Risk-based modelling of surface water quality: a case study
of the Charles River, Massachusetts

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Abstract

A model of phytoplankton, dissolved oxygen and nutrients is presented and applied to the Charles River, Massachusetts within a framework of Monte Carlo simulation. The model parameters are conditioned using data from eight sampling stations along a 40 km stretch of the Charles River, during a (supposed) steady-state period in the summer of 1996, and the conditioned model is evaluated using data from later in the same year. Regional multi-objective sensitivity analysis is used to identify the parameters and pollution sources most affecting the various model outputs under the conditions observed during that summer. The effects of Monte Carlo sampling error are included in this analysis, and the observations which have least contributed to model conditioning are indicated. It is shown that the sensitivity analysis can be used to speculate about the factors responsible for undesirable levels of eutrophication, and to speculate about the risk of failure of nutrient reduction interventions at a number of strategic control sections. The analysis indicates that phosphorus stripping at the CRPCD wastewater treatment plant on the Charles River would be a high-risk intervention, especially for controlling eutrophication at the control sections further downstream. However, as the risk reflects the perceived scope for model error, it can only be recommended that more resources are invested in data collection and model evaluation. Furthermore, as the risk is based solely on water quality criteria, rather than broader environmental and economic objectives, the results need to be supported by detailed and extensive knowledge of the Charles River problem.

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1. Introduction

1.1. Motivation

The reasons for and significance of uncertainty in predictions of water quality are widely recognised and documented elsewhere (Whitehead and Young, 1979; Hornberger and Spear, 1980; Beck, 1987; Reckhow, 1994; Reichart and Omlin, 1996;
Van Straten, 1998; McIntyre et al., 2002a). The inevitability of significant uncertainty, and the need to account for it in water quality management, has been recognised in the development of some decision-support tools, for example, QUAL2E-UNCAS (Brown and Barnwell, 1987), DESERT (Ivanov et al., 1996) and SIMCAT (UK Environment Agency, 2001). An alternative modelling philosophy is to aim to reduce uncertainty to an insignificant level through refinement of scale and process representation (Young et al., 1996; Beck, 1999). While so refined models have proven valuable in a number of applications (see the review of Ambrose et al. (1996)), there are four reasons why this modelling philosophy seems to be of restricted value in practice. (1) Field data are not usually adequate to identify the boundary conditions and parameter values of such models (Beck, 1997). (2) In any case, more data do not necessarily lead to better models or system understanding (Chatfield, 1995; Beck, 1999). (3) Human resource constraints often preclude intricate, data-intensive, modelling exercises (Reckhow, 1994). (4) Results of complex models are more easily misinterpreted, while not necessarily being any more reliable (Gardner et al., 1980; Van der Perk, 1997). Therefore, there remains a need to promote uncertainty estimation, and to continue to develop models and analytical tools which permit such analysis, and which reflect the resource constraints of users.

The modelling tool used in the current investigation is the Water quality Risk Analysis Tool (WaterRAT) developed by McIntyre and Zeng (2002). This software was designed to encourage exploration of the uncertainties arising from all sources of prediction error—field data, model formulations, model parameters, boundary and initial conditions, model scale and numerical approximations (see McIntyre et al. (2002a,b)). Furthermore, it allows the effects of these uncertainties to be evaluated in terms of risk of failing water quality targets, and provides a suite of models of varying complexity to suit the modelling task and resource constraints. This paper will review the utility of tools such as WaterRAT for water quality management, using the Charles River, Massachusetts as a case study.

1.2. Scope and objectives

The case study is approached in a way which addresses the difficulty of applying a water quality model to decision support on the basis of limited supporting data and modelling resources. This is done in the context of five tasks which are set for the study.

1. To condition the model using the water quality data observed at various control sections of the Charles River on the 20th August 1996.
2. To evaluate the conditioned model with respect to its success in representing the water quality observed on the 8th October 1996.
3. To identify the principal factors affecting water quality on the 20th August 1996.
4. To support the appraisal of options for reducing eutrophication in the Charles River, specifically limiting chlorophyll-α to less than 10 mg m⁻³ at a number of control sections. Proposed water quality interventions will be evaluated on the basis of associated risk of failure to achieve the specified target.
5. To identify ways to reduce the element of risk which stems from model prediction uncertainty.

Arguably, confronting these tasks rigorously would require careful consideration of different modelling tools, and selection of one or more approaches. Furthermore, a critical review of data reliability including evaluation of sources of sampling and measurement errors would normally be recommended, followed by iterative model structure adjustments and parameter calibrations. However, within the scope of this paper, none of these practices are adopted. Instead, this investigation starts from the premise that modelling resources are limited so that only one model structure can be used, and that the readily available data (see Section 2.2) must be interpreted without researching quality control issues. Additionally, the view is taken that the in-river data are too sparse to be usefully analysed using traditional maximum likelihood techniques (McIntyre et al., 2002a). Instead, this investigation is founded on the methodologies of regional sensitivity analysis (RSA; Hornberger and Spear, 1980) and generalised likelihood uncertainty evaluation (GLUE; Beven and Binley, 1992), whereby qualitatively derived
constraints are used to supplement the information in the sparse data set. RSA has previously been applied to a dynamic river eutrophication model by Whitehead and Hornberger (1984). In adopting these approaches, we set out to address the question “If human resources and observed data are limited, as they typically are, what degree of support can be given to strategic management of water quality?”

The study does not take account of a large number of factors presently affecting policies for management of the Charles River, nor of many observations outwith the 1996 study. The study is primarily a demonstration of methods, and all results should be seen in this context.

1.3. The case study

The headwater of the Charles River is located in the hills of eastern Massachusetts in the USA. The river flows approximately 130 km through the state, through numerous towns and over a succession of dams, before discharging into Boston harbour. Water quality problems associated with the Charles River in previous decades were industrial pollution and combined sewer overflows, which led, among other unwelcome effects, to nutrient enrichment and eutrophication. Storm-water interceptions and other interventions in the 1990s have greatly improved the overall ecology and amenity value of the river, although they have failed to control eutrophication satisfactorily. Further measures are currently being implemented by installing phosphorus-stripping facilities at a number of wastewater treatment plants (CRWA, 2000). However, such control of point sources will not necessarily solve the problem, as phosphorus from non-point sources may enter the river directly or via tributaries. Furthermore, the phytoplankton may be resilient to low phosphorus concentrations. There is therefore a need for decision-support tools which can estimate the residual eutrophication given various options for point and non-point interventions.

This study looks at the 40 km length of the Upper Charles River, between the Populatic Pond in Medway County and the Cochrane Dam in Dover County, on two days in the summer and autumn of 1996 (the 20th August and the 8th October), when data were collected at nine sections along the river (CDM, 1997), shown in Fig. 1. The determinants measured include,

- phytoplankton (Ag),
- dissolved oxygen (Ox),
- 5-day biochemical oxygen demand (Cf),
- organic phosphorus (Ps) and orthophosphates (Po),
- organic nitrogen (Ns), nitrates (Ni) and ammonium (Na).
- flow (Q), water depth (H) and water temperature (T).

These measurements were made three times on each day to estimate a daily mean and an expected diurnal range. In addition, the major point sources to the river (two wastewater discharges and seven tributaries) were monitored, and daily pollution and hydraulic loads were estimated. An additional pollution and hydraulic load was assumed to be evenly distributed along the studied length of river, based on measurements at a number of minor inlets to the river. Both the 20th of August and the 8th of October were chosen from periods when the river was considered to be near steady-state, and a steady-state assumption is maintained in this exercise.

2. Model structure and methods

2.1. Specification of the model structure

We begin with the premise that a model structure which is adequate for the tasks, can be adopted, and all the uncertainty in the model structure can be represented by parameter uncertainty. While not analytically ideal, this premise is consistent with the constraints of time and resources which are normal in practice, and the adequacy of the model structure will be reviewed and discussed as part of the model evaluation. The philosophy of parsimonious modelling has been rejected, as an important task is to explore the risk stemming from model components which are not identifiable during conditioning, but are relevant to future scenarios. Importantly, it should be noted that the selected structure, summarised later, is not intended to represent our full prior knowledge of phytoplankton dynamics and nutrient
cycling, but is a simplification based on our prior experience of what the principal components of the system are likely to be. Notwithstanding the simplifications, the model is of a similar complexity to the commonly used QUAL2E model (Brown and Barnwell, 1987).

The selected model structure includes all the monitored determinants previously listed. The in-river nutrient and oxygen cycling processes are represented by the set of differential equations presented later, and the interactions of the water quality determinants are summarised in Fig. 2. The descriptions below are purposefully brief—a more in-depth description and discussion of the formulations are given in McIntyre and Zeng (2002) and Chapra (1997). All notation is listed at the end of this paper.

2.1.1. Phytoplankton

\[
\frac{dA_g}{dt} = k_{ga} A_g - k_{da} A_g + \Phi(A_g) + \Delta(A_g)
\]

where \( t \) is time (in units of days); \( A_g \) is phytoplankton concentration measured as Chlorophyll-\( a \) (gm\(^{-3}\)); \( \Delta(A_g) \) represents the advective and dispersive transport of phytoplankton to and from adjacent control volumes of water; \( \Phi(A_g) \) represents the external load of phytoplankton; \( k_{ga} \) (day\(^{-1}\)) is the net photosynthesis rate of phytoplankton (includes effect of phytoplankton respiration); and \( k_{da} \) (day\(^{-1}\)) is the death rate of phytoplankton. \( k_{ga} \) is a function of water temperature \( T \) (\( ^{\circ} \)C), light availability \( I_s \) (J m\(^{-2}\) day\(^{-1}\)), nutrient availability and the maximum net photosynthesis rate at \( T = 20 \) \( ^{\circ} \)C, \( k_{ga20} \); \( k_{da} \) is a function of water temperature, and the maximum death rate at \( T = 20 \) \( ^{\circ} \)C, \( k_{da20} \); \( k_{ga} \) and \( k_{da} \) are defined by the minimum of nitrogen and phosphorus limitation, and the Arrhenius formula of temperature effect (see Chapra (1997, p. 40, 607, 610)). The Arrhenius coefficient \( \theta \), which defines the relationship between reaction rates and temperature (Chapra, 1997, p. 40), is assumed to have a common value over all the model components for this study.

Fig. 1. Charles River model boundaries, point sources and monitoring locations.
2.1.2. Dissolved oxygen

Dissolved oxygen \( Ox \) (gm\(^{-3}\)) is gained or lost through exchange with the atmosphere which occurs in direct proportion to the oxygen deficit \((Ox_\ell - Ox)\) at a rate \( k_{oa} \) (m day\(^{-1}\)), where \( Ox_\ell \) is the dissolved oxygen concentration in equilibrium with the atmosphere calculated as a function of water temperature (Chapra, 1997, p. 362). \( Ox \) is gained due to the process of photosynthesis, at a rate of one unit of \( Ox \) to \( r_{oa} \) units of chlorophyll-\( \alpha \) produced. In addition, \( Ox \) is lost due to bacterial respiration at a rate \( k_{oc} \) (day\(^{-1}\)) and is lost because of nitrification at the rate of nitrification \( k_{on} \) multiplied by the oxygen demand of a unit mass of ammonium nitrogen \( r_{on} \). Finally, dissolved oxygen is lost due to sediment oxygen demand (SOD) (gm\(^{-2}\) day\(^{-1}\)) which is a spatially varying model parameter;

\[
\frac{dOx}{dt} = \frac{k_{oa}}{H} (Ox_\ell - Ox) + r_{oa}k_{oc}Ag - k_{oc}Cf
- k_{on}r_{on}Na - \frac{SOD}{H} + \phi(Ox) + \Delta(Ox)
\]  

The aeration rate \( k_{oa} \) (gm\(^{-2}\) day\(^{-1}\)) is calculated through relationships with water velocity, depth and temperature (see Chapra (1997, p. 377)), and the effect of a weir or sluice on the aeration rate is modelled using an additional empirical relationship (see Chapra (1997, p. 380)). Error in these aeration formulae is allowed by assuming that any deviation from the relationship increases linearly with \( k_{oa} \) at a rate given by parameter \( k_{er} \).

2.1.3. Non-living organic carbon

Non-living organic carbon (i.e. excluding that in phytoplankton) is modelled using two conceptual fractions, all modelled in units of equivalent oxygen demand. The first is 5-day biochemical oxygen demand \( Cf \) representing the fast decaying dissolved organic carbon, and the second is \( Cs \) representing the slow-decaying particulate detritus, which slowly hydrolyses into \( Cf \).

\[
\frac{dCf}{dt} = k_{hc}Cs - k_{oc}Cf - k_{oa}r_{omp}Ni + \phi(Cf) + \Delta(Cf)
\]  

\[
\frac{dCs}{dt} = -k_{hc}Cs + \frac{v_{sc}}{H}Cs + k_{oa}r_{omp}Ag + \phi(Cs) + \Delta(Cs)
\]  

where \( k_{hc} \) (day\(^{-1}\)) is the hydrolysis rate of \( Cs \) which is dependent on \( T \) (as already described for \( k_{oa} \)); \( k_{oc} \) (day\(^{-1}\)) is the decay rate of \( Cf \) which is
similarly dependent on $T$ and is also limited by $Ox$ using the previously mentioned Michaelis–Menten formulation; $v_{ac}$ (m day$^{-1}$) is the sedimentation rate of $Cs$; $k_{dn}$ (day$^{-1}$) is the rate of denitrification of nitrate $Ni$, a process which consumes $r_{np}$ units of $Cf$ for each unit of $Ni$ (see Chapra (1997, p. 478)).

2.1.4. Nitrogen

Nitrogen is included in the model as non-living organic nitrogen $Ns$, ammonium (plus ammonia) $Na$, and nitrate $Ni$. Nitrite is omitted under the assumption that the conversion of ammonium to nitrite is the rate-limiting process (Chapra, 1997, p. 422). Nitrogen is allowed to be lost by sedimentation of $Ns$ at a rate $v_{ns}$ and by denitrification of $Ni$ at a rate $k_{dn}$ (day$^{-1}$) which is a function of $T$ as previously described (while denitrification generally occurs only in anoxic waters, the $k_{dn}$ term represents the effect of denitrification processes in the sediments—see Whitehead and Toms (1993)). Similarly, the rate of nitrification of $Na$ to $Ni$ is dependent on $Ox$ and is also limited by $Ox$ using the previously mentioned Michaelis–Menten formulation. Both ammonium and nitrate are assimilated at a rate $k_{pa}$ in proportion to the nitrogen–chlorophyll-a ratio $r_{na}$ in the phytoplankton. The phytoplankton consume $Ni$ and $Na$ in a proportion (which is defined by coefficient $\lambda$) to the relative availability of these two nutrients,

$$\frac{dNa}{dt} = -k_{ga}r_{na}\lambda Ag - k_{na}NA + k_{na}NS + \Phi(Na) + \Delta(Na)$$

(7)

$$\frac{dNi}{dt} = -k_{gn}r_{na}(1-\lambda)Ag + k_{na}NA - k_{dn}Ni + \Phi(Ni) + \Delta(Ni)$$

(8)

$$\frac{dNs}{dt} = k_{ga}r_{na}Ag - k_{na}NS - \frac{v_{ns}}{H}NS + \Phi(Ns) + \Delta(Ns)$$

(9)

2.1.5. Phosphorus

Phosphorus is represented by non-living organic phosphorus $Ps$ and inorganic phosphorus $Po$.

$$\frac{dPo}{dt} = -k_{ga}r_{pa}Ag + k_{hp}Ps + \Phi(Po) + \Delta(Po)$$

(10)

$$\frac{dPs}{dt} = k_{ga}r_{pa}Ag - k_{hp}Ps - \frac{v_{ps}}{H}Ps + \Phi(Ps) + \Delta(Ps)$$

(11)

where $r_{pa}$ is the ratio of phosphorus to chlorophyll-a and $v_{sp}$ is the effective sedimentation rate of $Ps$.

The pollution transport model (through which the $\Delta$ terms above are calculated) is a one-dimensional control volume solution of the advection–dispersion equation (see Chapra (1997, p. 215)). The control volumes are defined by a series of 44 cells (average length of 910 m) which make up the full length of the river. Adjacent cells with similar hydro-geometric properties are grouped together into reaches, giving the 12 reaches illustrated in Fig. 3. The flow routing model is a non-linear store whereby the flow out of each cell $Q$ (m$^3$ day$^{-1}$) is proportional to a power $b$ of the average depth in that cell $H$ (m), and a constant $a$ (m$^{3/2}$ day$^{-1}$),

$$Q = aH^b$$

(12)

The rate of change of water volume $V$ in each cell is simply the balance of flow from the upstream cell $Q_{up}$, flow out of the cell $Q$, and external sources $\Phi(Q)$,

$$\frac{dV}{dt} = Q_{up} - Q + \Phi(Q)$$

(13)

$H$ is a function of $V$ and the geometric properties of the cell. Each cell is conceptualised as having a symmetrical trapezoidal cross-section, so these properties are the cell length, the base width and the side-slope. The dispersion between cells is calculated from an empirical relationship with water velocity (Chapra, 1997, p. 245). The water temperature is prescribed on the basis of observations.

The set of ordinary differential equations described earlier is integrated using an adaptive time-step solver, which is described fully in McIntyre et al. (2002b). The integration was performed during the 12 days leading up to the observed days, on the assumption that the daily average pollution loads and other boundary conditions were constant during this period. Twelve days was found to be sufficient to allow the water quality to reach steady-state.

2.2. Specification of prior parameters and uncertainty in observed data

The model includes 24 uncertain parameters. The ranges of possible values of these parameters, prior to model conditioning, are taken from various reviews (Brown and Barnwell, 1987; Bowie et al., 1985;
Thomann and Mueller, 1987; Chapra, 1997). All prior parameter ranges together with references are listed in Table 1. All values within these ranges are taken to be independent and equally likely prior to conditioning.

As well as the high number of parameters, the sources of pollution are also not known precisely. To make justified inferences about the parameters, this additional source of uncertainty must be allowed for during the model conditioning. As is often the case, the available data for sources of pollution are daily means with no supporting quality control information to indicate the scope for procedural errors. Therefore, we initially assume that all sources are described as uniform distributions with ranges ±30% around the given mean value. If there is evidence in the data to suggest that this assumption is important and unreasonable, then this will become evident during model evaluation and sensitivity analysis.

The in-river water quality data consists of three measurements per determinant per monitoring section on both of the monitored days—one of the three measurements was taken early in the morning, one at mid-day and one in early evening. Therefore, the variability observed within each set of three will consist of errors (e.g. sampling errors) and diurnal variations. For this study, it is appropriate to use the mean of the three measurements to condition the model, as the model is assumed steady-state at a daily time scale, and is driven by mean daily inputs. The uncertainty in the estimation of the daily mean water quality is difficult to estimate due to the limited statistical significance of such small sets of data, and due to unknown procedural biases. The problem of describing data error structures using typically available data sets is a major obstacle to objectivity in water quality model uncertainty analysis (McIntyre et al., 2002a), and some degree of simplification and subjectivity is required. For the purpose of this investigation, the simplifying assumption is made that the uncertainty bounds on the observed mean water quality are represented by the maximum and minimum daily values—all values between these bounds are perceived to be equally likely. Exceptions to this rule are when the concentrations are below the detection limits, in which case the daily mean is taken as anywhere between zero and the detection limit, which occurs frequently for Na.

Therefore, as well as having a prior estimation of the uncertainty in all the model’s input variables (24 parameters plus 7 types of pollution for each of 9 point sources plus the headwater), we have an estimation of the uncertainty in the data (7 determinants at each of 8 downstream monitoring sections). These data are central to the first of our modelling tasks—to condition the model using the observations made on the 20th August 1996. Clearly, there is very large number of factors to be taken into account in confronting this task.

2.3. Multi-objective model conditioning

The initial objectives of the model are to adequately replicate the observed concentrations of the eight determinants observed on the 20th August, 1996. The degrees to which the eight objectives are met are measured by eight objective functions (OFs),
one for each determinant;

\[ \text{OF}_{1} = \text{replicate the observations of } Ag \]  
\[ \text{OF}_{2} = \text{replicate the observations of } Ox \]  
\[ \text{OF}_{3} = \text{replicate the observations of } Cf \]  
\[ \text{OF}_{4} = \text{replicate the observations of } Ns \]  
\[ \text{OF}_{5} = \text{replicate the observations of } Ni \]  
\[ \text{OF}_{6} = \text{replicate the observations of } Na \]  
\[ \text{OF}_{7} = \text{replicate the observations of } Ps \]  
\[ \text{OF}_{8} = \text{replicate the observations of } Po \]

To condition the model to meet each of these objectives individually, the values of the OFs are calculated for each of a number of randomly sampled sets of factors \( \{ \alpha \} \) within a Monte Carlo procedure. Each sampled set \( \{ \alpha \} \) contains a value of all the uncertain factors affecting the calculation of the OFs, including model parameters, pollution loads and in-river data. These values are independently and randomly sampled from within their limits of uncertainty. The number of sampled sets \( (R) \) is fixed according to the required thoroughness of the sampling (the issue of sampling error is discussed later). Calculation of the OF values involves running a simulation of the Charles River for each of \( R \) samples of \( \{ \alpha \} \) and calculating the corresponding OF values for all 8 determinants. For the \( j \)th sampled set of factors \( \{ \alpha_j \} \) and the \( i \)th
2.4. Graphical model evaluation

The justification of the model as a tool for sensitivity and scenario analysis depends on the model structure being a good conceptual representation of the actual water quality processes under all conditions of interest. To some extent, the structure is known to be reasonable a priori because the formulations (Eqs. (1)–(13)) are based on common knowledge of the principal processes affecting water quality. On the other hand, some processes known to have the potential to affect water quality are not represented. For example, sediment–water nutrient interactions are not represented explicitly, but might become important following nutrient load reduction, and therefore their omission casts doubt on the model’s reliability for appraising intervention scenarios. Ideally, the model structure would be evaluated under a wide range of conditions to identify the importance of these and other ‘missing’ structural components. Additional discussion of approaches to model structure evaluation is given in Wagener et al. (2002).

The traditional criterion for evaluating a model structure is its ability to achieve a satisfactory distribution of model residuals (i.e. the residuals between the model result and the corresponding observed data point) (see Kuczer (1983) and Beck (1987)). This approach is rejected here because the observations in this study (and many other distributed water quality studies) are not of sufficient quality and quantity to allow any useful statistical inference about the residuals. It is more useful to interpret observations subjectively alongside the prior knowledge contained in the model result. Arguably, in cases of unknown data reliability, it may be equally justifiable to invalidate the data on the basis of an a priori hypothesis of the model structure as vice versa (see the discussion of Chatfield (1995) on data-mining).

For this study, the model is evaluated using the Charles River data from the 20th August and the 8th October 1996. The spatial variations in water quality on these two dates are stochastically modelled using the conditioned point estimates of likelihood, with each determinant \( i \) modelled using its own likelihood measure \( OF_i \) (see Eqs. (14a–h)–(16)). For the 20th August, the variations modelled along the river have been conditioned on the same day’s observed data and
therefore, excepting serious structural error, would be expected to explain the data relatively well. For the later day, an additional Monte Carlo analysis is needed which incorporates the changed boundary conditions—pollution loads, hydraulic loads, water temperature and light intensity. Graphically comparing the modelled spatial variations with the in-river data indicates, on a subjective basis, the suitability of the model structure and the suitability of the definition of uncertainty given by Eqs. (15) and (16). That is, this evaluation seeks to answer the question “are the observations sufficiently described by the modelled confidence limits?” (see Section 3.1 for results).

2.5. Regional sensitivity analysis

RSA identifies the factors which have significant probability of influencing the degree of achievement of each of the objectives. It is an essentially probabilistic sensitivity analysis, as opposed to traditional derivative-based methods. This means that the measure of regional sensitivity assigned to each factor is not only dictated by the sensitivity of the model outcome to a unit perturbation in that factor, but by the relative responses due to all the factors, and due to the relative uncertainties in all the factors.

The employed RSA procedure is founded on the behavioural analysis described by Hornberger and Spear (1980) and Spear and Hornberger (1980), together with the generalised likelihood uncertainty estimation (GLUE) procedure of Beven and Binley (1992). The sensitivity analysis is employed in multi-objective mode, using a similar approach to that described by Bastidas et al. (1999) and Meixner et al. (1999). The procedure may be summarised as follows. The marginal frequency distribution of each of the factors for all eight objectives is derived. The marginal distribution function \( P_i(\gamma) \), indicates the probability that objectives \( i \) will be met across the range of factor \( \gamma \), given the uncertainty in all the other factors. \( P_i(\gamma) \) is derived by totalling the values of \( L \) (for objective \( i \)) within each of a number of equally sized bins of \( \gamma \), which is illustrated schematically in Fig. 4(a) and (b). The difference between the cumulative marginal distribution and the factor’s prior distribution (which is shown as uniform in Fig. 4) is summarised by the Kolmogorov–Smirnoff statistic, \( \text{KS}_i(\gamma) \) (see Ang and Tang (1975, pp. 277–280)). The significance of this statistic is illustrated in Fig. 4(c).

Fig. 4(a) draws attention to the fact that different likelihoods are found for any one value of \( \gamma \)—the likelihood is not solely a function of \( \gamma \), but also of the values of all the other factors in the sampled set \( \{ \alpha \} \). This is why joint and marginal distributions must be reported rather than uni-variate distributions. High correlation between factors will tend to diminish their regional sensitivity, and so the results of the RSA should be interpreted in conjunction with the factor covariance matrix.

Note from Eq. (15) that different realisations of the in-river data are being used as part of the sensitivity analysis. This is done to improve robustness of the sensitivity analysis to data uncertainty, and to indicate the importance of the data uncertainty compared to that of the a priori parameter uncertainty. For example, referring again to Eq. (15), if the OF is shown to be more sensitive to the X terms than the \( X \) terms, then it may be argued that the model cannot usefully be conditioned given the quality of
the available data (i.e. the task of replicating the observations is too poorly defined). The penalty for sampling the data errors is that there are more interacting factors so that less information is retrieved about the effect on the posterior marginals of high order factor interactions. This is an issue of sampling adequacy, which is discussed later.

For this sensitivity analysis, 10,000 samples are taken from the prior ranges using Latin hyper-cube sampling (MacKay et al., 1979). Latin hyper-cube sampling ensures optimum coverage of the individual ranges, and with 10,000 samples gives relatively comprehensive representation of two-, three-, and four-factor interactions, but sampling of higher level interactions is sparse. In theory, this means that if the overall significance of a factor is dependent on the simultaneous value of more than three other factors, then its evaluation will not be reliable. In practice, however, it tends to be only the lower interactions that affect the results of a sensitivity analysis (Hender-

son-Sellers and Henderson-Sellers, 1993). Therefore, 10,000 samples are assumed to be sufficient. Due to the semi-random nature of Latin hyper-cube sampling, values of the KS statistic beneath an arbitrary level will not be significant. While significance levels can easily be calculated as a function of the number of samples for fully random uni-variate experiments (see Ang and Tang (1975, p. 278)), this is not valid in the context of Latin hyper-cube sampling. Also, the KS statistic refers to the difference between the marginal posterior and prior distributions, but the sampling is from the multivariate prior distribution. While this does not preclude the KS test, it makes analytical derivation of the significance level very difficult. To address this issue of identification of meaningful significance levels for the KS statistic, a number of control factors—factors which are known not to have any significance—are included. Significant factors can then be identified as those whose KS statistics clearly above those of the control factors.

Although the KS statistic is a potentially insightful summary of model sensitivity, it can diminish the importance of local effects, especially at extreme values. Where significant factors are reported by the KS statistic, or where significant factors are expected but not reported, the sensitivity associated with that factor can be visualised by the scatter-plot of the likelihood or the marginal distribution (Fig. 4). This isolates important local sensitivities not identifiable from summary statistics.

The ultimate task of the Charles River model is to identify pollution management scenarios which lead to an acceptable risk of failing to limit phytoplankton (Ag) concentrations to below 10 mg m\(^{-3}\) of chlorophyll-a. It is not safe to assume that the model components which are important under this new objective, are the same as those identified for the objective of replicating the 1996 data, and another sensitivity analysis is warranted. The same algorithm is used, but in this case it is known precisely what the objectives are (<10 mg m\(^{-3}\) at each monitoring section), and so there is no need to treat X as a randomly sampled variable (although there may be practical cases where regulatory objectives are not so exact, with the qualitative ecological objectives set by the European Community’s Water Framework Directive (CEC, 2000) being a prime example).

The previously conditioned parameter sets and associated likelihoods \(\{\alpha_{1,j}, L_{1,j} : j = 1, R\}\) are employed to define the prior distribution for this second sensitivity analysis. This is based on the premise that model parameters represent the principal physical components of the system and will not change under future pollution load scenarios (as opposed to the pollution loads, for which the preferred changes are under investigation). The likelihoods are translated to the prior likelihoods for this second sensitivity analysis, \(L_{1,j} \rightarrow Lp_{1,j}, j = 1, R\) 

\[
L_{1,j} \rightarrow Lp_{1,j}, \quad j = 1, R
\]  

(17)

The sampled pollution loads within \(\{\alpha_{1,j}, L_{1,j} : j = 1, R\}\), which previously represented the perceived range of errors in the historic pollution load data, are overwritten by random samples from feasible ranges of future pollution reductions. These ranges are defined as from zero up to the average pollution loads measured in the summer–autumn of 1996 (i.e. from 100% reduction to no substantial change). This provides the basis for investigating Ag responses to pollution interventions.

Nine objectives are defined—the constraint Ag < 10 mg m\(^{-3}\) at each of nine control sections (Sections A to I in Fig. 1). The constraints are defined by upper and lower constraints \(X_{up}\) and \(X_{lo}\) (in this case, 0 and 10 mg m\(^{-3}\), respectively), and are
imposed on the model results $X_{ij}$ using Boolean OF,

$$\text{OF}_{ij} = 1 \quad \text{for} \quad X_{ij} \leq X_{ij} \leq X_{ij}$$

$$\text{OF}_{ij} = 0 \quad \text{otherwise} \quad (18)$$

Eq. (16) is then applied and $P_g$ and $K_S(g)$ are derived as before (although this time the prior marginals of the parameters are not uniform), and factors which will dictate our ability to achieve the Ag management objectives are speculated.

2.6. Risk-based appraisal of intervention strategies

Although the results of the second sensitivity analysis will indicate the pollution sources most affecting our ability to achieve the objective of eutrophication reduction, a useful question to ask is “on the evidence of the model (and given all the uncertainties involved) what is the probability that a specified intervention will produce the desired effect?” This question can be answered by further processing of the results of the RSA. Following application of Eq. (18) then Eq. (16), and derivation of the factor’s marginal distribution as in Fig. 4, $P_g$ is the probability of factor value $g$ given that $Ag < 10$ mg m$^{-3}$ at the $r$th control section. To derive the probability that $Ag < 10$ mg m$^{-3}$ given a value of $\gamma$ is a simple application of Bayes theorem,

$$P(Ag_i < 10|\gamma) = \frac{P(\gamma)P(Ag_i < 10)}{Lp(\gamma)} \quad i = 1, 9; \ j = 1, R \quad (19)$$

where $Lp(\gamma)$ is the prior likelihood of $\gamma$ and $P(Ag_i < 10)$ is the overall probability of success at control section $i$,

$$P(Ag_i < 10) = \sum_j Lp_j \text{OF}_{ij} \quad i = 1, 9; \ j = 1, R \quad (20)$$

$P(Ag_i < 10|\gamma)$ is not conditional on the value of any factor other than $\gamma$, and will reflect the risk that the uncertainty in the other factors will cause non-achievement of the target across the range of $\gamma$. For example, the risk of not achieving the target water quality at each control section can be plotted against the degree of a proposed pollution load intervention. This uni-variate report of risk could be extended into a bi-variate plot, although more realisations may be required to identify a usefully smooth risk surface. For this study, each potentially important pollution load intervention is analysed individually. The other pollution loads, as well as the model parameters, are kept as conditioned by the August 1996 observations.

3. Results and discussion

3.1. Preliminary model evaluation

The modelled spatial variation and 90% confidence limits of all eight determinants for the 20th August are shown in Fig. 5(a)–(h), together with the data of the observed water quality and their error bounds. It is seen that the model, with isolated exceptions, is successfully representing spatial variations in water quality on that date. The estimated confidence limits for the phytoplankton $Ag$ are interesting, as they are not constrained by the observations as much as might be expected relative to the other determinants. In particular, the lower confidence limit at the downstream reach diverges to a value 90% less than the observed data at the downstream boundary. It is speculated that this is due to the high order nature of the $Ag$ model (evident in Eq. (1)), together with the non-discriminating nature of the phytoplankton OF defined by Eq. (15). For example, a high numerical order would mean that the $Ag$ result could be a good replication of the observed data until the downstream stretch when it could swing rapidly to a poor replication. As the OF defined by Eq. (15) is aggregated over all of the monitored sections (except the headwater), such a result would be given significant likelihood. Hence, the lower confidence limit in Fig. 5(a) is not reflecting the observed data at monitoring section (I). This is a case where arguably, the discrimination between alternative sets of factors is not high enough, and Eq. (15) should be re-designed so that the model uncertainty is reduced, and the confidence limits are narrower. On the other hand, more discrimination would mean that the estimation of uncertainty is less robust to structural error, data bias, and inadequate sampling of the prior ranges of factors (the value of $R$). Narrower confidence limits are less likely to explain the effects of these sources of error. For example, as one point of data on Fig. 5(g)
Fig. 5. Modelled and observed spatial variations in water quality 20th August 1996. Observed data are shown as discrete squares, with vertical error bars. Model results (mean and 90% confidence limits) are shown as continuous lines over distance.
and another on Fig. 5(h) are not explained by the combined estimates of model and data error, it may be argued that the confidence limits on the $P_s$ and $Po$ models are not wide enough. Essentially, this issue needs to be addressed using the judgement of the modeller—to achieve a balance between robustness (presumed higher model uncertainty), and precision (presumed lower uncertainty) which is appropriate to

1. the modeller’s judgement of data precision and reliability,
2. the modeller’s judgement of model structure validity,
3. the answers the modeller requires from the model, and
4. the available modelling resources.

As the observed data in Fig. 5 were used to condition the model, this result does not demonstrate the model’s predictive capability. To attempt to do so, the conditioned model is applied to prediction of the water quality on the 8th October, and the results are shown in Fig. 6(a)–(h). The confidence limits are generally wider than in Fig. 5 indicating that the principal processes affecting water quality have changed from August to October, so that the result is more dependant on the poorly identified model parameters. This is clear for $Ag$, for which the upper confidence limit diverges to a value 625% greater than the observed data at the downstream boundary. Clearly, we are not able to accurately predict $Ag$ concentrations under the October conditions, given the information retrieved from the conditioning. Notwithstanding the lack of precision, we are able to predict with confidence that the $Ag$ concentrations on the 8th October are less than the target of 10 mg m$^{-3}$ of chlorophyll-$a$.

The purpose of Figs. 5 and 6 is not to evaluate the model structure alone, but to jointly evaluate the structure, the data and the success of the likelihood estimator defined by Eq. (15) in estimating model uncertainty. The inseparability of these three facets of model evaluation, which is endemic in modelling water quality using sparse and/or unreliable data, is best approached using subjectively orientated visualisation. Summarising model performance using objective measures is avoided here, as this neither provides a spatial context to the evaluation, nor reports the significance of estimated model and data uncertainty.

The approach was taken that the model should be conditioned individually for each of the eight determinants, so that there were eight joint distributions of model parameters. This is justified because it maximises the information retrieved about the sensitivities of the determinants, as individual entities, to all the factors. However, arguably such an approach fails to rigorously estimate the uncertainty in the model because, for every determinant, the information contained in the data of the other determinants is neglected. In fact, if the model had been required to explain the variations in all the determinants simultaneously as a function of one joint distribution of factors, the confidence limits would have inevitably been significantly wider. A related observation was made with respect to the $Ag$ spatial variation in Fig. 5. In that case, the model was expected to explain the variations in $Ag$ at the upstream sections simultaneous to explaining those downstream, leading to confidence limits which were not intuitive from the observations. This prompts a discussion of how to use multiple objectives to robustly represent model uncertainty, and to diagnose why and in what respects the model is failing to achieve all its objectives simultaneously. Such discussion is not pursued here, but the reader is referred, for in-depth discussion, to Wagener et al. (2002) and Yapo et al. (1998). For current purposes, it is proposed that the conditioned model is sufficiently explaining the spatial variation and error in the observed data, and that, in the context of limited resources and high uncertainty, the model conditioned by the phytoplankton observations may usefully be applied to the remaining tasks of this study.

3.2. Sensitivity analysis (1996 conditions)

Rather than tabulating the values of the KS statistic, the model sensitivities are reported graphically, in Fig. 7. Within this figure, there are six graphs which report the model sensitivities measured using the $Na$, $Ni$, $Ag$, $Po$, $Ox$ and $Cf$ data, as described in Section 2.5 (only the $Ns$ and $Ps$ results are not illustrated). The common $x$-axis of these graphs is the series of factors, comprising of model parameters, point loads and observed in-river data. On the $y$-axes,
Fig. 6. Modelled and observed spatial variations in water quality 10th October 1996. Observed data are shown as discrete squares, with vertical error bars. Model results (mean and 90% confidence limits) are shown as continuous lines over distance.
Fig. 7. Sensitivity of the eight model conditioning objectives (Eqs. (14a–h)) to the model factors. The Kolmogorov–Smirnov statistic, as a measure of sensitivity, is plotted as a solid line across the model factors. The significance level is shown as a broken line. The significant factors are labelled.
the value of the KS statistic corresponding to each of these factors is plotted, and these points are joined to give a trajectory, the significantly high peaks of which indicate significant factors. The significance level, which is shown on Fig. 7 as the horizontal dashed line, is defined by the maximum KS statistic identified for the control factors (factors to which the specific OFs are known to be independent). For clarity, only the evidently significant factors are labelled.

In Fig. 7, the mean observed water quality for determinant \( x \) at the \( i \)th control section (from Fig. 1) is signified by \( d_{ix} \). For example, \( d_{0,po} \) signifies the mean observation of orthophosphate at the ninth control section, i.e. Cochrane Dam. Similarly, the point load of determinant \( x \) at the \( i \)th point source (from Fig. 1) is signified by \( w_{ix} \). The special case of \( i = 0 \) signifies the point load from the headwater.

It is seen that the \( Na \) objective has been affected largely by the data uncertainty (perhaps predictable because ammonium was below the detection limit for all but one of the monitored sections). Lack of more precise measurements of \( Na \) has restricted the information that can be retrieved about lesser factors such as the model parameters. Nevertheless, four parameters are identified as significantly affecting the \( Na \) result (\( k_{in20}, k_{on20}, k_{da20}, \) and \( k_{gahsen} \)). Considering the role of these four parameters in the model concept (Fig. 2), all three arrows leading to or from the \( Na \) box may be considered ‘active’ components of the model. There is no evidence, therefore, upon which to reduce the complexity of the \( Na \) representation. Returning to Fig. 7, three point sources (\( Ns \) from the headwater, \( Na \) from the CRPCD wastewater treatment plant and \( Na \) from the Medfield wastewater treatment plant) are clearly most affecting the modelled \( Na \) pollution under the conditions of the 20th August, 1996.

The objective of replicating the \( Ox \) data is suggested by Fig. 7 to be dominated by parameters \( k_{pa20}, k_{da20}, k_{oa}, k_{oc20}, k_{he20}, k_{in20}, \) and \( k_{er} \). Thereby, with the exception of the SOD component, all the model components affecting \( Ox \) are implied as active and there is no justification contained in Fig. 7 for removing them from the model. That \( Ox \) should be largely affected by phytoplankton dynamics is somewhat predictable (at least for a water quality expert) from general knowledge of the issues affecting the Charles River (CRWA, 2000). However, Fig. 7 also indicates that the uncertainty in the phytoplankton’s chemical composition (parameter \( r_{wp} \)) may be more important to our success in modelling \( Ox \) (and hence the broader ecological status of the river) than, for example, improved knowledge of the organic pollution loads. This is an excellent example of the insight which the sensitivity analysis can offer.

The result for \( Cf \) indicates the dependency of \( Cf \) on nitrogen and phosphorus concentrations, which can only be caused by the role of \( Ag \) in the model of the carbon, nitrogen and phosphorus cycles. Why then is the \( Cf \) significantly influenced by the third point source of phosphates (\( w_{3,roa} \)) but \( Ag \) has not been implied as so? This is because there is some information contained in the \( Cf \) data which has improved the chance of \( w_{3,roa} \) standing out as an individual factor, and apparently less such information in the \( Ag \) data. This demonstrates that no inferences should be made about individual factors without taking into account all the available evidence, and that the most informative data are not always where they might be expected.

If the current objectives were limited to the replication of the \( Ni \) data, Fig. 7 indicates that barely two parameters would be justified, and only one point source (CRPCD wastewater treatment plant) would be significant in effect. The sensitivity of the \( Ni \) objective to \( d_{2,Ni} \), the \( Ni \) data at monitoring section 2 (shortly downstream of Mill River), is because this point of data is the most uncertain of all the \( Ni \) data. This is evident from Fig. 5. The significance of the point source from the CRPCD wastewater treatment plant (\( w_{1,Ni} \)) is predictable because this is such an intense source of nitrate (six times the average from the other point sources). It should be noted that a perceived uncertainty of ±30% rather than a statistically identified distribution was applied for this source, and the value of the KS statistic depends on this assumption. However, inspection of the scatter-plot of likelihood values against \( w_{1,Ni} \), Fig. 8, implies significant responses even, for example, in the ±5% bracket.

Finally, from Fig. 7, it is seen that the data uncertainty at the eighth analysed monitoring section (Section I in Fig. 1) is repeatedly implied to significantly affect the ability of the model to meet the objectives. In other words, the ‘goalposts’ are being moved too much, through sampling of \( X \).
in Eq. (15). This suggests that the uncertainty in the data at that monitoring section is limiting the information retrievable about the other factors, and that this section is a priority for more data collection and/or more precise measurement techniques. This suggestion may equally well be applied to the data shortcomings previously identified specifically for the \( Na \) and \( Ni \) models. Thus, it is proposed that application of RSA in the described manner has potential value in designing and updating field monitoring programs, and in the objective management of sources of data error. Clearly, significant investment would not be justified solely on the basis of a preliminary analysis, like that presented here. Instead, for example, the analysis could be repeated to incorporate hypothesised reductions in sampling and measurement error, to evaluate associated reductions in model uncertainty and improvements in decision-making (Section 3.4).

3.3. Sensitivity analysis (eutrophication reduction)

Fig. 9 presents the general trends and variabilities in the KS statistic. The overwhelming implication of the analysis is that the concentration of phytoplankton in the headwater \( w_{0,Ag} \) is generally responsible for the occurrences of failing to achieve the objective. For the sections further down the river, the growth and death rates of phytoplankton become more significant, as the phytoplankton have had more time to grow, or to die.

Various other phytoplankton parameters are implied to be relevant, so that the uncertainty in the phytoplankton properties is a source of risk which may lead to nutrient reduction interventions being ineffective. For example, this suggests that it is important to know the dominant species of phytoplankton (e.g. blue-greens, diatoms, etc.) in identifying low-risk interventions for eutrophication management, as species are known to have individual maximum growth rates, carbon to chlorophyll-\( a \) ratios, etc. Both the phytoplankton phosphorus and light half-saturation constants (\( k_{galp} \) and \( k_{galh} \)) are included in the significant parameters, implying that there is insufficient evidence to predict whether the system would be phosphorus or light limited, although there is evidence that it would not be nitrogen limited. The evidence for phosphorus limitation is corroborated by the observation that three point sources of phosphorus have significant KS values—at the CRP CD wastewater treatment plant, at the Stop River and at the Medfield treatment plant.

Fig. 9 shows the superimposed trajectories of the KS statistic for each of the eutrophication reduction objectives (keeping phytoplankton concentrations below 10 mg m\(^{-3}\) of chlorophyll-\( a \) at each of the nine control sections, A–I). Rather than attempting to distinguish between the nine individual objectives,
3.4. Appraisal of intervention strategies

Before appraising options for reduction of summer eutrophication, it is noted from Fig. 5(a) that a ‘do nothing’ strategy has little chance of working, assuming that 1996 conditions are typical. It is seen that all the observed phytoplankton concentrations are well above the target phytoplankton concentration of 10 mg m\(^{-3}\), and the lower 90% confidence limit of the model result just dips below the target at the downstream end of the studied reach (although, as previously argued, this limit is an outcome of the limitations of the likelihood measure, and may be overly optimistic).

Firstly, the risk associated with reducing the phosphate load from the CRPCD treatment plant was investigated. Even with 100% reduction in this load, results indicated insignificant probability of achieving the target at any of the control sections. Following this, the effect of reducing the total phosphorus load from the CRPCD treatment plant was investigated (the organic fraction of the total phosphorus load was lumped into the inorganic fraction). Again, this was ineffectual. The results are strong evidence that phosphorus stripping at the CRPCD treatment plant alone is unlikely to adequately control eutrophication. The residual phosphorus in the river is estimated as adequate to sustain undesirable phytoplankton growth under almost all feasible summer conditions. Additional or alternative measures are required. These results also emphasise the lack of detail given by the sensitivity analysis results in Fig. 9. Fig. 9 indicates the factors for which the successful factor values are significantly different from the unsuccessful values, not the level of success.

A further scenario involved leaving all phosphorus loads at their 1996 levels, and investigating the effect of reducing the concentration of phytoplankton in the headwater. The results are presented in Fig. 10 for the sections (A)–(I) indicated on Fig. 1. These suggest, for example, that reducing the headwater Ag by 60%
will guarantee to satisfactorily reduce \( Ag \) at control section (A) (although this is a trivial result, as section (A) is the headwater); has a 80% chance of success at control section (B); 30% chance at (C); 5% chance at (D); and no chance at any of the further downstream sections. Alternatively, 100% reduction in the headwater \( Ag \) is more or less guaranteed to be effectual upstream of South Natick Dam, and even has a 30% chance of success at the Cochrane dam.

For the final scenario, the concentration of \( Ag \) in the headwater was fixed at 50% of the average value observed in the summer of 1996, and the risk associated with reducing the CRPCD total phosphorus concentration was investigated. The risk associated with reducing the CRPCD total phosphorus load under these new conditions is plotted in Fig. 11. Firstly, it is noted that the \( Ag \) is almost bound to be below the target at section (A) which is consistent with the result in Fig. 10. In general, Fig. 11 shows that even after reducing \( Ag \) concentrations in the headwater phosphorus stripping at the CRPCD plant is, by itself, a high-risk intervention. For example, 95% reduction in phosphorus loading is suggested as having a 40% chance of adequately reducing phytoplankton at section (D), a 25% chance at section (E) and no chance of success further downstream, following the influences of Medfield WWTP, Sewall Brook and Bogastow Brook. However, this intervention is likely to be effective at sections (B) and (C).

Clearly, the specific objective of the planners is crucial in this case.

This demonstration has highlighted the considerable degree of uncertainty, or risk, attached to any water quality intervention. Importantly, the derived risk should not be interpreted as the expected frequency of failure. This would imply that the model parameters behave randomly as described by their conditioned joint distribution when, in fact, we simply do not know what their statistical properties or time-variance should be. Although predicted fluctuations in the water quality can be allowed for in the measure of risk (for example, by using a dynamic simulation or, as done here, by treating diurnal variations as random effects), a large part of the risk stems from the low reliability of model predictions. Therefore, interventions, which can be modelled with relative precision—which are not affected by highly uncertain components of the model—will be identified as preferable. For example, the reduction in chlorophyll-\( \alpha \) concentration which would be achieved by doubling the flow in the Charles River would be identified as a low risk intervention, as it does not rely on highly uncertain biochemical properties. However, given that much of the risk comes from the model’s limitations, it is sensible and probably economical to explore methods of improving the reliability of the model, rather than opt for a low-risk intervention.

A primary motivation for risk-based modelling is that management decisions should not be restricted to those which prioritise water quality interventions. A judicious decision may recognise that a sufficiently low-risk intervention is unattainable, and instead call for model improvements, review of water quality targets or further data collection. Further data collection has been identified as a priority for this investigation of the Charles River, due to the restrictions which the employed data (and their assumed errors) imposed upon model reliability. By implication, the reliability of any decisions about preferred interventions is degraded, and this is represented in the high-risk levels reported in Figs. 10 and 11. A useful extension to this investigation, therefore, would be to evaluate how the attainable quality of decision (reduction in risk) would respond to proposed investments in data.
4. Conclusions

A Monte Carlo-based framework of sensitivity analysis and risk evaluation has the capacity to support risk-based management of surface water quality through,

1. calculating the response of model outputs to uncertain or stochastic model inputs (boundary conditions, pollution loads and model parameters), allowing the distributions of model outputs to be reported at all points within the model’s space and time domains,

2. calculating the response required of model inputs to meet constraints imposed upon the model output, allowing the posterior distributions of model inputs to be reported. The imposed constraints are either defined by observed water quality (with the purpose of conditioning the model, and exploring the sensitivities of the system), or by prescribed water quality targets (with the purpose of appraising intervention scenarios, and identifying realistic targets).

This has been demonstrated in this paper using the upper Charles River, Massachusetts as a case study. A model structure has been selected based on a prior hypothesis of the principle water quality processes. The model has been conditioned using observations of water quality observed on 26th August 1996 at a number of control sections along the river. The model was conditioned with respect to each of eight objectives, one for each of the eight key water quality determinants, and was evaluated through visualisation of the spatial variation of modelled water quality and observations (Figs. 5 and 6). The superposition of confidence limits (estimated uncertainty in the model) and error bars (estimated uncertainty in the observed data) allowed informed judgement upon the relative reliabilities of the model structure and the measured data.

In pursuit of rigorous evaluation of risk, all uncertain factors potentially affecting the achievement of water quality objectives should be included in the sensitivity analyses. This may include model parameters, pollution and hydraulic sources, boundary conditions, and perhaps the water quality objectives themselves. It was shown (Fig. 7) that treating the water quality objectives as random variables allows the relative importance of data error to be indicated. This feature also has potential for integrating the effects of uncertain regulations into the appraisal of scenarios (e.g. which scenario is safest given qualitative or otherwise uncertain water quality criteria?), and in offsetting different targets against the cost of conforming (i.e. what are viable targets?).

Figs. 7 and 9 are examples of how the factors significantly affecting water quality are identified using the Kolmogorov–Smirnov statistic to summarise the results of a RSA. These results should be seen as indicators of the factors most likely to be affecting the respective objectives given the knowledge embodied in the model structure and parameter ranges. It is a useful approach to screening the model for unexpected sensitivities, and for identifying factors to be taken forward to more detailed analysis. For example, Fig. 9 clearly identified that reducing the headwater \( Ag \) and the \( Po \) load from the CRPCD treatment plant were priorities for further investigation—because there is indication that the former might be an effective way forward, and that the latter might be less so. Further investigation resulted in Figs. 10 and 11 which confirmed these suspicions in terms of risk of failure associated with various magnitudes of intervention.

The overriding and unavoidable limitation to the methods employed here, at least in applications where data are typically sparse and imprecise, is that results are partly subjective. This is because model evaluation must be based on judgement of the relative unbiasedness of the model structure and the observed data. Tools such as WaterRAT (McIntyre and Zeng, 2002) are needed to support the modeller in these judgements, and allow justifiable use of results in a decision-support role, within the practical constraints of data and modelling resources.
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Appendix A

Notation

Model parameters

- \( k_{hc} \) (\( k_{hc20} \)): slow carbon hydrolysis rate (max. rate at 20 °C)
- \( v_{sc} \): slow carbon settling velocity
- \( k_{oc} \) (\( k_{oc20} \)): fast carbon oxidation rate (max. rate at 20 °C)
- \( k_{nchs} \): fast carbon oxygen half-saturation
- \( k_{nra} \): reaeration rate
- \( k_{ner} \): error in aeration formula
- \( k_{we} \): weir aeration coefficient
- SOD: sediment oxygen demand
- \( k_{ln} \) (\( k_{ln20} \)): organic nitrogen hydrolysis rate (max. death rate at 20 °C)
- \( v_{sn} \): organic nitrogen settling velocity
- \( k_{on} \) (\( k_{on20} \)): inorganic nitrogen nitrification rate (max. rate at 20 °C)
- \( r_{on} \): oxygen demand of nitrification
- \( k_{nahs} \): inorganic nitrogen oxygen half-saturation
- \( k_{dn} \) (\( k_{dn20} \)): inorganic nitrogen denitrification (max. rate at 20 °C)
- \( r_{nap} \): fast carbon demand of denitrification
- \( k_{sp} \) (\( k_{sp20} \)): organic phosphorus hydrolysis rate (max. rate at 20 °C)
- \( v_{sp} \): organic phosphorus settling velocity
- \( k_{po} \) (\( k_{po20} \)): phytoplankton growth rate (max. rate at 20 °C)
- \( k_{phln} \): phytoplankton nitrogen half-saturation constant
- \( k_{phbp} \): phytoplankton phosphorus half-saturation constant
- \( k_{phal} \): phytoplankton light half-saturation constant
- \( k_{do} \) (\( k_{do20} \)): phytoplankton death rate (max. rate at 20 °C)
- \( r_{no} \): phytoplankton ratio Nitrogen:Chl-\( a \)
- \( r_{oa} \): phytoplankton ratio Oxygen:Chl-\( a \)
- \( r_{pa} \): phytoplankton ratio Phosphorus:Chl-\( a \)
- \( \lambda \): ammonium preference coefficient
- \( \theta \): Arrhenius coefficient for all reactions
- \( a \): linear flow residence time parameter
- \( b \): non-linear flow residence time parameter

State variables

- \( Ag \): concentration of phytoplankton
- \( Ox \): concentration of dissolved oxygen
- \( Cf \): concentration of 5-day BOD
- \( Cs \): concentration of slow reacting carbon
- \( Po \): concentration of orthophosphate
- \( Ps \): concentration of organic phosphorus
- \( Na \): concentration of ammonium
- \( Ni \): concentration of nitrate
- \( Ns \): concentration of organic nitrogen
- \( Q \): flow
- \( Q_{up} \): flow in upstream cell
- \( H \): water depth
- \( T \): water temperature
- \( V \): volume of water in control volume
- \( I_s \): light intensity

Sub-models

- \( \Delta(\cdot) \): mass flux due to transport processes
- \( \Phi(\cdot) \): pollution or hydraulic load
- \( f_i \): light limitation factor
- \( f_T \): temperature limitation factor
- \( f_N \): nutrient limitation factor

Analytical variables

- \( OF \): objective function
- \( X \): arbitrary model result
- \( \gamma \): arbitrary factor
- \( \alpha \): a sample set of factors
- \( L \): posterior likelihood
- \( L_p \): prior likelihood
- \( R \): number of Monte Carlo samples
- \( P(\cdot) \): Probability
- \( KS \): Kolmogorov–Smirnov statistic

References


