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Evaluating the Uncertainty in Water Quality Predictions - A Case Study

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Abstract

A method for assessing model result uncertainty is presented and applied to a case where a paper mill wastewater is discharged into an estuary in the Southeastern U.S.. Model result uncertainty was quantified by incorporating the uncertainty analysis into model calibration. The two-dimensional, laterally averaged model CE-QUAL-W2 was used to predict water quality conditions. The water quality model was calibrated against field measurements of longitudinal and vertical variations in salinity, dissolved oxygen, and biochemical oxygen demand (BOD) concentrations. A quantitative, multi-constituent criteria for acceptable calibration was used to identify plausible parameter sets. A collection of plausible parameter sets was then identified, and used to assess the uncertainty in dissolved oxygen prediction, and the uncertainty in predicted system response to a reduction in organic matter loading. A search procedure was also developed to minimize the calibration criteria statistic and to assess the range of model predictions. Plausible parameter sets differed widely in their parameter values, and they produced widely different dissolved oxygen concentration predictions. The system response to reduced loading, however, was found to be very similar between the plausible parameter sets.

Introduction

Water quality models are commonly used to determine suitable limits in wastewater discharge permits (e.g. Gong et al. 1997). To establish a permit limit, the model is used to provide quantitative impact assessments for various discharge scenarios. In substantiating the conclusions of these studies, modelers typically per-form an "uncertainty analysis," where the uncertainty of model predictions is quantified. The most common uncertainty analysis is the "sensitivity analysis", where variability in model results is measured as systematic changes are made to a single set of input

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parameters established through model calibration (e.g., Bowen et al. 1992, Chapelle et al. 1994). The calibrated parameter set may be determined either through the traditional "trial-and-error" approach, through an optimization procedure (e.g. Neuman 1973, Rinaldi et. al 1979), or by solving an inverse parameter identification problem (e.g., Yeh 1986, Panchang and Richardson 1993, Shen and Kuo 1996).

Although a sensitivity analysis is often insightful, it may not give an accurate estimate of model uncertainty, for the following reasons:

- parameter ranges may be unrealistically large or small, since they are typically chosen without considering whether they produce a calibrated model,
- inter-parameter covariances are typically ignored, and
- synergistic effects among parameters are typically not considered.

The underlying problem with the standard sensitivity analysis procedure is that it is done independently of model calibration. In this article we present the results of a modeling study where the uncertainty of model results have been explicitly quantified by incorporating the uncertainty analysis into model calibration. The procedure and the analysis is developed for application to water quality prediction from an earlier model uncertainty analysis for groundwater flow (Brooks et al. 1994).

In the method developed here, many "plausible" parameters sets are selected from a larger collection of candidate sets. Each plausible parameter set produces model results that meet a quantitative calibration criteria. Model prediction uncertainty is assessed by determining the degree to which model results vary between these plausible parameter sets. This variability is examined both by running the model repeatedly with different plausible parameter sets, and by using an automated search technique that looks through the multi-dimensional parameter space to determine the range of model predictions. The automated search method is pursued here in lieu of Monte-Carlo based methods (e.g. Beven and Binley 1992) that would involve much more computational effort. The uncertainty analysis method is applied to a case study where an estimate is made of the degree to which a reduction in BOD loading would increase the dissolved oxygen concentrations in a tidally influenced river.

Study Area and Model Description

The uncertainty analysis technique was applied to a water quality study performed to predict dissolved concentrations in the Sampit River, South Carolina for various wastewater discharge scenarios. The water quality study included both an extensive hydrodynamic and water quality field study (Hickey et al. 1997) and a modeling study (Gong et al. 1997) that used the 2-d, laterally averaged water quality model CE-QUAL-W2 (Cole and Buchak 1995). The Sampit is a tidally influenced river that drains approximately 500 km^2 of coastal South Carolina and is surrounded by an extensive

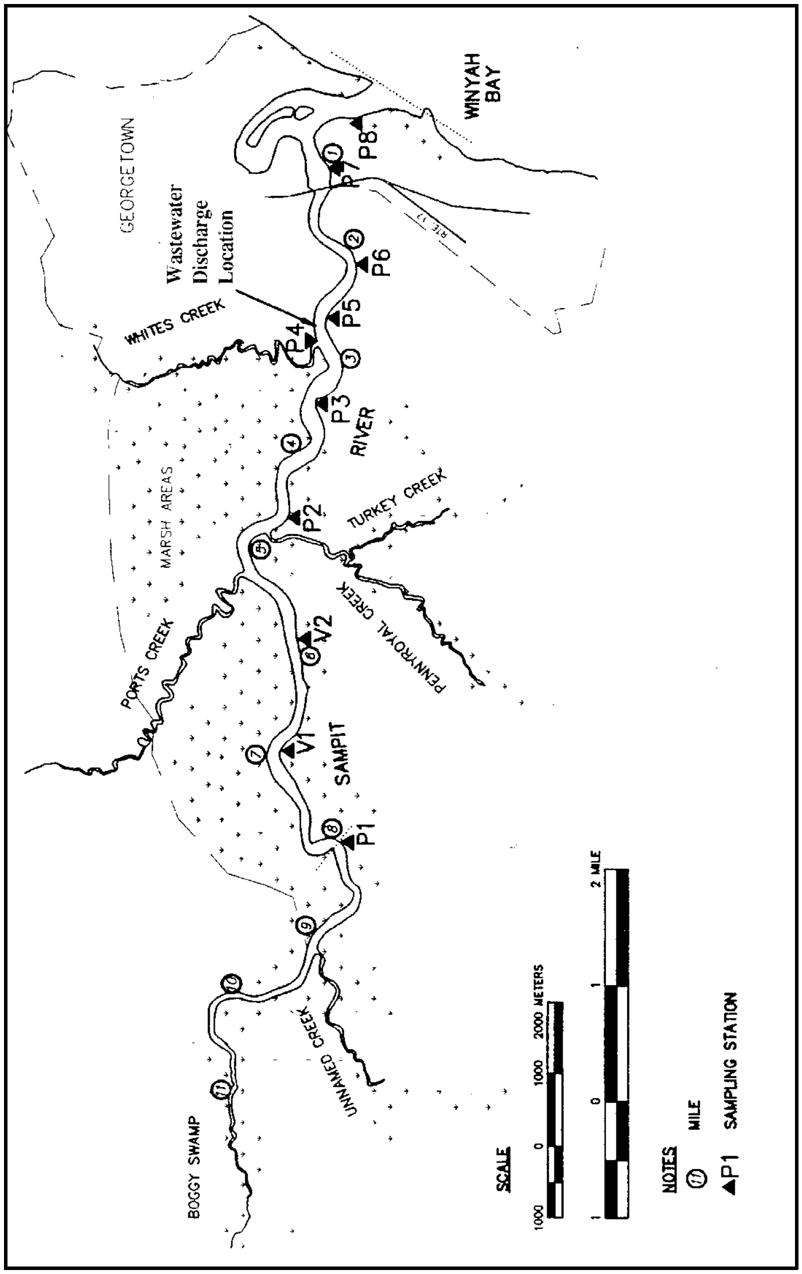

Fig. 1. Sampit River Study Area, Wastewater Discharge Location and Sampling Station Locations.

marsh system (Fig. 1). A paper mill wastewater enters the river on the ebb tide only, from a surface discharge located approximately 5 km upstream of the river mouth (Fig. 1).

The model analysis used a "pseudo steady-state" approach. Field studies and model simulations focused on summer conditions when dissolved oxygen (DO) concentrations are at a minimum. The state variables in the water quality model were temperature, salinity, ammonia, nitrate-nitrite, dissolved oxygen, and carbonaceous BOD.

Ensemble averages of multiple sampling rounds were calculated, and were considered to represent a summer, steady state condition. Upstream boundary conditions for water quality state variables were set to steady values equal to the ensemble averages from the monitoring program. Downstream boundary elevations included the M2 tidal component only. Wastewater discharges, which occur for one hour, once per day, just after high tide, were based on plant discharge records. Downstream boundary conditions and wastewater conditions for water quality state variables were varied in time, based on results of the water quality monitoring study and plant discharge records. A steady and homogeneous sediment oxygen demand was used to represent benthic organic matter decomposition.

Uncertainty Analysis Procedure

The uncertainty analysis procedure can be summarized as follows:

1. calibrate the hydrodynamic model,
2. establish a "base case" water quality parameter set through model calibration,
3. establish fitness measures and criteria (i.e. determine what makes a "plausible" parameter set),
4. select parameters to vary for uncertainty analysis,
5. set up a "grid" of candidate parameter sets,
6. evaluate the degree-of-fit at each grid point,
7. examine prediction uncertainty for plausible sets, and
8. perform automated search of parameter space to determine:
    a. range of model fitness values, and
    b. range of system responses.

Steps 3 - 8 of the procedure are described in this article. Steps 1 and 2 of the procedure for this application are described by Gong et al. (1997). From this earlier work, the base case set of parameters was determined. The uncertainty analysis then examined how well this base case, and many other candidate parameter sets, performed against two quantitative fitness criteria.

Quantitative Fitness Criteria

Two separate measures were used to determine the degree to which model predictions agreed with observations from a monitoring program. The observations used for comparison were averages of four sampling rounds taken at different tide stages (high and low water slack, maximum ebb and flood current) during a survey in late August, 1996. Ten stations were sampled within the study area (Fig. 1). Comparisons of three measured water quality constituents (salinity, DO concentration, BOD concentration) were compared against model predictions. Vertical and longitudinal variations in each constituent were considered with this analysis (Table 1).

Table 1. Observed Data

Parameter	Vertical Location	Station									
		P1	V1	V2	P2	P3	P4	P5	P6	P7	P8
Salinity (ppth)	Top	2.5	3.0	3.0	3.3	3.2	-	3.5	3.5	3.5	3.5
	Bottom	2.7	3.0	3.0	3.3	3.2	-	3.9	4.5	6.4	8.0
DO (mg/l)	Top	3.1	2.8	2.8	2.7	3.1	-	2.5	3.6	4.0	3.8
	Bottom	3.6	3.6	3.4	3.4	3.5	-	3.6	3.5	3.8	3.8
BOD (mg/l)	Top	2.8	-	-	2.1	3.0	2.0	2.2	1.9	2.0	2.3
	Bottom	2.1	-	-	2.6	2.6	1.9	2.1	2.0	1.5	2.1
Channel depth @ low-water slack tide (m)		4.0	5.5	5.5	7.0	6.0	4.5	5.5	8.5	8.0	7.5

A multi-constituent, normalized fitness measure was used as the first of the two fitness criteria. This average "lack-of-fit" measure is defined as follows:

$$LOF = \frac{1}{n} \times \Sigma \frac{rms(observed - predicted)}{avg\ \ predicted} \qquad \textbf{(1)}$$

where LOF is the average normalized lack-of-fit, and n is the number of constituents (n=3 in this case). Because the model prediction of most interest was dissolved oxygen, a second measure, the normalized DO fit was also used. This measure, DO_{LOF}, is defined as follows:

$$DO_{LOF} = \frac{rms(observed\ \ DO\ - \ predicted\ \ DO)}{avg\ \ predicted\ \ DO} \qquad \textbf{(2)}$$

Selection of Variable Parameters

Approximately 20 adjustable parameters might be included in the uncertainty analysis. Because of computational limitations, and based on the work of Brooks et al (1994), it was decided to consider only 3 - 7 parameters as variables for the uncertainty analysis. The following considerations were used to select the variable parameters:

! select parameters that seem relatively uncertain, based on consideration of the field program and hydrologic conditions, and

! select those parameters that most likely affect the state variables that are used as part of the quantitative analysis of degree-of-fit (salinity, DO, and BOD in this case).

Five variable parameters were selected based upon this analysis (Table 2). A parameter specific range was selected for each of the five parameters. The ranges varied from a factor of 10 to 25 around the base case values. Two of the five parameters, BOD loading and freshwater runoff, were varied by factors relative to the base case. The five dimensional parameter space was then "gridded" by specifying three or four levels for each parameter. Every combination of parameter levels was then considered as a candidate parameter set, giving a total of 324 candidate sets (Table 2). The two fitness measures were then determined for each of the candidate parameter sets.

Table 2. Specification of Variable Parameters

Parameter	No. of Values	Grid Levels	Units
Longitudinal Dispersion	3	**1**, 5, 25	m^2/s
Sediment Oxygen Demand	4	0.04, 0.10, **0.40**, 1.0	$g/m^2/d$
BOD decay rate	3	0.032, **0.10**, 0.32	day^{-1}
Relative BOD Load	3	0.32, **1.0**, 3.2	* base case
Relative Freshwater Runoff	3	0.10, 0.32, **1.0**	* base case
Note: base case levels of each parameter are in **bold**			

Automated Search Procedure

An automated search procedure was developed to search through the entire parameter space for "optimal" parameter sets. To accomplish this, a utility program was written to create input files for arbitrary combinations of the five variable parameters. Two automated searches were conducted, having the following objectives:

1. minimize the multi-constituent lack-of-fit, (LOF), defined in Eq. 1, and
2. maximize the increase in DO concentrations for a 30% reduction in BOD load while maintaining an acceptable lack-of-fit.

Searches for minima and maxima were conducted with the Nelder and Mead simplex method (Dennis and Woods 1987). Since the functions to be maximized or minimized are not linear, the search procedure found only local extrema. Multiple searches were therefore performed to investigate variability in these local values. The search for the maximum DO increase was performed by maximizing the function, I_{max}, given as:

$$I_{\max} = \max[\frac{DO_{70\%} - DO_{100\%}}{A} - \exp(LOF - B)] \quad \textbf{(3)}$$

where $DO_{70\%}$ and $DO_{100\%}$ are the 5th percentile DO concentrations from the model predictions for 70% and 100% BOD loading respectively, A = DO normalization concentration = 0.02 mg/l, LOF is the multi-constituent lack-of-fit for the particular parameter set (see Eq. 1), and B is a LOF criteria value that was set equal to the LOF determined for the “base” set of parameters. The exponential term serves as a cost function that gets exponentially large as the lack-of-fit increases. This procedure is a computationally efficient approximation to a constrained optimization problem (Brooks et al. 1994).

Results

Grid Point Runs

Water quality modeling results were gathered from the five-dimensional parameter grid having 324 points, which represented variations in five independent model parameters. For the entire collection of 324 candidate parameter sets, the multi-constituent lack-of-fit (LOF) varied from 36% to 280% (Fig.2), with a median LOF of 60%. The DO specific fit measure (DO_{LOF}) varied from 32% to 77%, with a median value of 54%. The “base” case, which was grid point 1,3,2,2,3 (see Table 2), produced an LOF of 48.3% and a DO_{LOF} of 55.1%.

The lack-of-fit levels for the base case were chosen as the criteria for an acceptable lack-of-fit between model predictions and observations. A “plausible” parameter set was therefore one that produced an LOF of no more than 48.3% and a DO_{LOF} of no more than 55.1%. Looking separately at the criteria, 28% met the multi-constituent criteria, and 41% met the DO criteria, while 19% met both criteria (Fig. 2). Thus 62 of the 324 candidate parameter sets were considered to be plausible.

The plausible parameter sets were well distributed over the parameter space. No plausible parameter sets came from the highest SOD value of 1.0 $g/m^2/d$ or the highest relative runoff of 3.2 times the base case (Table 3). Only 4 of the 62 cases came from the highest BOD decay rate of 0.32 day^{-1}. Each of the remaining grid levels had at least 25% of the plausible parameter sets (Table 3).

A broad range of dissolved oxygen values were predicted for model runs using the various candidate parameter sets. The variability was due to several factors. For a particular parameter set, the model produced a range of DO concentrations, as expected, depending on the time and location of the prediction. In addition, there was variability

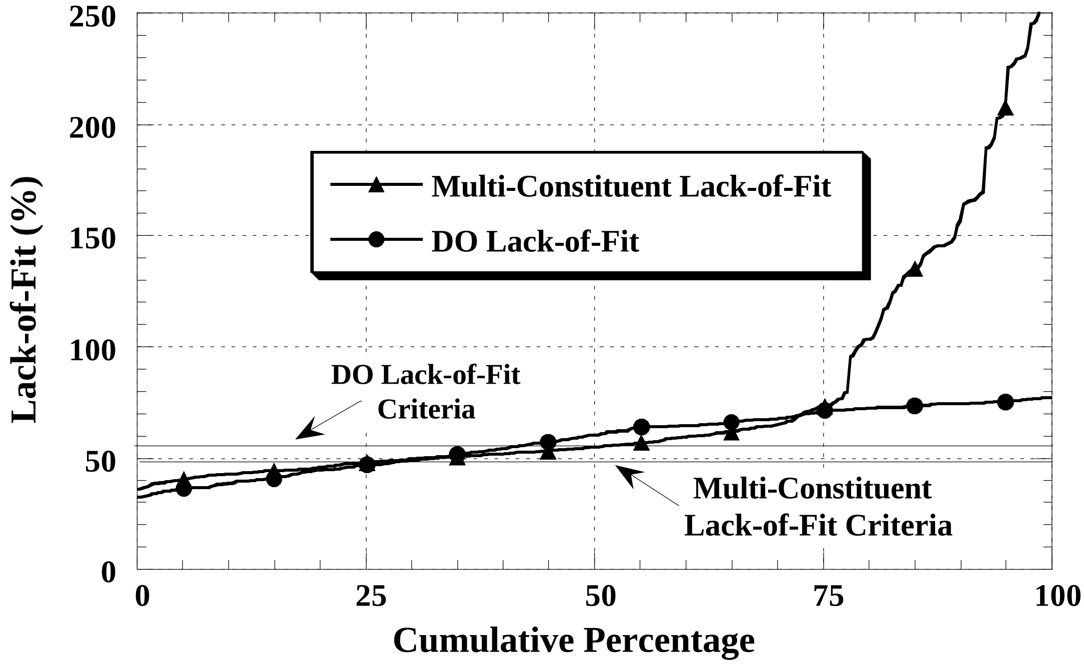

Fig. 2. Distribution of the Multi-Constituent and DO Lack-of-Fit Measures LOF and DO_{LOF} for all 324 Candidate Parameter Sets.

Table 3. Number of Plausible Parameter Sets for the Various Grid Levels of the Five Variable Parameters

Parameter	Number of Plausible Parameter Sets at Grid Level				Total
	1	2	3	4	
Longitudinal Dispersion	18	17	27	-	62
Sediment Oxygen Demand	23	23	16	0	62
BOD Decay Rate	27	31	4	-	62
Relative BOD Load	36	26	0	-	62
Relative Freshwater Runoff	23	21	18	-	62

in the model predictions between runs with different parameter sets. For instance, the spatially and temporally averaged mean DO concentration varied from 0.0 to 5.2 mg/l for all 324 candidate parameter sets, and from 2.2 to 3.8 mg/l for the 62 plausible parameter sets (Fig. 3). The variability in maximum and minimum DO concentrations for the 324 and 62 run tests showed a similar relationship, with decreased, although considerable,

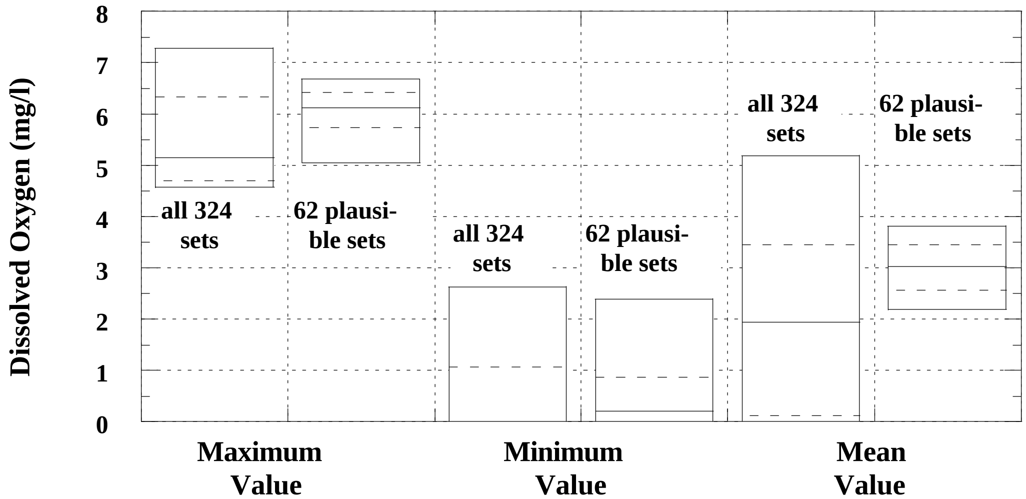

Fig. 3. Predicted Dissolved Oxygen Concentrations for all 324 Parameter Sets and for the 62 Plausible Parameter Sets. The bars indicate the range of values. The solid line through the interior of the bar represents the median value, while the dashed lines represent the 25th and 75th percentile values.

variability for the 62 run test. For the set of 62 plausible parameter sets, the maximum DO concentration varied from 5.0 mg/l to 6.7 mg/l, while the minimum DO concentration varied from 0.0 to 2.4 mg/l (Fig. 3).

As expected, runs with a BOD loading from the paper mill wastewater that was reduced by 30% from the base value had higher dissolved oxygen concentrations. The magnitude of the difference, however, was quite small. For the 62 plausible parameter sets, the median mean concentration increased from 3.01 mg/l to 3.06 mg/l (Fig. 4) when the wastewater BOD loading was reduced by 30%. Decreasing the loading resulted in a median minimum DO concentration that increased from 0.19 mg/l to 0.23 mg/l, while the median maximum concentration remained unchanged at 6.11 mg/l (Fig. 4). As a control, an additional set of runs simulated the river with no wastewater BOD loading. Higher DO concentrations resulted; the magnitude of the increase was consistent with the findings from the 30% BOD reduction cases (data not shown).

Decreasing the BOD loading by 30% increased the DO concentration; the magnitude of the increase varied between the plausible parameter set runs. For this comparison, the 5th percentile DO concentration was taken as the statistic of interest. This statistic was chosen because it depends both on the mean and variance of the DO distribution. It is also a useful statistic for consideration of wastewater discharge limits, where only infrequent violations of a water quality standard would be allowed. The increase in the 5th percentile DO concentration varied from 0.005 mg/l to 0.078 mg/l for the 62 plausible parameter sets (Fig. 5). The median increase in dissolved oxygen concentration was 0.035 mg/l.

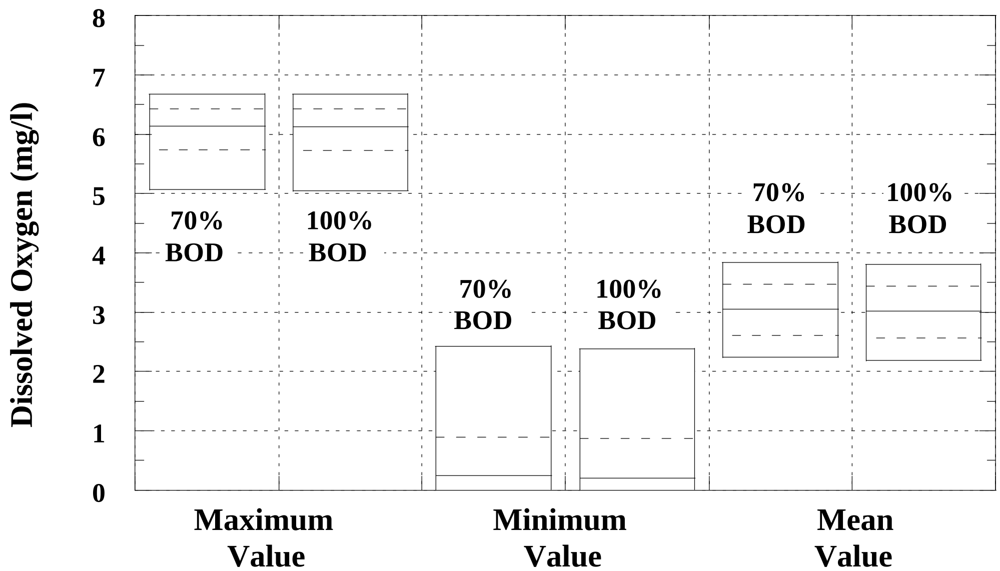

Fig. 4 Predicted dissolved oxygen concentrations for 100% and 70% BOD loading for the 62 plausible parameter sets. The bars indicate the range of values. The solid line through the interior of the bar represents the median value, while the dashed lines represent the 25th and 75th percentile values.

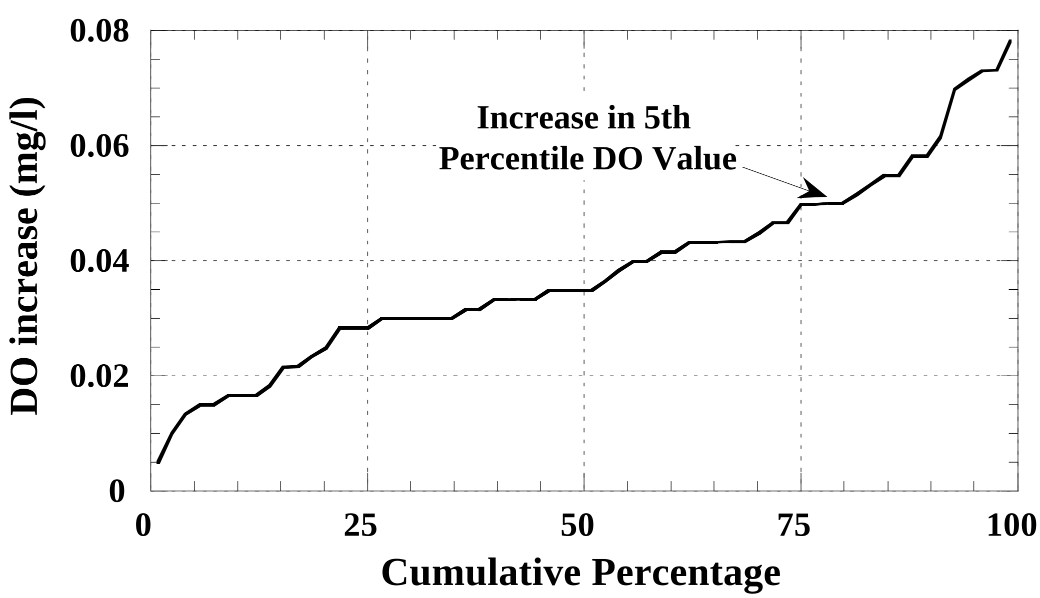

Fig. 5. Effect of a 30% load reduction of the 5th percentile DO concentration for the 62 plausible parameter sets.

Automated Searches

Two searches were conducted to find the set of parameters producing the minimum value for the multi constituent lack-of-fit, LOF. The first search started from the base case, grid point 1,3,2,2,3. The search routine finished after 150 iterations, with the LOF value decreasing from 48.3% to 30.6% (Table 4). A second search started from the grid point producing the lowest multi-constituent lack-of-fit (2,1,1,1,1). This search gave a different parameter set having a similar LOF value. In this case the LOF decreased from 36% to 34.5% and terminated after 137 iterations (Table 4).

Table 4. Results of automated searches to find the parameter set that produces the minimum lack-of-fit.

Search 1: starting from "base" case					
	Dispersion (m^2/s)	**SOD ($g/m^2/d$)**	**BOD decay (day^{-1})**	**BOD loading (* base)**	**Runoff (* base)**
Initial Values	**1.0**	**0.4**	**0.1**	**1.0**	**1.0**
Final Values	**1.5**	**-0.98**	**0.05**	**0.87**	**0.06**
Lack-of-Fit			**Number of Iterations**		
30.6%			**150**		

Search 2: starting from grid point with best fit					
	Dispersion (m^2/s)	**SOD ($g/m^2/d$)**	**BOD decay (day^{-1})**	**BOD loading (* base)**	**Runoff (* base)**
Initial Values	**5.0**	**0.04**	**0.032**	**0.32**	**0.10**
Final Values	**5.03**	**0.01**	**0.025**	**0.36**	**0.06**
Lack-of-Fit			**Number of Iterations**		
34.5%			**137**		

Automated searches were also conducted to find the set of parameters that gave the largest increase in DO concentration for a 30% decrease in wastewater BOD loading, while maintaining an acceptable level of fit. The search starting from the base case found a maximum DO increase of 0.17 mg/l after 191 iterations, more than twice the largest DO increase found in the grid point runs. The LOF value for this parameter set was 64.4 %. A second search was started from the grid point having the highest difference in the 5^{th} percentile DO concentration (3,1,1,1,1). This search found a maximum difference in the 5^{th} percentile DO concentration of 0.15 mg/l (Table 5). The LOF value for this case was 84.8%**.**

Table 5. Results of automated searches to find the parameter set that produces the maximum increase in DO concentration that results from a 30% load reduction.

Search 1: starting from "base" case					
	Dispersion (m^2/s)	**SOD ($g/m^2/d$)**	**BOD decay (day^{-1})**	**BOD loading (* base)**	**Runoff (* base)**
Initial Values	**1.0**	**0.4**	**0.1**	**1.0**	**1.0**
Final Values	**1.53**	**-0.28**	**1.22**	**2.52**	**-5.34**
Lack-of-Fit		**DO Increase (mg/l)**		**Number of Iterations**	
64.4%		**0.17**		**191**	

Search 2: starting from grid point with maximum DO increase					
	Dispersion (m^2/s)	**SOD ($g/m^2/d$)**	**BOD decay (day^{-1})**	**BOD loading (* base)**	**Runoff (* base)**
Initial Values	**25.0**	**0.04**	**0.032**	**0.32**	**0.10**
Final Values	**20.2**	**-2.35**	**8.44**	**4.3**	**-9.78**
Lack-of-Fit		**DO Increase (mg/l)**		**Number of Iterations**	
84.8%		**0.15**		**142**	

Discussion and Conclusions.

This study demonstrated the feasibility of using multiple parameter sets to perform a surface water quality impact assessment that includes a prediction uncertainty analysis. A previous modeling study (Gong et al. 1997) had identified one set of kinetic parameters (referred to as the base case) that produced an acceptable fit between water quality observations and model predictions. In our study, 324 candidate parameters sets were tested against two quantitative calibration criteria; 61 additional parameter sets were found to produce results that fit the observations as well as the base case. Any one of these 62 plausible parameter sets represents a reasonable description of the system under study, thus differences in the model results between the parameter sets truly represent one portion of model prediction uncertainty. Identification of this collection of plausible parameter sets therefore allowed for a prediction of model prediction uncertainty.

Model prediction uncertainty was found to be relatively large for predictions of water quality conditions, yet quite small for the prediction of the system response to an environmental manipulation. For instance, the range in predicted mean dissolved oxygen concentrations (100% BOD load) for the 62 plausible parameter sets was 1.6 mg/l (2.2 to 3.8 mg/l, Fig. 4), yet the range of increases in DO concentration for a 30% wastewater load reduction was only 0.073 mg/l (0.005 to 0.078 mg/l, Fig. 5). In addition, this study modeled only a single season (Summer 1996). Had interannual variability been considered, then prediction of water quality conditions would probably have been even less certain. Will model predictions of system response always be as certain as was seen in this case? Probably not, yet it does seem likely that system response prediction will generally be more certain than prediction of water quality conditions. This point should be kept in mind during project planning, when modeling project objectives and expectations are being discussed.

Selection of the variables to vary was found to be a difficult task. Like the earlier application of this method to groundwater flow (Brooks et al. 1994), it was found that it is practical to vary only a few variables, perhaps 3 - 7, depending on the simulation run time. Clearly this limit will grow as more computational power becomes available. In our study, where modeling was performed on a UNIX workstation, it took approximately one week to simulate all 324 cases. Unfortunately, since the number of candidate parameter sets grows exponentially with the number of variable parameters, it seems unlikely that anytime soon will we be able to consider all the parameters in a water quality simulation as variable. For this reason, future work on water quality modeling uncertainty analysis should address how best to pick the subset of parameters that are considered as variable.

Selection of the appropriate criteria for identifying plausible parameter sets is another difficult issue. In this study, the results of previous modeling (Gong et al. 1997) were used to establish the lack-of-fit criteria. Did the selection of the fitness criteria affect model prediction uncertainty? Clearly, uncertainty in predictions of water quality conditions would have decreased if the criteria had been more restrictive, i.e., if the maximum lack-of-fit for plausible parameter sets had been smaller. Would the uncertainty in prediction of system response also have decreased with a more restrictive criteria? The answer to this question seems neither obvious nor generally true. In this study, the system response (i.e., the increase in DO concentration with reduced waste-water loading) decreased slightly as the multi-constituent lack-of-fit increased (Fig. 6). Although a linear regression of the variables was significant at the 99% level, the variation in lack-of-fit explained only 16% (regression $R^2 = 0.4^2$) of the variability in system response. It is unclear whether the system response will always be so insensitive to changes in the fitness criteria.

As expected, the automated searches found parameter sets that produced better fits and larger system responses as compared to the grid point runs. The magnitude of the differences, however, was relatively small. The best fit for the grid point runs was 36%; it was 31% for the automated search. The maximum DO increase for the grid point runs was 0.08 mg/l; for the automated search it was 0.17 mg/l. A weakness of the current automated search method was identified during this study; there were no constraints on the magnitudes of the variable parameters. This was a problem, as the search to find the maximum DO increase produced negative parameter values (Table 5), which are not physically reasonable. Further development of this procedure to eliminate this problem is needed.

Both automated searches were found to require a large computational effort, as it required 100 - 400 model runs to locate a local minima or maxima. The search to find the maximum system response required the largest effort, as each function evaluation passed to the maximization routine was the result of two model runs, one at 100% BOD loading, and a second at 70% BOD loading. An additional difficulty of this search was the need to tune the normalization DO concentration (see Eq. 3) so that both the degree of fit and the DO increase were equally important in affecting the magnitude of the function to be evaluated.

In summary, when models are used for environmental management, prediction uncertainty should be quantified. Until now, modelers have generally relied upon a sensitivity analysis to estimate prediction uncertainty, while recognizing the method's limitations. This study has demonstrated the feasibility of a method that could provide a more accurate estimate of the uncertainty in water quality predictions.

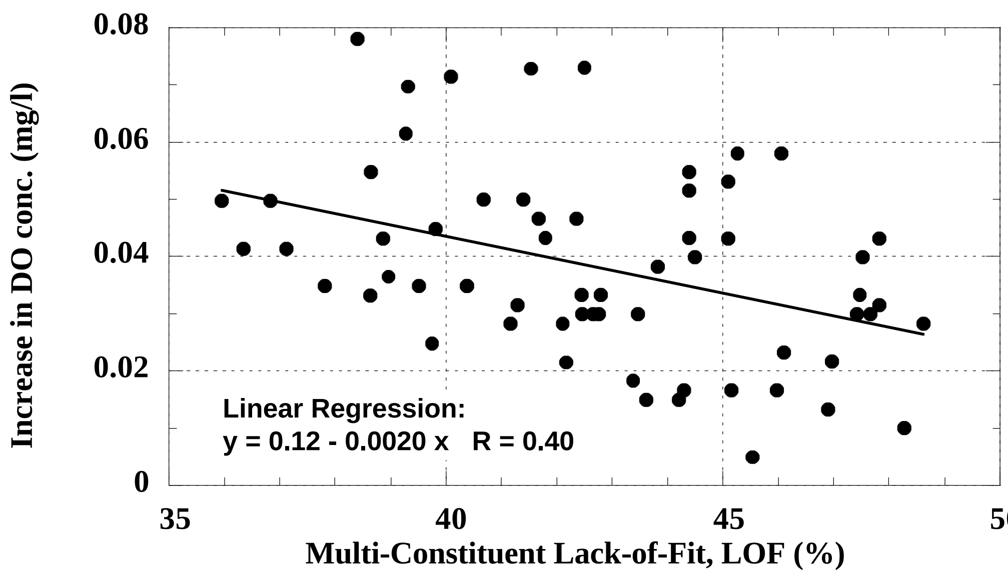

Fig 6. Effect of BOD loading reduction on DO concentrations for various levels of the multi-constituent lack-of-fit.

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