. The analysis led to the following conclusions that are important to the present development:

(i) Test simulations show that a model similar to ASM-1 can simulate water quality in rivers. Due to differences in spatial and temporal scale, concentration ranges, and environmental conditions in comparison to treatment plant situations, some changes must be introduced into the model (nutrient limitations must be included, rate coefficients controlling hydrolysis must be modified, etc.).

(ii) In riverine situations, the system's dynamics are controlled by the concentrations of particulate organic material and electron acceptors (dissolved oxygen or nitrate). The other variables often reach 'quasi-equilibrium' levels relatively quickly, and thus ASM-1 can be reduced to a phenomenological model similar to Streeter-Phelps.

(iii) In addition to eliminating existing inconsistencies, improved models will be needed primarily when there are abrupt changes in environmental conditions, loads, hydraulics, and other factors such that 'fast' variables are not able to attain their quasi-equilibrium levels, i.e. when the system is characterized by spatial non-uniformity and/or rapid temporal changes.

CANDIDATE STATE VARIABLES AND ANTICIPATED RESULTS

Process sub-models and state variables

As discussed above, the envisaged River Water Quality Model (RWQM) should describe the O, N, and P household in rivers. The need to ensure consistency and closed mass balances, as well as integration with the ASM-1 or ASM-2 models, suggests a change to COD as the basis for expressing state variables as in the activated sludge models. This also applies for algae biomass, which will necessitate the introduction of N/COD and P/COD stoichiometric ratios. The variables of the ASMs should obviously be included in the RWQM, to which should be added temperature, elements of P cycling (as exist in QUAL2E), sediment/benthos state variables, as well as algae and macrophytes. Certainly, the selection and combination of all these state variables requires special care: their number will be large–about fifteen for the water column only.

DO and NO_3 play important roles in switching on and off processes such as anaerobic decomposition, nitrification, and denitrification. A similar role is played by light conditions which necessitates modelling suspended solids. Suspended solids must be the sum of all the particulate matters, including bacteria and algae biomass, particulate bioavailable organic matter, and inert suspended matter. The latter includes inorganic suspended solids due to erosion and resuspension. This fraction is inert and not a part of the material cycles, but it can significantly influence light conditions. Also, there is a need to consider pH, at least in a simplified way, in order to properly describe unionized ammonia, nitrification, toxicity, and sediment processes.

The detailed characterization of wastewater discharges and other inputs to the river should be in harmony with the planned state variables since these inputs significantly influence effects on receiving water quality. In fact, monitoring in terms of the model state variables is one of the key elements to improve the weak predictive power of existing models.

For model calibration and validation routinely available observations should also be used. The principal determination of many variables (such as algae biomass) will remained unchanged. Thus, conversion between observed variables and state variables will be unavoidable (as it is with ASM-1). For this purpose, the measurement matrix **M** will be introduced to guarantee mass conservation in the model. **M** is defined by the equation $\mathbf{c}_m = \mathbf{M}\,\mathbf{c}$, where $\mathbf{c}_m$ is the vector of observed variables (its size is usually smaller than that of $\mathbf{c}$).

Decision support tool

With a model as complex as ASM-1 not only data scarcity, but also measurability of certain variables and parameters can be a problem (for instance heterotrophic biomass is generally not known). For this reason, the proposed development will lead to a set of conversion models from simple to complex rather than a single version, and there will be a need for the user to select those sub-models appropriate to a particular application. Guidelines will be provided on how to proceed with the selection of sub-models for particular applications. Model structure identification and calibration methods will be used and recommended.

The guidelines and modelling framework will incorporate several additional elements that can be visualized as a decision tree (or basis of an expert system). This is intended to give advice on how to decide on the type of the full water quality model and its usage. Major elements and criteria will include: mixing lengths; temporal and spatial scales; forcing functions; dynamics of flow and emissions; physical and numerical dispersion; representation of the physical system; hydraulic and transport equations to be employed; effluent composition; conversion sub-model complexity; design of data collection; selection of major parameters, constants, and associated empirical formulas; methods of calibration, validation, model selection, and uncertainty; and manner of application for management purposes (steady-state for a critical low flow condition, statistical approach similar to that of SIMCAT [NRA, 1990], or full dynamic procedure).

Case study applications

Case studies will be an important test of the RWQM concept and a key component of the development process. Mostly past studies will be used, but participation will be solicited from researchers working in the field. Previously planned case studies may be augmented with supplementary measurements of new variables.

CONCLUSION

River water quality models were developed in incremental stages over the course of decades without a consistent and clear conceptual basis. They are characterized by a lack of clear definitions, inconsistencies, and the inability to link them to wastewater treatment models, which is needed to prepare integrated management strategies. This paper is the last element of a 'trilogy' and presents—on the basis of the two preceding articles and the comparison of the ASM-1 and QUAL2E models—detailed objectives and anticipated products for the IAWQ Task Group on River Water Quality Modelling (RWQM). Planned products include the development of improved standardized (alternative) conversion sub-models for O, N, and P compatible with the ASMs; a decision tree to guide the user on how to proceed with modelling in a research or management framework; and case study applications. Above all, it is intended that the development process be open-ended and flexible to encourage the participation of interested professionals.

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