Predicting the Frequency of Water Quality Standard Violations: A Probabilistic Approach for TMDL Development

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To address the impaired condition of the water bodies listed under Section 303(d) of the Clean Water Act, over 40 000 total maximum daily loads (TMDLs) for pollutants must be developed during the next 10–15 years. Most of these will be based on the results of water quality simulation models. However, the failure of most models to incorporate residual variability and parameter uncertainty in their predictions makes them unsuitable for TMDL development. The percentile-based standards increasingly used by the EPA and the requirement for a margin of safety in TMDLs necessitate that model predictions include quantitative information on uncertainty. We describe a probabilistic approach to model-based TMDL assessment that addresses this issue and is suitable for use with any type of mathematical model. To demonstrate our approach, we employ a eutrophication model for the Neuse River Estuary, North Carolina, and evaluate compliance with the state chlorophyll *a* standard. Any observed variability in chlorophyll *a* that is not explained by the model is explicitly incorporated via a residual error term. This probabilistic term captures the effects of any processes that are not considered in the model and allows for direct assessment of the frequency of standard violations. Additionally, by estimating and propagating the effects of parameter uncertainty on model predictions, we are able to provide an explicit basis for choosing a TMDL that includes a margin of safety. We conclude by discussing the potential for models currently supported by the EPA to be adapted to provide the type of probabilistic information that is necessary to support TMDL decisions.

Introduction

Identification and listing of impaired waters is required of all states under Section 303(d) of the Clean Water Act. This process is generally accomplished through the assessment of samples collected as part of an ambient monitoring program. While states have used a variety of criteria for placing a waterbody on the 303(d) list, the U.S. EPA guidelines for state water quality assessments instruct that a water body be listed as impaired if more than 10% of the samples from that water body violate water quality standards (*1*). This percentile-based approach is intended to limit excessive pollutant levels while recognizing that, because of natural variability and measurement error, it is unreasonable to disallow *any* standard violations. Because guidance documents do not dictate the number of samples that must be taken, it is presumably intended that the 10% allowance refers to the whole distribution of values over a specified time and space. Barnett and O'Hagan (*2*) refer to this as an *ideal* standard, because it is not possible to measure the pollutant level at all points in a section of a water body at all times.

Implementation of an ideal standard requires an operational procedure to address whether the standard is being met. The only practical approach is to collect a limited number of samples that can be used, together with a statistical procedure, to infer the characteristics of the true distribution of relevant water quality characteristics. The use of a limited sample for statistical inference introduces uncertainty into the assessment of compliance, and the degree of uncertainty depends on the quality and quantity of samples collected. Therefore, decisions regarding the listing of a water body as impaired depend on the sampling scheme used as well as the degree of confidence required from the statistical test. Methods for using sample information to infer compliance with an ideal, percentile-based standard have been reported in the literature recently from both the classsical and Bayesian statistical perspectives (*3–5*).

Once a water body is listed as impaired, Section 303(d) requires that a total maximum daily load (TMDL) be developed for the pollutant causing the impairment. TMDLs establish the allowable pollutant loading to a water body and provide the basis for states to require watershed-based controls (*6*). Within the next 10–15 years, over 40 000 TMDLs must be developed for 21 000 water bodies nationwide (*7*). Whereas the process of placing a water body on the 303(d) list requires inferring current compliance with standards based on collected data, the TMDL development process requires predicting future compliance, after a pollutant load reduction, usually based on a water quality model. The appropriate use of models to address ideal percentile-based standards has not been previously discussed in the literature. Given the substantial social and economic implications of TMDL decisions, it is important to consider whether current water quality modeling practices adequately address the type of standards on which the TMDL program is based.

Most water quality models currently used for TMDL development are deterministic (*8*). That is, the model outputs are uniquely determined by the inputs, and predictions consist of a single value at a point in time and space. However, predicting natural system response to anthropogenic change is a highly uncertain endeavor (*9, 10*), and the relationship between pollutant loading and receiving water effects can never be perfectly known. Regardless of the accuracy and complexity of the modeled physical, chemical, and biological processes, there will be residual uncertainty due to natural variation, misspecification of boundary conditions, and measurement error. This is the reason that many models are observed to "under-represent" the dynamics of the system, missing the highest and lowest measured values (*11*). Many modelers interpret this to mean that they need to add more detail to their model. However, a few acknowledge that exact

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Abstract

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Implementation of an ideal standard requires an operational procedure to address whether the standard is being met. The only practical approach is to collect a limited number of samples that can be used, together with a statistical procedure, to infer the characteristics of the true distribution of relevant water quality characteristics. The use of a limited sample for statistical inference introduces uncertainty into the assessment of compliance, and the degree of uncertainty depends on the quality and quantity of samples collected. Therefore decisions regarding the listing of a water body as impaired depend on the sampling scheme used as well as the degree of confidence required from the statistical test. Methods for using sample information to infer compliance with an ideal, percentile-based standard have been reported in the literature recently from both the classsical and Bayesian statistical perspectives *(3-5)*

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Most water quality models currently used for TMDL development are deterministic *(8)*. That is, the model outputs are uniquely determined by the inputs, and predictions consist of a single value at a point in time and space. However, predicting natural system response to anthropogenic change is a highly uncertain endeavor *(9,10)* and the relationship between pollutant loading and receiving water effects can never be perfectly known. Regardless of the accuracy and complexity of the modeled physical, chemical, and biological processes, there will be residual uncertainty due to natural variation, misspecification of boundary conditions, and measurement error. This is the reason that many models are observed to "under-represent" the dynamics of the system, missing the highest and lowest measured values *(11)*. Many modelers interpret this to mean that they need to add more detail to their model. However a few acknowledge that exact mathematical representation of nature is impossible and model

predictions can represent only an average effect at some scale *(2)*. Predicting an average effect may be appropriate for assessing the ability of management actions to meet certain water quality standards expressed in terms of average levels. However, a deterministic model that purports to make exact predictions, without error, is inadequate in addressing the type of percentile-based standard that underlies the 303(d) listing. Such a model disregards the variability that is not explained by the model but is always present *(2)*. For models that are calibrated to "go through the middle of the data", this oversight will bias predictions toward an underestimate of the frequency of standard violations under future conditions, thereby weakening the basis for model-based TMDL decisions.

We describe a probabilistic approach to TMDL assessment that is suitable for use with any type of mathematical water quality model. The method explicitly incorporates residual variability into assessments, leading to more appropriate predictions of the frequency of standard violations. Additionally, we describe how to estimate the uncertainty in these percentile-based predictions that results from uncertainty in the choice of model parameter values. Such an assessment provides decision-makers and stakeholders with a measure of the degree of confidence they can have in model results and provides an explicit basis for the choice of a margin of safety in setting a TMDL.

To demonstrate our approach, we evaluated compliance with the state chlorophyll a standard in the Neuse River estuary, North Carolina, as a function of total nitrogen inputs. The Neuse estuary is currently believed to be in violation of the chlorophyll standard (40 μg/L), and the development of a TMDL for nitrogen is required. We describe the nitrogen-phytoplankton relationship with an empirical model fit to observational data *(12)*. Model predictions are then developed to assess the impact of various nitrogen load reductions on the expected frequency of

chlorophyll standard exceedances. Predictions include estimates of uncertainty which are expressed in a form that facilitates their use in selecting an appropriate margin of safety. We conclude by discussing the ability of detailed simulation models, such as those currently supported by the EPA, to provide the type of information that is necessary for TMDL decisions.

Probabilistic Modeling Approach

Most water quality models consist of a mathematical expression that relates pollutant concentration to a set of input, or predictor, variables and a set of coefficients, or model parameters. For example, following the direction of Chapra *(13)* we can write a general mass balance model for a pollutant in a well-mixed water body or stream segment as:

$$\text{Accumulation} = \text{loading} - \text{outflow} \pm \text{reaction},$$

where loading includes all inputs, outflow includes all outputs, and reaction includes all internal processes that add or remove the pollutant (all terms in units of mass/time). If the volume of the water body is approximately constant, then accumulation, the change in mass with time, can be written as:

$$\frac{dVc}{dt} \quad \text{or} \quad V\frac{dc}{dt},$$

where V = volume, c = pollutant concentration (mass/volume), and t = time. With inputs aggregated and described as a function of time, the loading term can be expressed as, $W(t)$ = mass loading rate (mass/time). With the assumption that the water body is well-mixed, the outflow term can be written as the product of the in-lake pollutant concentration times Q, the rate of water flowing from the lake (volume/time), or outflow = Qc. Reaction terms are commonly assumed to occur as first-order processes, where the reaction rate is proportional to the pollutant concentration or:

$$\text{reaction} = kVc,$$

where k is a rate coefficient (1/time). The final mass-balance equation can now be expressed as:

$$V\frac{dc}{dt} = W(t) - Qc \pm kVc. \quad (1)$$

Equation 1 is a general expression that can include any number of specific input, output, and *in situ* removal or addition processes. It can be applied to a whole lake or be used as a spatial discretization for advective systems such rivers and estuaries. In this model, concentration c is the dependent, or response, variable, and $W(t)$ is the independent, or input, variable. The quantities V, Q, k, and V are the parameters, or coefficients, of the model. When eq. 1 is solved, either analytically or numerically, the solution can be written in the general form:

$$c = g(X, \beta) \quad (2)$$

where g is a mathematical function (or functions) relating the pollutant concentration c to a set of all input variables X and a set of all model parameters β. Equation 2 is entirely general and can represent a series of detailed process-based functions or the expression of statistical relationships derived from historical data. In either case, once the function $g(X,\beta)$ is developed, predictions can be made regarding the value of the pollutant concentration c for any chosen values of input variables X and parameters β. Values of the model parameters are generally selected either informally so that predictions visually "go through the middle of the data" or formally using an optimization procedure to minimize prediction error *(13)*. Either way, model predictions based on $g(X,\beta)$ represent the expected value of c at the chosen values of X and β, not accounting for the variability that is not explained by the function $g(X,\beta)$. However, model-based assessments that consider only these expected values do not provide an adequate basis for estimating the frequency of standard violations. Accurate estimation of this figure depends on explicit consideration of the additional sources of variability, so that eq. 2 becomes:

$$c = g(X, \beta) + \varepsilon \quad (3)$$

where ε represents an error term that accommodates discrepancies between the predicted values of c represented by $g(X,\beta)$ and the observed values of c. This lack of fit, or unexplained variability, may occur because the proposed function is an imperfect system representation or because of intrinsic randomness or measurement error (most likely, for all of these reasons).

Characterization and incorporation of the residual error term is straightforward for a model that has been optimized to available data using maximum likelihood or least-squares regression. Adherence to the assumptions required for statistical inference with least-squares regression implies that the residual errors follow a normal distribution (after a suitable transformation, if necessary) with a mean of 0 and a variance, σ^2, the value of which is directly estimated from the data and is assumed to be a constant with respect to the value of c. Therefore, for any given set of input variables X and model parameters β, the response variable c can now be viewed as being normally distributed with a mean $g(X,\beta)$ and a variance σ^2:

$$c \sim N(g(X,\beta), \sigma^2). \quad (4)$$

As changes in the input variables X lead to changes in the model prediction $g(X,\beta)$, the mean of this distribution shifts up or down, while the variance remains constant (Figure 1). The probability of the response variable exceeding a numerical criterion c^*, given values of β, σ, and X, can then be calculated as:

$$p = P(c > c^* \mid \beta, \sigma, X) = 1 - F\left(\frac{c^* - g(X,\beta)}{\sigma}\right) \quad (5)$$

where p is the "exceedance probability" and $F(\cdot)$ is the value of the cumulative standard normal distribution. (While our model development focuses on violation of standards written as an upper limit, the approach is equally applicable to those written as a lower limit, such as those for

dissolved oxygen. In these cases, the desired probability is the complement of eq. 5, or p'.) To assess compliance with the relevant standard over a specified time period, such as an annual cycle, multiple sets of predictor variables, X, can be chosen that represent the variability over that time period, such as daily values. The exceedance probability is then calculated from eq. 5 for each predictor variable set and the results averaged to calculate the "expected frequency of exceedance" for that time period. This value can then be compared with the frequency considered tolerable for the given situation, such as the 10% value suggested by EPA's water quality guidance documents *(1)*.

Uncertainty Analysis

In addition to a single prediction of the expected frequency of standard violations, stakeholders and decision-makers will want information about the uncertainty in that prediction so that they might obtain a realistic expectation of the chances of achieving compliance with the percentile-based standard. If the uncertainty in model parameters can be expressed as a joint probability distribution, this type of uncertainty analysis is straightforward, as the uncertainty in the exceedance probability p (arising from uncertainty in the model parameter values) for a given value of X can be characterized by the probability density function:

$$f(p \mid X) = \int P(c > c^* \mid \beta, \sigma, X) f(\beta, \sigma) d\beta d\sigma \qquad (6)$$

where $f(\beta,\sigma)$ is a joint distribution representing parameter uncertainty. Because it may be an unfamiliar concept, it is worth reiterating that eq. 6 represents a *probability distribution of a probability value*. It is an expression of the uncertainty in the predicted exceedance probability, p, for a given value of X. Equation 6 can be solved, in conjunction with eq. 5, using a Monte Carlo procedure *(14)*. When multiple sets of predictor variables are used to represent a longer

time period of interest, the result is a distribution of the predicted frequency of standard violations over that time period. This distribution can be expressed either as a confidence interval (CI) on the exceedance frequency *(14)* or as a degree of confidence that the true value of the exceedance frequency is below a specified value (e.g. the 10% in the EPA guidelines). This latter quantity is termed the "confidence of compliance" (CC), *(5)* and its calculation provides an explicit means for determining an appropriate margin of safety based on the degree of confidence required by managers and stakeholders. This approach will be demonstrated in the context of the Neuse River example described below.

If the function $g(X,\beta)$ is linear and parameter values have been derived from maximum likelihood or least-squares regression, then the parameter distribution in equation 6 can be appropriately represented by a multivariate t distribution described by the maximum likelihood estimates, together with the associated covariance matrix. From a Bayesian perspective, this distribution is equivalent to the posterior parameter distribution under noninformative priors *(15)*. Alternately, in the true Bayesian spirit, informative priors based on cross-system data *(16)* or expert judgment *(17)* could be incorporated into the analysis, as well as a nonlinear model form. Either situation would require a more involved parameter inference method *(18)*.

Application to the Neuse River Estuary

Study Site and Model Description

The Neuse River estuary has recently received considerable attention due to recurrent algal blooms, bottom water hypoxia, and fishkills. It has been listed as an impaired water body on the Federal 303(d) list because, in certain segments, more than 10% of water quality samples analyzed for chlorophyll a have exceeded the state standard of 40 μg/L. The general belief is

that high chlorophyll levels are due to high watershed inputs of nutrients, particularly nitrogen *(19)*, and a TMDL for nitrogen is being developed to satisfy the state chlorophyll standard. To investigate the nitrogen-phytoplankton relationship that will serve as the basis for the TMDL, the state has funded a coordinated water quality modeling and monitoring effort (ModMon) *(20)*, of which this study is a part.

For this analysis, we used an empirical model to relate chlorophyll a concentration in each of five sections of the estuary (Figure 2) to estuarine water temperature and incoming Neuse River flow and total nitrogen concentration *(12)*. Model parameters were estimated using ordinary least squares regression with approximately five years of biweekly monitoring data. Parameter values indicated a positive relationship between chlorophyll and nitrogen input concentration for all estuarine sections, with the strongest relationship in the lower section, where nitrogen is most likely a limiting factor for algal growth *(21)*. Increased river flow was found to generally exert a negative effect on chlorophyll concentration in the upstream sections, possibly due to shortened residence times, lowered salinity, and increased turbidity. However, in the middle, bend, and lower sections, higher flow was associated with higher chlorophyll for flow values below an empirically-determined breakpoint but with lowered chlorophyll at flows above this value (Figure 3). This may be the result of increased nitrogen delivery from upstream sections at intermediate flow values and a flushing effect at higher flows. Additional model details and interpretation are discussed by Borsuk et al. *(12)*.

Probabilistic Prediction and Uncertainty Analysis

A time-series of predictions and observations shows model fit to observed data (Figure 4). The deterministic portion of the model visually "goes through the middle of the data" and

captures both short and long term components of variation. The R^2 value indicates that the model explicitly resolves approximately 55% of the variation in log-transformed chlorophyll. While this is a better fit than that of other, more complex simulation models that have been applied to the Neuse *(22)*, the deterministic component $g(X,\beta)$ cannot capture all of the variability in the observed data. Thus, the time series that represents the expected chlorophyll value for each day almost never exceeds the 40 μ/L standard for any of the estuarine sections (see Fig. 4). However, inclusion of the residual variability, represented graphically by a predictive interval, indicates that there is still some probability that samples collected on most days in the lower sections will exceed the standard.

The average frequency (and associated uncertainty) of exceeding a chlorophyll level of 40 μg/L over a specified time period can be calculated from eq. (6). The Neuse TMDL is to be expressed in terms of a percent nitrogen load reduction relative to 1991-95 *(22)*. Therefore, to assess standard compliance, our model predictions will focus on those years using observed daily values of flow, nitrogen concentration, and water temperature as predictor variables. To generate the distribution described by eq. (6), we used a Monte Carlo procedure. We first randomly drew 1,000 parameter sets from a multivariate normal parameter distribution with mean vector and covariance matrix determined from the regression estimation. We then calculated a mean predicted chlorophyll value from the regression model and a corresponding probability of exceeding 40 μg/L from eq. (5) for each of the 1825 (5*365) days, for each parameter set. These values were then each averaged across all days for each parameter set to obtain the daily average chlorophyll concentration and average exceedance frequency for the 1991-95 time period predicted by that parameter set. The distribution of exceedance frequencies across parameter sets was then used to represent the uncertainty in the exeedance frequency resulting from

parameter uncertainty. The bounds of the middle 90% of the values are reported as the 90% confidence interval (CI). The "confidence of compliance" (CC) is the proportion of the exceedance frequency distribution that lies below the EPA's 10% cutoff (Figure 5). This is a measure of the probability that the true exceedance frequency is below 10%, given the uncertainty in the model. To determine the necessary reduction in riverine nitrogen inputs, results were generated for the three estuary sections in violation of the chlorophyll standard (upper, middle, and bend) for total nitrogen concentration reductions of 0%, 10%, 20%, 30%, 40% and 50%.

Results (Table 1) indicate that, under the baseline scenario, the expected frequency of standard exceedances is above 10% for all three sections, consistent with the 303(d) listing. However, because of parameter uncertainty, the true exceedance frequency may be higher or lower as indicated by the 90% confidence interval. In fact, only for the bend section does the 10% value fall below the lower limit of this confidence interval. This is reflected by a confidence of compliance of less than 5%. As the nitrogen input concentration is reduced, both the average chlorophyll concentration and the exceedance frequency are also reduced, while the confidence of standard compliance increases. Only at reductions of 50% or greater do we predict the expected exceedance frequency to reach 10% for all three sections. However, it is important to note that even under this scenario, our confidence in complying with the 10% guidance is still only 50% for the bend section. If managers and stakeholders demand greater confidence that the actual exceedance frequency is less than 10%, an even greater nitrogen reduction is necessary. The difference between the nitrogen reduction necessary to achieve an exceedance frequency of 10% with 50% confidence and the reduction necessary to achieve a higher level of confidence is the required margin of safety.

Discussion

The interpretation of water quality standards to allow for violations at some frequency (e.g., 10%) and the requirement that TMDLs include a margin of safety both represent explicit acknowledgment of the importance of natural variability and prediction error. From an operational standpoint, these conditions imply that model-based TMDL predictions must consist of more than a single point or deterministic time series; instead, probability distributions or interval estimates are required. This error analysis must occur at two levels. First, any variability in water quality that is not explained by the model must be quantified to appropriately predict the frequency of standard violations (see eq. 5). Second, any knowledge uncertainty arising from the misspecification of the model or parameters must be probabilistically described to explicitly derive the margin of safety (see eq. 6). We have demonstrated how to characterize these two sources of error simultaneously for a model statistically fit to observational data. At this point, it is worth examining the extent to which other types of models, such as the simulation models currently supported by the EPA, can be used to provide this additional assessment.

Prediction error in water quality simulation models has traditionally been estimated in one of two ways. For a comprehensive assessment, error propagation using Monte Carlo simulation has been used to estimate the collective effect of individual error terms on the prediction error *(see summaries in 23,24)*. A second and simpler approach has been to compare predictions with observations and assume the differences between the two represent total prediction error. However, each of these methods has important practical limitations that may limit their applicability for TMDL development.

In a Monte Carlo analysis, it may be difficult to derive appropriate distributions describing the individual error terms. If a model is fit to observational data using least squares,

maximum likelihood, or Bayesian analysis, parameter and residual uncertainty are estimated explicitly. However, simulation models typically have too many parameters for statistical estimation. As a consequence, parameters are judgmentally chosen and model fitting becomes an art; more experienced modeler/artists will presumably produce better fitting models. Accurately quantifying the uncertainty, especially the parameter covariance structure, in such a situation is extremely difficult. However, because these models are generally calibrated to describe typical or average system behavior, it is reasonable to expect that a well-calibrated model will yield a prediction trajectory that goes through the middle of the time series of observations. This observation leads to the second common approach to error analysis.

The second approach to error analysis has been to statistically describe the nature of the differences between predictions and observations. Again, if a model is fit to data using classical statistical or Bayesian analysis, this error term has clear meaning; it describes a prediction interval centered on the fitted observations. However, if the model is fit using judgmental parameter selection, then correct interpretation of such an analysis is not straightforward. Depending on the judgment of the modeler, the resulting prediction interval may not be centered on the mean of the observations or have a constant error variance. For example, if, in order to address the 10% exceedance allowance, the judgmental parameters are selected to fit the upper extremes of the response variable (e.g., high chlorophyll a levels) then the chosen parameters are incompatible with a model structure designed to describe average system behavior. It is then not clear how the prediction-observation differences can be used for assessing uncertainty. Additionally, if a model is "overfitted" to calibration data, then the prediction-observation differences will likely underestimate the prediction error in new scenarios. The best way to

avoid this is to obtain independent verification data substantiated with a statistical comparison between calibration and verification data

Two-dimensional and three-dimensional simulation models can generate large numbers of predictions, so when an error analysis is not feasible, one option might be to simply plot the empirical distribution of all predictions and assess the distribution tail area for percent standard exceedances. However, as noted above, simulation models are typically specified and fitted to describe average behavior. This means that extremes are underestimated, so the tail area of a distribution of predictions can be expected to underestimate the true extent and percentage of extremes. This practice also does not provide any basis for selecting a margin of safety based on uncertainty in model specification.

Each of the above observations may explain the common practice of selecting the margin of safety using safety factors or conservative model assumptions. However, such a practice obscures the underlying basis for the margin of safety *(7)* and amounts to making decisions in the dark. If, on the other hand, a formal uncertainty analysis is performed, allowing model results to be expressed as the degree of confidence that a standard will be met for any given pollutant loading level, then decision-makers simply need to choose the percent reduction that corresponds to their desired level of confidence. The choice of required confidence is not an easy decision and should be based on careful consideration of the potential cost to stakeholders of continued impairment despite the attainment of the target pollutant load.

Given the substantial model forecast uncertainty in most water quality models, the practical consequence of the analysis in this paper is that TMDLs are likely to require considerable over-design to accommodate margin of safety requirements. Because the margin of safety depends on both the risk tolerance of decision-makers and the uncertainty in the water

quality model, the size of the margin might be reduced in either of two ways. Either: (1) decision-makers and stakeholders must settle for a lower degree of confidence in achieving their objectives, or (2) predictive uncertainty must be reduced. Assuming that a lower confidence level is not acceptable, then the size of the margin of safety is wholly reliant on the choice of a model and the appropriate assessment of predictive uncertainty. If the prediction error estimate is incomplete, biased, or in some way does not reflect the application scenario, then the error analysis is misleading. Since the size of the margin of safety has a direct impact on the pollutant load reduction required and, therefore, on the cost of watershed management, modelers and decision-makers should place a high priority on selecting and developing TMDL models that facilitate the assessment of prediction error *(7)*. This requirement should be considered no less important than any other model choice criterion.

The model that we present for TMDL development and error analysis is largely empirical. In general, however, we may prefer a TMDL model that has a strong mechanistic basis, as this provides additional assurance that the model will reflect the changes in pollutant loads associated with a TMDL forecast. Thus, an urgent research need is the development of process-based models that accommodate rigorous and complete error analysis *(*e.g. *12)*. Such models will allow for the direct assessment of the frequency of standard violations and facilitate the determination of an appropriate margin of safety – both essential tasks within the current TMDL framework.

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Table 1. Model predictions for the 1991-95 time period for total nitrogen reductions from 0 to 50%. Confidence of compliance values have been rounded to the nearest 10%, except when less than 5%.

Upper Section				
Nitrogen Reduction	Average Chl a (µg/L)	Expected Exceedances (%)	90% Confidence Interval	Confidence of Compliance (%)
0%	17.7	11	8 - 15	30
10%	16.7	10	7 - 13	50
20%	15.8	9	7 - 12	70
30%	14.9	8	6 - 11	80
40%	14.1	8	5 - 11	90
50%	13.4	7	4 - 11	90
Middle Section				
Nitrogen Reduction	Average Chl a (µg/L)	Expected Exceedances (%)	90% Confidence Interval	Confidence of Compliance (%)
0%	21.1	13	9 - 18	20
10%	20.4	12	8 - 15	20
20%	19.7	11	8 - 14	30
30%	19.1	11	8 - 13	40
40%	18.5	10	7 - 14	60
50%	18.0	10	6 - 15	60
Bend Section				
Nitrogen Reduction	Average Chl a (µg/L)	Expected Exceedances (%)	90% Confidence Interval	Confidence of Compliance (%)
0%	26.2	18	12 - 23	<5
10%	24.5	16	12 - 20	<5
20%	23.0	14	11 - 18	<5
30%	21.6	13	9 - 16	10
40%	20.4	12	8 - 15	30
50%	19.2	10	6 - 15	50

Figure 1. Hypothetical distributions of predicted pollutant concentration for two sets of input variables, X_1 and X_2. Shaded areas p_1 and p_2 represent the corresponding probabilities of exceeding a numerical criterion c*.

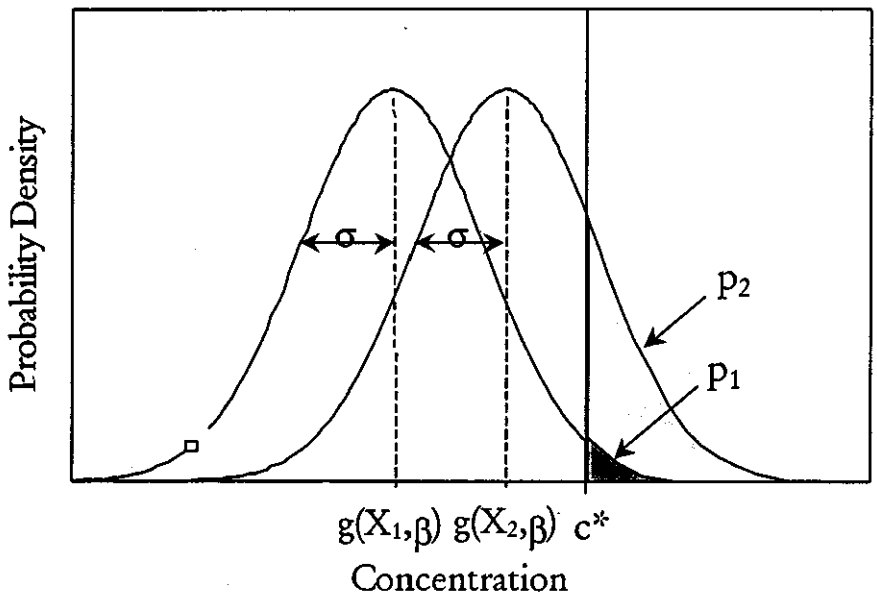


Figure 2. The Neuse River Estuary, North Carolina, showing the delineation into five sections for this analysis. Filled points indicate the location of water quality sampling stations.

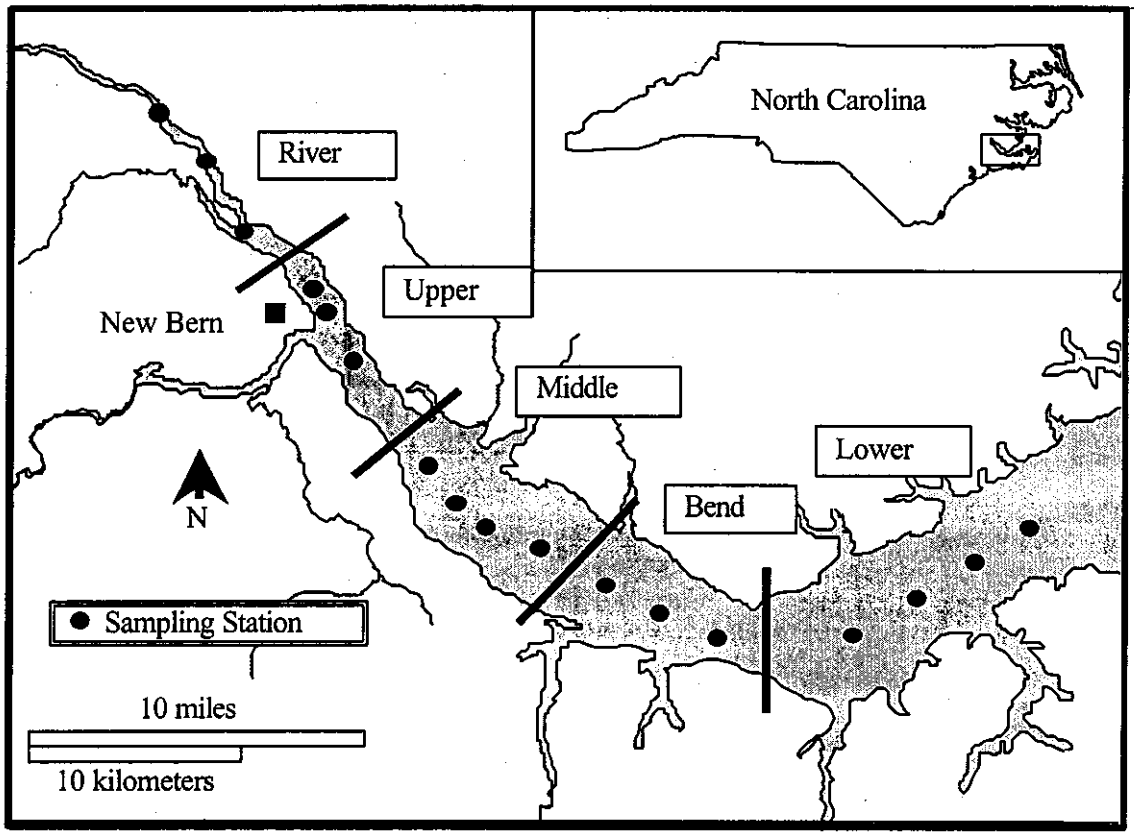


Figure 3. Partial residual plots indicating the effect of river flow on chlorophyll a concentration for each estuary section. Solid lines indicate the fitted model relationship, and points indicate the observed values after removing the effect of the other model terms.

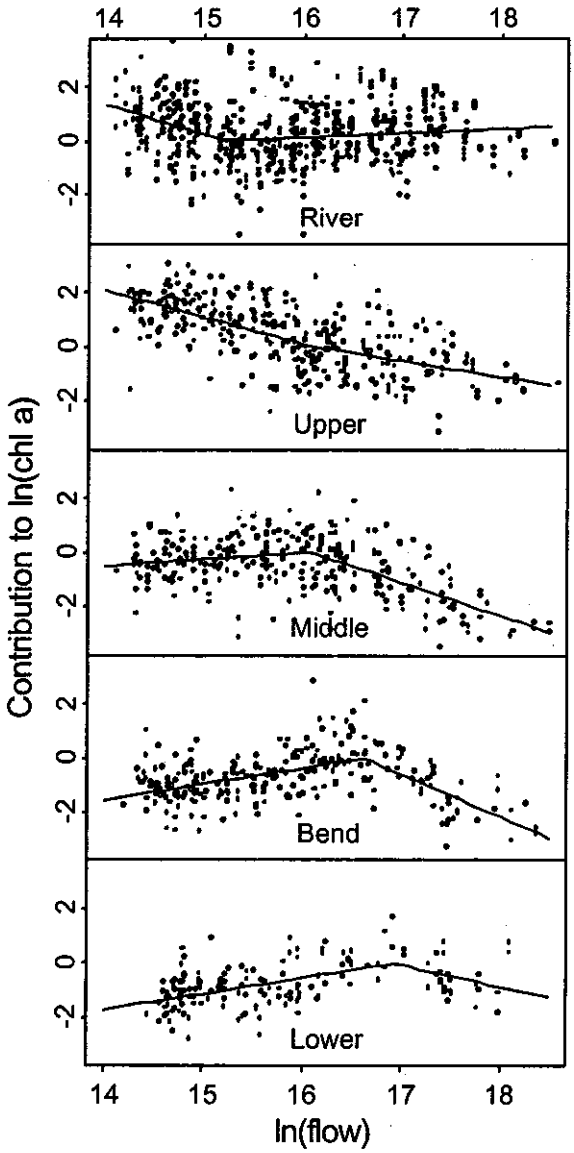


Figure 4. Time series plot of predictions and observations of chlorophyll a concentration for each estuary section (both after a natural log transformation). Points indicate observed values and solid lines indicate the mean and the 80% credible interval for the model predictive distribution. The horizontal dashed line indicates the 40 µg/L standard.

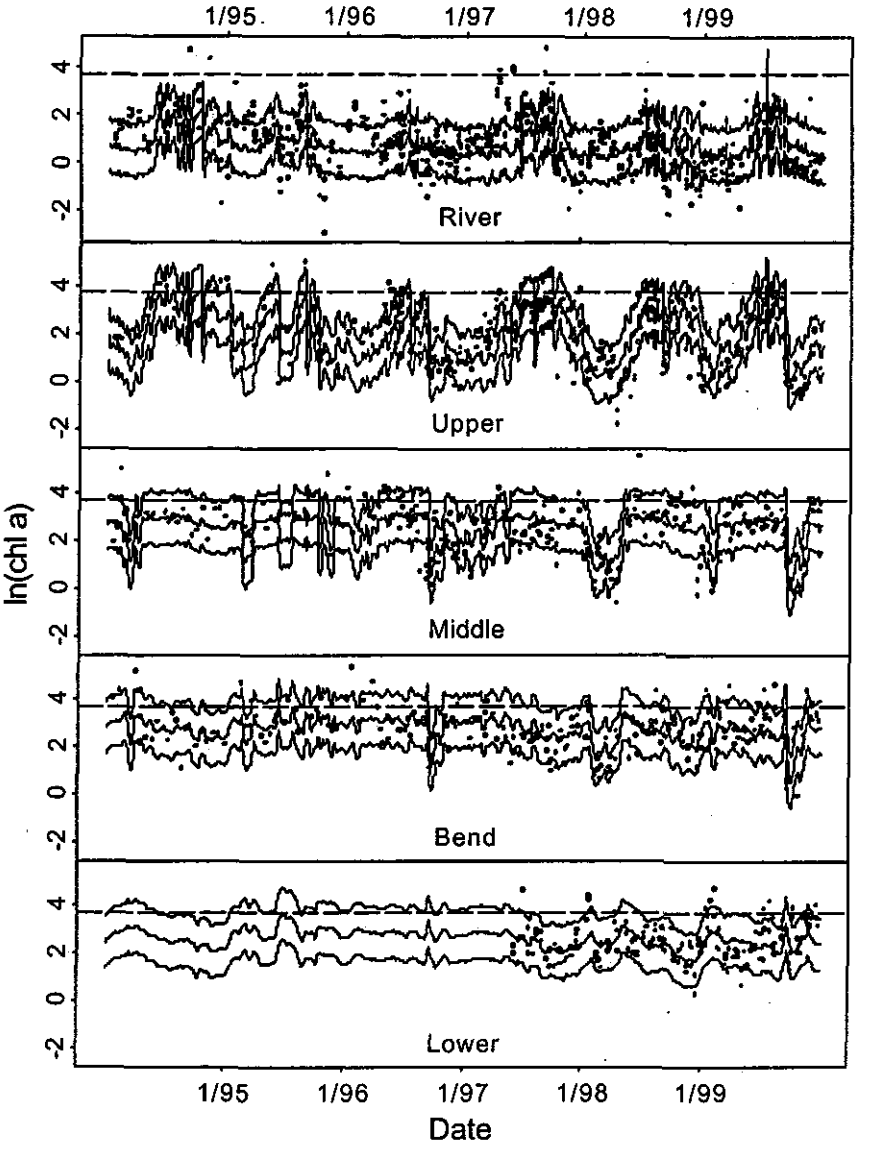
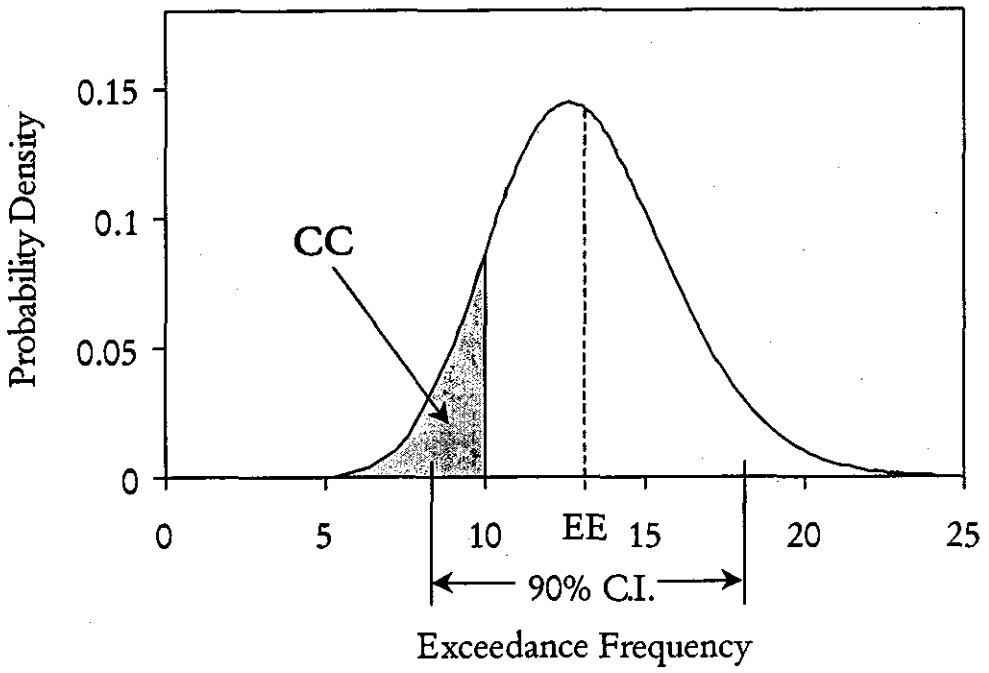


Figure 5. Hypothetical probability density for the exceedance frequency over a specified time period. The shaded area represents the probability that the true exceedance frequency is below the 10% EPA guideline and is termed the confidence of compliance (CC). The mean of the distribution is termed the expected exceedance (EE).



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- Background
- Research Interests
- Recent Publications
- Other Work
- Neuse Projects
  - Neuse River MODeling& MONitoring
  - Neuse NitrogenTMDL Modeling
- Eutromod
- Personal Interests
- Links to Other Sites
- ENV335 Water Quality Modeling Class
- Director's Forum (short essays on science and policy)
- National Academy of Sciences report on TMDLs

BACKGROUND

CURRENT POSITION:
Director, Water Resources Research Institute of The University of North Carolina

Professor, Duke University (reckhow@duke.edu)
Nicholas School of the Environment and Earth Sciences

Adjunct Professor, Department of Civil Engineering, North Carolina State University

EDUCATION:
S.B. Cornell University, Engineering Physics, 1971
S.M. Harvard University, Environmental Science and Engineering, 1972
Ph.D. Harvard University, Environmental Science and Engineering, 1977.

RESEARCH INTERESTS

For the past several years, my research has focused on surface water quality modeling and decision analysis. I am particularly interested in the treatment of scientific uncertainty, methods for combining information (in particular, Bayesian inference), statistical characterization of multivariate patterns in water quality, and recently,

probabilistic modeling approaches. This research has involved a number of Ph.D. students and faculty colleagues at Duke and other universities. In addition, I am interested in the more applied area concerning the development and presentation of mathematical models and statistical methods for use by practicing professional scientists and engineers.

RECENT PUBLICATIONS (since 1990)

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Reckhow, K.H. 1993. A Random Coefficient Model for Chlorophyll-Nutrient Relationships in Lakes. Ecological Modelling. 70:35-50.

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Reckhow, K.H. 1993. Lake Ecosystem Modelling (p. 315-318); Trophic State Criteria (p. 630-631); and Validation of Simulation Models: Philosophy and Statistical Methods of Confirmation (p. 656-660). all in: Concise Encyclopedia of Environmental Systems. P.C. Young, ed. Pergamon Press. Oxford, UK.

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TECHNICAL GUIDANCE DOCUMENTS

Reckhow, K.H., and W. Warren-Hicks. 1994. Biological Criteria: Technical Guidance for Survey Design and Statistical Evaluationof Biosurvey Data. Draft final report prepared for USEPA, Washington, DC. 63 pp.

Reckhow, K.H., K. Kepford, and W. Warren-Hicks. 1993. Methods for the Analysis of Lake Water Quality Trends. EPA 841-R-93-003. Washington, DC. 84 pp. (includes software). Available from EPA Publications.

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Gaugush, R. F., D.C. Blouin, J.P. Geaghan, K.H. Reckhow, and W.G. Warren. 1986. Statistical Methods for Reservoir Water Quality Investigations. Instruction Report E-86-2. US Army Corps of Engineers Waterways Experiment Station. Vicksburg, MS. 216 pp.

Reckhow, K.H., J.T. Clements and R.C. Dodd. 1986. Statistical Goodness-of-Fit Measures for Waste Load Allocation Models. Project completion report to the U.S. Environmental Protection Agency, Washington, DC. 68 pp.

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UNPUBLISHED MANUSCRIPTS

Water Quality Prediction, Mechanism, and Probability Network Models-**This is a postscript file of a recent (December, 1996) manuscript.**

Reaction Rates and Uncertainty in Water Quality Models Issues in Parameter Selection: Phytoplankton Settling Velocity **These are postscript files of short discussion papers (November, 1996) on uncertainty and the scientific basis for model specification.**

Uncertainty in Water Quality Modeling and Assessment-**This is a postscript file of a manuscript (November, 1996) on uncertainty.**

EUTROMOD

Eutromod is a spreadsheet-based model that is used for the prediction of nutrient runoff and lake eutrophication for individual lakes in the US. With the model, phosphorus and nitrogen runoff may be predicted using either nutrient loading functions or nutrient export coefficients. The nutrient loading functions are based on the rational formula for dissolved nutrients, and the universal soil loss equation for sediment-attached nutrients. The sediment delivery ratio is addressed with user-defined trapping zones.

Lake eutrophication response is predicted based on a set of regional statistical models. Respose variables include:total phosphorus concentration, total nitrogen concentration, chlorophylla level, Secchi disk depth and in some cases - probability of hypolimnetic anoxia and probability of blue-green algal dominance. The spreadsheet program, and a users manual, may be ordered from the North American Lake Management Society, NALMS, at 608-233-2836 or at the NALMS homepage.

PERSONAL INTERESTS

Some Interesting Sites:
Duke Sports Online
Carolina Godiva Track Club

Family:
Ellen
Sarah
Michael

LINKS TO OTHER SITES

School of the Environment, Duke University

Civil and Environmental Engineering, Duke University

Civil Engineering, North Carolina State University

ENV335 WATER QUALITY MODELING CLASS

Fall, 2000

Instructor: Dr. Kenneth H. Reckhow, A317ALSRC,613-8026, reckhow@duke.edu
Office Hours: Wednesday 1:30 - 3:30; Friday 9:30-11:30

CLASS SCHEDULE and LECTURE TOPIC (Readings)

1 Introduction (Reckhow & Chapra, Chapter 1)

2 Basic modeling concepts (Reckhow 1994b; Chapra and Reckhow, Chapter 10)

3 Probability network models (Reckhow 1996)

4 Stream DO models (Chapra 1997, Lectures19-21)

5 Uncertainty analysis (Reckhow andChapra, Chapter 2)

6 Mechanistic models - QUAL2E (Chapra1997, Lecture 26, 36)

7 Pollutant runoff models (Novotny and Olem, Chapter 9)

8 Lake eutrophication models (Chapra 1997, Lecture 29)

9 Trend analysis (Reckhow, Kepford, and Warren-Hicks

1994)

10 To be determined

11 Statistical modeling

12 Toxic substances (Chapra 1991)

13 Final issues

Course Objective: To acquaint students with problems and approaches in surface water quality modeling, with particular attention to model choice and applications for management.

Course Requirements: Six problem sets, weekly written literature reviews, readings, and active participation inclass discussion.

Standard Class Format: first half lecture and second half discussion.

Expected Assignment Schedule: Each assignment will have two weeks for completion; the first assignment will be given on the first day of class. Assignment topics and expected sequence are:
1. model selection criteria
2. probability network models
3. stream DO model error analysis
4. pollutant runoff models
5. water quality trend analysis
6. statistical modeling

Readings: There is no class textbook; instead, copies of all readings will be distributed in class.

Additional useful websites:
EPA TMDLs
ODU list of WQ model sites
USGS Water Research Abstracts

Literature Reviews: Each week, a paper from the recent professional literature will be assigned for reading and critique. Written reviews (approximately three pages) will be due the following week, and the second half of that class will be devoted to a discussion of the paper and related issues.For each reading, the written review should provide a brief summary, your own comments on the paper, and answers to questions; these will provide the initial basis for class discussion.

Last updated: October 21, 2002