

KEY SOURCES OF UNCERTAINTY IN QUAL2E MODEL OF PASSAIC RIVER

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ABSTRACT: Application of stream water-quality models in decision making has been hampered by a lack of data appropriate for minimization of model-simulation uncertainty. A method for determining data needed to reduce model-prediction uncertainty is illustrated in this paper. First-order reliability analysis is applied to determine (1) the model parameters that significantly affect model-prediction uncertainty; and (2) the constituents for which model-prediction uncertainty is unacceptable. Additional data are required to reduce uncertainty in the parameters that significantly affect constituents with high prediction uncertainty and consequently in model prediction. The method is demonstrated for multiconstituent water-quality modeling on the Passaic River in New Jersey applying QUAL2E. The model-prediction uncertainty of dissolved oxygen, biochemical oxygen demand, ammonia, and chlorophyll *a* is considered. For this example, only the reaeration rate and the algal maximum-specific-growth rate contribute significant uncertainty to model prediction. The effect of reducing the uncertainty in the reaeration rate and algal maximum-specific-growth rate on the uncertainty on predicted dissolved oxygen and chlorophyll *a*, respectively, is demonstrated.

INTRODUCTION

Planning and management activities require the assessment of hydraulic and water-quality conditions beyond the range of observed field data. Water-quality models must be formulated that are general enough to (1) describe observed conditions; and (2) predict planning scenarios that may be substantially different from observed conditions. In stream water-pollution control, water-quality models are applied to assess the maximum pollutant releases allowed from wastewater treatment plants and nonpoint-source-pollution controls so that pollutant levels in the receiving stream meet water-quality standards. Billions of dollars have been spent on wastewater treatment plant construction and improvement to meet maximum release levels selected in part on the basis of water-quality modeling. Yet, despite the large investment, water quality in many streams has not substantially improved. Uncertainty in simulations from water-quality models has contributed to the unexpectedly poor results of some stream water-pollution control plans.

Collection of water-quality data is relatively expensive. Thus, water-quality models developed for many rivers have been calibrated and verified with data collected prior to model development during surveys designed to check basinwide water quality for regulatory compliance. These data are typically inadequate for the following reasons:

- Many key water-quality constituents or inputs are not measured because the purpose of data collection is a general survey of water-quality conditions in the stream system and not the development of a water-quality model; e.g., the Potomac River water-quality model (ICPRB 1991).
- There is a tendency to sample certain water-quality constituents because they are easy to sample, not because they increase knowledge of key water-quality processes (Reckhow 1979).
- The frequency of data collection is usually insufficient.

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These inadequacies force water-quality modelers to make weakly supported assumptions regarding model parameters or inputs, thus increasing model-prediction uncertainty and adversely affecting decision making for water-pollution control.

This paper describes and demonstrates a method for determining the data required to reduce model-prediction uncertainty. First-order reliability analysis (FORA) is applied to analyze the uncertainties in simulation of stream water quality for the Passaic River in New Jersey with a complex, multi-constituent model, QUAL2E (Brown and Barnwell 1987). FORA application provides insight on model performance in terms of key parameters requiring detailed study and the overall model-prediction uncertainty. The objective of this study is to examine the uncertainty in a typical example stream water-quality model applied by regulatory agencies for waste-load allocation and other purposes. Thus, model identification effects on model-prediction uncertainty, discussed in detail by Beck (1987), are not considered in this paper. Further, the goal of this study is to identify the reaction coefficients that significantly affect the uncertainty of estimates of various key, water-quality constituents so that the uncertainties in these coefficients can be reduced by a carefully designed sampling program. Therefore, reliability analysis with respect to reaction coefficients is described, and the uncertainties in the other model parameters (hydraulic and geometric characteristics, initial conditions, pollutant loads, etc.) are omitted from the analysis.

METHODS FOR DETERMINATION OF KEY SOURCES OF UNCERTAINTY

A number of researchers [e.g., Gardner et al. (1981); Beck (1987); Yeh and Tung (1993)] have shown that traditional sensitivity analysis, wherein basic variables are perturbed one at a time and the sensitivity of model output to the perturbation in each variable is observed, is not appropriate for determining the sources of uncertainty that most affect model output and, thus, require more detailed study. The sensitivity coefficient for a given parameter does not account for the likelihood that the parameter is different from its "best" value. Therefore, a highly sensitive parameter that is known with low uncertainty may have much less effect on the uncertainty of model output than a much less sensitive parameter that is highly uncertain. Reliability-analysis methods based on multiple simulations (e.g., Monte Carlo or Latin Hypercube simulation) and FORA allow consideration of the combined effects of parameter sensitivity and parameter uncertainty in the determination of the key parameters affecting model-prediction uncertainty.

Simulation-Based Methods

For the simulation-based methods, two approaches may be used to infer the key parameters. In the first approach, the correlation between the parameter values and the model-output values is assessed, and the parameters with significant positive or negative correlations are determined to be important. Correlation analysis may be performed in four ways. The simple correlation coefficient (CC) and partial correlation coefficient (PCC) between parameter values and model-output values can be calculated to examine the linear relations between the model parameters and the model output. The CC and PCC can also be calculated for the ranked parameter values and ranked model-output values to examine possible nonlinear relations between the model parameters and the model output. Gardner et al. (1981) note that if the modeler is interested in the underlying error-propagation properties of a model, the PCC is the most useful. In the field, all hydraulic and water-quality characteristics are subject to variability and are measured with error. These field-data errors cannot be controlled, and their effect on prediction uncertainty cannot be removed as in PCC analysis. Thus, in the design of field sampling programs, the ranking of parameters according to the CC is most relevant. Gardner et al. (1981) provide an example of CC and PCC analysis of model-parameter values and model-output values for a nonlinear stream-ecosystem model. Jaffe and Ferrara (1984) provide an example of rank correlation analysis for a model of sediment-water column interactions for hydrophobic pollutants. Yeh and Tung (1993) provide a comparison between standard correlation analysis and rank correlation analysis for a model of the movement of borrow pits in alluvial streams.

A second approach applies regional sensitivity analysis (RSA) (Hornberger and Spear 1981) to determine the key model parameters. In RSA a reasonable range for model output is hypothesized. Model parameters for simulations with output falling in the reasonable range are recorded as set A, and model parameters for simulations with output falling outside the reasonable range are recorded as set B. Empirical probability distributions are developed for model-parameter values for simulations in each set. These empirical probability distributions are compared [e.g., using the Kolmogorov-Smirnov test; Law and Kelton (1991), pp. 387–391]. If sets A and B are significantly different for a given parameter, that parameter significantly affects model-prediction uncertainty. Otherwise, that parameter is not important to model-prediction uncertainty.

First-Order Reliability Analysis (FORA)

In FORA, a Taylor series expansion of the model output is truncated after the first-order term

$$C = g(\mathbf{X}_e) + \sum_{i=1}^p (x_i - x_{mi})(\partial g/\partial x_i)_{\mathbf{X}_e} \quad (1)$$

where C = concentration of the constituent simulated in the selected water-quality model; $g(\)$ = functional representation of the procedures simulating constituent C in the water-quality model; \mathbf{X}_e = the vector of uncertain basic variables (model-input variables, model parameters, etc.) representing the expansion point; p = number of basic variables x_i ; and the subscript \mathbf{X}_e indicates that the partial derivative is taken at the expansion point.

In FORA applications to water-resources engineering, the expansion point is commonly the mean value (or some other convenient central value) of the basic variables. Thus, the expected value and variance of the performance function are

$$E[C] \approx g(\mathbf{X}_m) \quad (2)$$

$$\text{Var}(C) = \sigma_C^2 \approx \sum_{i=1}^p \sum_{j=1}^p (\partial g/\partial x_i)_{\mathbf{X}_m} (\partial g/\partial x_j)_{\mathbf{X}_m} E[(x_i - x_{mi})(x_j - x_{mj})] \quad (3)$$

where σ_C = standard deviation of C ; and \mathbf{X}_m = vector of mean values of the basic variables. If the basic variables are statistically independent, the variance of C becomes

$$\text{Var}(C) = \sigma_C^2 \approx \sum_{i=1}^p [(\partial g/\partial x_i)_{\mathbf{X}_m} \sigma_i]^2 \quad (4)$$

where σ_i = the standard deviation of basic variable i . In some cases, the derivatives may be determined analytically.

To estimate the cumulative distribution function (CDF) and probability density function (PDF) of C , it is typically assumed that C is normally distributed, and the exceedance probability P_E (complement of the CDF) for a given target concentration C_T , is estimated as

$$P_E = 1 - \Phi\{(C_T - E[C])/\sigma_C\} \quad (5)$$

where $\Phi\{ \}$ is the standard normal integral. The normal (Gaussian) assumption has several practical advantages that are discussed in detail by Yen et al. (1986) and Melching (1995).

In comparison with the simulation-based methods, simplicity is the primary advantage of FORA. When the Taylor series expansion is taken at the mean of the basic variables, only the first two statistical moments of the basic variables and simple sensitivity calculations are required in FORA. However, when applied to engineering design problems, the method has several theoretical and/or conceptual problems (Melching 1992; Cheng 1982). The main problem of the method is that a single linearization of the model-output function at the central values of the basic variables is assumed to represent the statistical properties of model output over the complete range of basic variable values. For nonlinear systems, this assumption becomes more inaccurate as the basic variables depart from the central values. For engineering design, the method may be especially inaccurate because design failure should result only because of extreme values of the basic variables describing the system. The assumption to use a normal distribution for the model output is only weakly supported, and the method cannot include available information on basic variable probability distributions.

FORA, with the expansion at the mean values, has been applied successfully in water-quality modeling, despite the conceptual problems. Burges and Lettenmaier (1975) and Melching and Anmangandla (1992) have found reasonably good agreement between results from FORA and Monte Carlo simulation for estimation of statistical characteristics of dissolved-oxygen (DO) concentrations simulated with the Streeter-Phelps (1925) model. Yoon (1994) found reasonably good agreement between results from FORA and Monte Carlo simulation for estimation of statistical characteristics of DO, biochemical oxygen demand (BOD), ammonia, and chlorophyll a concentrations simulated with the QUAL2E model (Brown and Barnwell 1987). In the Monte Carlo simulations done by Burges and Lettenmaier (1975) and Yoon (1994) all parameters were normally distributed, whereas in the Monte Carlo simulations done by Melching and Anmangandla (1992) cases where all parameters were normally, lognormally, uniformly, and Gamma distributed were considered.

In FORA, the fraction of model-output variance contributed by each basic variable can be determined directly from (4) (or similar formulations for correlated basic variables). This FORA approach to determining key model parameters has been applied to several water-quality models. Chadderton et al. (1982) applied FORA to determine the relative contributions of reaeration rate, deoxygenation rate, initial DO concentration, and BOD load on output uncertainty for the

Streeter-Phelps (1925) model for streamflow conditions typical for natural streams. Scavia et al. (1981) applied FORA to determine the relative contributions of seven of 22 model parameters, initial conditions, and loads on output uncertainty for a nonlinear, seasonal-food-chain, nutrient-cycle eutrophication model of Saginaw Bay, on Lake Huron, in Michigan. Brown and Barnwell (1987) applied FORA to determine the relative contributions of all parameters in QUAL2E on the uncertainty of estimates of carbonaceous BOD and DO concentrations for the Withlacoochee River in Georgia and Florida.

Comparison of Methods

Yeh and Tung (1993) compared the results of correlation analysis, rank correlation analysis, and FORA in determining the key parameters for a model of the movement of borrow pits in alluvial streams. The correlation approaches and FORA resulted in considerably different lists of key parameters. Correlation approaches are used to assess the global importance (i.e., importance over a wide range of possible basic variable values) of a basic variable (McKay 1988; Yeh and Tung 1993), whereas FORA is used to assess the local importance (about the best estimate of model output) of a basic variable. The choice of the most appropriate method depends on the model use. If a model is being developed or validated, global measures are probably of greater importance than local measures. For fine tuning model output from models that are considered well identified and well calibrated, local measures are probably of greater importance than global measures. In the case studied in this paper, it is assumed that the model is well identified and well calibrated and reduction of prediction uncertainty is

sought. Therefore, the local measures of parameter importance obtained from FORA are selected. Monte Carlo simulation is applied to test accuracy of the key parameter identification in FORA.

EXAMPLE APPLICATION

Description of the Passaic River

The freshwater portion of the Passaic River upstream of Dundee Dam drains approximately 2,090 km² in northeastern New Jersey. The watershed of the Passaic River and the modeled portion of the Passaic River system are shown in Fig. 1. The Passaic River may be divided into three geographic regions: the upper, middle, and lower regions (NJDEP 1987). The upper region is approximately 45 km long, including the major downstream section of the Dead River and the Passaic River main stem between the confluence with the Dead River and the confluence with the Whippany River. The middle region of the Passaic River is approximately 24 km long and extends from the confluence with the Whippany River to the confluence with the Pompton River. The lower region of the Passaic River is approximately 26.9 km long and extends from the confluence with the Pompton River to the end of the freshwater reach at Dundee Dam. The river upstream of Chatham in the upper region is significantly steeper than the river downstream of Chatham (0.37% slope upstream and 0.028% slope downstream). The low-flow hydraulics in the downstream portion of the upper region and in the middle region are controlled by pool and riffle sequences. The middle region is also substantially affected by five major wetlands (Great Piece Meadows, Hatfield Swamp, Troy Meadows, Black Meadow, and Bog and Vly Meadow). Over 90% of the lower region is in

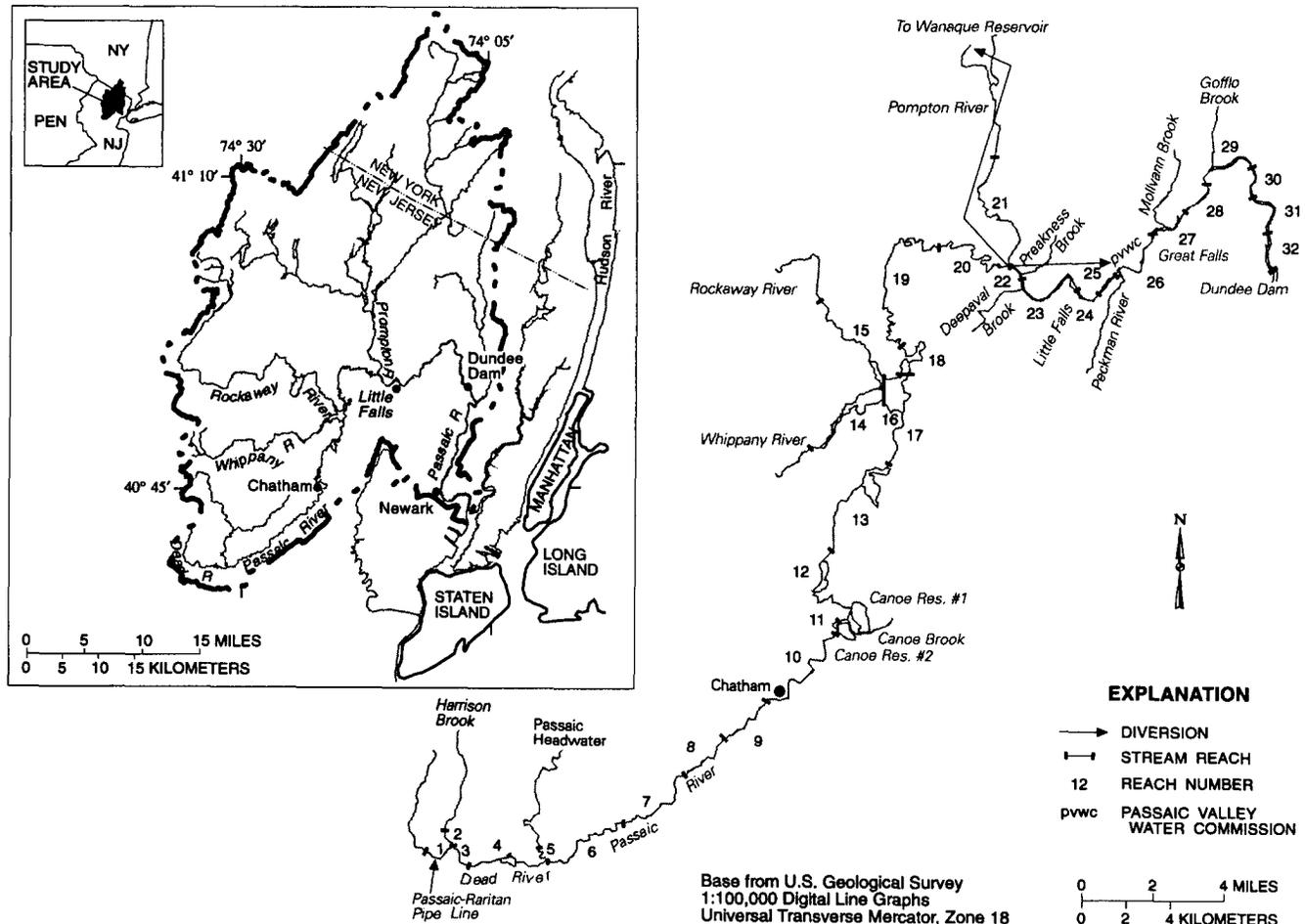


FIG. 1. Location of Model Reaches Simulated in QUAL2E-Passaic and Diversions to and from Passaic River in Northeast New Jersey

backwater from three low-head dams and the river resembles ponds in several areas.

Relatively large wastewater flows are discharged to the Passaic River and its tributaries. There are eight major municipal wastewater treatment plants (WWTPs) in the upper region, one major municipal WWTP in the middle region, and two major municipal WWTPs and 35 industrial WWTPs in the lower region. It was estimated that during the 1981 drought more than 80% of the streamflow at the Passaic Valley Water Commission at Little Falls was effluent sewage from upstream WWTPs (NJDEP 1987). The majority of these WWTPs discharge into the Passaic River or its tributaries at locations close to the river. The main stem of the Passaic River and short reaches of its main tributaries (Dead River, Whippany River, Rockaway River, and Pompton River) are simulated in the model developed by the New Jersey Department of Environmental Protection (1987).

The model prediction uncertainty of four water-quality constituents was considered: DO, carbonaceous BOD (CBOD), ammonia, and chlorophyll *a*. These constituents were selected because they are significant problems in the Passaic River, as discussed in detail by the New Jersey Department of Environmental Protection (1987) and summarized briefly below. DO concentrations in much of the mainstem of the Passaic River are below 4 mg/L and anoxic conditions have been observed. CBOD was selected because of its strong effect on DO concentrations. Persistently high levels of ammonia are present in the upper and middle regions of the Passaic River. Consequently, the molecular ammonia level (a measure of ammonia toxicity) may often be above the stipulated limit (0.05 mg/L) in almost the entire length of the river considered in this study. Large portions of the lower region of the Passaic River are highly eutrophic because of large wastewater flows and extensive backwater effects. Thus, chlorophyll *a* is important as a surrogate for algae populations.

QUAL2E Stream Water-Quality Model

In QUAL2E model simulations (Brown and Barnwell 1987), the stream is conceptualized as a string of completely mixed reactors that are linked sequentially by advective transport and dispersion. Sequential groups of these reactors are defined as reaches. Each reach is divided into computational elements with identical length, hydrogeometric properties, and biological rate constants. The hydrogeometric properties and biological rate constants may change between reaches, but the computational-element length remains constant throughout the simulated stream. Up to 15 water-quality constituents in any combination selected by the user can be simulated in QUAL2E. Constituents that can be simulated in the model are DO, CBOD, temperature, algae as chlorophyll *a*, components of the nitrogen cycle as nitrogen (organic nitrogen, ammonia, nitrite, and nitrate), components of the phosphorus cycle as phosphorus (organic and dissolved phosphorus), coliforms, an arbitrary nonconservative constituent, and three arbitrary conservative constituents. The primary application of QUAL2E is simulation of DO concentration in a stream and the interactions between DO and CBOD, the nitrogen cycle, algae (dependent on the nitrogen and phosphorus cycles), sediment oxygen demand (SOD), and atmospheric reaeration. Details on these interactions as simulated in QUAL2E are presented in Brown and Barnwell (1987).

QUAL2E was applied to the Passaic River by the New Jersey Department of Environmental Protection (1987). This model, referred to as QUAL2E-Passaic, was applied in this study. QUAL2E-Passaic includes 32 reaches (Fig. 1) and 257 computational elements each 0.4 km long to simulate approximately 96 km of the main stem Passaic River and small portions of the main tributaries. Uncertainty analysis subroutines

are included in QUAL2E (QUAL2E-UNCAS) with options for sensitivity analysis, FORA, and Monte Carlo simulation. The uncertainty-analysis procedures illustrated in this paper can be applied to any stream system of interest with QUAL2E-UNCAS with the number of reaches allowed in QUAL2E-UNCAS computations increased from 25 as necessary. Computation of the CDF of model output by FORA is not performed in QUAL2E-UNCAS, and the user must apply (5) manually with the mean and standard deviation computed in QUAL2E-UNCAS. Whereas the CDF of model output is computed in the Monte Carlo simulation option in QUAL2E-UNCAS. The work reported in this paper is part of a larger study of uncertainties in water-quality modeling (Yoon 1994), and information for some aspects of the larger study could not be computed with QUAL2E-UNCAS. Therefore, programs for application of FORA and Monte Carlo simulation were developed for this study (Yoon 1994) and applied to QUAL2E-Passaic.

Estimation of Model-Parameter Uncertainties

The most important aspect of applying reliability-analysis methods, such as FORA and Monte Carlo simulation, for assessment of model-prediction uncertainty, is to characterize properly the uncertainty in the individual basic variables. The uncertainty of each parameter was estimated from a literature review (Zison et al. 1978; Bowie et al. 1985; Brown and Barnwell 1987) and engineering judgment. QUAL2E-Passaic (NJDEP 1987) was calibrated for water-quality constituent-concentration data collected during an intensive 3-day synoptic study of the Passaic River in August 1983. Multiple measurements of each water-quality constituent of interest, flow, and temperature were made at 32 locations throughout the Passaic River representing each of the computational reaches. The model was verified for two sets of synoptic data collected for each constituent at each location in October 1983 and September 1984. The verification for September 1984 is particularly noteworthy because advanced waste treatment became operational at the Bernards Sewage Treatment Plant on the Dead River between October 1983 and September 1984. The advanced waste treatment resulted in a massive change in loads substantially affecting constituent concentrations as far as 20 km downstream. Therefore, the September 1984 verification represents a "significantly perturbed condition relative to the calibration data" providing the type of data set recommended by Thomann (1982) to provide an adequate test of the model. Thus, QUAL2E-Passaic was considered an adequate model for simulation of water quality in the Passaic River and the majority of estimated coefficient of variation (COV) values were selected at the high end of the range for typical QUAL2E applications in Brown and Barnwell (1987, p. 86). The estimated COVs for each model parameter are listed in Table 1.

Some parameters are assumed to have little uncertainty, whereas SOD and reaeration-rate coefficients are assumed to have COVs of 30% and 50%, respectively. Wilson and Macleod (1974) reviewed 16 published equations for estimation of the reaeration-rate coefficient and checked for agreement with field and laboratory data covering widely different physical and hydraulic conditions. They found that even the best of the available equations gives unreliable estimates. House and Skavroneck (1981) compared reaeration-rate coefficients estimated with 20 published equations to observed values from the propane-area modified-tracer method on two streams in Wisconsin. The Langbein and Durum (1967) equation, used in QUAL2E-Passaic, was one of the five most accurate equations applied considered by House and Skavroneck (1981) with a mean error of 49% in the estimates of reaeration-rate coefficients for the Wisconsin streams. The physical characteristics of the Passaic River are different from those of the Wisconsin

TABLE 1. Estimated Coefficient of Variation Values for Input Parameters Based on Literature Review

Parameter (1)	Definition (2)	Coefficient of variation (%) (3)	Notes* (4)
a	Evaporation coefficient a	10.0	1
KBOD	5-day to ultimate CBOD conversion coefficient	10.0	5
b	Evaporation coefficient b	10.0	1
d	Dust attenuation coefficient	10.0	1
α_5	Oxygen-uptake by ammonia oxidation	5.97	2
μ_{max}	Algal maximum-specific-growth rate	10.0	1
TFACT	Algae/temperature solar radiation factor	10.0	1
α_6	Oxygen uptake by nitrate oxidation	2.89	2
α_4	Oxygen uptake by algae	5.10	2
KNITRF	Nitrification inhibition coefficient	3.93	2
K_1	CBOD decay rate	25.0	1
K_3	CBOD settling rate	25.0	1
K_4	SOD rate	30.0	3
K_2	Reaeration rate coefficient	50.0	4
β_1	Rate constant for the biological oxidation of ammonia to nitrate	25.0	1
α_0	Chlorophyll a to algae ratio	5.0	1
α_1	Algal settling rate	10.0	1
λ_1	Non-algae light extinction coefficient	5.0	1

*1 = based on the typical range for the coefficient of variation for such parameters reported by Brown and Barnwell (1987, p. 86); 2 = based on assuming a triangular distribution with the modeled value at the apex over the reasonable range for this parameter reported by Brown and Barnwell (1987, pp. 54–56); 3 = based on a review of U.S. rivers by Bowie et al. (1985, p. 189); 4 = based on the performance of the Langbein-Durum equation for small streams in Wisconsin determined by House and Skavronck (1981); and 5 = based on engineering judgment.

streams for many reaches. However, the uncertainty determined for the Wisconsin streams was taken as representative of a case where the Langbein and Durum equation works well. Calibration of QUAL2E-Passaic indicated that the Langbein and Durum equation works well for the Passaic River. Therefore, the COV of the reaeration-rate coefficient was estimated to be 50% for the Passaic River.

In this paper, correlations between model parameters were assumed to be zero. This is probably not true, especially for the reach-varying parameters; however, no data are available on the likely magnitude of these correlations. Therefore, rather than selecting a correlation value without documentation, consideration of uncorrelated parameters was selected. If parameters are positively correlated, this assumption results in underprediction of the overall model-prediction uncertainty resulting from uncertainty in model parameters. However, as described in the following, the uncertainties in a few key parameters almost completely dominated the uncertainty of the simulated DO, CBOD, ammonia, and chlorophyll a concentrations. Further, these key parameters most likely have strong correlations between reaches. Thus, the key parameters identified in FORA would be unlikely to change if parameter correlations were considered.

Determination of Key Sources of Uncertainty

FORA was applied to determine the parameters that significantly contributed to uncertainty in QUAL2E-Passaic estimation of the lowest DO concentration and the highest CBOD, ammonia, and chlorophyll a concentrations throughout the Passaic River corresponding to 7-day, 10-yr low flow with typical effluent discharges. The derivatives required in FORA were determined numerically by increasing the parameters val-

TABLE 2. Contribution of Key Model Input Parameters to Output Variance of QUAL2E-Passaic

Parameter (1)	Contribution (%) (2)	Remarks (3)
(a) Lowest DO concentration (reach 3)		
Reaeration coefficient	49.351	Reach of interest
Reaeration coefficient	25.087	One reach upstream
Ammonia oxidation rate	12.299	Reach of interest
SOD	4.428	One reach upstream
Ammonia oxidation rate	4.015	One reach upstream
(b) Highest CBOD concentration (reach 2)		
BOD decay rate	81.800	Reach of interest
BOD settling rate	13.088	Reach of interest
(c) Highest ammonia concentration (reach 2)		
Ammonia oxidation rate	96.152	Reach of interest
SOD rate	3.848	Reach of interest
(d) Highest chlorophyll a concentration (reach 32)		
Algal maximum-specific-growth rate	93.170	System-wide
Algae/temperature solar radiation factor	5.655	System-wide

ues one at a time by 5%, determining the change in concentration of the constituent of interest, and dividing the change in concentration by the increase in the parameter value. The application of a 5% increment in the parameter values was recommended by Brown and Barnwell (1987) for uncertainty calculations in QUAL2E-UNCAS. The locations of the lowest DO concentration and the highest CBOD, ammonia, and chlorophyll a concentrations were reach 3, element 1; reach 2, element 1; reach 2, element 1; and reach 32, element 6, all shown in Fig. 1. In the FORA, all system-wide parameters and the reach-varying parameters for the reach in which the key output concentrations resulted (reach N) and the reach upstream (reach $N - 1$) were considered model parameters that could potentially have a significant effect on simulation uncertainty.

The contribution in percent of key model parameters to the variance in the lowest DO concentration and the highest CBOD, ammonia, and chlorophyll a concentrations throughout the Passaic River estimated in QUAL2E-Passaic for the 7-day, 10-yr low flow with typical effluent discharges is listed in Table 2. Five parameters account for more than 90% of the estimation variance in the key constituents: reaeration rate and ammonia-oxidation rate for DO, CBOD-decay rate and CBOD-settling rate for CBOD, ammonia-oxidation rate for ammonia, and algal maximum-specific-growth rate for chlorophyll a .

Parameters related to CBOD would normally be expected to significantly affect the lowest DO concentration. WWTPs discharging into the Passaic River and tributaries already meet rather stringent standards for secondary treatment and removal of CBOD. Specifically, the permitted CBOD discharges from the WWTPs discharging into the Passaic River range from 8 to 35 mg/L with an average of 20 mg/L; less than 24 mg/L represents advanced treatment levels (NJDEP 1987). Thus, with a relatively high level of CBOD removal already achieved, CBOD related parameters have little effect on uncertainty in the estimated lowest DO concentration. Further, the effect of ammonia oxidation on the lowest DO concentration supports the current requirement to install nitrification processes at WWTPs throughout the Passaic River Basin.

In sensitivity analysis, the key parameters are identified by calculating and ranking the sensitivity coefficients. The sensitivity coefficients are often normalized to provide a more balanced ranking. The normalized sensitivity coefficients $SN_{j,i}$ are defined as

$$SN_{ji} = (\Delta C_j / C_{j0}) / (\Delta x_i / x_{i0}) \quad (6)$$

where ΔC_j = change in the estimated concentration of constituent j resulting from change Δx_i in parameter i with all other parameters kept at their original values; C_{j0} = estimated concentration of constituent j when all parameters are at their original values; and x_{i0} = original value for parameter i . The rankings of the most important parameters determined in FORA were compared with those from normalized sensitivity analysis for DO and chlorophyll a concentrations. The results from FORA and normalized sensitivity analysis are the same for the five parameters having the largest effect on uncertainty of estimated chlorophyll a concentrations. For estimates of DO concentration, however, the rankings obtained from normalized sensitivity analysis and FORA differ substantially as presented in Table 3.

The key model parameters affecting the variance in esti-

TABLE 3. Comparison of Ranking of Key Parameters Affecting Estimated DO Concentrations Applying Normalized Sensitivity Analysis and FORA

Model parameter (1)	Rank among 17 Parameters Estimated by	
	Normalized sensitivity analysis (2)	FORA (3)
Reaeration rate (reach 3)	2	1
Reaeration rate (reach 2)	4	2
Ammonia oxidation rate (reach 3)	3	3
SOD rate (reach 2)	15	4
Ammonia oxidation rate (reach 2)	7	5
Oxygen uptake by ammonia oxidation	1	6
Algal maximum-specific-growth rate	4	7
Nitrification inhibition coefficient	4	12

TABLE 4. Locations Selected for Uncertainty Analysis

No. (1)	Reach- element (2)	River kilometer (3)	Remarks (4)
1	2-1	0.80	Highest CBOD and ammonia concentrations
2	3-1	2.40	Lowest DO concentration
3	6-13	12.40	—
4	8-7	20.40	—
5	9-11	30.00	—
6	12-12	42.40	—
7	18-4	53.20	—
8	20-3	64.40	—
9	25-1	74.80	—
10	29-5	84.40	—
11	32-6	94.00	Highest chlorophyll a concentration

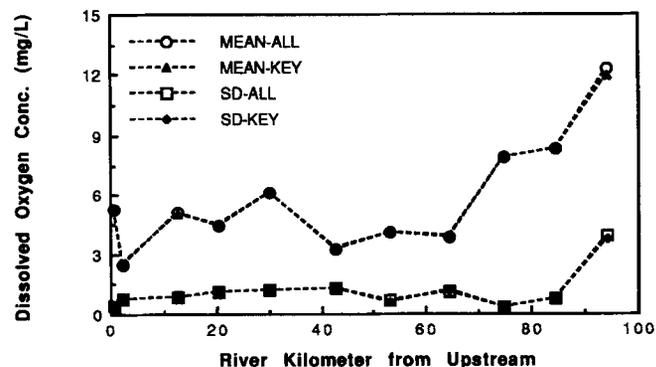


FIG. 2. Monte Carlo Simulation Estimates of Mean and Standard Deviation of DO along Passaic River for Cases with All Model Parameters Variable and Only Key Model Parameters Variable

mates of the lowest DO concentration and the highest CBOD, ammonia, and chlorophyll a concentrations were assumed to affect significantly the variance in estimated DO, CBOD, ammonia, and chlorophyll a throughout the Passaic River. Eleven locations were selected to study model-prediction uncertainty throughout the Passaic River (see Table 4). The locations were fairly evenly distributed throughout the river and with diverse values of the model parameters.

The key model parameters significantly affecting model simulation uncertainty determined in FORA were tested with Monte Carlo simulation. Results were compared from two sets of Monte Carlo simulations: (1) All 10 systemwide and eight reach-varying model parameters were considered uncertain; and (2) only the parameters listed in Table 2 were considered uncertain. The values for these parameters were generated independently in space. All model parameters were assumed to be normally distributed. To obtain reasonable estimates of the mean and standard deviation of the simulated constituent concentrations, 1,000 Monte Carlo simulations were made for cases (1) and (2). When randomly generating the values of the model parameters, occasionally a value is generated that is physically unrealistic. Simulation applying unrealistic parameter values resulted in computational problems. Therefore, the Monte Carlo simulation procedure was modified to omit physically unrealistic parameter values that resulted in computational failure.

The mean and standard deviation of the estimated DO, CBOD, ammonia, chlorophyll a concentrations at the 11 locations listed in Table 4 are illustrated in Figs. 2–5, respectively, for the two sets of Monte Carlo simulations. The results of the two cases are generally in close agreement for all con-

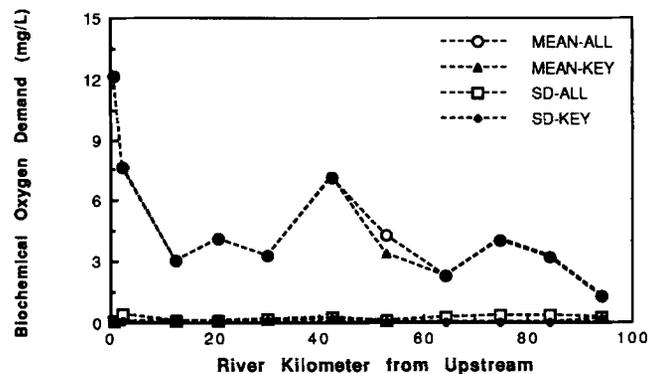


FIG. 3. Monte Carlo Simulation Estimates of Mean and Standard Deviation of CBOD along Passaic River for Cases with All Model Parameters Variable and Only Key Model Parameters Variable

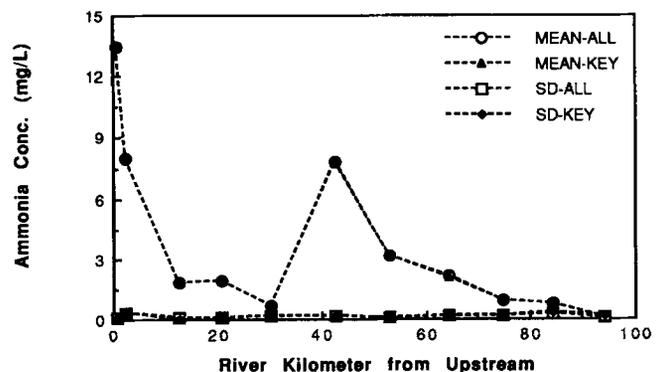


FIG. 4. Monte Carlo Simulation Estimates of Mean and Standard Deviation of Ammonia along Passaic River for Cases with All Model Parameters Variable and Only Key Model Parameters Variable

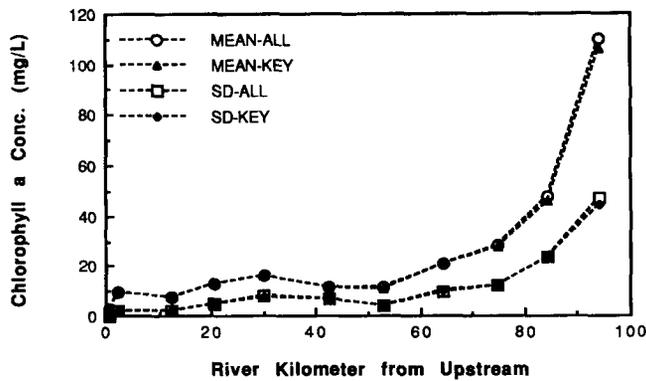


FIG. 5. Monte Carlo Simulation Estimates of Mean and Standard Deviation of Chlorophyll *a* along Passaic River for Cases with All Model Parameters Variable and Only Key Model Parameters Variable

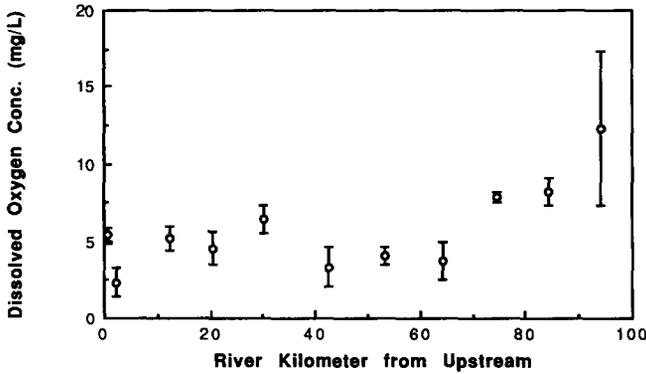


FIG. 6. FORA Estimates of Mean ± 1 Standard Deviation Error Bar for QUAL2E-Passaic Simulations of DO in Passaic River

stituents as shown in Figs. 2–5. The largest difference is 0.15 mg/L in the standard deviation of CBOD. Overall, these results indicate that the key parameters determined by FORA are appropriate for QUAL2E-Passaic simulation of DO, CBOD, ammonia, and chlorophyll *a* concentrations.

Constituent Prediction Uncertainty along the River and Sampling Design

FORA was applied to estimate the mean and standard deviation of the estimated DO, CBOD, ammonia, and chlorophyll *a* concentrations at the 11 locations listed in Table 4. The mean and one standard deviation error bars are presented in Figs. 6–9 for DO, CBOD, ammonia, and chlorophyll *a* concentrations, respectively. For chlorophyll *a* at upstream locations, CBOD, and ammonia, the one standard deviation error bars are so small that they lie within the symbols for the mean in Figs. 7–9. DO (Fig. 6) and chlorophyll *a* (Fig. 9) concentrations have large uncertainties along the river. Thus, the parameters significantly affecting the prediction uncertainty of these constituents require additional sampling to reduce parameter uncertainty.

CBOD (Fig. 7) and ammonia (Fig. 8) concentration estimates have very small standard deviations indicating that model-parameter uncertainty has insignificant effects on prediction uncertainty for these constituents in the QUAL2E-Passaic estimations. This does not mean that these constituents are reliably estimated in QUAL2E-Passaic because uncertainties in CBOD, organic nitrogen, and ammonia loads could significantly affect overall prediction uncertainty. However, it does indicate that (1) additional sampling is not required; and (2) special sampling programs need not be designed to more accurately determine the model parameters that simulate the CBOD and ammonia reactions in the Passaic River. The orig-

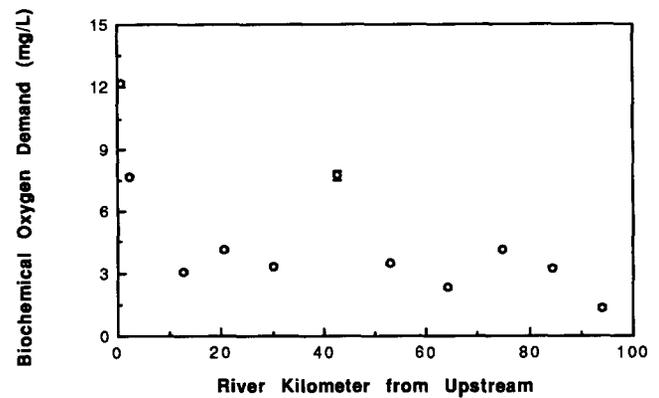


FIG. 7. FORA Estimates of Mean ± 1 Standard Deviation Error Bar for QUAL2E-Passaic Simulations of CBOD in Passaic River

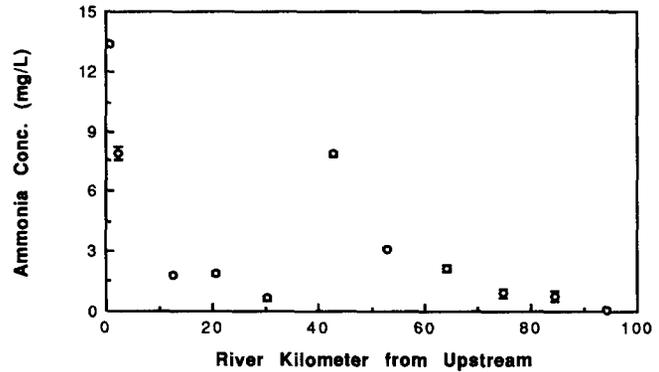


FIG. 8. FORA Estimates of Mean ± 1 Standard Deviation Error Bar for QUAL2E-Passaic Simulations of Ammonia in Passaic River

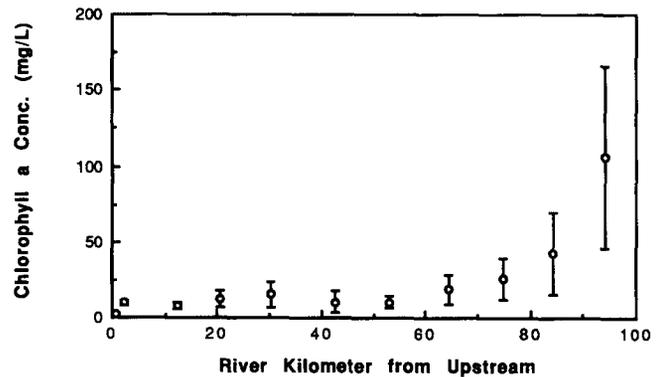


FIG. 9. FORA Estimates of Mean ± 1 Standard Deviation Error Bar for QUAL2E-Passaic Simulations of Chlorophyll *a* in Passaic River

inal stream survey data are adequate to define these parameters. Thus, the set of five parameters identified as significantly affecting model-output uncertainty can be reduced to two parameters for which additional data could be important: reaeration-rate coefficient and algal maximum-specific-growth rate. The ammonia-oxidation rate effect on DO is significant, but ammonia concentration is predicted with low uncertainty with respect to parameter uncertainty and additional data probably would not improve the estimate of the ammonia-oxidation rate.

The reaeration rate can be measured directly in streams by tracer methods. These measurements are relatively expensive to make, but the potential reduction in model-prediction uncertainty obtainable with these measurements is high. Bennett and Rathbun (1972) report that the expected error of reaeration rates determined by tracer methods is 15%, whereas it is about 65% for reaeration rates determined by DO balance methods

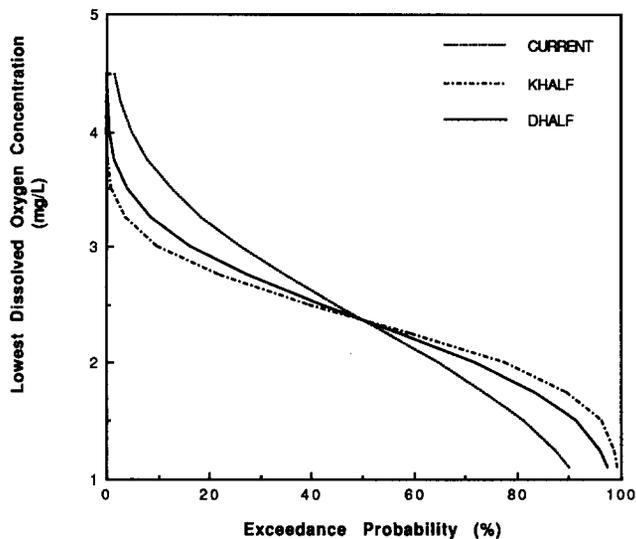


FIG. 10. FORA Estimates of Exceedance Probability for Lowest DO along Passaic River for Current Level of Model-Parameter Uncertainty and Two Cases of Reduced Model-Parameter Uncertainty

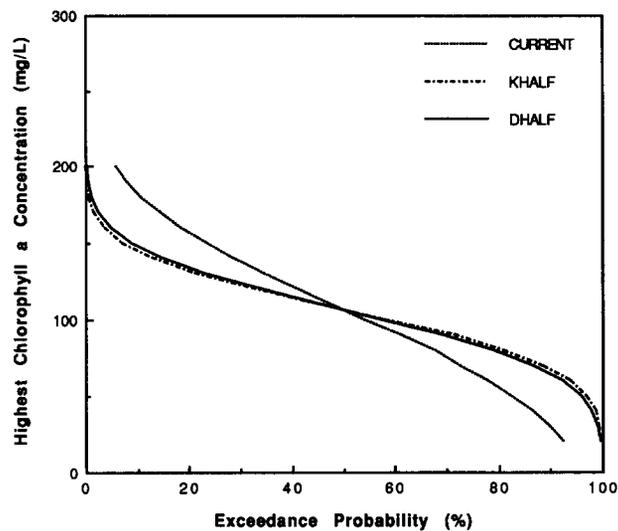


FIG. 11. FORA Estimates of Exceedance Probability Curves for Highest Chlorophyll *a* along Passaic River for Current Level of Model Parameter Uncertainty and Two Cases of Reduced Model-Parameter Uncertainty

(essentially equivalent to model calibration). Thus, the cost of developing a reaeration-rate estimation equation or verifying one of the standard equations for a specific river compared to the relative reduction in prediction uncertainty is a promising area for study. Yoon (1994) has studied the cost and reliability of developing site-specific reaeration-rate estimation equations in detail.

In the Passaic River, the uncertainty in chlorophyll *a* simulation is significantly large only in the downstream portion of the river (Fig. 9). Thus, additional sampling to reduce the uncertainty in the algal maximum-specific-growth rate should be focused on in the downstream reaches of the river between 80 and 100 km from upstream.

Effects of Reduction in Parameter Uncertainty

Model-output uncertainty can be decreased by reducing the uncertainty in key input parameters. FORA was applied to compute the exceedance probability of the lowest DO concentration and highest chlorophyll *a* concentration for the 7-day,

10-yr low flow with typical effluent discharges for three levels of parameter uncertainty:

- CURRENT—the COV for each parameter as given in Table 1 (the “current” level of parameter uncertainty)
- KHALF—the COVs of the parameters listed in Table 2 reduced by 50% and the COV for all other parameters kept at the value shown in Table 1 (reflecting improved knowledge of the key parameters, identified in FORA, from carefully designed field sampling)
- DHALF—the COV of the dominant parameter (reaeration-rate coefficient for DO and algal maximum-specific-growth rate for chlorophyll *a*) reduced by 50% and the COV for all other parameters kept at the value shown in Table 1 (reflecting improved knowledge of two dominant parameters from carefully designed field sampling)

The exceedance probabilities estimated by FORA for these three cases are illustrated in Figs. 10 and 11 for DO and chlorophyll *a*, respectively. The exceedance probability curve would be a step function if the model simulation is completely deterministic and perfectly reliable. As shown in Figs. 10 and 11, the reduction of the uncertainty in a single dominant parameter can greatly reduce the uncertainty of predictions of DO and chlorophyll *a* made in QUAL2E-Passaic. For example, reducing the uncertainty in the reaeration-rate coefficient from the CURRENT condition to the DHALF condition increases the confidence that the lowest DO concentration will be greater than 1 mg/L from 90 to 98%. The effect of reducing the uncertainty in a single parameter is larger for chlorophyll *a* than for DO because algal maximum-specific-growth rate contributes 93% of the variance of estimated chlorophyll *a* concentrations, whereas reaeration rate contributes 74% of the variance of estimated DO concentrations (Table 2).

CONCLUSIONS

This paper has illustrated that a simple method based on FORA may be applied to determine key sources of uncertainty affecting prediction uncertainty for complex water-quality models. The method is as follows:

1. A literature search is done and discussions are held with experienced surface water-quality modelers to determine the relative uncertainty in each of the model parameters.
2. FORA is applied to determine which of the parameters in the multiconstituent water-quality model contribute significant uncertainty to the simulation of key water-quality constituents. The identified parameters become the focus of data collection to improve model-prediction uncertainty.
3. FORA is applied to determine the prediction uncertainty for the key water-quality constituents. If any of these constituents have acceptably low prediction uncertainty, further data collection to more accurately determine the parameters significantly affecting simulation of this constituent will not result in improved simulation.

FORA is applied for computational efficiency, producing results equivalent to those from more computationally intensive and theoretically correct reliability methods, such as Monte Carlo simulation (Yoon 1994).

The reliability-analysis method was applied to determine the key parameters affecting prediction uncertainty for dissolved oxygen, carbonaceous biochemical oxygen demand, ammonia, and chlorophyll *a* along the Passaic River in New Jersey simulated with QUAL2E. The reliability analysis considered uncertainties in 10 systemwide and eight reach-varying model parameters. The uncertainty of estimated concentrations of

CBOD and ammonia owing to model-parameter uncertainty alone was found to be acceptably small. Data collection to refine parameters significantly affecting these constituents would not greatly reduce model-prediction uncertainty. The uncertainty of estimated concentrations of DO and chlorophyll *a* resulting from model-parameter uncertainty alone was found to be significant. However, for each constituent, a single model parameter had a dominant effect on prediction uncertainty (reaeration-rate coefficient for DO and algal maximum-specific-growth rate for chlorophyll *a*). Reduction of the uncertainty in reaeration rate and algal maximum-specific-growth rate were shown to significantly improve model-prediction uncertainty of DO and chlorophyll *a*, respectively.

Prediction uncertainty of four water-quality constituents with a complex multiconstituent water-quality model involving 18 model parameters was found to be significantly improved by reducing the uncertainty in only two of the model parameters. It is hoped that these results will encourage water-quality modelers and planners to do similar reliability analyses leading to more efficiently planned sampling programs to reduce model-prediction uncertainty.

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APPENDIX II. NOTATION

The following symbols are used in this paper:

- C = concentration of the water-quality constituent simulated in the selected water-quality model;
- C_{j0} = estimated concentration of constituent j when all uncertain basic variables are at their original values in normalized sensitivity analysis;
- C_T = target concentration whose exceedance probability is sought;
- $g()$ = functional representation of the water-quality model procedures used to simulate a given water-quality constituent;
- P_E = exceedance probability;
- p = number of uncertain basic variables (model-input variables, model parameters, etc.);
- $SN_{j,i}$ = normalized sensitivity coefficient of constituent j to uncertain basic variable i ;
- \mathbf{X}_e = vector of uncertain basic variables (model-input variables, model parameters, etc.) representing expansion point;
- \mathbf{X}_m = vector of means of uncertain basic variables (model-input variables, model parameters, etc.);
- x_{i0} = original value for uncertain basic variable i in normalized sensitivity analysis;
- ΔC_j = change in estimated concentration of constituent j resulting from change Δx_i in uncertain basic variable i with all other parameters kept at their original values;
- Δx_i = change in uncertain basic variable i ;
- σ_C = standard deviation of water-quality constituent simulated in the selected water-quality model;
- σ_i = standard deviation of uncertain basic variable i ; and
- $\Phi()$ = standard normal integral.