A Tool for Evaluating Risk to Surface Water Quality Status

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Abstract: Water quality Risk Analysis Tool (WaterRAT) is recently developed software for supporting surface water quality management. The software contains a library of river and lake quality models, aiming to give flexibility over specification of model scope, complexity and scale. Various sources of uncertainty can be included in the analysis, including uncertainty in boundary conditions, initial conditions, parameters, model structure and management objectives. Water quality can then be modelled allowing for these sources of uncertainty. Important data uncertainties can be indicated, and so data collection programmes can be suitably refined. In this paper, the motivation for the WaterRAT tool and the methods it employs are presented, its features are described, and its utility for uncertainty evaluation and sensitivity analysis is demonstrated using a river water quality management problem. Emerging challenges for modellers, which cannot yet be addressed using WaterRAT, are discussed.

***Keywords**:* Water quality; simulation; uncertainty; Monte Carlo

1. INTRODUCTION

There is increasing motivation and opportunity to use simulation model predictions as a basis for managing water resources, including the protection of surface water quality. The motivation comes from the generally high priority given to protecting the aquatic environment. In particular, new directives governing water quality specify that river basins should be viewed as integrated units, potentially requiring consideration of large numbers of factors with complex, interacting effects on water quality. The opportunity for using simulation models is coming from at least three directions: reducing constraints on computer power and therefore model size and complexity; new attempts to observe and understand processes affecting water quality management; and the increasing number of qualified modellers.

Arguably, a fourth reason to be optimistic about a more useful role for simulation modelling in the future is the increasing attention that is now being given towards resolving, or at least assessing, model uncertainty. The fundamental reason for uncertainty is our inability to observe and understand the controlling processes and represent them numerically at the relevant scales. Implicit to that are a number of modelling issues that are well-discussed elsewhere (see Beck 1987, McIntyre et al. 2003a) but might be summarised as: the need to simplify the real environment into a conceptual model; equally plausible alternative simplifications lead to different predictions; the need to calibrate model parameters leading to biases and equifinality; limitations in our measurement techniques leading to errors in point estimates of data; errors in integrating or interpolating data to the relevant modelling scale; and numerical errors in solutions to differential equations. While there is no clear consensus about how these issues should be addressed, it is generally agreed that the consequent model uncertainty is high, and that water quality modellers need to give more attention to estimating and reporting this uncertainty.

This paper introduces the Water quality Risk Analysis Tool (WaterRAT), a tool for exploring uncertainty in forecasts of river and lake quality. This software was developed as part of a European Commission project, Total Pollution Load Estimation and Management (TOPLEM), which aimed to produce a software system for managing water pollution in a Chinese catchment where supporting data are sparse. This paper will briefly describe WaterRAT, summarise a case study, and discuss the limitations of this and other software in the context of future modelling needs.

2. DESCRIPTION OF WATERRAT

2.1 Summary

WaterRAT (McIntyre and Zeng 2002) is a spreadsheet-based modelling tool that includes a library of surface water quality models, presently including a choice of one-dimensional river models and two-dimensional lake models. WaterRAT is built within Microsoft Excel, so that WaterRAT's own data processing modules can be supplemented by those of Excel. The input and output is via a series of spreadsheets and model specifications are made via Visual Basic menus and dialogue boxes. The library of simulation models comprises a series of Dynamic Link Libraries.

The model library includes alternatives for modelling pollution transport, water temperature and water quality, and also offers a choice of modelled determinands. These include total organic carbon, biochemical oxygen demand, phytoplankton, dissolved oxygen, nitrogen and phosphorus, a toxic substance, floating and suspended oil, and total suspended solids. This is supported by sediment models which include biochemically and physically-driven sediment-water interactions. A thermodynamic model simulates water temperature and ice cover.

2.2 Spatial and temporal resolution

For river modelling, the river is represented as a series of well-mixed control volumes between which pollution transport processes are simulated using the advection-dispersion equation supported by two alternative hydraulic models (a quasi-steady friction formula and a non-linear store). Each control volumes must be prescribed certain spatially-varying parameters which depend on the transport model selected. The lake models work on the same control-volume principle, except that they are able to represent the vertical variation in water quality due to effects of thermal stratification as well as length-wise variations.

The output time-step is defined by the user, and may be anything greater than one minute. The available input time-series data will be automatically interpolated to this time-scale, using either linear interpolation, a cubic spline or a step function, as chosen by the user. The numerical integration in the time domain uses a Fehlberg adaptive time-step scheme. This is an important feature for Monte Carlo simulation, where randomly sampled inputs lead to numerical stability and accuracy criteria which can vary widely, both over the time-domain and from one model realisation to the next (McIntyre et al., 2004). The spatial grid is prespecified, making the user responsible for reconciling the spatial resolution with the temporal tolerance, so that numerical dispersion and spatial averaging errors are not excessive.

2.3 Boundary conditions, initial conditions and model parameters

Dynamic boundary conditions include the meteorological, pollution and flow source and abstraction data. All meteorological time-series (rainfall, evaporation, dew-point, air temperature, wind speed, and surface light intensity are needed as inputs to various alternative models) are assumed to be uniform over the river or lake. Any number of sources of flow and/or pollution can be input, subject to computer memory. A negative flow is interpreted as a loss, and any associated pollution loads are neglected.

Static boundary conditions are specified for each control volume. For the river models examples of these are: channel cross-section shape; a leakage rate; sediment oxygen demand; active sediment area; and hydraulic or routing parameters. For the lake models, the bathymetry is defined by a volume-level relationship for the lake. Initial conditions can be either entered via a spreadsheet as a model input, or they can be estimated using a specified ‘warm-up’ period. During this period the dynamic boundary conditions are assumed steady-state at those of the specified start time of the simulation.

With the exception of meteorology, all model parameters, initial conditions, boundary conditions (including sources of flow and pollution) can be considered as uncertain inputs. Prior to running the model, the user signifies that an input is uncertain by specifying a distribution instead of an assumed value. Each distribution may be propagated to prediction uncertainty, or included in the calibration or sensitivity analysis. This means that the model calibration and predictions need not be conditional on the precision and reliability of input data, and that the relative significance of input uncertainties can be revealed through sensitivity analysis.

2.4 Model conditioning, sensitivity and uncertainty analysis

Uncertainty in inputs may be specified as independent uniform distributions using a maximum and minimum bound, or as any joint distribution using a series of discrete samples. In the latter case, each sample is weighted with a relative probability.

Random sampling from these distributions (i.e. Monte Carlo simulation) can be used as a basis for model conditioning and sensitivity analysis. For example, the unconditioned distribution can be updated by multiplying the prior probability of each sample by a posterior probability. The posterior probability associated with a sampled set of inputs may be defined as their perceived likelihood based on how well they simulate the observed data. This is the same as Generalised Likelihood Uncertainty Estimation (GLUE; Beven and Binley 1992). However, WaterRAT's facilities encourage integration of boundary and initial condition uncertainty, which is not normally done within the GLUE framework. Alternatively, the posterior may be defined by the probability that the sampled set of inputs will lead to a successful outcome in terms of meeting a water quality target. Thereby, the probability of achieving or failing a water quality objective due to combinations of uncertain inputs may be quantified.

Any posterior likelihood may be plotted against each individual uncertain input as a marginal distribution. This is a well-established technique for assessing regional sensitivity of calibration objective functions to parameter uncertainty. However, previous applications generally assume inputs other than parameters to be known with certainty, and all results are conditional on this assumption. Also, it seems that the same method has not previously been applied to assess how the probability of failing management objectives is sensitive to uncertain inputs. Such inputs may be manageable in practice (e.g. point sources of pollution), or less manageable (e.g. initial sediment quality), or may be essentially unmanageable (e.g. parameters representing the physical properties of the environment).

Whereas sensitivity analysis can highlight which uncertain inputs are most likely to influence the model results, prediction of space and time-series is needed to show where and when this influence is significant. Using Monte Carlo sampling, a specified number of samples are taken either from the prior uniform distributions of inputs, or from the sets sampled during prior conditioning. In this latter case the likelihood of the model result obtained from each sample is weighted by the likelihood of that sample (as calculated during conditioning), following the GLUE methodology. A distribution of model output can then be derived.

WaterRAT also offers first order methods of sensitivity analysis and uncertainty propagation.

3. CASE STUDY

3.1 Background, model and data

The case study presented here is of the Charles River in Massachusetts. This study represents the data availability that might be expected in the USA and Europe (rather than the original WaterRAT application in China where data was especially limited). The Charles River in the 1990s suffered from undesirable concentrations of phytoplankton, largely due to pollution with nutrients. The principal management option was investment in phosphorus removal at a number of wastewater treatment works (WWTWs) along the river. This modelling study revisits that situation, to identify the key uncertainties affecting the reliability of the phosphorus removal option, and to quantify the probability of failure due to the effect of data and model uncertainties.

The model is of flow, water depth and temperature, and nine water quality determinands:

- Phytoplankton, measured as chlorophyll-a
- Slow-reacting organic carbon
- Fast-reacting organic carbon
- Organic nitrogen
- Ammonium
- Nitrate plus nitrite
- Organic phosphorus
- Inorganic phosphorus
- Dissolved oxygen

A system of partial differential equations represents the interactions between these 12 variables, including 24 uncertain parameters to be conditioned. A full description of the model is not important for the objectives of this paper, but is available in McIntyre et al. [2003b].

The conditioning and model assessment were based on data from the 20th August 1996 and the 10th October, 1996. On both dates the water quality was assumed to be at steady-state. Measurements of the water quality variables were available from nine sections along the river, and daily pollution loads from the headwater and eight sources (sewers and tributaries). Error bounds in all these data were estimated; this estimate was largely subjective due to the limited number of measurements.

3.2 Model conditioning

Model conditioning was performed by random sampling from the joint prior distribution of uncertain inputs, and assigning a posterior probability to each sample based on its performance in meeting the objective. This was done in two stages – conditioning upon chl-a data (measured on the 20th August) to reduce uncertainty in parameters, and then further conditioning to the constraint chlorophyll-a < 10mgm^{-3}, to identify the probability of achieving this objective across a range of phosphorus (P) load reduction scenarios.

The first stage of conditioning is essentially the GLUE method, using the objective function (OF_1) given in (1). Using (2), OF_1 is multiplied by the prior probability Lp and rescaled to give a relative measure of likelihood L of the sampled input set

(α). This is based on the simple, subjectively-founded premise that the better the model fits reality, the more reliable it will be for predictions.

$$OF_1(\alpha) = \sum_j \left(A_j(\alpha) - \overline{A}_j(\alpha)\right)^{-2} \quad (1)$$

$$L(\alpha) = \left[\sum_N Lp \cdot OF_1\right]^{-1} Lp(\alpha) OF_1(\alpha) \quad (2)$$

where subscript j indicates the j^{th} monitored section on the river, A is the model output of chl-a, $\overline{A}$ is the measured chlorophyll-a, and N is the number of samples (7000 in this case). Importantly, α is a sampled set of inputs to the objective function calculation, which includes a sampled set of model parameters, a sampled realisation of pollution loads and a sampled realisation of $\overline{A}$, all from within their a priori perceived bounds of error. The joint posterior distribution of the model parameters may be obtained by integrating over the other inputs - an improvement upon the normal practice of fixing the other inputs during conditioning.

The posteriors (L) from (2) become the new priors (Lp) for the second stage of conditioning. The 7000 sampled parameter sets, each with an associated Lp, are recalled and the model is run using each. Other model inputs are randomly sampled from within new ranges that are relevant to the forecasting problem. In this case, these ranges are of a feasible P load reduction (W) at a selected site, together with the estimated uncertainty in the other inputs. The relevant objective function is the intended constraint on chlorophyll-a in August, defined in (3).

$$\begin{aligned} OF_2(\alpha) &= 1 \quad \text{for chl-a} < 10\text{mgm}^{-3} \\ OF_2(\alpha) &= 0 \quad \text{otherwise} \end{aligned} \quad (3)$$

Following calculation of OF_2 for the 7000 model runs, (2) is applied again (but with OF_2 instead of OF_1). Subsequently, each value of L is the combined probability of a set of inputs and the objective being achieved (given, of course, the various modelling assumptions that have been involved to this point). WaterRAT outputs all the values of L, Lp, corresponding input samples and summary statistics of the conditioned distribution.

Integration over all other uncertain inputs allows the marginal distribution of each input to be presented. For example, for our investigated point source reduction W, $P(W|A<10)$ can be calculated across the range of W. Baye's theorem allows the modelled probability of achieving the objective to be calculated across W:

$$P(A<10|W) = \frac{P(A<10).P(W|A<10)}{Lp(W)} \quad (4)$$

where,

$$P(A<10) = \sum_N Lp \cdot OF_2 \quad (5)$$

and

$$Lp(W) = 1/N \quad (6)$$

For the Charles River study, Equations 3-6 were applied to the constraint A < 10mgm^{-3} independently at each of nine strategic locations (A-I) along the river. Various sites for P load reductions were analysed. For example, Figure 1 shows the probability of achieving the target as a function of the percentage P load reduction at the headwater.

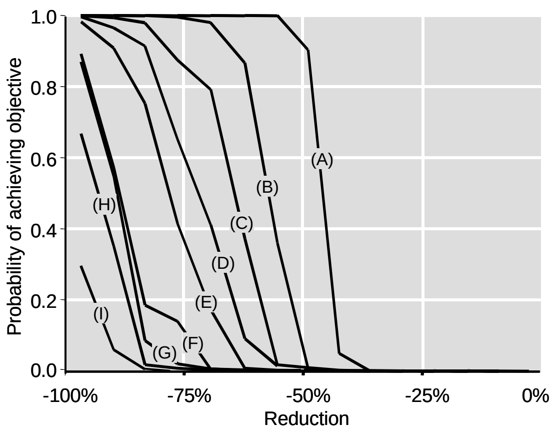

Figure 1. Modelled probability of A < 10mgm^{-3} at nine sections (A-I) on the Charles River as a function of percentage reduction in *P* load from the headwater.

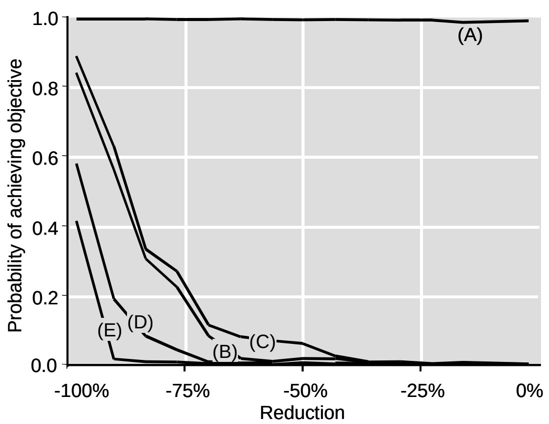

Figure 2. Modelled probability of A < 10mgm^{-3} at nine sections (A-E) on the Charles River as a function of percentage reduction in *P* load from the CRPCD wastewater treatment works.

Figure 2 shows the same for *P* load reduction at the large CRPCD treatment works on the upper Charles River, given a 50% reduction at the headwater (F-I are consistently zero in this case and so are not shown). Even substantial reductions at either location would be a high-risk option for controlling chlorophyll-a especially at the further downstream sections, given the uncertainties about how the system will respond.

3.3 Sensitivity analysis

One method of sensitivity analysis is the well-established method of regional sensitivity analysis first applied to water quality models by Spear and Hornberger [1980]. This summarises the difference between the prior and posterior marginals using the univariate Kolmogorov-Smirnov (KS) statistic.

An example output is given in Figure 3, the KS statistic comparing the distributions prior to and after conditioning to the A < $10 mgm^{-3}$ constraint. In Figure 3, the x-axis contains all the uncertain inputs, divided into model parameters and P loading rates, and the y-axis is the value of the KS statistic. There are nine trajectories – one for each of the nine sections (A-I) on the river. For the purpose of this discussion only the evidently most important inputs are labeled. It is clear that the uncertainty in the load of *P* from the headwater, and that in the model parameters (representing the biochemistry) dominate the uncertainty in the outcome. The regional influence of variations in *P* loadings from wastewater treatment works is small in comparison.

4. DISCUSSION

4.1 Review of WaterRAT

The aim of WaterRAT is to allow integration and exploration of many sources of uncertainty. For example, the case study included sampling realisations of input and output data from within perceived error bounds, so that the parameter conditioning and subsequent analysis were not conditional on the accuracy of any measured data. The sensitivity analysis indicated that the reliability of management decisions is controlled by parameter uncertainty, and uncertainty about the contribution of the headwater (i.e. distributed sources from the upper catchment). Judicious planning might therefore in this case involve further data collection and modelling, prior to engineering interventions.

The obvious scientific weakness of the case study is the assumption that the model structure is correct. A nominal remedy would be to repeat the analysis with a more complex model from the WaterRAT library (e.g. including sediment-water interactions) and compare the outcomes. However, it is speculated that this would lead to the same overall conclusion, considering the limitations of the data. Although discrete trials of alternative model structures is unlikely to resolve the issue of model structure error, it indicates their potential significance. Should the data allow, more rigorous analysis methods of evaluating structural error are available, outwith WaterRAT (e.g. Wagener et al. 2002).

In WaterRAT, the procedure used for sampling from uniform priors is Latin hyper-cube sampling. Initial versions of WaterRAT also included Monte Carlo Markov Chain sampling methods, which might be expected to be better for Bayesian model analysis (Vrugt et al. 2003). However, the advantage was not evident when using typically sparse data such as those from the Charles River.

WaterRAT also includes a genetic algorithm for deterministic optimistation, and first order methods as an alternative to Monte Carlo analysis.

4.2 Current challenges

Amongst others, a primary challenge facing surface water quality modellers is how to obtain useful estimates of uncertainty in much larger models than those in WaterRAT. Spatially distributed catchment models may include hundreds or thousands of uncertain model inputs and outputs. Current methods of uncertainty analysis for complex environmental models are centered around Monte Carlo simulation, due to the ease of application to complex non-linear simulation models. While new computing power is allowing models to expand in size, it is far from allowing comprehensive Monte Carlo sampling of all possible models and model input scenarios. This is despite new algorithms based on Markov Chains aimed at giving a more efficient exploration of the uncertainties (e.g. Vrugt et al. 2003). Furthermore, the importance of extreme values has been largely overlooked in design of algorithms, which tend to focus resources on the modes of the posteriors.

Research at Imperial is currently investigating pathways to resolving these challenges.

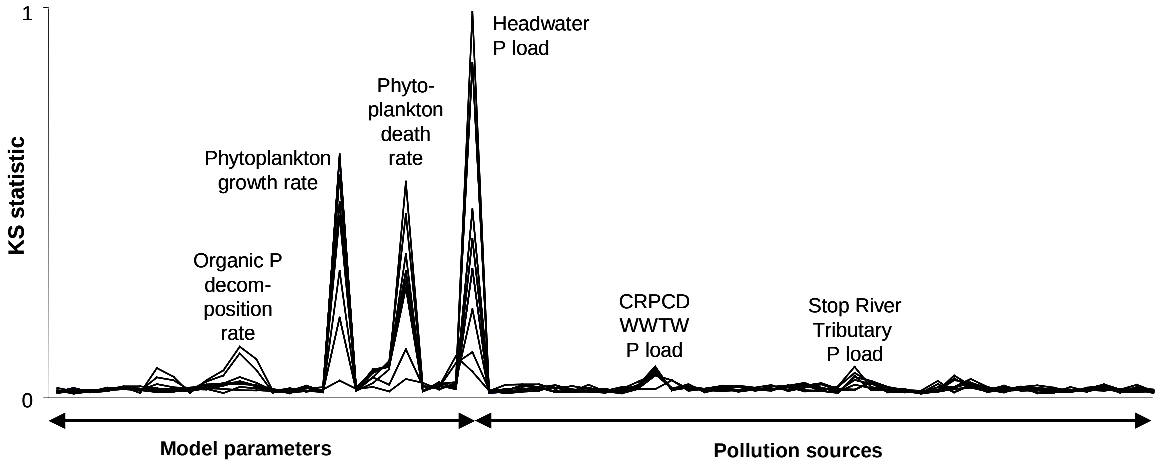

Figure 3. Sensitivity of the probability of achieving target water quality to the various model inputs, measured by the Kolmogorov-Smirnov (KS) statistic.

5. CONCLUSIONS

The WaterRAT software, developed at Imperial College has been introduced. A case study (the Charles River, Massachusetts) has been used to highlight some capabilities and limitations of the software. The significance of many different sources of uncertainty can be included in Bayesian analysis and regional sensitivity analysis. The analyses can be used to indicate priorities for protecting water quality via further modelling, data collection and engineering interventions. The main limitation to the WaterRAT software is that it provides no tools to assess model structure error, apart from discrete comparisons of alternative model structures. Also, at present it only includes models of rivers and lakes rather than of the wider catchment. Finally, the paper briefly discussed research priorities for water quality modelling, arguing that new methods of analysis will be needed to face the challenges of distributed modelling and extreme value analysis.

6. ACKNOWLEDGEMENTS

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7. REFERENCES

Beck, M.B., Uncertainty in water quality models, *Water Resources Research*, 23(8), 1393-1441, 1987.

Beven, K.J. and Binley, A.M., The future of distributed models; model calibration and predictive uncertainty, *Hydrological Processes*, 6, 279-298, 1992.

McIntyre, N. and Zeng, S., TOPLEM River and lake water quality models. Report. PL972722 D4.3(10), Imperial College London, 2002.

McIntyre, N., Wagener, T., Wheater, H.S. and Zeng, S., Uncertainty and risk in water quality modelling and management, *Journal of Hydroinformatics*, 5, 259-274, 2003a

McIntyre, N., Wagener, T., Wheater, H.S., Chapra, S., Risk-based modelling of surface water quality- A case study of the Charles River, Massachusetts, *Journal of Hydrology.*, 274, 225-247, 2003b.

McIntyre, N., Jackson, B., Wheater, H.S., Chapra, S. Numerical efficiency in Monte Carlo simulations - a case study of a river thermodynamic model, *ASCE Journal of Environmental Engineering*, 130, 4, 456-464, 2004.

Spear, R. C. and Hornberger, G. M., Eutrophication in peel inlet - 2. Identification of critical uncertainties via generalized sensitivity analysis, *Water Research* 14(1), 43-49, 1980.

Vrugt, J., Gupta, H., Bouten, W. and Sorooshian, S., A shuffled complex evolution Metropolis algorithm for optimization and uncertainty assessment of hydrologic model parameters, *Water Resources Research*, 39(8), SWC1:1-1:16, 2003.

Wagener, T., McIntyre, N., Lees, M.J., Wheater, H.S. and Gupta, H.V., Towards reduced uncertainty in conceptual rainfall-runoff modeling: dynamic identifiability analysis, *Hydrological Processes*, 17(2), 455-476, 2002.