Hydrophysical and Ecological Modelling of Deep Lakes and Reservoirs

Summary Report of a IIASA Workshop, December 12-15, 1977

Sven E. Jørgensen and Donald R. F. Harleman, Editors

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Preface

An important subtask within IIASA's Resources & Environment Area (REN) is the development and application of Models for Environmental Quality Control and Management. The initial objectives of this task are to assess existing models, to develop improved hydrophysical and ecological models as tools for the analysis of water quality problems and to apply these models to lakes, reservoirs and river systems.

In 1976, research on the modelling and control of water quality in rivers was initiated with a case study of the Rhine. This was followed in September 1977 with the IIASA Workshop on Mathematical Modelling of Water Quality. As a result of this workshop it was decided to focus immediate attention on the water quality problems of natural lakes and man-made impoundments (reservoirs). In addition, it was felt that IIASA could make an important contribution to the use of models for water quality control and management purposes by attempting to bridge the gap between the hydrophysical and ecological modelling disciplines. Accordingly, it was decided to convene two specialized workshops, one on deep lakes and reservoirs and one on shallow lakes and reservoirs.

This report summarizes the results of the first of these workshops on deep lakes and reservoirs, held December 12-15, 1977. The workshop was attended by 20 people representing 11 countries and by 9 IIASA staff members from 5 countries. Prior to this workshop, a set of questions relating to ecological and hydrophysical modelling problems were formulated by the IIASA staff. The questions were sent to the expected participants with the request that they come prepared for their discussion. The participants included experienced modellers from both the ecological and hydrophysical areas and the entire group participated in all of the presentations and discussions of the two areas. The smallness of the group made possible a useful exchange of ideas and viewpoints.

For some of the questions discussed, there were no unique answers or even a clear consensus among the participants. Nevertheless, an attempt was made to record the "sense" of the discussion.

A number of these questions were also discussed at the April 1978 Workshop on Shallow Lakes and Reservoirs. The results are contained in the report of that meeting.

Summary

A series of questions related to the geophysical and ecological modelling of deep lakes and reservoirs were formulated and distributed in advance of the workshop. This workshop report summarizes the discussion of each of the questions relating to the following topics: element cycles, nutrient uptake and grazing rates by phytoplankton and zooplankton, single versus multi-layer models, vertical mixing and diffusion, lake circulation and methods of parameter estimation.

Acknowledgments

The editors would like to express their thanks to all those who contributed to this Workshop whether by formal presentations or through participation in the discussion. Special thanks are due to the participants who acted as general reporters and prepared written summaries. The editors accept full responsibility for errors of omission or commission.

Our appreciation is extended to Ms. Ann Wadia and Ms. Hilary Aziz for their assistance in preparing this publication.

Contents

Introduction

On September 13-16, 1977, a workshop on the general subject of Water Quality Modelling was held at IIASA. At this meeting the most recent theoretical developments in the subject, as well as developments in the application of hydrophysical and ecological models to various water bodies were discussed. One important recommendation of the workshop was that a number of more specialized workshops be convened in the near future. The first of these, on Hydrophysical and Ecological Modelling of Deep Lakes and Reservoirs, was held December 12-15, 1977, at Laxenburg.

The subject of deep lakes and reservoirs chosen for this workshop implies a basic concern with stratification and interactions at the free surface boundary rather than with conditions of full vertical mixing and bottom sediment interactions. The latter subjects will be the focus of a second workshop on Shallow Lakes and Reservoirs to be held April 11-14, 1978.

Topics suggested for discussion at the December workshop included:

- Boundary conditions--surface exchange and transmission of light and heat, oxygen and CO_2 inflows and outflows;
- Hydrothermal models--wind induced currents and circulation, wind mixing, thermocline formation and temperature distribution, retention time in stratified lakes and reservoirs;
- Water quality models--limiting nutrient and total cycle models--model complexity; and
- Field data collection and model verification techniques--coordination of field work and modelling, choice of parameters.

The intent of the workshop was to bring together qualified scientists and engineers, working on both the physical and ecological aspects of deep lakes and reservoirs, for an intensive period in which ideas, information and experience could be exchanged. A small number of invited papers were presented; however, the major effort was devoted to the discussion of a set of questions that were distributed in advance to the workshop participants. The discussion questions were divided into types ecological, hydrophysical, and general. Workshop participants, acting as general reporters, prepared written summaries of the discussion. At the close of the conference these summaries were submitted for final coordination and editing. Professor Jørgensen was editor for the

ecological section and Professor Harleman for the hydrophysical and general sections.

These workshops are within the framework of IIASA's studies on Models for Environmental Quality Control and Management of the Resources and Environment Area, Task 2, and are under the general supervision of Professor Oleg Vasiliev, a Deputy Director of IIASA.

Introduction to Questions Related to Ecological Modelling of Deep Lakes and Reservoirs

S.E. Jørgensen

The literature on ecological modelling in lakes contains a large number of different ecological models. In Table 1 a survey of some of the most generally applied lake models is given. They cover a wide range of complexity: consider only one nutrient while others consider four; consider the lake as one box, while others use several segments and layers. The growth of phytoplankton can be described by use of constant stoichiometrics, but chemostat experiments show that the nutrient cycles are independent.

Unfortunately, only a small number of the models have been validated, a step absolutely necessary if models are to be used as predictive tools.

Not only is the complexity different from model to model, but also the mathematical expressions used for description of ecological processes vary from model to model. Which of the many models and the many equations used in the different models are the best to apply? This question is difficult to answer, as there is no such thing as a general lake model. An ecological model of a lake system must be generated in accordance with the goals set up for the model. A more complex model is not necessarily better, even though we know that the ecosystem is more complex than the most complex models. A complex model introduces more parameters, which must be calibrated, thereby introducing errors that the simpler model may avoid.

Biology is not an exact science like physics or thermodynamics. It is therefore possible for the same biological process to find different mathematical descriptions by different authors. A more detailed examination of the different expressions will usually reveal that the difference is a matter of environmental factors included or excluded in the examination of the biological process. Theoretically, as many details as possible may be included in the description of biological processes in a lake. The question is whether these will provide additional advantages for the total model, taking into consideration the objective of the models.

From the above discussion the following conclusions can be drawn:

- The complexity of a model must be selected in accordance with the objective of the model.
- A more causal description of the biological processes should be preferred to a more or less detailed or empirical

Table 1. A survey of ecological lake models.

Model	Number of State Variables per Layer of Segment	Nutrient Considered	Segments	Dimension(D) or Layers(L)	Constant Stoichiometrics (CS) or Independent Nutrient Cycle (NC)	Calibrated(C) and/or Validated(V)	Number of Case Studies in Literature
Vollenweider	1	P(N)	1	1L	CS	C+V	many
Imboden	2	P	1	2L,1D	CS	C+V	3
O'Melia	2	P	1	1D	CS	C	1
Larsen	3	P	1	1L	CS	C	1
Lorenzen	2	P	1	1L	CS	C+V	1
Thomann 1	8	P,N,C	1	3L	CS	C+V	1
Thomann 2	10	P,N,C	1	7L	CS	C	1
Thomann 3	15	P,N,C	67	7L	CS	-	1
Chen & Orlob	15	P,N,C	sev.	7L	CS	C	min. 2
Patten	33	P,N,C	1	1L	CS	C	1
Di Toro	7	P,N	7	1L	CS	C+V	1
Biermann	14	P,N,Si	1	1L	NC	C	1
Canale	25	P,N,Si	1	2L	CS	C	1
Jørgensen	17	P,N,C	1	1-2L	NC	C+V	3
Cleaner	40	P,N,C,Si	sev.	sev.L	CS	C	many
Nyholm	7	P,N	1-3	1-2L	NC	C+V	13

description. Detailed descriptions should not be introduced into the model if they involve additional parameter values that are not known within a narrow range and that therefore must be calibrated. If however, such a detailed description is required of the model, it is necessary to study the details in the laboratory or in the ecosystem to obtain the necessary basic knowledge, including a good estimation of the applied parameter values.

- It is of great advantage for the calibration procedure to know the parameters within certain limits. A model with many parameter values and a limited number of observations can always be calibrated to fit the data. Therefore, it is recommended not only to have narrow ranges for the parameters, but also to have many observations available for calibration of a limited number of parameter values.

- All models should be validated against an independent set of observations.

Discussions on Ecological Topics

Edited by S.E. Jørgensen

Validity of constant stoichiometric models versus element cycle models. How many element cycles are needed in a eutrophication model?

Reported by S.E. Jørgensen.

Element cycles are to a certain extent independent. A phenomenon such as the luxury uptake of phosphorus demonstrates the independence of the nitrogen and phosphorus cycles. It is also known that the excretion rate of zooplankton and fish are different for nitrogen and phosphorus. Furthermore, the ratio of maximum phosphorus concentration to minimum phosphorus concentration in phytoplankton is about 5, while the corresponding ratio for nitrogen is about 2. Consequently, in most cases it is recommended that the independent element cycle description of phytoplankton growth be used in a eutrophication model, especially when the model is to be used as a predictive tool. The constant stoichiometric model may hold for a given case study, where the ratio of nitrogen and phosphorus concentration in a lake is constant even if different from the ratio recorded in the phytoplankton, but if the loading of one of the nutrients is changed, it is expected that the ratio of nitrogen to phosphorus in the phytoplankton will change. To account for changes in loading the best procedure is to use independent element cycles for nitrogen and phosphorus.

However, the disadvantage of independent element cycles is that more parameters are introduced into the model. This drawback can partly be eliminated, as the minimum and maximum concentrations of the elements in phytoplankton are well known. For example, the phosphorus concentration varies between 0.5 and 2.5% on a dry matter basis.

In lake studies where the ratio of the elements is kept rather constant, the stoichiometric model might be used as a less complex alternative to the independent element cycle description. Lake models containing an independent element cycle description of the eutrophication process can be found in *Ecological Modelling*, 4, No. 2-3, January 1978.

How should the following chain of processes be modelled:
organic N $\rightarrow$ NH_4^+ $\rightarrow$ NO_2^- $\rightarrow$ NO_3^-?

Reported by M. Watanabe.

The difference between various models for this chain of process was demonstrated by Harleman. He presented two examples and compared the results of using different models with chemostat data. Two models were compared, namely a linear kinetics model (first order), and a nonlinear kinetics model (Monod type) with bacterially mediated reactions as illustrated schematically in Figure 1. It was concluded that only the nonlinear model, with bacteria, gave an acceptable fit to the chemostat data. A detailed

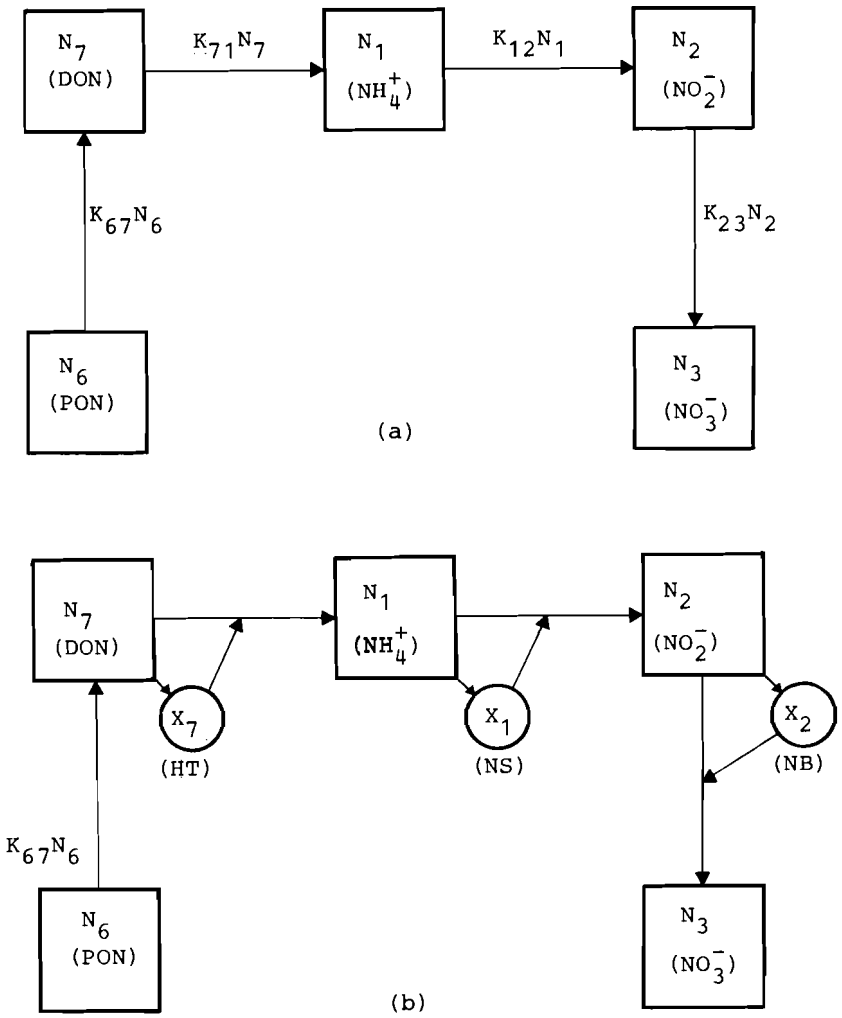

Figure 1. Schematic diagrams of (a) linear and (b) nonlinear models for bacterial hydrolysis and nitrification process (X_7, X_1, and X_2 are bacteria).

discussion may be found in the IIASA Research Memorandum RM-78-34, *A Comparison of Water Quality Models of the Aerobic Nitrogen Cycle* by D.R.F. Harleman.

However, problems are raised by the application of this more complex model for the chain of processes considered:

- How do we find the several rate coefficients? It seems necessary to use chemostat data with rate coefficients determined by fitting the model to the laboratory observations.

- Normally one does not know the initial conditions for the bacterial equations, as bacterial data are generally not available. This is one of the drawbacks of the more comprehensive description. On the other hand, it might in some situations be necessary to use the feedback mechanism contained in the bacterial model to be able to fit model data with observations.

However, in a normal lake situation the number of bacteria will generally be rather constant compared with the situation in the chemostat, where the initial bacterial concentration is low and the number of bacteria is increased exponentially in the first experimental phase. Consequently, it was not possible to agree upon whether the simple first order model description of the chain processes should be used rather than the more complex models described above. It can, however, be concluded that the concentration of nitrite in natural lakes is very small, since the nitrification process is rather fast.

From these arguments a linear model for nitrification process may be satisfactory. It is recommended, generally, to carefully study the role of chemostat experimental data and how such data can be implemented in ecological models.

What equations are most suitable for describing the nutrient uptake rates by phytoplankton of phosphorus, nitrogen, (NH_4 + NO_2 as well as NO_3), carbon, silica? How do we model the growth and mortality of phytoplankton with single and multiple nutrients? Should a linear equation, a Monod kinetic equation, or the intracellular concentration of nutrient be used? What light and temperature expressions are proper?

Reported by A. Knoblauch.

Investigation of algal growth kinetics in chemostats indicates that a steady state growth is indeed a Michaelis-Menten function of external substrate concentration. However, if we consider predicted changes in cell concentration of *Scenedesmus* under phosphorus limiting conditions, the concentration of phytoplankton will be an order of magnitude larger by the use of the Michaelis-Menten description than observed. However, if we modify the uptake

to reflect internal concentration, as found by Rhee, the correct predicted range of the cell quota is obtained. Former investigations of this observation indicated that when the cells are at equilibrium, the Michaelis-Menten function of the external substrate is a reasonably good simplification. This investigation showed also that phosphorus is more important than nitrogen or at least silica in the kinetics. As also indicated in the discussion of question 2, the more complex element cycle model is chiefly of importance under changed nutrient loadings, while the simple Michaelis-Menten function of external substrate can be used in lakes, in which the nutrient concentration is not changed drastically.

When phytoplankton can take up H_2CO_3, carbon will not be a limiting factor except in some very rare cases.

The type of function used for the limiting function, was not important (e.g. multiplication or weighted average etc.) but in all circumstances it is incorrect to include light as a limiting factor in a minimum function expression.

What equation should be used for describing the grazing rate? Should more than one species of zooplankton be included?

Reported by S.E. Jørgensen.

Up to ten grazing expressions are used by different authors. If the species present in a given lake are known , it is possible to select which one of these expressions give the best description of the grazing. However, in most cases we are interested in an average situation--what is the average grazing rate when we consider all the species present in a lake system? In this case a simple Michaelis-Menten expression should be available, but if the concentration of phytoplankton is rather low, a threshold limit must be introduced into the expression. Many zooplankton species are filter feeders and are not able to graze when the concentration of feed is too low.

What are the bottom-boundary conditions for deep lake models, e.g. the exchange of nutrient between the sediment and the water phase?

Reported by D. Di Toro.

If the condition at the bottom sediment interphase is aerobic the phosphorus is probably bound by an iron system. If, however, the condition becomes anaerobic, the phosphorus is released. It is important in this context to state how much of the sediment phosphorus is available for release, since this is a rather large fraction of the total annual loading of phosphorus.

A more comprehensive phosphorus sediment model was introduced at this stage by Jørgensen, in which it is necessary to

distinguish between exchangeable phosphorus and nonexchangeable phosphorus. Exchangeable phosphorus decomposes and dissolves in the interstitial water as interstitial phosphorus, which diffuses into the overlying water. However, under aerobic conditions considerably more phosphorus is adsorbed on the sediment and therefore the concentration of interstitial phosphorus will be low. Mineralization, i.e. the decomposition of exchangeable phosphorus into interstitial phosphorus, is also different under aerobic and anaerobic conditions. The rate is one order of magnitude higher under aerobic conditions than under anaerobic conditions. The profile of the phosphorus in the sediment indicates which part of the settled phosphorus is exchangeable and which part is nonexchangeable. Of course, this model does not take all problems into consideration; questions such as groundwater infiltration might be of importance in some instances.

Should more than one species of phytoplankton be considered? Blue-green algae are a problem in some lakes. How can we, for example, distinguish in the model between "other algae" and blue-green algae?

Reported by S.E. Jørgensen.

In some cases blue-green algae are a serious pollution problem and it is then necessary to distinguish between them and other algae. When lack of silica is a major limitation, it is necessary to distinguish between diatoms and other algae. This requires one more state variable for one additional species of algae, but it should not be too difficult to distinguish between blue-green algae and others, since blue-green algae differ from the others in the following manner:

- Lower settling velocity;
- Lower growth rate;
- No grazing by zooplankton, or almost no grazing;
- Higher P uptake rate;
- Higher optimum growth temperature (22 to 23 ^{o}C compared with most other species, which have their optimum between 16 and 19 ^{o}C).

The main problem in modelling algae succession is the accurate description of the death rates and decay, rather than the growth.

How should the settling of phytoplankton and detritus be included in a model?

Reported by N. Thomas.

The role of turbulence was discussed. It is possible to determine the flux of material through a plane by use of the

following equation:

$$F = vC + V_a C \ ,$$

where F is the flux through a plane,
v, the velocity due to turbulence,
V_a, the velocity in a certain direction, and
C, the concentration.

Turbulent eddies are able to circulate plankton and thereby influence the sinking rate. The phytoplankton sinking rate can be measured in the laboratory, but the results cannot be used as a parameter value in ecological models, as they differ by a factor of 10 from those applied in most lake models: laboratory measurements give settling velocities of 10 to 50 m per 24 hours, depending on the state (health) of the algae, while the rate used in most ecological models ranges from 0.1 to 0.5 m per 24 hours. If the high rate measured in the laboratory is used in models, it is impossible to explain how phytoplankton populations could be maintained.

Measurement of the sinking rate in a lake by use of settling traps shows that the sinking rate is higher while phytoplankton are decaying than while growing. Hence a biological process must be the explanation for the discrepancy between measured and actual sinking rates. For example, the phytoplankton might be able to change their density, and some studies in a shallow English lake indicate that phytoplankton sink only after blooms.

The following points must be taken into consideration if a more causal description of the settling is needed:

- Large and small algae settle at different rates;
- Turbulence;
- Upwelling and downwelling;
- Below the thermocline phytoplankton appear to sink at a faster rate: examination of data from Lake Ontario indicated that a part of the plankton would have to sink 200 m in 30 days or 7 m in 24 hours.

Further studies are necessary to give a more causal and detailed description of settling. As the settling describes the removal of phytoplankton, it is important to make these studies.

How do we select the number of state variables necessary for solving a specific problem? More state variables involves the introduction of more parameters, and more measurements must be carried out, while few state variables may not describe in enough detail the structure of the system. How do we find the balancing point? What is the role of chemostat data?

Reported by N. Adachi.

Two topics were discussed. One was a methodology for identification of the model structure and the other was the relation between model structure and the quality of observed data.

Harleman showed by a case study how it is possible to select the number of state variables. He started with a very simple model and increased the number of compartments. The simple model did not provide an acceptable fit with the observations; but the introduction of eight state variables explained the results of reported chemostat data. (Recent work by A. Leonov.)

Jørgensen presented an attempt to use a quantitative index for the solution of this problem. The idea is to apply a concept of sensitivity to identification of the model structure. An ecological buffer capacity, β, is introduced, defined as the ratio between a loading change and the recorded change in the response. If a change in phosphorus loading is considered and we want to study the phosphorus in the phytoplankton,

$$\beta = \frac{\Delta P \text{ (input)}}{\Delta P \text{ (in phytoplankton)}} \quad .$$

β and exergy are linearly dependent. The exergy can be found from the thermodynamic equation, and from the exergy information about the β value can be got. The β value can be used to decide the number of state variables necessary in a given ecological model. If we have a model with n state variables, we may ask whether it is necessary to add one more state variable. What is the difference in the response when we calibrate the model with the n state variables and when we use n + 1 state variables? Since the β value measures the response of the model, it is possible by calculating β for the two instances, with n and with n + 1 state variables, to get an idea of the consequent difference in response. If β is increased only slightly by adding one more state variable to the model, there is no reason to make the model more complex. Note that β always increases with increasing complexity. This is understandable when it is remembered that the models are calibrated to fit the same data, except for the state variable in question. In the example above we are not calibrating the model to fit with the phosphorus in the phytoplankton; this state variable is kept free. When we add a state variable to the model, we must take some phosphorus from the phytoplankton compartment to the additional compartment to cover this state variable. Thus β will increase when compartments are added to the model. Thus, the β value is only a tool used in the calibration phase to measure the change in

response when considering the necessity of increasing the complexity of the model.

Model structure depends on the accuracy required of the model, so it is important to consider the accuracy with which it is possible to simulate a specific ecosystem. This brings up the question of how much we can rely on the observed data. The observations have standard deviations related to the sampling, the chemical analyses of the samples, and the actual methods used for defining biological values. It must be assumed that ecological observations generally will have a standard deviation of from 10 to 25%. This must be taken into consideration when the accuracy of the model is estimated as the model can never be better than the observations on which it is based.

Is it possible to model the behavior of toxic substances, such as heavy metals in an ecosystem? Is it possible to consider limitation by several factors at the same time?

Reported by S.E. Jørgensen.

To model the distribution and effect of toxic substances, it is not just a matter of adding a few more state variables to the eutrophication model, but rather of changing the entire model structure. The exchange of toxic substances between sediment and water is of great importance. This depends on pH, dissolved oxygen, and the concentration and our present knowledge of these processes is rather limited. From the literature it is known that 90 to 95% of the accumulation of toxins in the biomass is by direct uptake from the water phase. Further research is necessary before a viable model can be obtained.

It was pointed out by Chahuneau, concerning limitation by several factors at the same time, that there is an interaction between the factors, e.g. temperature and light, which means that it is not possible to describe actual laboratory observations by means of the independent expressions generally used in the ecological modelling of lakes. It seems necessary to study the interaction of limiting factors as well as feedback mechanisms more carefully in the future to get a more causal description of the ecological processes.

Introduction to Questions Related to Hydrophysical Models of Deep Lakes and Reservoirs

D.R.F. Harleman

Hydrophysical models for lakes and reservoirs are at a fairly advanced level of development in contrast to the state of ecological modelling. Nevertheless, a number of interesting problems and questions remain to be resolved on models that describe the physical processes of water movement, mixing, and diffusion and the transmission and distribution of light and heat into the water body.

Many of these relate to the dimensional complexity of the hydrodynamic model ranging from the fully three-dimensional representation of lake circulation to the simplest "one box", i.e. horizontally and vertically mixed, models. From a conceptual and computational viewpoint, the entire spectrum of hydrophysical lake models is feasible. The primary questions are concerned with choosing the appropriate degree of complexity. As with ecological models, the choice is generally dictated by the objectives of the modelling effort. In the more complex models, the choice is also usually limited by the lack of detailed synoptic field observations needed for calibration and verification.

One area that has received relatively little attention is the coupling between hydrophysical and ecological models. It is not uncommon to see a highly sophisticated model coupled to a simple "one box" system that completely overlooks the hydrophysical processes. The reverse is equally prevalent in the literature of lake and reservoir models. One of the objectives of the present workshop and the set of questions formulated for discussion, was to bring together representatives from these two groups and have them participate in the discussion of problems in both areas.

Discussions on Hydrophysical Topics

Edited by D.R.F. Harleman

What is the validity of two-layer (epilimnion and hypolimnion) or multilayer models versus models with continuous vertical distribution of temperature, light intensity and water quality parameters? In the case of two-layer models should the depth of the upper layer vary with time? How do we model the mixing and exchange between two layers?

Reported by G. van Straten.

Opinions were divided on the problem of whether a two-layer or multi-layer model would be an acceptable alternative to a continuous model for describing the vertical distribution in a lake or reservoir. The behavior of vertical profiles of nutrients and oxygen in deep lakes is sometimes so complex that it would prohibit the use of the simpler discrete layer models (Imboden). The drawbacks of the discrete layer models are summarized below:

- It will be difficult to assess correct values for the exchange coefficients between layers, since the appropriate value will be essentially a function of layer dimensions. In addition, little is known about the dependency of the exchange coefficients on wind velocity (Kahlig).

- Instability of density distributions due to heat transfer through the surface, wind mixing, and changes in inflows and outflows introduces a highly dynamic behavior, resulting in the absolute need to consider the layer thickness as a function of time. In addition, two-layer models would not be able to handle the complex phenomena associated with inflow of water with a different temperature (Watanabe).

- Biochemical processes relevant to ecological modelling are usually significantly temperature dependent. The resolution in temperature prediction of a discrete layer model may not be sufficient to cope with this effect in enough detail. A similar argument applies to the light independent growth rate, which must be integrated over total layer depths (Watanabe).

- In thermal models, a special difficulty is introduced with two-layer models, since heat exchange with the atmosphere is a function of surface temperature, which is not computed

correctly due to averaging over the layer thickness. This may lead to accumulating errors in long run simulations.

Of course, some of these difficulties can be avoided by using the measured vertical temperature distribution as a forcing function.

Another approach advocates the use of the temperature distribution as a means of determining the exchange coefficient between adjacent layers. This can be done, since the transfer of mass and heat are essentially analogous (except perhaps near a very strong thermocline). The advantage will be that the effects of upwelling and internal waves, which are very difficult to model, are also automatically included (Di Toro). However, in lakes that do not turn over during the winter period due to the absence of large storms, examination of the vertical temperature, which tends to become essentially uniform due to cooling, may lead to erroneous conclusions on mixing (Imboden).

Techniques exist for determining the thermocline in continuous vertical distribution models from energy budget considerations by comparing potential energy from density gradients originating from heat exchange and kinetic energy transferred by wind action (Harleman). Attempts to apply such an approach to explain enhanced algal growth during periods when the layer above the thermocline was thin were not successful in a shallow lake (van Straten).

During the thermocline period, the predicted thermocline goes down much faster than in nature (Imboden). This is mainly due to the fact that thermocline prediction models do not take into account the energy associated with mixing due to density inversion.

It can be concluded that relatively simple two-layer or multi-layer models can only be applied with a chance of success in relatively uncomplicated situations, such as no or low inflow and outflow, and relatively low variability in thermocline depth. Otherwise, continuous models cannot be circumvented.

In the case of continuous vertical distribution, how do we model vertical mixing and exchange: by vertical diffusion coefficients, if so, constant diffusion or time and spatially varying, or by vertical mixing related to hydrodynamic parameters such as mean velocity, turbulent energy, wind stress, etc.? What is the relative importance of lake or reservoir inflows and outflows in the vertical exchange as opposed to vertical mixing by diffusion or wind?

Reported by M. Watanabe.

A short presentation about the relative importance of inflows or outflows in vertical exchange or mixing in lakes and reservoirs was given by Harleman. By nondimensionalizing the one-dimensional vertical heat transport equation, the following two dimensionless quantities are obtained: $D/A^{1/2}$, a geometric factor, and AE/QD,

the ratio of the rate of heat transport by diffusion to the rate of heat transport by advection. D is the depth from the surface at which the outlet is located; A, the horizontal cross-sectional area at the depth of the outlet; E, the vertical eddy diffusivity (of order 50 to 100 times the molecular diffusivity of heat); and Q the inflow-outflow rate. In reservoirs, generally AE/QD << 1, and vertical advection dominates vertical diffusion. In lakes, with small inflow and outflow, AE/QD >> 1, and diffusion dominates advection. In reservoirs that satisfy the above criteria, vertical temperature profiles are relatively insensitive to the eddy diffusion coefficient and the assumption of a constant value for E is reasonable. The opposite is true in lakes, if AE/QD >> 1. Under this condition it is important to consider the dynamic mixing and entrainment in the vicinity of the thermocline caused by wind stress at the lake surface. Details of this discussion are contained in R.M. Parsons Laboratory, M.I.T. Technical Report No. 227 by Hurley, Jirka and Harleman entitled *Vertical Heat Transport Mechanisms in Lakes and Reservoirs.*

Van Straten showed some case studies of Lake Grevelingen and reported that mass diffusivity and heat diffusivity were quite different in magnitude. Frequently mass and heat diffusivities are assumed to be the same, which may cause some problems. Filatov presented some of his work on turbulence and showed the distribution of turbulence energy in a stratified flow. Vasiliev gave a summary of the state of the art on turbulent exchange coefficients. Turbulent exchange coefficient can be expressed:

- As a function of Richardson number;
- By a two parameter turbulent model; and
- As a function of hydrodynamic parameters.

Under what conditions is it necessary to model the hydrodynamics of the lake circulation (equations of motion, wind and bottom stress, eddy diffusivity, Coriolis effects)?

Reported by T. Simons.

There are hydrodynamic models currently available capable of simulating the large-scale water movements in deep lakes and reservoirs. In particular for the North American Great Lakes, these models have been validated to a considerable degree and similar experiments are being carried out in the USSR. Numerical models coupling such three-dimensional hydrodynamic models with ecological models were reported at this meeting by Chen and Simons.

The question of the conditions or circumstances under which it would be advisable to extend ecological models of deep lakes and reservoirs to three dimensions cannot be answered without defining the goal of the modelling exercise.

If the purpose of the model is to simulate the basin-wide characteristics (some suitably defined spatial average), then the

currently available evidence indicates that a basin-wide averaged model is acceptable. This is based on comparisons of simulations of such models and averaged solutions from three-dimensional models run under similar circumstances. The apparent implication is that the response of the present ecological models is sufficiently linear that an average of the solutions over the whole basin approximates the solutions to the equations applied to the spatially averaged basin. If a basin consists of a number of subbasins, each with quite specific environmental characteristics, then it is clearly necessary to apply ecological models to each subbasin separately. The question then remains how to simulate the exchange between the subbasins. It is likely that in many cases a quasi-empirical diffusion formulation can simulate this exchange. Whether this should be done on the basis of hydrodynamical models or observations does not appear to be a priori clear.

For a large basin that shows very large horizontal gradients in nutrients and biomass (for instance, between near shore zones and deep water), the *local* response can be simulated by coupling an ecological model with a fully three-dimensional physical model. The only other alternative would be to derive a complete picture of the circulation from observations, which is obviously not practical. This is particularly true because the most important physical effects are such relatively short-term phenomena as upwelling in rather localized areas. Such physical processes cause transports of nutrients that may lead to very large loadings to low-nutrient zones.

Given the fact that the technology for three-dimensional hydrodynamic-ecological modelling is available, one might agree that we should adopt the general policy of modelling large basins with this kind of model since it obviously gives more information than a one-dimensional model. In practice, however, the limited data base and computing facilities will probably make it preferable to use simpler models, thus allowing for an order of magnitude increase in the number of calibration runs.

Is verification of the transient vertical temperature distribution an adequate indication of vertical mixing and exchange processes?

Reported by D. Imboden.

In many cases it is, but not in all. One may distinguish three cases:

(1) The water at the deepest point of the lake is warmed up above 4 °C during the summer; the lake reaches a homogenous temperature distribution during the fall; and the whole lake cools during the winter.

(2) Vertical temperature gradients never disappear in the lake below some depth.

(3) The deep water of the lake remains around 4 °C during the whole year and the lake goes through two (or more) situations of homogeneous temperature distribution.

For cases 1 and 2, the temperature profile does give clear evidence of either the presence (case 1) or absence (case 2) of complete vertical mixing turnover. In case 3 the question of total mixing cannot be decided from temperature profiles alone, but additional parameters (oxygen, phosphate, etc.) may help to trace the mixing process.

Methods for estimation of eddy diffusion from temperature profiles during the stratification period become very sensitive to errors in the data or in the underlying assumptions in cases when the vertical temperature gradients are small (lower hypolimnion of deep lakes and reservoirs). For instance, during the cooling or heating period, the vertical temperature regime may become strongly dependent on the local depth of the lake even in small lakes, which introduces horizontal temperature gradients. On the other hand, precise and dense temperature measurements are very good (and relatively cheap) data for estimating mixing processes.

How does the vertical temperature structure affect the detention time of a lake or reservoir?

Reported by M. Markofsky.

In deep reservoirs that experience horizontal thermal stratification, the time a given inflow (e.g. the inflow of March 1, May 10, etc.) remains in the reservoir is highly dependent on the thermal stratification. Due to the larger thermal inertia of a reservoir compared with that of the inflowing stream, the temperature of the stream rises faster than the reservoir temperature in the spring. The opposite occurs in the fall. Thus inflowing water in the spring tends to enter at the reservoir surface, whereas in the fall they enter at some intermediate depth corresponding to their inflow temperatures. Depending on the elevation of the inflow due to the thermal stratification, the inflowing water may remain in the reservoir for a long or short period of time. For example, for a deep outlet the water entering in the spring (at the surface) tends to remain in the reservoir for a longer time than the water entering in the fall (at depth). A mathematical model developed at M.I.T. was used to simulate this phenomenon.

Laboratory studies were also conducted in a 11 m long plexiglass flume with sloping bottom. The inflow and outflow rates, inflow temperature and surface heating simulated with heat lamps were varied throughout an experiment of approximately six hours. The outlet concentration resulting from pulse injections of dye at a given time during the heating or cooling cycle was measured. Comparison of laboratory measurements with prediction showed good agreement. Predictions for Fontana reservoir (TVA System, USA) showed similar trends.

More information can be found in: Markofsky, M. and Harleman, D.R.F., *A Predictive Model for Thermal Stratification*

and Water Quality in Reservoirs, R.M. Parsons Laboratory, TR 134, M.I.T., January, 1971; Markofsky, M. and Harleman, D.R.F., *Prediction of Water Quality in Stratified Reservoirs*, J. Hyd. Div. ASCE Hy 99, May, 1973.

The interaction between water quality and reservoir hydrodynamics related to thermal stratification is currently being studied at the University of Karlsruhe.

Wilmot commented that it would have been interesting in the laboratory studies to stop the inflow to the reservoir and investigate the effects of density currents resulting from the sloping reservoir bottom due to surface heating only. Markofsky replied that experiments conducted without inflow and outflow (only variable surface heating) showed horizontal stratification. Secondary density effects were not noticed in the temperature profiles. Watanabe mentioned that this may be due to the vertical walls in the laboratory flume. Sloping walls might have shown such an effect. van Straten indicated that scale effects in the laboratory could also be significant. Markofsky stated that the laboratory model served as a prototype for the mathematical model, which was then used for field prediction. Thus, no scaling in the formal sense of the word (i.e. Froude, Reynolds) was made.

What problems arise in the application of existng lake models by new users?

Reported by W. Kinzelbach.

Kinnunen reported on the application of an ecological model by Chen--made available by the US Environmental Protection Agency under the name of EPA-ECO--to a Finnish lake. The task is linked to a World Bank loan to Finland and comprises the prediction of algal density and dissolved oxygen, and a general description of the ecosystem on different trophic levels. The use of ecological models is quite a new practice in Finland. An independent development of a new model is out of the question because of limited time. However, the number of existing models advanced to a stage of being readily applicable or adaptable to a new site is very small. In fact, only one model was found. As there was no consultation with the author of this model, the familiarization with it took quite a long time.

Since a user should understand a model in its last details before applying it, Kinnunen suggested that in order to speed up and render more efficient the process of scientific software transfer, one should find a way to bring author and user of a model together. Further, the need of ecological modelling should be made clear to decision makers. Harleman suggested that this information transfer lends itself to being a task for IIASA. He identified two areas in which IIASA could be more active--collection and extensive documentation of models; organizing the dialogue between author and potential user.

Jørgensen added that the range in complexity of existing models was satisfactory, and that the main requirement in the near future is the validation of models. He suggested that comparison of models on the basis of new data sets be done at IIASA and made available as IIASA publications, thus giving the potential user a means of decision in his choice of a model.

Vasiliev proposed to find an appropriate organizational form of dialogue between potential users and model builders.

How can we consider the horizontal nonuniformities of geometric hydrophysical and ecological characteristics? Under what conditions should horizontal mixing and exchange be considered and how should it be implemented?

Reported by W. Wilmot.

Horizontal nonuniformities in the hydrophysical-ecological system were discussed for the first time by Chen on the opening day. He described experiments in which a three-dimensional model of the circulation in Lake Ontario, developed by Bennet, was coupled to his own ecological model. The physical model was spatially averaged over zones considered sufficient to represent the ecosystem. The physical solution was also averaged over the basic time step of the ecological model.

Simons raised the question on the third day of the meeting of whether it was necessary to obtain the three-dimensional circulation if the long-term whole lake ecological response is being sought. The consensus was that since the ecological equations for the whole lake are roughly linear, the hydrodynamics could be included as fluxes necessary to satisfy heat and mass balances. Simons stated that from his experience with circulation models, only the highly transient response of a lake could be modelled. The long-term average fluxes remain unknown. Chen felt that since the linearity/nonlinearity of the ecological model and spatial variability are not well known, work on this should continue. Imboden pointed out that lakes often contain basins of essentially different ecological nature. The consensus again was that since fluxes from one basin to another are unknown and difficult to compute, unless there is a net flow through the system, as in a reservoir, some kind of flux related to the difference in concentration should be used. The advective-diffusive nature of this flux would be ignored and just parameterized.

Reservoirs where a net inflow-outflow exists were discussed by Harleman and Markofsky. Their results showed that it took very little throughflow for advective process to dominate vertical "diffusive" processes.

Horizontal variability/exchange processes could be important for "near-field" studies, as pointed out by J. Simons. It is the feeling of the reporter that horizontal dispersion is primarily due to horizontal advection. If the aim is to parameterize subgrid horizontal dispersion then the best way to do it is to

relate the dispersion to the vertical shear of the large-scale circulation and the vertical mixing. The shear causes a "cloud" of some substance to be horizontally elongated without change of volume. The vertical mixing causes a decrease in concentration in the "cloud".

Simons ended this discussion by offering the opinion that near field studies required a whole lake three-dimensional circulation model, because it was impossible to establish boundary conditions in the interior of the lake, which would be consistent with the lake circulation.

Discussions on General Topics

How should time dependent meteorological factors be included in lake models?

Reported by P. Kahlig.

In steady state models, time dependent meteorological factors (e.g. cloud cover) are usually handled by a succession of steady states. In some time dependent models, meteorological variables are supposed to be periodic (e.g. annual cycle of equilibrium temperature). In three-dimensional models, time dependence of meteorological factors can usually be included from the outset (e.g. wind speed, air temperature, relative humidity, atmosphere pressure, and cloud cover).

Vasiliev stated that the time scales involved give some hint for deciding whether time dependent meteorological factors should be included: ecological processes exhibit a relatively large time scale, a little larger than the time scale of hydrophysical processes, while meteorological processes have the smallest time scale. If in a particular case, the meteorological time scale turns out to be very small, it may not be justified to include the time dependence of meteorological factors. If meteorological records have to be taken from distant stations, the inclusion of detailed time dependence may not be justified.

Is it possible to set up a more general procedure for handling a specific lake modelling problem? The procedure should focus on the method of selecting the process equations, the number of observations required and on the method of parameter estimation, and of verifying, calibrating, and validating the model.

Response by M.B. Beck.

The difficulty of questions of a general nature is that the underlying problems are usually of a quite fundamental, if not philosophical, character and that perhaps an equally general answer is expected. In my answer, however, I shall not be very general, referring only to a few specific items of interest, and I shall hardly touch upon philosophical issues. Rather I intend to introduce topics that are not discussed elsewhere.

On the matter of a general procedure for modelling, the techniques available from system identification (see, for example, Eykhoff 1974) have some relevance. However, what is suggested here is not a general procedure but more an all-purpose "bag of tools" for analysis. System identification has emerged and matured quickly over the past ten or fifteen years and textbooks to synthesize and unify the subject are still lacking.

If one is fortunate enough to be able to design specialized experimentation for (dynamic, unsteady-state) modelling exercises, then a consideration of certain features of the given lake system is crucial to the eventual success of the modelling effort. Two factors that must be determined are the rate at which sample measurements of the state of the system should be taken, and for how long the experiment should last. Two very rough rules of thumb state (Gustavsson 1975):

- The sampling interval should be at most as long as the minimum time constant of interest; or alternatively the interval should be one sixth of the period of the fastest "sinusoidal"-type variation expected in the behavior of the system.

- The length of the experiment should ideally cover a period at least ten times the largest time constant of interest; to some extent this is because the degree of subsequent parameter (coefficient) estimation error is inversely proportional to the length (number of samples) of the experiment.

Thus, if a time constant is, say, the detention time for water in the lake, and assuming that this can also be crudely translated into time-scales for biological growth of a species and rates at which nutrients are cycled, one has the beginnings of an experimental design.

The selection of process equations, or the model structure identification, is one of the fundamental problems of modelling complex and/or poorly defined systems. Model structure identification partly concerns the choice of the number of state variables in the model and with identifying the correct form of the mathematical expressions in the equations. A simple example will illustrate this: the problem of choosing between, say, a linear first-order growth-rate function and a Monod growth-rate function. Alternatively, one may visualize model structure identification as being analogous to the choice of whether a straight line or a curve should be fitted to a set of experimental data. Having decided upon the form of such a growth function, the subsequent problem of parameter estimation is one of obtaining values for the coefficients (e.g. first-order growth-rate constant, or maximum specific growth-rate and limiting substrate saturation constant) that appear in the identified functional form. What I have said elsewhere on model structure identification (Beck 1978) must be strongly qualified here. Hitherto my experience has been of assuming in situ time-series field data to be available, and of assuming that a posteriori model structure identification can be carried out by reference to those field data, that reasonably low-order models are being employed (about 5 or 6 state variables), and that analysis is restricted to lumped-parameter, ordinary differential equation models. How many of these conditions hold for ecological modelling case studies is clearly debatable.

It has emerged from the workshop that one widely used procedure for adjusting parameter values so that the model fits the

data is the method of "trial and error deterministic simulation". In other words, starting with initial guesses for the parameter values taken either from the literature or from laboratory chemostat experiments, the model is repeatedly run through the field data; and between each run some of the parameter values are modified on the basis of the analyst's judgment of the model's performance (see Figure 1). One restriction of such an informal

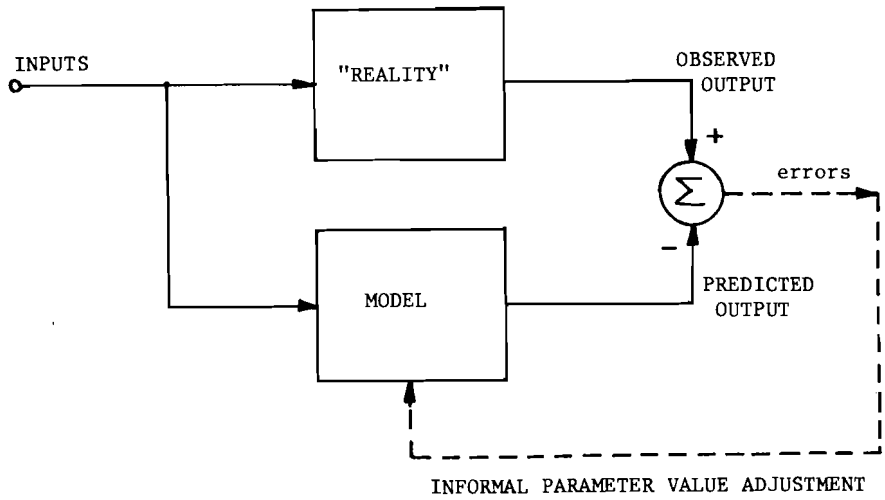

Figure 1. Parameter estimation by comparing trial and error deterministic simulations with the field data.

method is that it is essentially deterministic and does not take account of stochastic events always present in the field data. Two forms of random noise are usually recognized, one of which deals with unknown, or unmeasured, disturbances of the system behavior, while the other refers to chance measurement error (see Figure 2). Given certain assumptions about the statistical properties of the noise processes, most formal algorithms of parameter estimation operate upon the measured input information, the observed system responses, model predictions of those responses, and the corresponding errors between observations and predictions, and use this information to make corrections to the a priori parameter estimates in the model. Of course, it is not so much that the analyst is unaware of the stochastic aspects of the problem but more that the formal algorithms may assist in being more systematic about the estimation of parameter values. Some of the estimation algorithms will in any case not converge unless reasonable a priori estimates are provided, which would usually be estimated by prior trial and error simulation. Again, the potential scope of current estimation algorithms must be qualified by the statement that they are by and large restricted

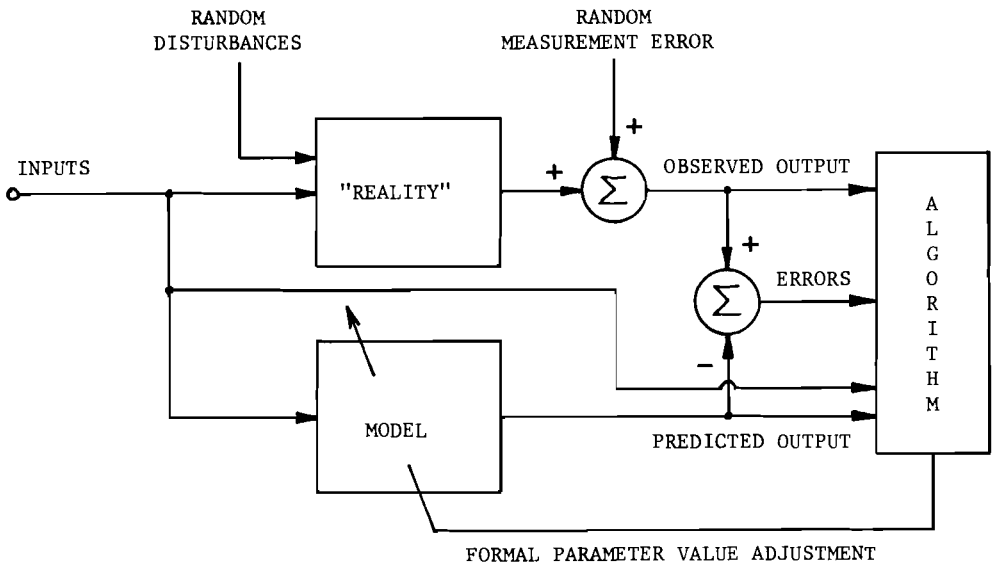

Figure 2. Formal parameter value adjustment by using systematic parameter estimation algorithms.

in practice to lumped-parameter model forms. These algorithms, however, are not necessarily constrained by requiring field data with a uniform sampling interval.

It is useful here to digress briefly on a topic raised earlier in the workshop. Because of the uncertainties (stochastic aspects) in the nature of the modelling problem, one can argue that models are still required even if all the variables to be predicted can be freely measured. For whether one models a system's behavior along the lines of Figure 1 or Figure 2, a large part of the modelling exercise is devoted to precisely this activity of filtering out the uncertainty (noise) in the observed patterns of behavior. Now, a very good question that arises from this is: having removed the uncertainty in order to model the process, do we reinsert some measure of the uncertainty when making predictions from the model? My thoughts are directed here more towards model prediction error covariances than the computation of a number of deterministic "scenario" forecasts. One imagines that if large capital investment sums are related to the application of the model, then it would be helpful for the decision maker to be advised of the confidence in the model forecast.

Let us turn to two aspects of model verification, where model verification means determining whether the "correct" model has been obtained from the given single data set. To avoid confusion in terminology model validation here is the checking of the accuracy with which the same model predicts the behavior observed

in different, independent data sets. Suppose, first, that the model structure has been identified, the parameters estimated, and thus a sequence of final model response errors can be computed (Figure 3). Certain assumptions are generally made about the statistical properties of the noise sequences in Figure 3. According to these, the model response errors should also conform to

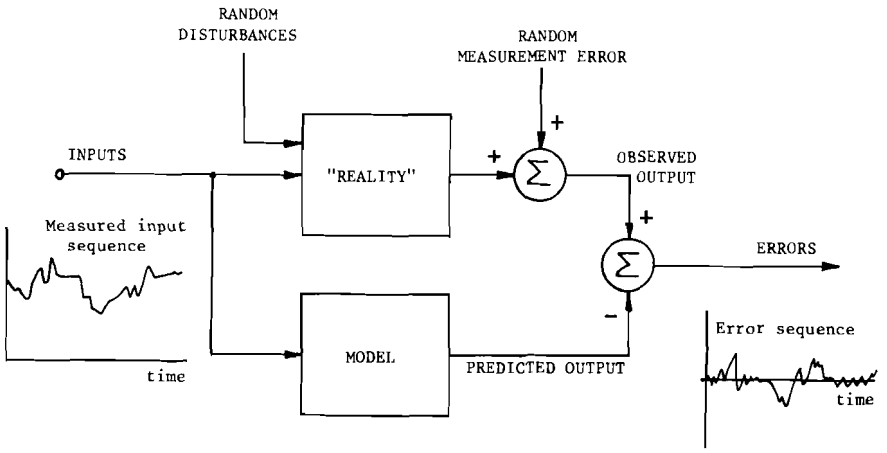

Figure 3. Model verification by checking the statistical properties of the model fitting error sequences and by testing that the errors are independent of all measured input sequences.

certain statistical properties, in particular those of white noise, i.e. the errors are not correlated with themselves in time and they are statistically independent of the measured system input disturbances (forcing functions). Indeed, cross-correlation of the model response errors with the measured input sequences is a very useful analytical technique that can be used to good effect in the process of model structure identification. A strong correlation between a given input and errors of a given output, for example, suggests that the model structure should be modified to accommodate additional significant relationships between these two variables. If the error sequences do approximate the statistical properties of white noise, then one can conclude that the model has been verified subject to the various assumptions that have been made.

Besides these more straightforward aspects of model verification, other questions of considerable interest remain unanswered.

For instance, how, in model assessment, does one determine which model is "best" in some sense, upon what criteria should this judgment be based, and can we measure whether a "significant" addition of model complexity is matched by a correspondingly "significant" addition in model accuracy. Although a number of aspects of these questions may be answered by the argument that the choice of the correct model depends upon the intended model application, it is still useful to consider the questions in a fairly general, abstract context.

Most systems analysts are intuitively aware that the quality of a model is judged by some balance between model accuracy and model complexity. So to assess models by fitting error statistics alone assumes a somewhat narrow view of model assessment, especially when the number of observations is probably too small to lend significance to such an analysis of variance. The crucial problem is the development of some more representative measure, which can be applied with ease and which allows the comparison of quite differently structured models, e.g. partial differential equations, ordinary differential equations, difference equations. In this respect recent results of Maciejowski (1977) are of considerable interest. By using the theory algorithms and by borrowing ideas from algorithmic information theory, Maciejowski is able to construct a measure of model "goodness" derived from a comparison of the lengths of two specially defined computer programs (see Figure 4). The first program, or base program, simply generates a look-up table for the original data sequence. The second program embodies the

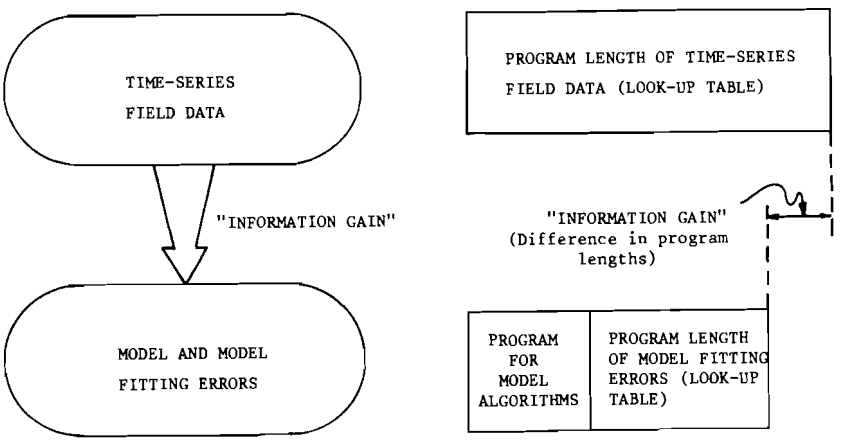

Figure 4. Assessment of the quality of a model as an overall function both of model complexity and of model accuracy.

algorithms that compute the set of model predictions and generates a look-up table of the associated model fitting errors. The length of the second program is, therefore, a function both of model complexity and of model accuracy. Thus the shorter the length of the candidate model's program the better is said to be the capability of that model to represent the observed process behavior. It would be premature to speculate on the likely success of this approach; at present one can say that preliminary results are encouraging.

Much of the foregoing has assumed a fairly pragmatic approach to modelling in that the analysis of the system is carried out by reference to a set of field data. The remainder of my comments, which deal primarily with the selection of the number of state variables, and the role of chemostat data, are not so constrained to the limitation of this kind of assumption. The discussion will, nevertheless, be closely allied with certain restricted objectives for model application.

In Figure 5, a four state (compartment) model is given where the state x_1 is directly disturbed by some input function u(t) and where the state x_2 is available for measurement as output y(t). Now assume that in terms of model performance assessment or model application the accuracy of the given model can be essentially described by its ability to reproduce the response in y(t) resulting from a step or impulse variation in the input u(t). Control theory has a law of large systems, which is probably relevant to the modelling of lake ecosystems and which can roughly be described as follows. For many highly complex, nonlinear systems the detailed (microscopic) characteristics of process dynamics tend to aggregate as a small number of relatively simple, even linear, macroscopic dominant modes of behavior as observed through the system's input-output relationships.

One can draw a parallel here with what has occurred earlier in the subject of nuclear power plant modelling and control (Atari and Shah, 1972). On a somewhat grander scale than envisaged in Figure 5, it was not uncommon to find dynamic models of the nuclear plant consisting of about 200 state equations. The question then posed is: how can this high order of the model be reduced to a much more manageable level--for control system design purposes--while preserving a conceptual link between each section of the reduced model and each subsystem in the original model to which that section approximates? Thus, what is required in effect is a systematic model order reduction technique. According to Atari and Shah (1972) such techniques are available, for they eventually reduced a model of 200 state variable equations to a model with only 18. For computational reasons, therefore, it might be desirable to search for a simpler manner in which to relate y(t) to u(t), where this relationship involves a smaller number of state variables. But the objectives for model application may not always be those that require merely the input-output relationship of Figure 5 to be preserved.

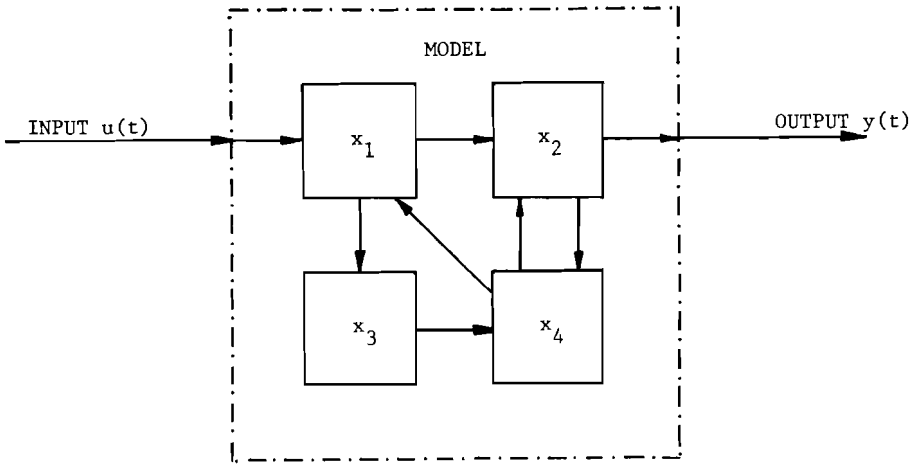

Figure 5. Selection of the number of state variables and identifiability problems in an example compartmental system model.

The example of Figure 5 can also be used to illustrate a possible corollary of the law of large systems. How many state variables are required to characterize an observed input-output relationship? Here it might happen that the addition of more and more compartments to the ecological model soon enters the area where the net result of including such minor modes of behavior becomes indistinguishable from the effect of stochastic variations in the observed relationship between u and y. Or alternatively--to illustrate a different view of the same point--given that one wishes to use the model of Figure 5, an a priori analysis of the model may reveal two important features:

- Those parameters in the model that can be uniquely estimated from an experiment in which u and y are measured;

- An appropriate combination of possible input and output measurements that will allow the unique estimation of all the model parameters.

All of these items relate to what might be called identifiability problems (see, for example, Cobelli et al, 1978). For instance, we should have an identifiability problem in the model if it were possible only to estimate the sum of two rate constants k_1 and k_2 as a value $\hat{a}$

$$(k_1 + k_2) = \hat{a} \quad .$$

There is no unique solution to this equation and many pairs of values for k_1 and k_2 will sum to the value $\hat{a}$.

This example of an identifiability problem leads conveniently to a consideration of my final point concerning the role of chemostat data. It is clear that if the parameter values for a model are estimated from in situ field data, apparently unrealistic values for coefficients may be obtained from the estimation algorithms. This would certainly be possible if there were hidden identifiability problems in a complex nonlinear model. Such a gross discrepancy between in situ estimates and estimates for the same constants from chemostat data must raise a rather fundamental question in the analyst's mind--whether to reject the validity of the model and experimental field data or whether to reject the assumption that laboratory chemostat rate-constant values are transferable to the field system. Nor should it be forgotten that presumably implicit in the chemostat coefficient values is the assumption that a correct mathematical form, i.e. model, of growth kinetics attaches to the particular culture of microorganisms grown in the chemostat. Without such an assumption, how does one determine rate coefficients from observations of substrate and organism concentrations? And since I have no well formed answers to my own questions, it is probably appropriate, though unsatisfactory, to conclude here.

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