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MONTE CARLO SIMULATION AND FIRST ORDER ERROR ANALYSIS: TWO POSSIBLE METHODS TO COPE WITH UNCERTAINTIES IN WATER QUALITY MODELING, APPLIED ON A SPECIFIC MODEL

Sjors van de Kamer

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PREFACE

Nowadays it is a quite common feature in ecology to use models to analyze, correct and reduce ecological data, to study detailed ecological processes, to integrate ecological, i.e. multidisciplinary, research and to assist managers in their decision making process. Although the first three objectives perhaps are, or at least promise to be, very fruitful, in this paper we will focus on the last one, namely on water quality models meant to simulate the future behaviour of a river or lake system. Our contribution will not be another simple or comprehensive model. Attention will be paid to the issue maybe best described as sensitivity analysis. That is to say the analysis of the propagation of uncertainties in the field data (partly because of natural variability), in the forcing functions and in the model equations with their parameters. These uncertainties result in an error in the model prediction.

As a matter of fact, many modelers pay little attention to error analysis, in spite of many recent publications on this topic. A decent calibration procedure is often skipped for the sake of convenience or for so-called practical reasons. As a result any meaningful sensitivity analysis is impossible and the confidence that can be placed in their model output is unknown. One objective of this paper is to illustrate the practical possibility and practical necessity of sensitivity analysis in water quality modelling. Sooner or later it must strike the model user that models which predict only one trajectory, always predict the wrong one even without providing any information about the degree of wrongness.

This report has been written and all the work involved has been done during a part of a three month summer visit of the writer to IIASA. He was a participant in the young scientists summer program 1982. He owes special thanks to Kurt Fedra for putting him on the track and letting him use one of his water quality models. Perhaps the results presented here will influence the further development and application of this model.

ABSTRACT

Two methodologies to cope with uncertainties in water quality data and models are considered, namely Monte Carlo simulation and first order error analysis.

To illustrate the methods, results of applications on a water quality model, which in fact is an 8 state variable, 14 parameter submodel of a comprehensive model for lake Neusiedl, are presented.

Monte Carlo simulation based methods are shown to be useful for calculating valuable model predictions based on an adequate calibration.

CONTENTS

1. INTRODUCTION

In this paper we deal with some aspects of water quality models, meant to be used as a tool for management purposes. Usually these models are time dependent, non linear and consist of differential equations based on mass conservation and parameterized processes. In spite of uncertainties in initial conditions, forcing functions, parameters and model equations, they are often applied in order to provide a unique trajectory, being the future behaviour of the water quality. Although this seems to be a statement a manager can handle, the real confidence that can be placed in the output is unknown. Considering the possible impact of management decisions, both financially and ecologically, as well as the costs of model development and application, surprisingly little effort is usually made to determine the value of the model output. The argument that the problem is solved when models are only used to simulate different scenarios in order to compare their relative results, is not sound. One should not compare two probability density

functions by means of two realizations. So one of the main properties of water quality models should be their ability to deal with the propagation of uncertainties. In fact it would not be surprising if in the long term confidence in models were to be affected by lack of a decent sensitivity analysis.

Presenting a model output as a probability density function (e.g. Fedra et. al., 1981) or together with its variance (e.g. Di Toro and van Straten, 1979) will reveal its uncertainty. Thus a model result is not a number without value. On the other hand, the stochastic model output might appear to be too uncertain to be valuable for management purposes. In that case, the modeler should be able to indicate the best way to reduce the uncertainty, when possible, by revealing the major sources of error. In fact, it always will be desirable to have the uncertainty as small as possible. Thus, the model also becomes useful as a tool for suggesting research needs.

As already stated, the uncertainties in the model predictions originate from errors in initial conditions, inputs, parameters and model equations. It is often possible to quantify the errors in the first two. The last two are determined in the process of calibration and model testing. Hence, Chapter 1 will deal with calibration. Chapter 2 will continue with the propagation of errors. Finally, some attention is paid to the detection of the most troublesome parameter(s). Every chapter will be illustrated by exercises on the lake Neusiedl model of Kurt Fedra. This model is explained in the Appendix. A full description will be given in Fedra (a).

2. CALIBRATION AND MODEL TESTING

2.1 Uncertain Parameters

Calibration basically requires knowledge about the system's behaviour in a former period of time. Since field data always reflect measurement errors and the stochastic variability of the system itself, it would be unwise to try for a perfect fit on these data as a result of calibration and model testing. Nevertheless, in order to test the model, criteria are required to decide whether the model output is in accordance with the field data or not. Usable criteria are proposed in Fedra et al. (1981). From the field data, constraints are deduced, defining the so-called behaviour space. Model equations and parameters have to be found in such a way that the model results lie within the behaviour space. Given the uncertainty in the data only an uncertain description of the system is possible. Most likely more than one model is capable of satisfying the behaviour conditions. So, accepting only one model structure - it seems justifiable to choose the simplest one, which is able to provide the required level of detail in the output, taking into account the inputs of interest; see, e.g. Fedra (1982) - it is obviously insufficient to consider one unique parameter vector.

2.2 Monte Carlo Method

In Fedra et al. (1981) a generally applicable method is described to perform the calibration procedure. The method is partly based on the work of Spear and Hornberger (1980). First ranges of model parameters are specified for the particular model structure based on empirical evidence and previously quoted values. Then these

ranges are randomly sampled by a Monte Carlo technique. The sample parameter vectors giving rise to a model response, which is found to satisfy the behaviour constraints (see 2.1), are considered to be acceptable. Their relatons and interdependencies can be analyzed and the vectors can be used for computations under changed conditions. In fact, the acceptable parameter vectors define a multidimensional probability density function. Of course it is possible to extend the method by including, apart from the parameters, the forcing functions and initial conditions.

2.3 Minimizing a Loss Function

A more common way to calibrate is to accept the parameter vector, which minimizes some loss function, describing the discrepancy between behaviour and model output. Some of these methods allow the estimation of the covariance structure of the parameters. Di Toro and van Straten (1979) showed it to be of the utmost importance to have this information in order to perform an adequate sensitivity analysis. Their method, using a weighted squared error loss function, provides a parameter vector and its covariance matrix. In contrast with the Monte Carlo based method, with this method it is necessary to assume a certain error structure (Gaussian, independences, etc.), as well as the applicability of the asymptotic properties of maximum likelihood estimators and the covariances for the number of observations available. Apart from that, the presentation of only one parameter vector might lead to misinterpretations. Finally, note that after the estimation of the parameter vector the model test still has to be performed as well as a check on the credibility of the vector.

2.4 Other Methods

The most common way to calibrate a model is by "tuning". Apart from benefits during model development, this method does not provide enough information to support a sensitivity analysis. It has additional disadvantages in being irreproducable, based on the subjective perception of the analyst and probably expensive both in computer time and in man hours.

In recent years the Kalman Filter algorithm has been used for calibration purposes. See e.g. Beck (1979) and Scavia (1980). This method is beyond the scope of this study. Also the properties of probabilistic model structures, involving direct a priori use of probability density functions are not considered.

2.5 Calibrating the Illustrative Model

To illustrate the theory, some exercises were performed, using the lake Neusiedl model of Kurt Fedra (Fedra (a)). A submodel of his model, called the lake submodel, serves throughout this study as an example of a water quality model on which the theory is applied. So, e.g. in this section the calibration of the lake submodel is described. (Further explanation about the Neusiedl model and the lake submodel is given in the Appendix. Note that the lake submodel is only a small part of the Neusiedl model. Note further that empirical data up to and including 1979 have been incorporated in the Neusiedl model). The rest of this model has only been used in this study to generate input sets - climatic records (temperature, radiation, eddy diffusion coefficient, flow) and records of loads (soluble and particulate phosphorus loads) - and initial conditions for the submodel. For one year different input sets may be generated, due to the

stochastic perturbations in the Neusiedl model, which represent uncertainties and natural fluctuations. In this paper we will concentrate on the years 1976 and 1980. The Neusiedl model has been fed with data up to and including 1979. Therefore, the perturbations are larger after 1979, and the variance between the input sets of 1976 is less than between those of 1980.

In order to calibrate the submodel with its 14 parameters (see Appendix and Table 1) with 1976 data, according to the method using Monte Carlo simulations, first 10 input sets were generated by the Neusiedl model. These sets reflect empirical observations, within the way the Neusiedl model operates. One of these 10 sets was assumed to be measured without errors. The choice was done in such a way as to avoid the selection of an exceptional set. Also the initial conditions, generated by the Neusiedl model were assumed to be without error. In other words, 1976 is considered to be a year in which the error in both input data and initial conditions is zero due to very extensive measurements. So, in the calibration procedure only parameters were sampled, input set and initial conditions have been fixed. The parameter ranges were defined as shown in Table 1. They are based on "best knowledge" rather than on an extensive literature search or experiments. The behaviour constraints for the 1976 results were mainly based on the initial conditions generated by the Neusiedl model for 1977. These constraints apply to the state variables at the end of 1976. Additional constraints were based on the very scarce field measurements of 1976. They apply to the average values of some of the state variables (see Table 2). The constraints, based on the initial conditions of 1977, were more or less arbitrarily chosen in such a way that a 2 percent chance was created for a

Table 1. The parameters of the lake submodel.

Symbol		Unit	Range
p_1	sedimentation rate in reeds	$(month)^{-1}$	0.3 ± 50%
p_2	mineralization rate in reeds	$(month * {}^{0}C)^{-1}$	0.018 ± 50%
p_3	reed production rate	$(month * {}^{0}C)^{-1}$	0.012 ± 50%
p_4	reed carrying capacity	$mg\ P * m^{-2}$	18000 ± 10%
p_5	reed mortality rate	$(month)^{-1}$	0.01 ± 50%
p_6	fraction of reed nutrients obtained from water	-	0.25 ± 50%
p_7	sedimentation rate in lake	$(month)^{-1}$	0.033 ± 50%
p_8	mineralization rate in lake	$(month * {}^{0}C)^{-1}$	0.025 ± 50%
p_9	algal mortality rate	$(month)^{-1}$	0.5 ± 50%
p_{10}	algal production rate	$(month * {}^{0}C)^{-1}$	0.12 ± 50%
p_{11}	Michaelis Menten constant for P	$mg\ P * m^{-3}$	10 ± 10%
p_{12}	immobilization rate of organic P in sediment	$(month)^{-1}$	0.0033± 50%
p_{13}	mineralization rate of detritus in sediments	$(month * {}^{0}C)^{-1}$	0.0025± 50%
p_{14}	eddy diffusion coefficient for reed sediment/water interface	-	0.0022± 50%

Table 2. The behaviour constraints for calibration of the lake submodel on 1976. The 8 state variables of the lake submodel are defined in the Appendix.

A) Based on the initial conditions of 1977, the values of the state variables at the end of 1976 are constrained by:

14000	<	Y_1	<	16000	50000	<	Y_5	< 15000
70	<	Y_2	<	100	50	<	Y_6	< 120
50	<	Y_3	<	450	20	<	Y_7	< 75
10000	<	Y_4	<	20000	5	<	Y_8	< 15

B) In addition, based on field measurements, the average 1976 values are constrained by:

$$60 < \overline{Y}_6 < 100$$

$$10 < \overline{Y}_7 < 30$$

$$10 < \overline{Y}_8 < 20$$

sampled parameter vector to be acceptable. Fairly loose constraints appeared to be necessary. So, in fact we adjusted the behaviour constraints. Otherwise the chance that a parameter vector would be acceptable was too small to create an interesting example. In other words we a priori accepted the model. Normally however, one should start with defining the behaviour space. After that the model testing can take place. One hundred acceptable parameter vectors were generated. Their correlation matrix is shown in Table 3. Some typical marginal distributions are presented in Figure 1.

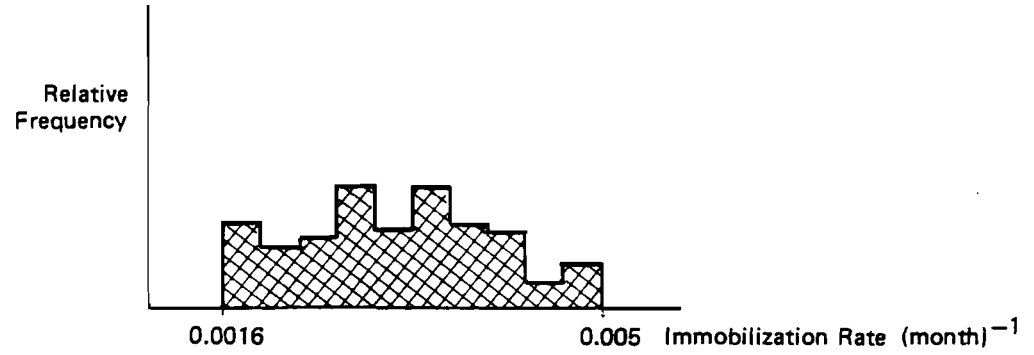

Figure 1A. Marginal distribution of parameter 12, immobilization rate of organic P in sediment.
Mean = 0.0032 (monthly)$^{-1}$

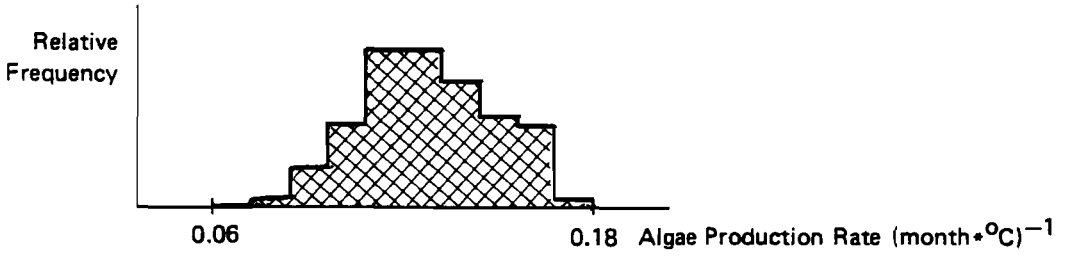

Figure 1B. Marginal distribution of parameter 10, algae production rate.
Mean = 0.13 (month*^{o}C)$^{-1}$

Table 3. Correlation matrix of the acceptable parameters. Only significant correlations ($\alpha < 0.05$) are shown.

	1	2	4	5	6	7	8	9
2	-0.36							
6				-0.24				
7	-0.22			-0.25				
8					-0.23	0.22		
9						0.25	0.44	
10						0.26	0.44	0.96
12		0.25						
13					-0.26	-0.20		
14		-0.25	0.36					

A program SIMUL was written to perform several kinds of simulations with the lake submodel. SIMUL is able to read input sets, initial conditions and parameter vectors, and to run the lake submodel. SIMUL was used for the first time to check whether or not the acceptable parameter vectors were giving rise to highly inacceptable values of the model state variables, running the year 1976 one hundred times, the initial conditions of each run being the final results of the run before. The state variables were stabilizing on an acceptable level.

3 ERROR PROPAGATION

3.1 Biased Model Output

One important feature to note is the bias in the values predicted by a deterministic model. See e.g. Gardner and O'Neill (1979). Letting f_i (p,u) - throughout this paper - represent the dependency of model result i from parameter vector p and input set u, this bias results from the fact that in general:

$$E\{f_i(p,u)\} \neq f_i(E\{p,u\}) \qquad (1)$$

Only when f_i is a linear function of p and u, equality holds. This however is not the case even in the most simple water quality model. To analyze this feature for the model under consideration, the model output for 1976, based on the mean parameter vector, as well as the mean output, based on all one hundred acceptable parameter vectors, was calculated. The results are tabulated in Table 4. The analysis was restricted to the calculation of the maximum yearly algal biomass (algmax), the yearly average algal biomass (algav) and the yearly average detritus (detav). These are considered to be representative for the water quality. The resulted bias, expressed as a percentage of the model output's standard deviation is:

30% for algmax

25% for algav

3% for detav

These results are in good agreement with those of Gardner and O'Neill (1979). Their subsequent conclusion is that the bias will not lead to serious problems. We would rather not a priori

neglect the bias in the output of a model under consideration. The more so as a possible reduction of the standard deviation, e.g. after model improvements, does not necessarily imply a proportional reduction of the bias.

3.2 Variance of the Model Results

Using all of the one hundred parameter vectors, the model results for 1976 are probability density functions. Figure 2 shows the functions for algmax and detav. The variance of the results is easy to calculate (Table 4). Accepting biased model results, one may confine oneself to only one calculation, using

Table 4. Simulation results (see 3.1).

	result of one simulation using the mean parameter vector	mean and standard deviation of the simulation results using the acceptable parameter vectors	
		m	s
alg max	48.1	45.5	8.0
algav	16.0	15.4	2.5
detav	74.8	75.0	6.9

the mean parameter vector. In fact, as stated, this is mostly done, using a single parameter vector, which is not necessarily the mean. As is easily verified, in this case a first order approximation of the variance can be obtained from:

$$\mathrm{var}\{f_i(p)\} = \sum_{j=1}^{N} \sum_{k=1}^{N} \left(\frac{\partial f_i}{\partial p_j}\right) \left(\frac{\partial f_i}{\partial p_k}\right) \mathrm{cov}\,(p_j, p_k) \qquad (2)$$

N is the number of parameters involved.

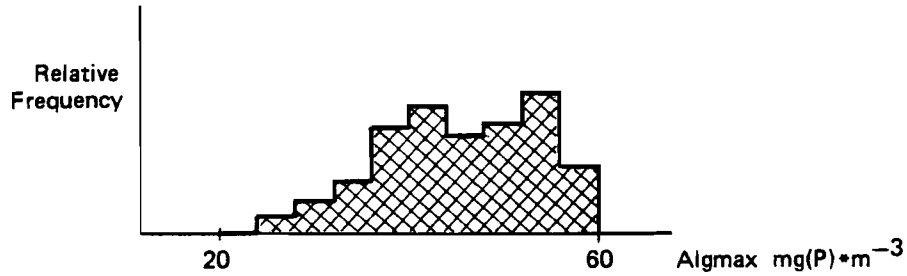

Figure 2A. Probability density function of algmax. Mean equals 45.4 mg*m^{-3}; standard deviation equals 8 mg*m^{-3}

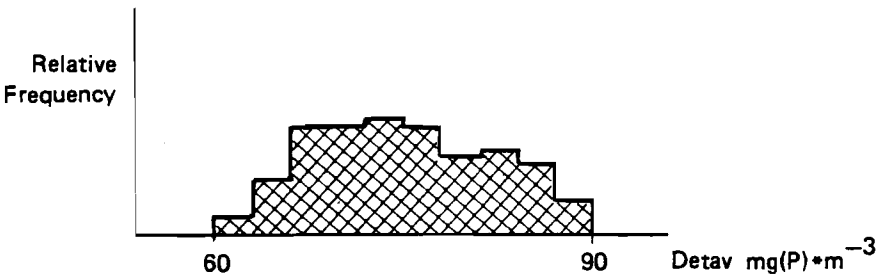

Figure 2B. Probability density function of detav. Mean equals 75 mg*m^{-3}; standard deviation equals 7 mg*m^{-3}

Equation (2) can be rewritten as:

$$\mathrm{var}\{f_i(p)\} = \sum_{j=1}^{N} \left(\frac{\partial f_i}{\partial p_j}\right)^2 \mathrm{var}(p_j) \; + \; + \sum_{\substack{j=1 \\ j\neq k}}^{N} \sum_{k=1}^{N} \left(\frac{\partial f_i}{\partial p_j}\right)\left(\frac{\partial f_i}{\partial p_k}\right) \mathrm{cov}(p_j, p_k) \qquad (3)$$

Since often the cross covariances between parameters are being neglected, it is worthwhile to compare the model result variances using:

$$* \; \mathrm{var}(f_i) = \sum_{j=1}^{N} \left(\frac{\partial f_i}{\partial p_j}\right) \mathrm{var}(p_j), \qquad \text{method A.}$$

* equation (2) method B.

Table 5 shows the results, presenting also as a reference the standard deviations based on the Monte Carlo method.

Table 5. Standard deviations of model outputs, based on different methods (see 3.2).

	s Monte Carlo	s Method B	s method A
algmax	8	9	32
algav	3	3	12
detav	7	7	13

The deviations based on equation (2) and those based on the Monte Carlo method, appear to be in very good agreement. As also found by Di Toro and van Straten (1979), neglecting the cross covariances leads to enormously inflated results.

3.3. Predictions

When simulating the future behaviour of a system, one has to cope with uncertainties in the parameter vector, but also in the input sets or forcing functions. If the uncertainties in the parameter vector are independent of those in the input set, the variance of the model output will be approximated by:

$$\mathrm{var}\{f_i(p,u)\} = \sum_{jk}\sum \frac{\partial f_i}{\partial p_j}\frac{\partial f_i}{\partial p_k}\,\mathrm{cov}(p_j,p_k) \; + \; \sum_{jk}\sum \frac{\partial f_i}{\partial u_j}\frac{\partial f_i}{\partial u_k}\,\mathrm{cov}(u_j,u_k) \qquad (4)$$

To return to our example for the lake submodel, input sets for 1980, reflecting uncertain input values, are available (see 2.5). Some characteristics of the sets are shown in Table 6. Three different Monte Carlo simulation series were performed resulting in stochastic model output for 1980. In the first series only the parameter vectors were sampled, holding the input set fixed. In the second series input sets were sampled, holding the parameter vector fixed at its mean. In the third series both the parameter vectors and the input sets were sampled. Of course only the stochastic model results, based on the third series, represent the predictions for 1980. For all three series the initial conditions are assumed to be perfectly known. But it is useful to compare these predictions with the results of the two other series in order to estimate

the relative impact of the two lumped sources of error. The standard deviation of a model result, produced by the third series, is called the total error of the result. Figure 3 shows the model results algmax and detav, based on series 1 and 3. As can be

Table 6. Input statistics for April.

A) Coefficients of variation (%).

		s/m *100
1	temp	11
2	rad	6
3	flow	160
4	eddy	6
5	pprin	7
6	psrin	6
7	pplin	5
8	pslin	6

B) Correlation matrix. Only significant correlations ($\alpha < 0.05$) are shown.

	5 pprin	6 psrin	7 pplin
6	0.96		
7	0.74	0.84	
8	0.38	0.58	0.86

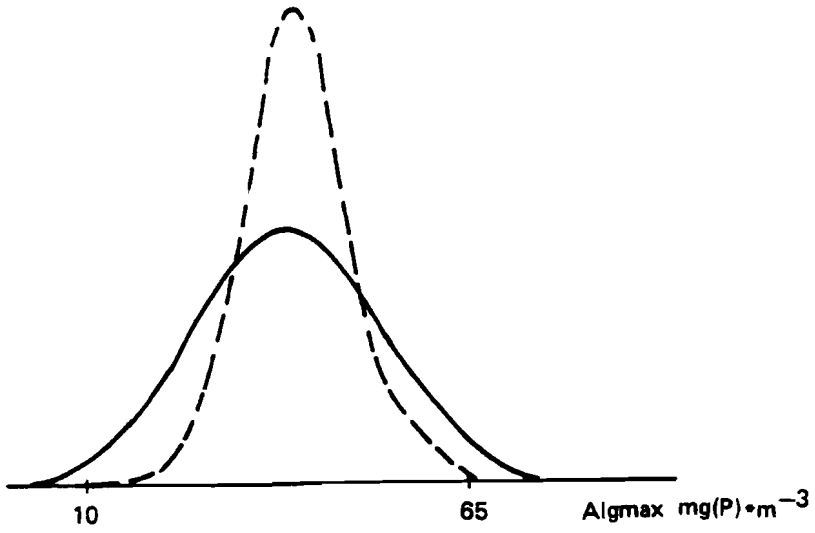

Figure 3A. The probability density functions of algmax. The solid line is a Gaussian approximation, reflecting uncertainties in parameters and input. The dashed line is the approximation with fixed input and uncertain parameters.

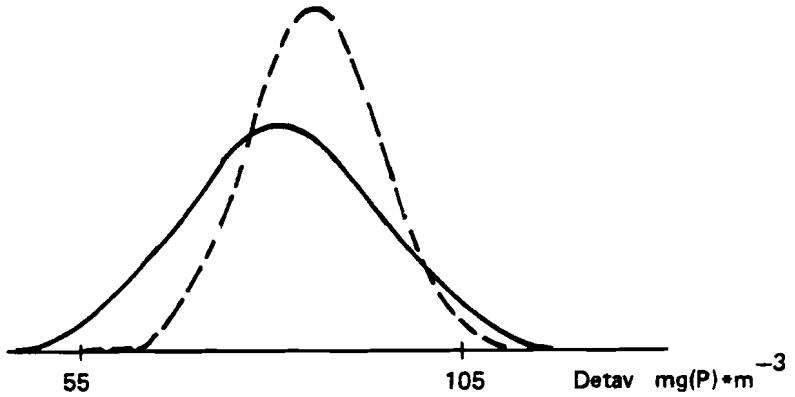

Figure 3B. The probability density functions of detav. The solid line is a Gaussian approximation, reflecting uncertainties in parameters and input. The dashed line is the approximation with fixed input and uncertain parameters.

deduced from Table 7, the standard deviation of the model results roughly doubles when the uncertainties in the input set are taken into account in addition to those in the parameter set. From the data of the same table it can be verified that equation (4) holds for algmax and algav. For detav presumably nonlinearities cause the approximation not to be valid.

Based on additional simulation series, Table 7 also shows the impact of the uncertainties in the climatic record. The uncertainties in temperature and flow are not only mainly responsible for the additional error caused by the uncertainties in the input set, but also for the total error in the model results! The effect of the uncertainties in the record of loads is small. With the exception of temperature and flow, the reduction of the uncertainty of a single input variable does not significantly affect the total error in the model results.

Table 7. Simulation results (see 3.3). Shown are the standard deviations.

	Sampled parameters, fixed input	Sampled input, fixed parameters	Both sampled	Only temp and flow fixed	Only climatic record fixed
algmax	7	11	13	8	7
algav	2	3	4	3	2
detav	8	14	14	13	11

Calculations further showed that an increase of 50% in the average loads will only cause a change in the means of the model predictions (algmax, algav or detav) of about 1.5 times the prediction's total error. A 10% increase in the average loads will cause a change of 0.3*S. On the other hand, comparing two years, using one and the same climatic record, a 50% increase in loads will give rise to roughly a change of 3*S.

4. PARAMETERS AND MODEL EQUATIONS

4.1 Reducing Parameter Ranges

In this chapter the uncertainty of the parameter vector is considered to be the only source of errors for predictions. It is assumed to be impossible to formulate more restrictive behaviour constraints. Clearly a complete reduction of the a priori uncertainty of the parameter vector then will lead to a unique trajectory. It is not immediately clear, however, whether a particular reduction of the a priori uncertainty of a subset of the parameters will have any real effect. Often enough the effect of the variance of a parameter p_j on f_i is estimated - based on method A of chapter 3 - by:

$$\left(\frac{\partial f_i}{\partial p_j}\right)^2 \mathrm{var}(p_j) \qquad (4)$$

The resulting impressive reductions in the variance of f_i, based on this method, are for the lake submodel example listed in Table 8. But Monte Carlo simulations showed that no significant reduction of the model output error is achievable by decreasing the variance of any single parameter, thereby contradicting the values in Table 8. Although this result is due in part to the

Table 8. Reductions in % based on method A.

parameter	reductions		
	algmax	algav	detav
7	0.1	0.1	2
8	0.6	0.3	27
9	39	46	19
10	60	53	51
11	0.5	0.4	0.4

limited number of runs possible, clearly e.g. a reduction of the variance of parameter 10 (algal production rate) alone will be useless in view of the high correlation with parameter 9 (algal mortality rate).

A better way of dealing with clearly cross-correlated parameters is based on method B of Chapter 3. The variance of f_i can be rewritten as:

$$\mathrm{var}(f_i) = \sum_{jk} \sum \left(\frac{\partial f_i}{\partial p_j}\right)\left(\frac{\partial f_i}{\partial p_k}\right)\mathrm{cov}(p_j, p_k) =$$

$$= \left(\frac{\partial f_i}{\partial p}\right)^T C \left(\frac{\partial f_i}{\partial p}\right)$$

* with C being the parameters covariance matrix.

Because C is a hermitian matrix there exists a matrix A such that:

$$var(f_i) = (\frac{\partial f_i}{\partial p})^T_A \Lambda A^T (\frac{\partial f_i}{\partial p}) = B_i^T \Lambda B_i$$

$$var(f_i) = \Sigma \lambda_j b_{ij}^2 \qquad (5)$$

* with Λ being a diagonal matrix with the eigen values of C.

* with A being the matrix of eigen vectors.

The equations above show the possibility to remove the cross correlations by a transformation. The uncorrelated combinations $\sum_i a_{ij} p_i$ have variances λ_j. When a few terms of equation 5 happen to account for a large part of the total variance and for each term the corresponding combination reveals only a small subset of the parameters to contribute to the variance λ_j, application of the method provides much insight. In our example for each of the model outputs considered (algmax, algav, detav), only two terms of equation (5) turned out to contribute 85% of their total variance. Further analysis showed the parameters 9 and 10 together to be responsible for more than 90% of the variances λ_j corresponding to the two terms of algmax and algav. At the same time it showed the senselessness of reducing only the variance of one. As far as detav is concerned the parameters 8 and 7 contribute more than 80% of the variances λ_j corresponding to the two terms of detav. The possible use of a Monte Carlo based method to show the impact of the simultaneous reduction of variances of parameters could not be considered because of the limited number (100) of acceptable parameter vectors. After reduction a too small subset of the acceptable vectors would remain to sample from. However, this method is considered in principle to be most fruitful.

4.2 Altering Model Equations

The effect of alterations in model equations (and consequently model parameters) on the variance of the model output is poorly understood. Gardner et al. (1980) states that more complex models often generate greater uncertainty in the output. However, their statement is based on dubious reasoning. As they themselves make clear, a smaller uncertainty in a model prediction variable may require a more complex term in the model. And in fact, in their case, one of the two model prediction variables does. Scavia et el. (1981) point out a similar dilemma: sometimes aggregation of model state variables will pay off in reduction of variance of the output, sometimes disaggregation will pay off. Intuitively others advocate the simplest model possible (Fedra, Somlyody (pers. comm.)). On the other hand, incorporation of extra knowledge of biological, chemical and physical processes, derived from laboratory and field experiments, should be fruitful (see Scavia et al., 1980; see also Beck, 1981, for an interesting discussion on this topic and related topics). The above discussion suggests the following conjecture:

> Without adding essential knowledge of processes any increase in the complexity of a model improves the possible fit on field data, but enlarges the uncertainty of predictions. So the conjecture includes the warning to be careful with the incorporation of more detail just to improve the fit on field data. The value of adding new knowledge of processes to the model presumably only emerges, when its incorporation leads to predictions with less uncertainty. The concept

of extra process knowledge may be illustrated by the following example, which in fact is a continuation of an example given in Fedra (1982, pp 11-14).

Let $y(t) = a\ t + b$ be model 1

The original parameter ranges are given by:

$$0.5 < a < 2.5 \qquad 0 < b < 2$$

The behaviour space is defined as:

$$2.5 < y(2) < 5 \qquad 7 < y(8) < 9$$

Calibration, based on 1000 Monte Carlo runs, of model 1 results in:

	mean	var
a	0.85	0.008
b	1.33	0.165

$\text{cov}(a,b) = -0.026$

Consequently: $\text{mean}\ (y) = 0.85\,t + 1.33$

$\text{var}\ \ (y) = 0.009\,t^2 - 0.052\,t + 0.165$

Let $y(t) = at + c\ \sin(t) + 1$ be model 2.

The parameter ranges are given by:

$$0.5 < a < 2.5 \qquad 0.8 < c < 1$$

("process b" is now better known)

The behaviour space is identical to the one of model 1.

Calibration of model 2 results in:

	mean	var
a	0.77	0.005
c	0.90	0.003

$\text{cov}(a,c) = -0.0003$

Consequently:

mean (y) = 0.77 t + 0.90 sin(t) + 1

var (y) = 0.055 t^2 + 0.003 $\sin^2$(t) - 0.0006 t sin(t)

The conclusion is clear. Model 2 gives a marginally larger or a much smaller variance for y. For instance, the prediction for t = 12 is:

	model 1	model 2
y(12)	11.5	9.8
s	0.92	0.85

It should be stated that the reduction of the uncertainty in the output may not be worth the trouble of adjusting the model. Fortunately, in case of extra process knowledge (including parameter ranges) the effects of model adjustments are calculable.

5. CONCLUSIONS AND DISCUSSION

Monte-Carlo methods provide a possibility to deal with the impact of uncertainties on the predictions of a water quality model, meant to be used as a management tool. In spite of their huge demand for computer time these methods are considered to be of practical importance, partly because they are efficient in terms of modelers time and because computer time is becoming cheaper and cheaper. Some basic rules for more efficient use of Monte Carlo methods are given in Fedra (1982). Nevertheless, together with the tentative character of this study and its short time span, the computer time required was a reason to keep the number of simulation runs rather small. Particularly the quality of Chapter 4 would have been improved, if this number had been larger.

The conclusions with respect to the lake submodel, serving as an example throughout the paper, are not surprising. The prediction of next year's water quality is to a certain extent similar to the prediction of next year's weather, since e.g., temperature plays a dominant role. The standard deviations of the outputs from predictive model considered amount up to 30% of their means. So the most successful application will be the comparison of the stochastic simulation results for different (long term) scenarios. Perhaps some simplifications in that part of the lake Neusiedl model calculating the phosphorus loads, are possible, since only major changes in the loads have any effects. However, cumulative effects of sequential years with high loads have not been considered. Some curious discrepancies have been found between the lakes state at the year end and the following year's initial conditions. Therefore, some of the behaviour constraints had to be fairly loose. Apart from that, the simplicity of the lake submodel is justifiable. It was shown how bizarre it is from the point of view of predicting, to pay extra attention to the algal production aspect, given the obscure mortality aspect.

The impact of the quality of the calibration procedure is evident. To deal with error propagation, the use of a method, based on Monte Carlo simulations, is certainly successful and avoids a biased output. Linear approximation of the variance of the model results has to take the cross-covariances into account. To identify the weakest parts of a model it is useful to find the parameter subset, giving rise to a large part of the total variance. Again cross-covariances should not be

neglected and the method based on Monte Carlo simulations gives straightforward results.

Because ultimately a predictive model should be part of an interactive computer aided planning program, i.e. an interactive graphics supported tool to assist managers in their decision making process (see Loucks et al, 1982), the model should be as simple as possible. Otherwise the interactive process of simulating logically sequent scenarios is impossible. A reason for starting, at any rate, with a simple model has been given in Chapter 4. More complex models certainly do not guarantee models with a higher predictive value. It would therefore be recommendable to accept a more complex management model only after its higher predictive value has been shown.

APPENDIX: THE LAKE NEUSIEDL MODEL

The appendix is mainly based on a draft version of Fedra (a).

A.1 The Approach

Lake Neusiedl is an extremely shallow (1.5m) lake of about 150 km^2 surface, embedded in a belt of dense reeds (Phragmites), covering approximately 150 km^2. It is situated south-east of the Austrian capital Vienna, in the province of Burgenland. The lake's catchment extends over approximately 1300 km^2.

Since the early seventies, a conspicuous deterioration of the lake's water quality has been observed, resulting in a decreasing attractivity for recreation. Tourism however, is one of the most important elements in the economy of the region.

The specific management problems of the lake system arise from three major conflicting objectives in the development of the region, namely:

a) The development of tourism (affecting landscape and increase of waste and sewage production);

b) intensification of industrial and agricultural production (involving direct and indirect forms of pollution);

c) the preservation of environmental quality.

For the analysis of lake Neusiedl, Kurt Fedra extended the "classical" approach of load-response modeling of lakes, which requires the loading to be specified as an input, towards a more comprehensive examination of the lake as an integrated element within its physical as well as its socio-economic watershed. The pollution affecting the lake is treated explicitly. Therefore, this approach implies, besides the use of a classical water quality submodel for the lake and the surrounding reed belt, a group of additional sub-programs to simulate the system. The additional programs generate and transport nutrients to the lake as a function of land use, agricultural and industrial activities, wastewater treatment and tourism, the last of which in turn influenced by the lake water quality.

The model is operating on a monthly time step: after initialization and optional interactive parameter editing, the program for each month generates a climatic record. The program then generates a record of loads, calling a series of subroutines which estimates different sources of pollution, taking phosphorus as a proxy for pollution affecting water quality. These two can be considered to be the monthly input for the lake subprogram, evaluating the lake's water quality. It is important to note that experimental data up to and including 1979 underlie the records and that the two records are affected by stochastic perturbation on most of the estimates, used in the model, in an attempt to account for uncertainties and natural fluctuations.

The program provides a spatial resolution on the community and treatment plant level, and has been set up within an interactive dialogue oriented framework. This allows for interactive design of management policies. For each month economic indicators (revenues from tourism, costs of reed management and wastewater treatment) and a detailed listing of the lake's and reed system's status can be displayed. The model system has been designed as one step towards an intelligent and friendly decision support system.

A.2 The Lake Submodel

A simple approach was chosen to model the overall nutrient dynamics of the lake/reed system. The conceptualization of the system is given by two coupled elements, namely the reed and the open lake. Each of the two subsystems receives input of soluble and particulate nutrients and they are coupled by a small net flow from the reed system to the open lake, balancing the lakes outflow under the assumption of a stable volume, and eddy diffusivity along their common borderline.

To be more specific, the lake submodel calculates for every month t the state of the lake/reed system y(t). From this state a qualitative water quality indicator, like "good, "bad" or "disgusting" - based on the algal biomass, detritus and temperature - is determined. The monthly calculations require:

a) the climatic record for month t:

* temp (temperature)
* rad (radiation)
* flow (inflow = outflow of water)
* eddy (eddy diffusion coefficient, based on wind)

b) the record of loads for month t:

* pprin (load of particulate phosphorus into the reed)
* psrin (load of soluble phosphorus into the reed)
* pplin (load of particulate phosphorus into the lake)
* pslin (load of soluble phosphorus into the lake)

c) the state of the previous month, y(t-1)

d) the amount of reed harvested and constants like the lake volume.

The submodel's calculation of the next state is entirely deterministic, except for the determination of a turbidity value in f_2 (see below).

The state vector y consists of 8 elements, satisfying the following differential equations, containing 14 parameters (p_i).

reed biomass in p: $\frac{dy_1}{dt} = rprod - rmort - harv.$

detritus p in reed : $\frac{dy_2}{dt} = pprin - rmin - rsed - ppexch * C_1 - pptran$

available p in reed: $\frac{dy_3}{dt} = psrin + rmin + sedexc * C_2 - ruptk = psexch * C_1 - pstran$

detritus p in reed sediment: $\frac{dy_4}{dt} = rsed * C_3 - rsmin - sloss + rmort$

interstitial available p: $\frac{dy_5}{dt} = rsmin - rest - sedexc * C_3$

detritus p in lake: $\frac{dy_6}{dt} = pplin + ppexch * C_4 + amort - sedl + - dmin - ppexp$

available p in lake: $\frac{dy_7}{dt} = pslin + psexch * C_4 + dmin - aprod + - psexp - prec$

algal biomass in p: $\frac{dy_8}{dt} = aprod - amort - aexp.$

The description of the processes (when temp > 0):

$rprod = f_1(y_1, y_3, y_5, p_3, p_4, temp, rad)$ $sedexc = (y_5 - y_3) * p_{14}$

$rmort = y_1 * p_5$ $ruptk = C_1 * rprod * p_6$

$rmin = temp * y_2 * p_2$ $rest = rprod * (1 - p_6)$

$rsed = y_2 * p_1$ $rsmin = temp * y_4 * p_{13}$

$ppexch = - eddy * (y_6 - y_2)$ $amort = y_8 * p_9$

$psexch = - eddy * (y_7 - y_3)$ $sedl = y_6 * p_7$

$pptran = y_2 * flow * C_5$ $dmin = temp * y_6 * p_8$

$pstran = y_3 * flow * C_5$ $ppexp = y_6 * flow * C_6$

$psexp = y_7 * flow * C_6$ $aprod = y_8 * temp * rad * \frac{y_7}{y_7 + p_{11}} * p_{10}$

$aexp = y_8 * flow * C_6$ $prec = f_2(y_7)$

C_i are constants, e.g. C_1 is the ratio $\frac{\text{volume lake}}{\text{volume reed}}$

The parameters, p_i, are presented in Table 1.

A.3 A New Framework for the Lake Submodel

In view of the objectives of this paper the lake Neusiedl model was considered to be what it essentially is, namely an input generator for the lake submodel, and the lake submodel itself. The complete lake Neusiedl model was used to generate input, both for 1976 and 1980, consisting of:

a) the initial conditions

b) input sets. Each set consists of the climatic records and the records of loads for 12 months. On behalf of the 1980 simulations 100 different (because of the stochastic perturbances) sets were generated, on behalf of 1976 ten sets.

A simulation program SIMUL was written to perform the simulations, described in this paper. SIMUL is a controller able to read input from the input sets, which runs the lake submodel. Compared to the original model two changes were made:

a) the random disturbance of the turbidity value was skipped;

b) the amount of reed harvested each month was put at zero.

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