Working Paper

Uncertainty Analysis and Parameter Estimation for a Class of River Dissolved Oxygen Models

Ilia Masliev
László Somlyódy

WP-94-9
February 1994

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Preface

Central and Eastern European countries face rapid and profound economic transition and the need of solving pressing environmental and water pollution problems at the same time. Imposing Western effluent standards would lead to financial consequences which are unrealistic in the short run. For this reason, the development of ambient water quality criteria based, river basin least-cost policies is suggested which can be gradually extended later on. The pre-condition of such a strategy is the usage of water quality models relating emissions and receiving water quality, as well as their respective changes. River water quality models incorpotate a number of parameters which should be estimated from often scarce and error corrupted data. This paper deals with parameter estimation and validation for simpler dissolved oxygen models in the frame of a policy-oriented study of the Nitra River basin in Slovakia aimed at selecting the most appropriate catchment-wide wastewater treatment strategies. The Nitra River basin serves as a case study in the context of the ongoing research conducted in the IIASA Water Project, with the broader objective to develop models, methodologies and policy conclusions of interest in the CEE region. This is one of a series of papers that describe the components of the study.

Abstract

Water quality models are essential to the development of least-cost water quality control strategies based on ambient criteria. Such policies are particularly important if financial resources are limited which is currently the case in Central and Eastern European countries. In turn, the derivation of realistic model parameters is a pre-requisite of successful model application. Often, longitudinal water quality profile measurements are performed for the above purpose, but the traditional evaluation of this data encounters significant difficulties due to measurement and other uncertainties. Thus, probabilistic methods are preferred. This paper discusses two of them: the Hornberger-Spear-Young procedure using Monte Carlo simulation and a Bayesian approach. Both methods are rather generic, but they are applied here solely for the traditional Streeter-Phelps model and its extensions, describing oxygen household of rivers. For the purpose of illustration, water quality measurements from the highly polluted Nitra River in Slovakia are employed as a part of a policy oriented study. The BOD decay rate obtained was rather high due to partial biological wastewater treatment and small water depth, but overall, derived parameter values were in harmony with literature findings. Alternative dissolved oxygen models (2-3 state variables and 2-5 parameters) could be evenly calibrated to the data set. Ranges of probability density functions (PDFs) for model parameters were rather broad calling for a well-suited formulation of a water quality management model.

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UNCERTAINTY ANALYSIS AND PARAMETER ESTIMATION FOR A CLASS OF DISSOLVED OXYGEN MODELS FOR RIVERS

I.Masliev[1] and L.Somlyódy[2]

1 INTRODUCTION

Environmental legislation is generally based on effluent water quality standards, ambient criteria or a combination of the two. Effluent standard based legislation defines uniform emission reduction at all the sites. Receiving water quality is a(n unknown) consequence as well as investment and other costs. This type of policy requires no analysis and is easy to enforce if money is available. In contrary, ambient standard based legislation directly formulates goals according to actual water uses and desired environmental conditions. An analysis is required to understand the economic implications of the proposed legislation. The use of water quality models to relate emissions and downstream water quality is a pre-requisite. This approach allows for the development of a number of non-uniform control policies, including a least-cost one. This is particularly important under financial constraints, as it is currently the case in the post-socialist countries of Central and Eastern Europe (CEE) and the former Soviet Union. Such an approach also opens opportunities to address the issue of scheduling and allows for the transition from the least cost strategy to a more sustainable scenario.

The development of a least-cost policy for the highly polluted Nitra River, a second order sub-basin of the Danube in Slovakia (watershed area is about 5000 km^2) is the major objective of an ongoing cooperative study of International Institute for Applied Systems Analysis (IIASA), Water Research Institute in Bratislava, and the Váh River Basin Authority (see Somlyódy et al, 1993; Somlyódy et al, 1994). Among other tasks, the work incorporates the development of a sequence of dissolved oxygen models (according to problem specification) and their calibration and validation. The Nitra River will be used to demonstrate some of the methodologies developed for parameter estimation.

The selection of proper parameter values in water quality models is a crucial step in the development of a catchment wide control policy. The standard methodology is based upon the analysis of longitudinal profiles of concentrations for modelled substances and the computation of model parameters on a reach-by-reach basis (see e.g. Technical Guidance, 1983). Due to large uncertainties in the generally scarce data and to model simplifications, this procedure often produces misleading and even confusing results.

A number of methods have been developed for parameter estimation and uncertainty analysis in water quality modelling (e.g. Beck, 1979a; Beck and van Straten,1983, Beck, 1987). Most of them use minimization procedures with corresponding loss functions such as the least

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squares method (Beck, 1979a). The family of recursive methods such as Kalman filter were also applied for parameter estimation in water quality modelling (examples include Beck, 1979b; Rinaldi et.al., 1979). These methods came up with a single "best" set of parameter values which were then used for forecasting the system's behavior. Lately, it has been understood that given all the uncertainties mentioned above, the ability to uniquely estimate key model parameters is questionable in many cases. Hornberger and Spear (1980) developed the Monte Carlo methodology based on the so called behavior definition which derives sets or ensembles of parameter vectors rather than a single "best" value. This approach was extended (Fedra et al, 1981) to allow those ensembles to be treated as samples from a probability distribution which are used for the forecasting purposes in a stochastic fashion. This methodology and its extensions will be referred to as the Hornberger, Spear and Young (HSY) approach, similar to Beck (1987). Other probabilistic methods such as Bayesian estimation of probability distribution in the parameter space can also account for uncertainties in the modelling process.

In this paper, a class of traditional dissolved oxygen models is formulated, which can be used for water quality management. Major features of the conventional and probabilistic approach to the problem of parameter estimation are outlined. The HSY method and the application of a Bayesian procedure will be discussed. Both methods will be employed for longitudinal water quality profile observations performed in the Nitra catchment in August 1992 and June 1993 (Masliev et al, 1993). As noted before, the results are used to develop a policy framework (for details see Somlyódy et al,1993 and 1994).

2 WATER QUALITY MODELS

A range of conventional river water quality models is applied in this study. The number of state variables affecting the household of dissolved oxygen is between one and three, while the number of parameters varies between one and five. More specifically, the applied models include (see Thomann and Mueller, 1987):

- The original DO-BOD Streeter-Phelps model (two parameters)
- The same model with the incorporation of sedimentation of the particulate organic material (three parameters)
- As before, but with sediment oxygen demand (four parameters)
- A three state variable model with nitrogenous BOD (five parameters)

It is also noted that in addition to the relatively simple models listed above, the complex QUAL2e model was also applied to analyze nitrogen and phosphorus cycles in more detail (Breithaupt and Somlyódy, 1994). However, this model has not yet been involved in the parameter estimation procedure which is discussed here.

The set of partial differential equations for the three state variable-five parameter model can be written as follows (under the well-known assumptions):

$$\frac{\partial(A\,L)}{\partial t}+\frac{\partial(QL)}{\partial x}=-K_r\;A\;L; \qquad (1)$$

$$\frac{\partial(A\,N)}{\partial t}+\frac{\partial(Q\,N)}{\partial x}=-K_n\;A\;N; \qquad (2)$$

$$\frac{\partial(A\,C)}{\partial t}+\frac{\partial(Q\,C)}{\partial x}=k_a B(C_s - C) - K_d\ A\,L - K_n\ A\,N - BK_{SOD}, \tag{3}$$

where L- carbonaceous biological oxygen demand (CBOD), mg/l;
N - nitrogenous biological oxygen demand (NBOD), mg/l;
C - dissolved oxygen concentration, mg/l;
x - coordinate along the river, m;
t - travel time, d;
Q- streamflow, m^3/d.
A - cross-section area, m^2;
B - stream width, m;
k_a - oxygen exchange coefficient (see later), m/d;
K_d - CBOD oxygenation rate, 1/d;
K_r - CBOD decay rate, 1/d;
K_n - NBOD oxygenation rate, 1/d;
K_{SOD} - sediment oxygen demand, $g/m^2/d$.
C_s - saturation concentration of dissolved oxygen , mg/l;

The exchange coefficient across the water-atmosphere boundary, k_a was calculated using the O'Connor and Dobbins (1956) empirical relationship:

$$k_a = k_{a0}\ f(T)\ \sqrt{(U/H)}, \tag{4}$$

where: k_{a0} - the reaeration coefficient, m $s^{1/2}$ / d;
f(T) - dimensionless temperature correction factor,
U - flow velocity, m/s,
H - aeration depth in m, defined as the A/B ratio.

The reaeration rate K_a (1/d) is defined as k_a/H and is dependent on the flow and stream morphometry at the current location.

The solution of Eq(1)-(4) requires the computation of flow. For this purpose a steady-state one-dimensional river network hydraulic model is applied. The solution is obtained from analytical integration of the governing equations. Consecutive reaches specified by tributaries, emissions, and morphometric changes are processed from upstream to downstream. For discharges and confluences, the assumption of immediate mixing is employed.

3 PARAMETER ESTIMATION UNDER UNCERTAINTY

3.1 Standard methodology for parameter estimation: analysis of longitudinal profiles

As recommended by the EPA technical guidelines for waste water allocation studies (Technical Guidance, 1983), a dedicated measurement program should be conducted for model parameter estimation. The observations should cover a low-flow period for the river in question and should incorporate ambient water quality measurements together with the effluent emissions.

The longitudinal water quality profiles should be plotted and analysed in a reach-by-reach basis. Mass balance evaluations should be performed, and the loss of mass in a given reach should be explained by the process(es) assumed (e.g. first order decay for self-purification). Knowing the travel time for a given reach, it is a seemingly straightforward procedure to come up with the value of the parameter in question (e.g. the decay rate).

Figure 1 illustrates typical difficulties for the upper 50 km reach of the Nitra River, when attempting to implement this procedure. As can be seen, the BOD removal rate fluctuates unrealistically, differing significantly from values reported in the literature (including even negative estimates). These hypothetical abrupt changes in the microbiological activity in the river water cannot be caused by changes in external conditions, since this part of the river is comparatively uniform with regard to morphometry, bed composition, slope etc.

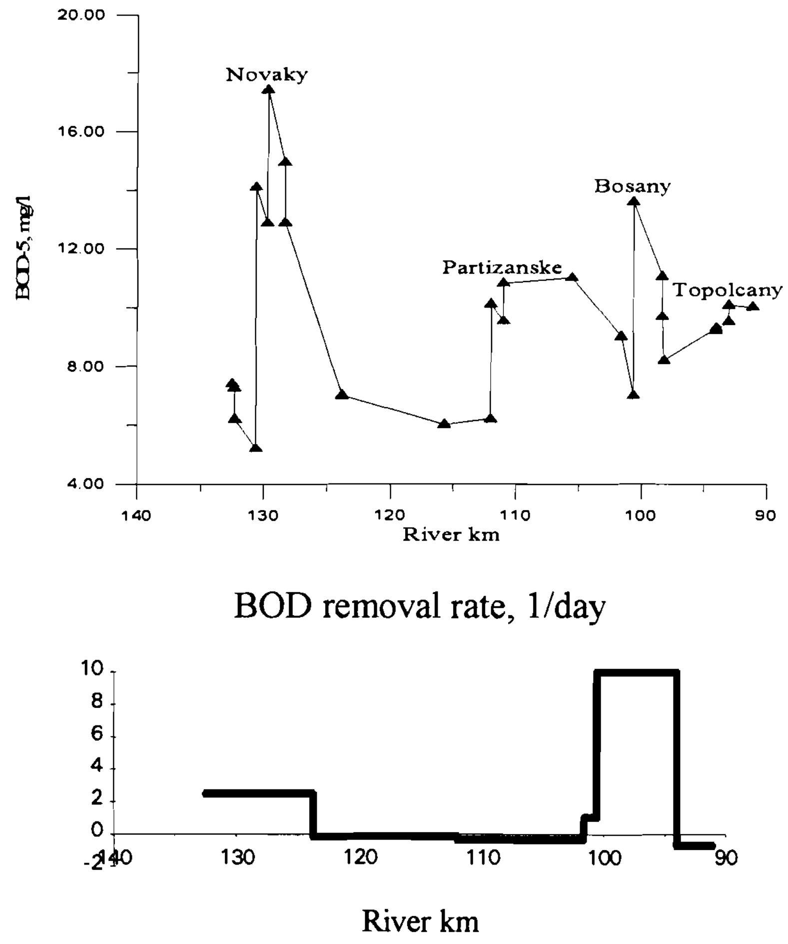

Figure 1. Longitudinal profile and the evaluation of the removal rate of BOD-5 (upper part of the Nitra River).

The evaluation of the longitudinal profiles for the Nitra River clearly shows that there is a need for the application of more advanced methodologies which will to properly handle the inherent uncertainties of the system.

3.2 The HSY approach

This method looks for an ensemble of parameter vectors rather than a unique, best value.The components of the ensemble are accepted or rejected on the basis of the knowledge about performance of the system, expressed by the "behavior definition" (e.g. lower and upper bounds of state variables). This knowledge can be "vague," allowing large uncertainties to be explicitly incorporated in the calibration procedure. Such a method is in harmony with the generally scarce water quality data and relatively poor understanding of processes that affect water quality. All the parameter vectors (elements of which are selected randomly from pre-specified uniform distributions of "feasible" domains) that comply with the defined behavior are considered "acceptable" and can be used later for forecasting of future system responses.

The probability distributions obtained can be applied for a policy-oriented risk analysis (Fedra et al, 1981). However, some caution is required in the interpretation of the results, because the parameter set depends on the specification of the a priori distribution in the parameter space and the behavior definition. The same reasoning applies to other techniques dealing with the uncertainty issues, including the Bayesian estimation to be outlined later.

The implementation of the HSY approach, in this case, logically breaks down into two distinct tasks: generating the samples in the parameter space and screening the resulting simulations. In the sampling unit, both the emission data and the river water quality observations are disturbed by a random component with normal distribution and zero mean. This should effectively model our "uncertainty." The extent of this disturbance is controlled by the analyst (model user) according to his experience and intuition. Samples of the model parameters are uniformly distributed within user-defined bounds, which can be deduced from the literature.

In the screening unit, as noted before, only those scenarios which correspond to the "behavior definition" specified by the analyst are selected. The extensive set of parameter values can be treated as a sample having a certain probability distribution (with the provisions mentioned above).

The software implementation of this appoach was targeted to IBM compatible personal computers. Microsoft Windows 3.0/3.1 (TM) operational platform for the DOS operation system was selected as the interface engine in order to make the tool easy to use (see Fig. 2 for illustration).

The main functional capabilities of this software tool are as follows:

- Read the tables with data about the river system in question, parse river distances and reconstruct the tributary tree.
- Display the river tree symbolically for checking purposes and for visibility.
- Perform the pseudo-random disturbances in coefficients, emissions and observation data, letting the user modify the extent of variability.
- Perform water quality routing through the river system network.
- Select/reject routed trajectories as they pass the measurement points on the basis of user-defined "windows of acceptability".
- Transfer the resulting data to a Microsoft Excel spreadsheet for analysis and display through the Object Linking and Embedding client-server library (OLE).

The validity of the analysis was checked by a "foolproof" test; the water quality model was evaluated on the river system tree with known coefficients, which were subsequently restored with the use of parameter calibration software to an error of not more than 5% (see Figure 7).

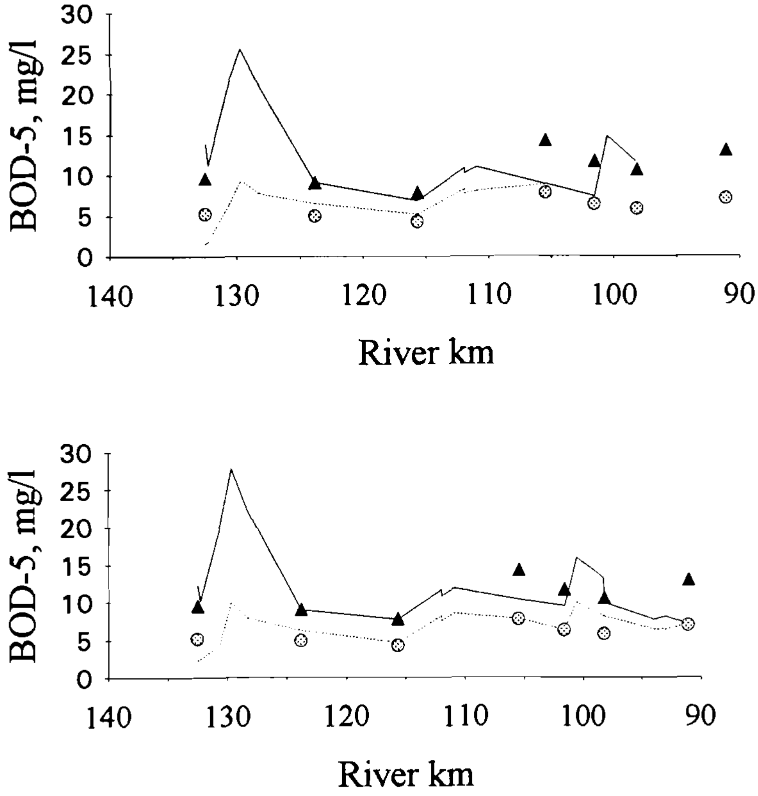

Figure 2. Display of Microsoft Excel charts with longitudinal profiles of BOD-5 generated during the HSY procedure.

—— and .... - bounds on the set of accepted simulations (compliant behavior)
● and ▲ - bounds of behavior definition (acceptance windows)

Above: all generated simulations failed to comply with specified behavior definition.
Below: a trajectory passed the behavior definition windows and will participate in the final analysis.

3.3 An alternative to the Monte Carlo procedure: Bayesian estimation

The approach described above is based upon Monte Carlo simulations and therefore requires simulation repetition. If the number of parameters to be estimated is not large (3-4), then the PDF for the parameters can be obtained with the help of the well-known Bayesian estimation procedure (see e.g. Box and Tiao, 1973). The implementation of the Bayesian estimation involves the following steps:

- selection of the a priori PDFs for the parameters to be estimated ;
- obtain the a posteriori PDFs under the condition that they match the set of observed data using Bayes formula; and
- store the a posteriori PDFs for subsequent use as the a priori distribution for the next set of observations (the next reach or the next year dataset, etc.).

The whole procedure can be subsequently applied for all river reaches (not necessarily following the water quality routing sequence).
The main features of the Bayesian estimation procedure are as follows:

- The a posteriori probability distribution can be stored and reused whenever more data is available.
- The "validation" data set can be used to derive a "validation" a posterior distribution for the parameter and it can be compared with the "calibration" PDF using statistical criteria (t-test, Kolmogorov, Mann-Whitney and so on).
- PDFs obtained via the Monte Carlo technique can be used as the Bayesian a prior distribution and vice versa;
- the Bayesian estimator is very fast for limited parameter space (it does not require extensive repetition of simulation).

Some of the drawbacks to Bayesian estimation are:

- "Curse of dimensionality": the probability distribution values grow in accordance to the power law with respect to the number of parameters that are estimated.
- The discretization of the parameter space is arbitrary.

The use of the Bayesian procedure for the estimation of the BOD removal rate is outlined in the Appendix in more detail.

4 APPLICATION TO THE NITRA RIVER BASIN

Data gathered during a comprehensive measurement campaign in the Nitra River basin at the end of August 1992 (Masliev et al. 1994) was used to formulate a characterization of the oxygen balance. This period was characterized by extremely low streamflow in the river. For the purpose of calibration and possible validation of the water quality models, the river was subdivided into two stretches: the upper part from Novaky to Nitrianska Streda (river km from 132.50 to 91.10) and the lower part from Luzianky to Komoca (river km from 65.25 to 6.50). The validation procedure is based on the June 1993 dataset.

4.1 The HSY approach

There can be several application strategies for the HSY approach to the Streeter-Phelps model. One is to estimate parameters in a sequential fashion, utilizing the fact that Eq (1) can be solved independently from the rest of the system. Thus we can estimate the BOD removal rate first and then use the average of the resulting sample for substitution into Eq (3). The other possibility is to sample from the two-dimensional parameter space (BOD removal rate, K_d, and the reaeration coefficient, k_{a0}). The third possibility is to fix the ratio of the two parameters and then estimate one of them. In this study, we apply the two first methods.

For estimation of the BOD removal rate, the coefficients of variance for the BOD measurements in the mainstream and emissions likewise were set to an arbitrary 30% reflecting our degree of (un)certainty. The "filtering window" was set to the same 30% of the mean value as well. The resulting frequency plots for BOD removal rate is plotted in Figure 3 for the upper and lower stretches of the river.

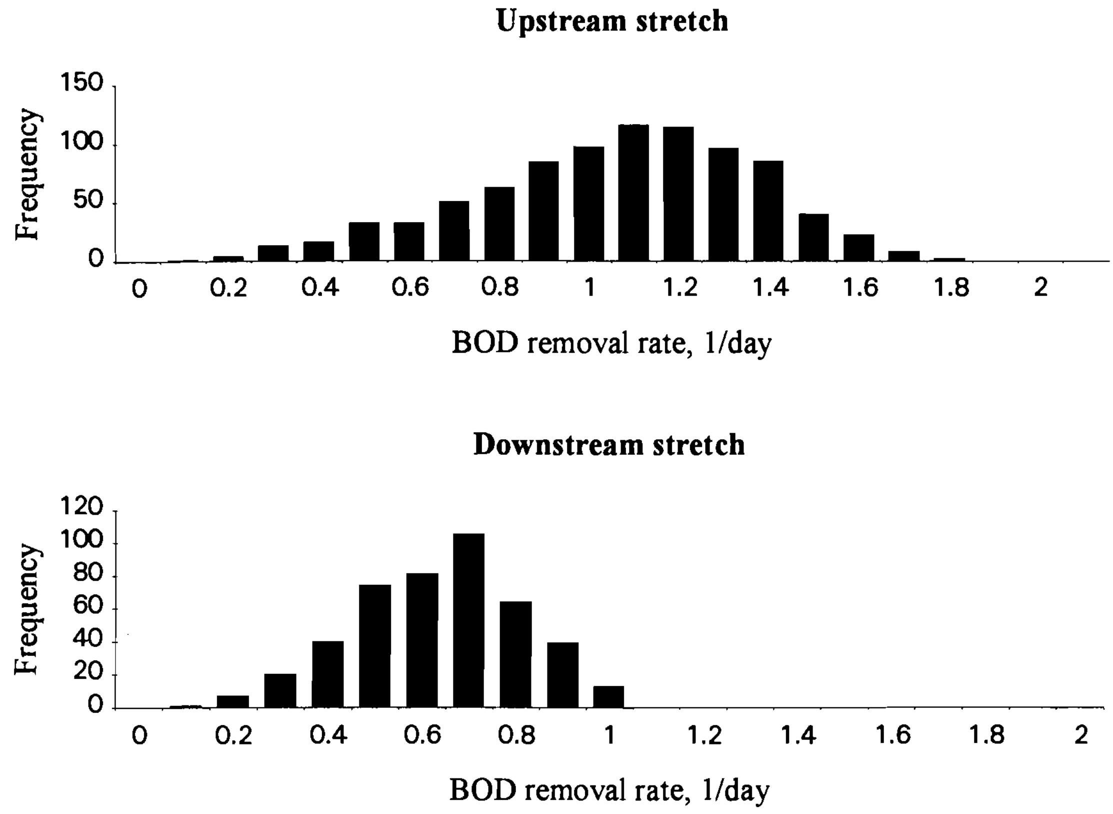

Figure 3. Frequency plots for the BOD removal rate in the upstream and downstream stretches of the Nitra River obtained with HSY technique (August 1992 experiment).

The probability distributions of the BOD removal rate for the upper and lower reaches have means of 1.1/day and 0.7 /day, respectively. These values appear to be higher than the usually assumed 0.2-0.3/day range for biologically treated wastewater effluents (Thomann and Mueller, 1987). The explanation can be twofold. One might be the presence of highly overloaded municipal sewage treatment plants (often by 100% or more) which maintain only partial treatment. On the other hand, systematic analysis of BOD removal rates performed by O'Connor and others (Technical Guidance, 1983) points to a relationship between stream morphology (water depth in particular) and the rate of microbiological utilization of organic waste. Shallow streams tend to have higher BOD removal rates due to increased water contact of water with microbiota attached to the stream bed. This interaction might explain the difference between BOD removal rates in the upper and lower stretches of the Nitra River (the lower stretch has a smaller slope and the river is approximately twice as deep as upstream). The subsequent discussion is focused on the upper part of the river. The findings are similar for both upstream and downstream stretches, the latter serving as a validation test.

The HSY method was used in a sequential fashion used first. For the original Streeter-Phelps model (assuming $K_r = K_d$ in Eqs (1) and (3)), the parameter k_{a0} (see Eq (4)) was calibrated with the BOD removal rate set to the previously found value 1.1/day. The mean value of the reaeration coefficient was found to be 0.37 (corresponding to a reaeration rate of 1.9/day at the

Chalmova measurement point; river km 123.9), which is less than some literature values (Thomann and Mueller, 1987). The ratio of the two parameters is 1.7. The underestimation of the reaeration coefficient suggests that some dissolved oxygen sinks were overlooked.

The incorporation of the sediment oxygen demand of 1.5 $g/m^2/d$ into the oxygen balance equation led to a mean reaeration coefficient of 0.63. Finally, for the model with nitrogenous BOD and sediment oxygen demand, a mean value of 0.77 for the reaeration coefficient was estimated (see Figure 4, Table I).

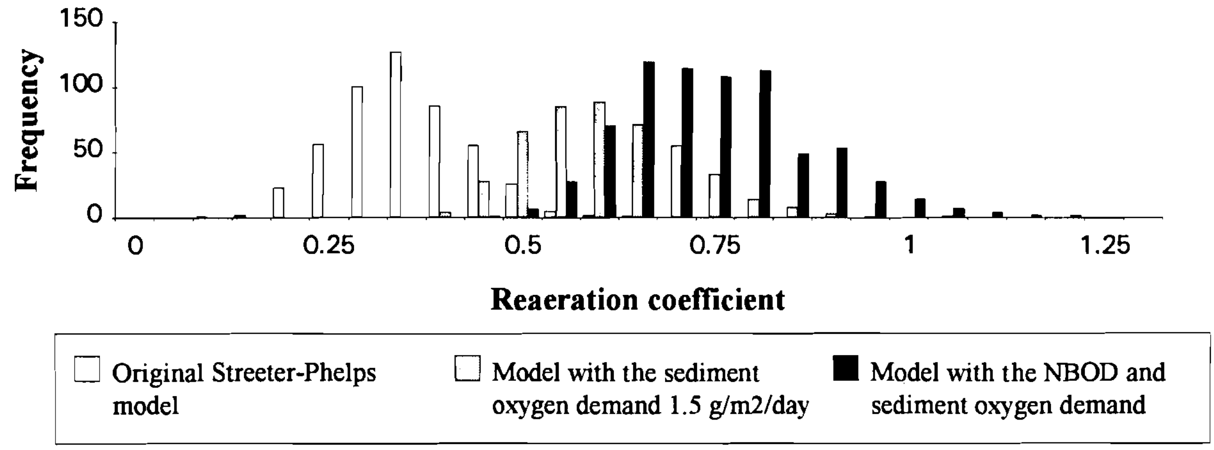

Figure 4. Frequency plots for the reaeration coefficient of the three DO water quality models (upper part of the Nitra River).

Table I Summary of mean parameter estimates for the upper stretch of the Nitra River (HSY method, sequential calibration)

Mean parameter values	K_r, 1/day	k_{a0} -	K_n, 1/day	K_{SOD}, $g/m^2/day$
Streeter-Phelps model	1.1	0.37	-	-
Model with SOD	1.1	0.63	-	1.5
Model with NBOD	1.1	0.48	0.24	-
Model with SOD and NBOD	1.1	0.77	0.24	1.5

If the BOD removal rate and reaeration coefficient are estimated simultaneously rather than in a sequence, the margins of acceptance criteria should be broader (because of the increase in the dimensionality of the event space). An analysis for the original Streeter-Phelps model was performed with acceptance boundaries set to 50% of the measured DO and BOD concentrations. This procedure leads to a small change in the mean reaeration coefficient and mean BOD removal rate .

From the scatterplot on the Figure 5, one can see that the estimates for the BOD removal rate and reaeration coefficient are correlated, which is in harmony with the structure of Eq (3). Linear regression was applied which explained this dependency reasonably well (the R^2 value is about 0.6). The K_a/K_d ratio for the Chalmova location is 2.1, well within the literature bounds for rivers (see e.g. Jolánkai, 1992).

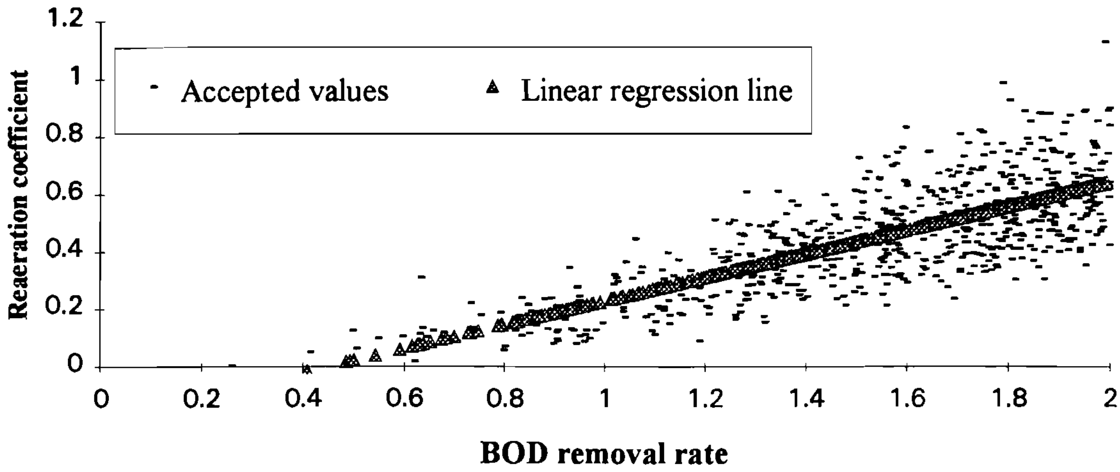

Figure 5. Correlation of the two major parameters from the joint Monte Carlo estimation (upper part of the Nitra River).

The four calibrated dissolved oxygen models were used to simulate water quality in the Nitra river. All produce dissolved oxygen profiles which fit the measured data reasonably well (Figure 6).

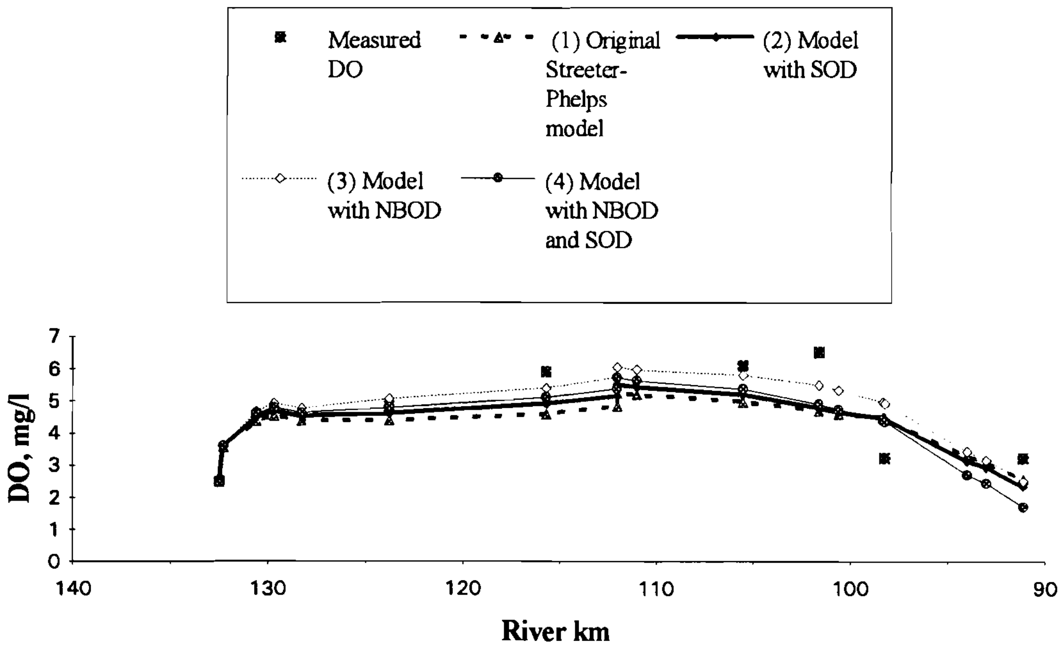

Figure 6. Simulation of DO for the upper stretch of the Nitra River by a sequence of calibrated models.

4.2 Testing the Bayesian estimation procedure for the BOD removal rate

To test the Bayesian estimation procedure, the linear BOD decay model (Eq (1)) was evaluated for the upper part of the Nitra River. Synthetic sets of data were generated from the analytical solution with known BOD decay rates from 0.2 to 1.0 1/d. First, the Monte Carlo calibration procedure was employed followed by the Bayesian approach. Coefficients of variation for all BOD "measurements" were set to 1% for both tests.

The resulting frequency plots for the test BOD removal rate 0.2/day are plotted in figure 7. The mean and variance of the two probability distributions are rather close to each other. Both PDFs center around the generation parameter with the standard error not exceeding 5% of the mean. As for the shape of PDFs (figure 7), the Bayesian method leads to more symmetrical and smoother distributions. This is understandable, since the Monte Carlo procedure approaches the "true" distribution asymptotically. The Bayesian procedure, on the other hand, always comes up with the "true" probability distribution (however discretized in our case to 50 frequency classes).

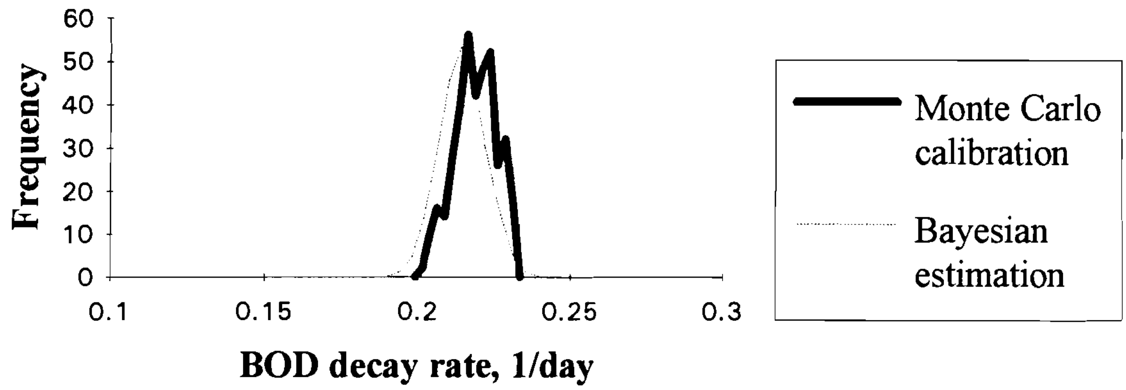

Figure 7. Frequency plot for PDFs of BOD decay rate.

Finally, Bayesian estimation was applied to the data of the August 1992 experiment (Fig. 8). The mean value of the BOD decay rate for the upper stretch of Nitra was found to be equal to 2.2/d (a very high value) with standard deviation of 0.55/d. The lower stretch of the Nitra River was found to have a mean of 1.3/d and deviation 0.5/d. In both cases, a coefficient of variance of 0.3 was used (similar to those used in the Monte Carlo analysis). As can be seen from Fig. 8, the mean value and the entire distribution of the Bayesian estimate is shifted towards the higher values in comparison to the Monte Carlo procedure. No clear explanation exists in this respect, except that the underlying idea of the two approaches is completely different.

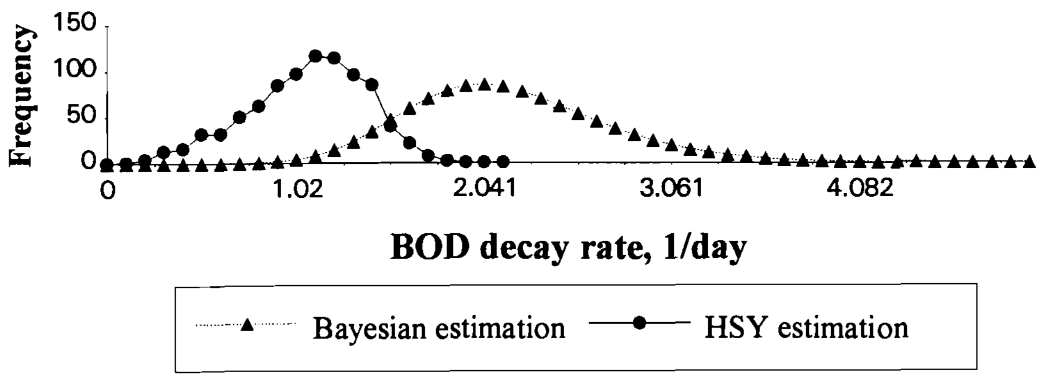

Figure 8. Probability density plots for the BOD removal rate obtained from the HSY technique and Bayesian estimation (upper stretch of the Nitra River).

4.3 Validation procedure on the basis of the June 1993 dataset

For validation purposes the parameters for the Streeter-Phelps model were estimated on the basis data from the June 1993 experiment (Masliev et al, 1994). The data for the upstream stretch of the Nitra River (Novaky - Partizanske) were processed with the help of the Hornberger-Spear-Young approach outlined above (3.2).

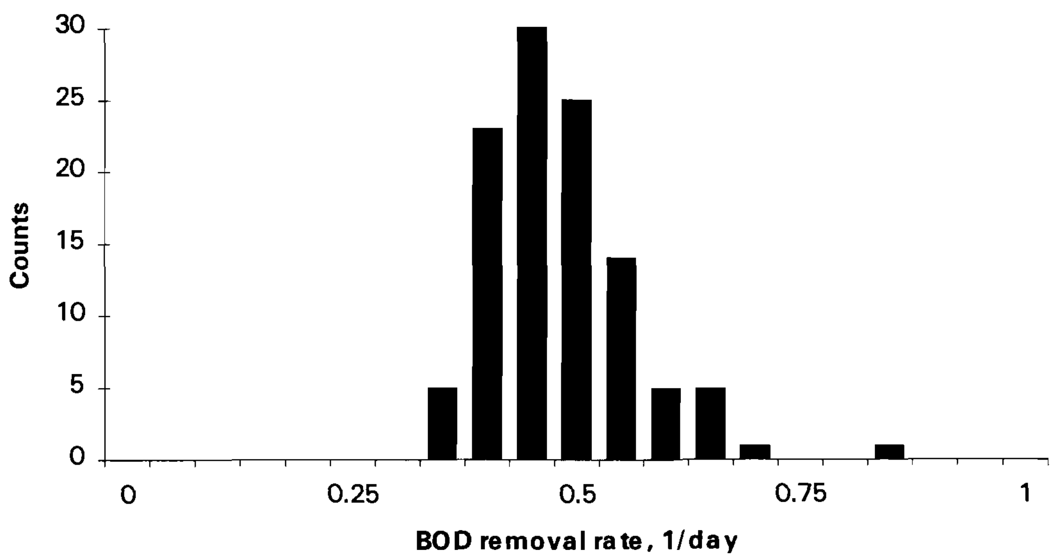

Figure 9. Frequency plot for the BOD-5 removal rate estimate for the upper stretch of the Nitra River (the June 1993 experiment).

Frequency plot for the resulting PDF is shown in figure 9. The mean value is 0.5/day, less than the value 1.1 1/day obtained during the evaluation of the August experiment. One reason might be a ignificant increase in the streamflow (1.4 m^3/s against 0.6 m^3/s in August). The larger streamflow implies an increase in water depth, thus affecting the BOD removal rate.

The reaeration coefficient was evaluated using the sequential approach, i.e. setting the BOD removal rate to 0.5/day. The resulting frequency plot for the estimation of the reaeration coefficient is shown in figure 10. The August 1992 estimation is also shown on the same plot for comparison. Note that the two distributions have similar appearance.

The mean value of the reaeration coefficient is 0.41 (the estimation for the August 1992 dataset is 0.37). Over all, the two estimates pass the estimation-validation test reasonably well.

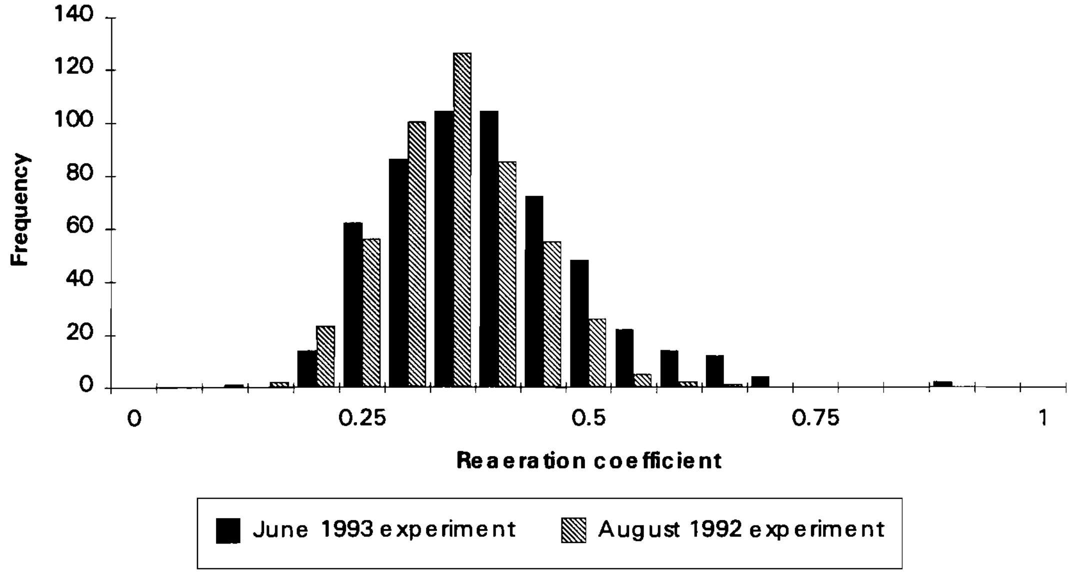

Figure 10. The frequency plots for the reaeration coefficient estimation PDFs for the upper stretch of the Nitra River. The June 1993 and August 1992 experiments.

5 CONCLUSIONS

The following conclusions can be drawn from this study.

(1) Deterministic evaluation of longitudinal water quality profile observations can often lead to unrealistic parameter values.

(2) The Hornberger-Spear-Young (HSY) approach forms an attractive, robust and generic methodology to account for uncertainties. For linear systems the Bayesian method has several promising features, but it deviate systematically from that of the HSY procedure. Further research is needed for a detailed explanation, although the difference in the underlying principles should be the principle reason.

(3) The BOD decay rate obtained for the Nitra River case study was high due to partial biological waste water treatment and small water depth. Parameter values of the Streeter-Phelps model and its extensions were in harmony with the recommendations of the literature. Different model variants can be calibrated to the available data set with a degree of similarity.

(4) The PDFs of the model parameters were characterized by rather broad ranges. For this reason, an appropriate formulation of water quality control policy models and the application of a risk analysis framework is necessary.

REFERENCES

Beck, M.B.(1979a). Applications of system identification and parameter estimation in water quality modeling. International Institute for Applied Systems Analysis (IIASA), Working Paper WP-79-99, 17 pp.

Beck, M.B.(1979b). Model structure identification from experimental data. In E.Halfon (Editor), Theoretical Systems Ecology. Academic Press, New York, pp. 259-289.

Beck, M.B. (1987). Water Quality Modeling: A Review of the Analysis of Uncertainty. Water Res. Res., 23, pp. 1393-1442.

Beck, M.B. and van Straten, G. /ed./(1983) Uncertainty and forecasting of water quality. Berlin: Springer-Verl.

Box, G.E.P. and Tiao, C. (1973). Bayesian inference in statistical analysis. Addison-Wesley, Reading, Mass.

Breithaupt, S. and Somlyódy, L. (1993). Modeling oxygen and nutrient households of the Nitra River Basin (Slovakia). International Institute for Applied Systems Analysis (IIASA), Working Paper (forthcoming).

Fedra, K., van Straten, G. , and Beck, M.B. (1981). Uncertainty and arbitrariness in ecosystem modeling: a lake modeling example. Ecological Modeling 13 , pp.87-110.

Jolánkai, G. (1992). Hydrological, chemical and biological processes of contaminant transformation and transport in river and lake systems. A state-of-the-art report. UNESCO, Paris.

Hornberger, G.M. and Spear, R.C. (1980). Eutrophication in Peel Inlet, I. Problem-defining behavior and a mathematical model for the phosphorus scenario. Water Res., 14: pp. 29-42.

O'Connor, D.J. and Dobbins, W.E. (1956) The mechanism of reaeration in natural streams. Proc. of Am. Soc. of Civ. Eng., J of Sanit. Eng. Division 82, pp. 1-30.

Masliev, I., Petrovic, P., Kuníková, M., Zajícová, H., and Somlyódy L. (1994) Longitudinal water quality profile measurements and their evaluation in the Nitra River basin (Slovakia). International Institute for Applied Systems Analysis (IIASA), Working Paper (forthcoming).

Rinaldi, S., Soncini-Sessa, R., Stehfest, H., and Tamura, H. (1979). Modeling and control of river quality. McGraw-Hill, NY.

Somlyódy, L., Kularathna, M., and Masliev, I. (1993) Water quality management of the River Nitra basin (Slovakia): Evaluation of various control strategies. International Institute for Applied Systems Analysis (IIASA), Working Paper WP-93-63.

Somlyódy L., Masliev I., and Kularathna M. (1994). Development of water quality management policies for the Nitra River basin (Slovakia). International Institute for Applied Systems Analysis (IIASA), Working Paper (forthcoming).

Technical Guidance Manual for Performing Waste Load Allocations. Book II, Streams and Rivers. Chapter 1, Biochemical Oxygen Demand/Dissolved Oxygen. U.S. E.P.A, Office of Water Regulations and Standards, Monitoring and Data Support Division, Washington D.C., October 1983.

Thomann R.V. and Mueller J.A. (1987). Principles of Surface Water Quality Modeling and Control. Harper and Row Pub., NY.

APPENDIX
BAYESIAN ESTIMATION OF DECAY RATE FOR THE LINEAR DECAY MODEL

Let us illustrate the use of the Bayesian estimator with the linear BOD decay example. Assume that BOD concentration measured at the beginning of the reach, $L_0(t=0)$, is a random value with the probability distribution function (PDF) $P(L_0<x)$ with a density $p_{L0}(x)$:

$$P(L_0 < x) = \int_{-\infty}^{x} p_{L0}(t)dt. \qquad (1)$$

Most commonly, a normal distribution is used to describe measurements errors, i.e. $p_{L0}(x)=N(L_0, \sigma_0)$ - normal PDF with mean L_0 and standard deviation σ_0.

Parameters also are treated as random values in the Bayesian approach. We will assume that for a BOD decay rate of K some apriori PDF does exist:

$$P(K < y) = \int_{-\infty}^{y} p_K(t)dt \qquad (2)$$

The initial apriori PDF for the paramerer is selected usually as a uniform distribution bounded by established literature ranges. If the parameter had been evaluated on the basis on some data sets, the aposteriori PDF based on this data can be used as the apriori for the next step. Of course if there is some additional information about the parameter besides the admissible interval it can also be utilized in the apriori PDF.

The linear model of BOD decay looks like

$$L_1=L(t=\tau)=L_0\exp(-K\tau), \qquad (3)$$

where τ is travel time in days between two river locations.

Let us write a probability function for L_1:

$$P(L_1 < z, y < K) = \int\int_{L_1(L_0=x,K=y)<z} p(x,y)\, dx\, dy =$$

$$= \int_{-\infty}^{K} p_K(y)\, dy \int_{x < L_1^{-1}(z,y)} p_{L0}(x)\, dx =$$

$$= \int_{-\infty}^{K} p_K(y)\, dy \int_{-\infty}^{\frac{z}{\exp-(y\,\tau)}} p_{L0}(x)\, dx =$$

$$= \int_{-\infty}^{K} p_K(y)\, dy \int_{-\infty}^{z} \frac{1}{\exp-(y\ \tau)} p_{L0}(\frac{x}{\exp-(y\ \tau)}) \tag{4}$$

According to the definition of conditional probability, the function

$$p(z\,|K=y) = \frac{1}{\exp-(y\ \tau)} p_{L0}(\frac{z}{\exp-(y\ \tau)}) \tag{5}$$

is the conditional PDF for L_1=L(t=τ). We can provide for a measurement error at the comparison location by combining the PDF defined in (5) with additional "white noise" N(0,σ_1) representing our uncertainty in calibration data. The resulting intermediary PDF will be marked with an additional prime: p'(z|K=y). Finally, the Bayesian estimator for aposteriori PDF for parameter K will look like

$$q(y) = \frac{p(z \mid K=y)p_K(y)}{\int p(z \mid K=t)p_K(t)dt}. \tag{6}$$

Implementation of this procedure requires discretizing the admissible range for the parameter (usually derived from literature) to a set of intervals. The integral in (6) is approximated by a sum over the number of intervals.

This procedure can be repeated for subsequent reaches of the river, not necessarily following the simulation of river water quality. However, for purposes of consistensy it is felt that simulation sequence is preferred.

It can be noted that from a computational point of view, many properties of the Bayesian estimator are similar to the dynamic progranmming method used for water quality management purposes (Somlyódy et al, 1993).