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RIVER WATER QUALITY MODELLING: II. PROBLEMS OF THE ART

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ABSTRACT

The U.S. EPA QUAL2E model is currently the standard for river water quality modelling. While QUAL2E is adequate for the regulatory situation for which it was developed (the U.S. wasteload allocation process), there is a need for a more comprehensive framework for research and teaching. Moreover, QUAL2E and similar models do not address a number of practical problems such as stormwater flow events, nonpoint source pollution, and transient streamflow. Limitations in model formulation affect the ability to close mass balances, to represent sessile bacteria and other benthic processes, and to achieve robust model calibration. Mass balance problems arise from failure to account for mass in the sediment as well as in the water column and due to the fundamental imprecision of BOD as a state variable.

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 II of a three-part series that analyzes river 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. This paper looks at the limitations and problems of the current state of the art. Part III (Somlyódy *et al.*,) 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.

PRACTICE OF WATER QUALITY MODELLING

The current practice in water quality modelling is largely driven by legislation and regulations. Accordingly, the practice of water quality modelling varies from jurisdiction to jurisdiction as the regulatory framework also varies.

U.S. framework

The most widely known and used computer program for river water quality modelling is the QUAL2E model developed by the U.S. Environmental Protection Agency (Brown and Barnwell, 1987). QUAL2E has a long history, having been preceded by another version of QUAL2 (Roesner *et al.*, 1981) and the similar but simpler QUAL1 model (TWDB, 1971). QUAL2E simulates dissolved oxygen and associated water quality parameters in rivers and streams under conditions of steady streamflow and pollutant discharge. While QUAL2E has clear limitations—stormwater flow events and other situations with unsteady hydraulics cannot be modelled—its formulation derives directly from the U.S. regulatory framework for which it was developed and for which it is generally well suited.

U.S. federal laws establish a two-tier system in which effluent limitations are first set based on available technology and then, if this degree of restriction is insufficient to meet water quality standards for a particular river, a further reduction in emissions is determined through a wasteload allocation. A wasteload allocation is the computation of the maximum amount of waste that can be discharged to the river while still meeting water quality standards under the low-flow conditions specified as a part of the stream standards (usually 7Q10, the seven-consecutive-day low flow with a probability of occurring once in ten years). Wasteload allocations are performed for conditions of constant low flow and maximum permitted effluent discharge rate. QUAL2E is intended specifically for the steady-streamflow, steady-effluent-discharge conditions specified in the water quality regulations for wasteload allocation.

The early and widespread use of QUAL2E and its predecessor models makes it a standard against which other models are typically compared. The capabilities and state variables of the model are described in the accompanying paper by Rauch *et al.* (submitted). Important for this critique (see Somlyódy *et al.*, submitted, for further details) the model follows the traditional formulation of stream dissolved oxygen based on carbonaceous biochemical oxygen demand.

European frameworks

Few other countries have established water quality management laws in which water quality modelling is as integral a part of the process as in the U.S. Although water quality modelling is often used, it is typically as a planning tool in special studies of particular rivers. These models are frequently developed on a custom basis for each individual application. Thus, without the standardizing requirements as created in the U.S. wasteload allocation system, alternative modelling standards have yet to emerge in most other countries. Consequently, the operating standard for river water quality modelling is QUAL2E in Europe and elsewhere as well as in the U.S.

In Europe, for example, water quality modelling is far less prevalent in the regulatory process. For municipal discharges, the EU requirements emphasize effluent criteria set for 'normal' and 'sensitive' areas (which are defined based on eutrophication potential). Decision makers typical employ dilution ratios (based on simple mass balances for the discharges to a river stretch) to assess expected water quality. Therefore, modelling the quantity of flow in the river is generally more important than modelling the quality. Nonetheless, there is a gradually increasing emphasis on quality modelling, largely as the result of important developments in the UK, Germany, Denmark, and The Netherlands. UK environmental agencies use simple stochastic models (for example, SIMCAT [NRA, 1990]) to summarize the two-week survey data typically collected by the agencies and to help the agencies decide on future restoration activities or permits/consents for dischargers on the catchment scale. Monte Carlo simulation is incorporated in the procedure to compensate for the inherently large uncertainty in the sparse data set. Also, in the UK, the Urban Pollution Management (UPM) procedure (FWR, 1994) has been developed and relies upon a suite of quality models of different levels of complexity, ranging from simple steady-state calculations implemented via a spreadsheet, to fully dynamic water quantity and quality models. The Danish Engineering Union was early to publish a detailed procedure for computation and assessment of water pollution, focusing on intermittent oxygen depletion due to a combined, sewer overflow (Spildevandskomiteen, 1985). In Germany, the ATV is currently developing a comprehensive water quality model (ATV,1996). In a number of countries, there is a similar increasing emphasis on modelling and water quality models are increasingly being used on a case-by-case basis for specific environmental impact assessments or scenario analysis. Computer programs in use include QUAL2E, WASP (Ambrose *et al.*, 1988), Mike-11 (DHI, 1992), Salmon-Q (Wallingford Software, 1994), and DUFLOW (Aalderink, 1995).

We anticipate further progress in the use of models in Europe due to changes in legislation that increasingly emphasize the affordability of treatment and cost-efficient policies. The ongoing trend is to use effluent standards and ambient criteria as in the U.S. that require river basin planning and water quality models to evaluate receiving water quality impacts. Examples include Austria and several CEE countries including Poland, the Czech Republic, Slovakia, and Hungary.

PROBLEMS IN THE CURRENT MODELLING STANDARD

Problems in model application

The limitations of the QUAL2E formulation become apparent when attempting to simulate conditions other than the steady-streamflow, constant-emission conditions for which it is intended. QUAL2E is best suited for point sources of pollutants. For even these problems, however, the model is unsuitable for rivers that experience temporal variation in streamflow or where the major discharges fluctuate significantly over a diurnal or shorter time period. (Other available models, including MIKE11, ATV, and AQUASIM, are able to simulate transient conditions [Rauch *et al.*, submitted]).

More significant are the limitations of the model when examining the contribution of nonpoint sources of pollutants to river water quality degradation. Nonpoint sources have assumed greater relative importance in water quality management as point sources have come under increasingly stringent control. Unfortunately, nonpoint source loads are often driven by rainfall events and thus both the wasteload and streamflow vary significantly over time. Both types of variation may deviate significantly from the assumptions of QUAL2E.

These limitations for point and nonpoint sources compromise the ability to model such problems as rivers regulated by hydropower or other dams that cause significant diurnal fluctuations in streamflow; combined sewer overflows and urban stormwater effects; the effects of diurnal variation in the flow of municipal effluents; and the effects of industrial effluents discharged on a batch basis or with significant variation in flow during different working shifts. For many of these problems, there is currently no readily available, widely accepted water quality model.

The limitations of the model are compounded in many applications by inexperience or insufficient knowledge on the part of the model user. The QUAL2E user's manual (Brown and Barnwell, 1987) is basically a description of the model formulation and input formats for a model user who is implicitly assumed to be experienced and knowledgeable. However, the widespread dissemination and ready availability of QUAL2E encourages use that sometimes falls short of this implicit expectation. In some cases, the model user simply lacks the depth of understanding needed to evaluate the applicability of the model to the problem at hand.

Problems in model formulation

As with all models, QUAL2E incorporates certain simplifying assumptions and approximations. These pose specific limitations for some applications but more generally reduce the robustness of the model representation of basic water quality processes. The problems also impinge on the intended goal of this Task

Group to integrate river water quality models with the more fundamentally based ASM models in order to develop control strategies that integrate river water quality with wastewater treatment. The following lists several problems in the basic representation of water quality processes.

QUAL2E and most river water quality models treat the river as a one-dimensional system. Implicit in this formulation is the assumption that any emissions to the river are instantaneously mixed across the full cross-section of the river. Actual experience is that discharged effluents, particularly if released from a shoreline outfall, may be distinguishable within the river flow for considerable distances downstream and that transverse mixing is often a slow process. Transverse mixing distances are roughly proportional to the square of the width, and become very large in larger rivers. For example, the mixing distance on the Danube River at Budapest is about 200 times the width. In terms of water quality, the result is the prediction of average river concentrations that may be much less than those observed in the field in the core of the effluent plume.

A basic principle of stream water quality models is the conservation of mass. Thus, a very fundamental concern with the existing approach is the fact that using BOD as a state variable intrinsically means that mass balances cannot be closed because BOD is ill defined and does not account for all biodegradable organic matter. Rather than being a unique material, BOD is the result of a bioassay measurement, the yield of which changes with the type of substrate consumed. Hence, the amount of substrate consumed and biomass produced, and the rates of those processes, can vary significantly. Existing models, with a single BOD substance and decay rate, cannot account for these variations. An extreme example occurs with the highly refractory waste generated by paper mills. The BOD of paper-mill wastewater is sufficiently different from municipal wastewater that practitioners such as Whittemore (1983) have experimented with two-stage decay and similar artifices to properly simulate degradation.

Concerns over BOD aside, virtually all models attempt to observe mass-balance principles within the water column, but often fail to close mass balances involving interaction with the sediment. Thus, for example, oxygen-demanding materials that settle to the streambed are lost from the model mass balance, yet their effect continues to be modelled through a sediment oxygen demand (SOD) flux term in the model equations that is unrelated to BOD sedimentation. In QUAL2E, the following constituents are lost from the mass balance upon settling to the bottom: phytoplankton, organic nitrogen, organic phosphorus, and BOD. A more fundamental formulation would consider a complete mass balance and track mass in both the water column and sediment.

A related issue is the treatment of benthic demands (flux terms). Most river water quality models employ user-specified fluxes such as SOD to model the effect of the benthos. However, if the complete mass balance approach were used, benthic fluxes could be determined based on the mass settled to the stream bottom and the population of mediating microbiota. Three mechanisms contribute to oxygen uptake from the sediments:

(i) Sedimenting solids form sludge banks that usually undergo both anaerobic and aerobic decomposition. Aerobic decomposition on the bank surface consumes oxygen from the overlying water column.

(ii) Sessile bacteria degrade organic matter and consume dissolved oxygen from the water.

(iii) Endogenous respiration and lysis lead to a decay of biomass under oxygen consumption.

A modelling approach that represents these basic phenomena could provide a more robust model formulation able to evaluate such changes as the transition from a discharge of untreated wastewater (and creation of a sludge bank) to secondarily treated wastewater (and eventual depletion of benthic sludge). Similar approaches are also possible for simulating the contribution of macrophytes to the stream dissolved oxygen concentration.

Mass balance approaches are also lacking for the pelagic bacteria that mediate biodegradation in the river water. These bacteria are typically not treated as state variables in the model but their effect is encapsulated within a single first-order degradation coefficient. As a result, changes in their population and character are not considered. Sedimentation, growth, and death affect bacterial population and are influenced by changes in the environment and emissions. The resulting dynamic changes in the degradation coefficient cannot be explained by the standard model approach.

QUAL2E and most other existing river water quality models also lack a phenomenological submodel of the sessile microbiota that mediate nitrification and some of the benthic demands discussed above. Biological degradation of organic compounds and biochemical transformations of inorganic compounds in rivers are affected by bacteria or algae attached to substrates at the river bed as well as by those suspended in the water column. Since small rivers have a much larger ratio of wetted surface area to volume of water, the contribution of attached bacteria to the total transformation in small rivers may be particularly significant. If conversion process rates are dominated by the activity of attached bacteria, a river water quality model must be able to describe the population dynamics of these bacteria in order to be able to predict changes in conversion rates that follow from changes in pollution loads. The processes governing such population dynamics are attachment and detachment of bacteria, and substrate limitations in the depth of the developing biofilms or in deeper interstitial zones.

The following example from the river Necker in Switzerland (Uehlinger *et al.*, 1996) illustrates these processes. The Necker has a gravel bed that creates a substrate for sessile algae. By comparing the results of a series of empirical models with measurements of algal surface densities over a measurement period of 1 years, the most important factors influencing the dynamics of algal surface densities in this river were identified. These factors were growth limitation with increasing biomass density, a slow increase in the algal detachment rate with increasing discharge, and nearly complete elimination of the algal population during bed-moving floods. Figure 1 shows a comparison of measured and calculated algal surface densities over the whole measurement period and illustrates that it is feasible to formulate sessile algal growth, limitation, and detachment processes in a river water quality model, although the description is empirical and not necessarily transferable to other rivers.

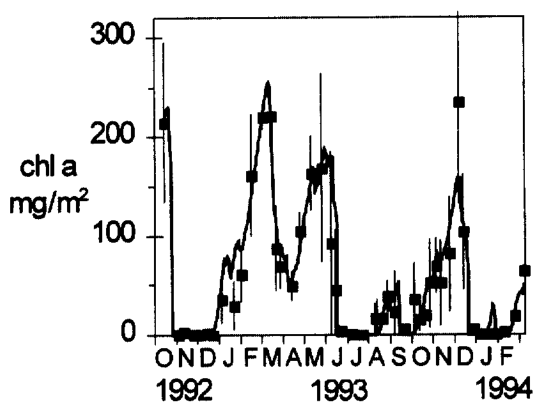

Figure 1. Comparison of measured (dots with error bars) and calculated (solid line) algal biomass densities for the most successful empirical algae model (Uehlinger *et al.*, 1996).

Problems in model calibration

Regardless of the formulation chosen for the river water quality model, calibration of the model to the specific river is a key step in model use. Several aspects of stream water quality may complicate or impede water quality model calibration. Ironically, one is the improvement of stream water quality over the years in many countries. Many rivers now experience such good water quality (at least for conventional water quality parameters) that there is no clear response to pollutant loading (that is, no depletion of dissolved oxygen or 'DO sag'). This leaves no clear 'signal' against which to calibrate the water quality model. These streams may still experience water quality problems on an occasional basis such as extreme low flow or severe rainstorm events. However, the normal absence of a DO sag creates the need to gather data for model calibration during unusual or extreme conditions. Thus, a complete calibration process must include both dynamic loading conditions as well as loads that do not cause major changes in DO or other parameters.

A key parameter in dissolved oxygen models for rivers is the reaeration coefficient, K_2, a parameter to which model predictions are highly sensitive. Typically, K_2 is taken to be a function of temperature and simple hydraulic parameters such as the stream depth and velocity (McCutcheon 1989; Bowie *et al.*, 1985). In typical stream DO model applications, K_2 is specified as a constant determined by calibration to each data set. However, intermittent discharges such as those associated with urban drainage, combined sewer overflows, or rainfall-derived nonpoint sources cause changes in streamflow and thus also in the reaeration coefficient. The implication of this type of variation is that determination of a constant reaeration coefficient by calibration likely results in a value that is not transferable to other conditions. This difficulty is compounded in small rivers, where determination of the reaeration coefficient is generally problematic.

The uniqueness of the model calibration is also an issue given that there are parameters that can counteract such that several sets of parameter values lead to the same modeling results. For example, the BOD decay coefficient, K_1, and the reaeration coefficient, K_2, can be adjusted to compensate for each other such that multiple acceptable calibration combinations typically are possible. Similarly, Li (1962) has shown that a distributed inflow from nonpoint sources may mimic the effect of altered reaeration and degradation rates. His analytical solutions for a uniformly distributed inflow of constant BOD showed this inflow term to be mathematically indistinguishable from changes in the reaeration and BOD decay rates.

Problems in data collection

A basic impediment to successful water quality modelling is the lack of adequate data for model calibration and verification. Thomann (1982) discusses issues of model calibration and verification and stresses the importance of using independent field data sets, preferably reflecting different field conditions, for calibration and verification. The need for independent data places a burden upon the model user to conduct multiple field measurement programs over a variety of streamflow and meteorological conditions. As discussed above, the data sets most useful for calibration and verification may be achievable only during extreme or unusual conditions when there is a clearly measurable pollutant stress exerted on the river.

Field data collection is often limited by such practical considerations as the financial and personnel resources available for data collection. Usually, data collection focuses on an intensive field survey of short duration—typically one, two, or three days. Protocols for surveys intended to support wasteload allocation studies with QUAL2E are given by Mills *et al.* (1986). These established procedures need to be modified for studies directed toward nonpoint sources or rainfall-driven events. Timing data collection to occur during such special events (either high flow or low flow) is difficult unless a dedicated field crew is available on a stand-by basis for the desired event to occur.

Despite attempts to create protocols for the design of data collection campaigns for model calibration and testing, these procedures are hardly ever followed. Rather, *ad hoc* designs are made for a particular study. The experimental designs are typically characterised by a too low measuring frequency, both in time and in space, to accommodate calibration of complex dynamic conversion models. Usually only daily grab samples are taken at different locations along the river. In other approaches a plug of liquid is followed (by labeling it with some inert dye) and samples are taken at regular times. Rarely, dispersion effects are determined by measuring the behaviour of the tracer. Increasingly, river quality modellers are aware of the lack of data and propose procedures such as (i) model-based design of the experimental set-up, (ii) high-frequency sampling at sufficient locations including the assessment of mixing and dispersion effects, and (iii) microcosm studies that follow the conversions taking place in a representative sample of river water.

A different problem is raised by the aims of this Task Group, namely to develop models based upon state variables similar to those used in the ASM models. The change to state variables such as bacterial biomass implies that model state variables may not be measurable in the field. However, this problem also arises with ASM as well as models in other disciplines. The solution has been to focus in calibration and verification on those variables that can be measured and, when feasible, one should use surrogate measurements for variables that are otherwise not directly measurable. Moreover, the inclusion of a closed mass balance provides an additional data constraint that can compensate when certain state-variable fractions cannot be measured directly (although the presence of large counteracting fluxes will diminish the accuracy with which smaller fractions can be discriminated).

Problems in predictive capability

The problems identified in the foregoing sections diminish the capability of water quality models to be truly predictive, particularly when significant changes alter the river's pollutant load, streamflow, morphometry, or other basic characteristics. These problems arise when the changes to the river affect model parameters that are fixed based on an observed river condition that no longer controls the parameter. If, like most models at present, the model lacks the phenomenological structure to change model parameters to reflect changes in the river, then there is no predictive ability for at least those particular kinds of changes.

A classic example of this situation is when a large-volume discharge that was untreated begins to receive secondary treatment. Standard water quality models cannot predict the resulting changes in light penetration due to a clearer effluent or sediment oxygen demand due to the depletion of sludge banks, nor can they predict the transition of the river from anaerobic to aerobic conditions or the accompanying cessation of denitrification. Denitrification occurs primarily in anoxic water zones and sediments and thus denitrification rates are higher in highly polluted rivers with major mud deposits (Billen *et al.*, 1985; Chesterikoff *et al.*, 1992). For this reason, it has been argued that a reduction in the organic load from sewage treatment plants without an accompanying increase in plant denitrification capacity may actually increase the nitrogen load passed downstream in the river. This happens because the in-river denitrification rate is reduced after restoration (Billen *et al.*, 1985, 1986; Chesterikoff *et al.*, 1992). It is impossible to quantify these processes without a model for the river sediment. Similar difficulties face those trying to predict the effects of physical stream changes such as adding or removing a dam or the restoration of natural stream conditions as advocated in recent U.S. initiatives (U.S. EPA, 1995).

CONCLUSION

The current standard for river water quality modelling is the QUAL2E model developed by the U.S. EPA. QUAL2E was specifically designed to conduct wasteload allocations—the determination of allowable maximum effluent loads under steady low streamflow. While QUAL2E and similar models are adequate for the specific regulatory situations for which they were developed, there is a need for a more comprehensive modelling framework for non-regulatory problems (e.g., research and teaching) and for those water quality management problems not addressed by QUAL2E (e.g., stormwater flow events, nonpoint sources, and transient streamflow).

Problems with current modelling practice include those of model application, model formulation, model calibration, data collection, and predictive ability. Problems in model application include the aforementioned management problems not addressed by QUAL2E as well as potential misuse by inexperienced users. Limitations in model formulation are continued reliance on BOD as the primary state variable, despite the fact that BOD does not include all biodegradable matter, and poor representation of benthic flux terms. As a result of these limitations, it is impossible to close mass balances completely in most existing models. Model calibration is hampered by the need for river characterization under unusual or infrequent conditions, a problem that is compounded by the general inadequacy of field data collection frequency in time. These various limitations in current river water quality models impair their predictive ability in situations of marked changes in the river's pollutant load, streamflow, morphometry, or other basic characteristics.

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