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PROCEEDINGS OF WORKSHOP ON HYDROPHYSICAL AND ECOLOGICAL MODELS OF SHALLOW LAKES AND RESERVOIRS

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FOREWARD

On September 13-16, 1977 a Workshop on the general aspects of *Water Quality Modelling* was held at IIASA. The most recent theoretical developments in the field of Water Quality were discussed at this meeting. At the same time the application of hydrophysical and ecological models to various water bodies was considered. One important recommendation of the Workshop was that a number of more specialized workshop be convened in the near future. The first of these on *Geophysical and Ecological Modelling of Deep Lakes and Reservoirs* was held December 12-15, 1977 in Laxenburg. The second of these on *Hydrophysical and Ecological Models of Shallow Lakes and Reservoirs* was held during the period 11th to 14th April, 1978 and was followed by a one day Task Force Meeting on *Lake Balaton* on April 17, 1978. In addition to these meetings a Seminar on *Waste Heat Management in Rivers* was held November 8-9, 1977.

The subject of deep lakes and reservoirs chosen for the December 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 subject of Shallow Lakes and Reservoirs chosen for the April Workshop implies a basic concern with the condition of full vertical mixing and bottom sediment interactions.

Topics discussed at the Workshop included:

- *Characteristic Features of Shallow Lakes and Reservoirs:* influence of wind and wave action; longitudinal and vertical mass transport processes; exchange of nutrients between the water body and the sediments; influence of sediment types on the transformation processes of chemical compounds.

- *Hydrophysical Models:* horizontal and vertical transport and diffusion processes, interaction across the water-sediment interface.

- *Ecological Models:* evaluation of available data by simple models; sensitivity analysis; improvement of the quantity of data, further development of ecological models of shallow lakes taking into account the binding and mobilization of nutrients in the sediments.

- *Water Quality Models:* limiting nutrients/carbon, nitrogen, phosphorus, element cycle models/simple and complex models.

- *Field Data Collection and Model Verification Techniques:* coordination of chemical and biological field measurements with water quality models, choice of parameters.

- *Possible Case Studies*

The intent of the Workshop was to bring together qualified scientists--hydrophysicists, chemists, biologists--and engineers, working on both the physical and ecological problems of shallow lakes and water reservoirs, for a brief but productive period in which ideas, information and experience could be exchanged.

The Workshop was held within the framework of IIASA's studies on Models for Environmental Quality Control and Management (Resources and Environment Area, Task 2) which is particularly concerned with hydrophysical and ecological models for water quality assessment. The Workshop served as an excellent opportunity to discuss future research needs in the subject area, with the background of a sound assessment of the present state of scientific knowledge concerning mathematical modelling of water quality.

Discussions during the Workshop were also directed towards the following issues:

1) Establishment of an international collaboration for the advancement of hydrophysical and ecological modelling of lakes and reservoirs;

2) Problems that require special concentration of scientific efforts in selected research areas;

3) The character of the end product of the joint research effort and forms of its presentation.

It is planned to report the work in the form of Research Memoranda and reports containing all the relevant information.

At the workshop 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 three areas: A. Ecology, B. Hydrophysics, and C. General Questions. Workshop participants, acting as rapporteurs, prepared written summaries of the discussions which apper in this Working Paper and later will appear as the Introduction to the complete Conference Proceedings. The Proceedings, edited by Prof. S.E. Jørgensen, is now being processed an an IIASA Conference Proceedings.

Prof. O.F. Vasiliev
Task Leader,
Task on Environmental Quality
Control and Management

Proceedings of Workshop on Hydrophysical and Ecological Models of Shallow Lakes and Reservoirs

INTRODUCTION

S.E. Jørgensen

A wide range of models for focusing on the eutrophication problems is available today, for example:

1. One to four nutrients may be considered.
2. Constant stoichiometrics are used in some models; in other models independent nutrient cycles are used.
3. One and up to several layers may be considered.
4. One and up to several segments may be considered.
5. Unfortunately most of the models have not been validated nor calibrated; only a few models have been both calibrated and validated.

Indeed, it can be said that no general model exists and the selection of a suitable model must be carried out in each individual case by reference to the nature of the problem at hand. Most models are based on biological-chemical knowledge of the actual processes taking place in the lakes. A black box approach does not seem to be appropriate for modelling a lake system, since no general knowledge about the aquatic system would thereby be obtained. From the experience gained in modelling lake systems, it seems that a multi-disciplinary scientific team is required.

One of the drawbacks of many models is the problem of data and, it should be stated that no model is better than the data on which it is built. We might even pose the question: is the ability of making good models better than the ability of getting good data? We should admit that the description of an ecosystem by means of a model is structured from the data and it is not possible to give a more accurate description of the ecosystem then the accuracy of the data (standard deviations, sampling accuracy etc.) allows. These general items mentioned above will be touched upon in several of the questions listed in the agenda of this workshop.

What is actually the state-of-the-art of lake modelling today? We can answer that it is not possible, by use of a "total" model, to find a new and better scientific description of a specific process in an aquatic ecosystem; but it is possible to select a better and new description of a specific process by means of a submodel based on intensive in situ measurement or by examination of an individual mechanism in the laboratory. This does not mean that total models are not useful. They can be used to over-view several interacting processes and to build a total model seems to be a necessary step in obtaining an applicable management tool.

Submodels, however, are more useful as a scientific tool. We know that selection of the right model is a matter of balance: for instance we must include all important processes, yet, of course, not all the fine details. Consequently, the problem determines the model. If too many state variables are included the model will be unwieldy. We might not have the basic data and we might introduce inaccuracy by introducing too many parameter values. But if we, in contrast, make the model too simple, we might not describe the dynamics of the system in the correct fashion.

Laws about reactions of ecosystems are missing and a more and more reductionistic approach to modelling seems not to be a feasible way to proceed.

Rather we need a holistic approach which contains ecological principles. Current ecological models can be compared with the description of gasses in a room by means of velocity, direction, groups of molecules. The models of tomorrow will correspond to the use of the general laws of gases containing terms equivalent to Avogadro's number etc.

Several of these problems at the focus of present-day water quality modelling will be discussed in the course of these Workshop Proceedings.

QUESTIONNAIRE FOR WORKSHOP ON HYDROPHYSICAL AND ECOLOGICAL MODELS OF SHALLOW LAKES AND RESERVOIRS

A. ECOLOGY

1. Validity of constant stoichiometric models versus element cycle models. How many element cycles do you need in a eutrophication model?

Reported by G. van Straten.

Generally preference was given to the element cycle models or at least to variable stoichiometrics. The reason for this is mainly that cycling of the nutrients - phosphorus, nitrogen and silica, are to some extent independent owing to such phenomena as luxury uptake. It seems that the use of an element cycle type of model would be absolutely necessary in the following two instances:

1) If a switch during the season occurs from one limiting nutrient to another (e.g. luxury phosphorus uptake, when silica is a limiting factor).

2) When the internal nutrient cycle is important compared with the external loading. Since internal cycling in most cases is of more significance for shallow lakes than for deep lakes, the element cycle models may be more urgent in the shallow lake situation.

In addition, the question was raised whether the P/N ratio in the cell had some influence on the settling rate. If this is the case then no constant stoichiometric model can be used. Finally, in some cases only an independent element cycle model was able to predict either the time or the peak height of an algal bloom maximum correctly. On the other hand some simulation results have been reported, which show only a minor difference between the two types of models. This minor difference is especially relevant if the changes in phytoplankton concentrations are small. A serious disadvantage of the independent element cycle model is the introduction of more parameters into the model.

In special cases it may therefore be beneficial to use the constant stoichiometric with actually measured values for the biomass/nutrient ratio. The best example of this is for the purpose of designing an algal growth basin to be operated under steady conditions. On the other hand many of the parameters in the independent element cycle models are actually well known, such as the minimum and maximum concentration of phosphorus, nitrogen, carbon and silica, so that then the independent element cycle models may have more unknown parameters. Calibration can thus be carried out for rather restricted small intervals of feasible values for the parameters. The conclusion of this discussion is that the use of constant stoichiometric models can be a reasonable approximation if no great changes in intercellular nutrient biomass ratio is to be expected. A detailed and more correct description, however, can only be obtained from a nutrient-cycle type of model at the expense of an increasing number of parameters, all of which have to be determined, although the parameters are known within quite small limits.

2. Which equations are most suitable for describing the nutrient uptake rates by phytoplankton of (a) phosphorus, (b) nitrogen (NH_4 + NO_2^- as well as NO_3^-), (c) carbon, (d) silica? How do we model the growth and mortality of phytoplankton with single and multiple cellular concentration of nutrient? Which light and temperature expressions are proper?

Reported by M.W. Lorenzen.

The following equations for nutrient uptake in phytoplankton growth were presented:

$$\text{growth} = \mu\text{max} \cdot f(T) \cdot f(PA) \cdot f(NA) \cdot f(CA) \cdot f(A),$$

where A refers to algal concentration and T, P, N and C are temperature, phosphorus, nitrogen and carbon. The nutrient uptake can be described by use of the following equation: (e.g., given for phosphorus)

$$UP = UP_{max} \frac{PA_{max} \cdot PHYT - PA}{PA_{max} \cdot PHYT - PA_{min} \cdot PHYT} \cdot PHYT \cdot \frac{PS}{KP + PS} ,$$

where S represents dissolved nutrient.

A differentiation between ammonia and nitrate uptake was included by the use of the following equation:

$$UN = UN(Nit) + UN(NH_4^+)$$

$$UN(Nit) = UN_{min}(Nit) + \left(1 - \frac{Nit}{NH_4^+}\right)(UN_{max}(Nit) - UN_{min}(Nit))$$

The effect of temperature was presented as the funtional relationship shown in Figure A1.

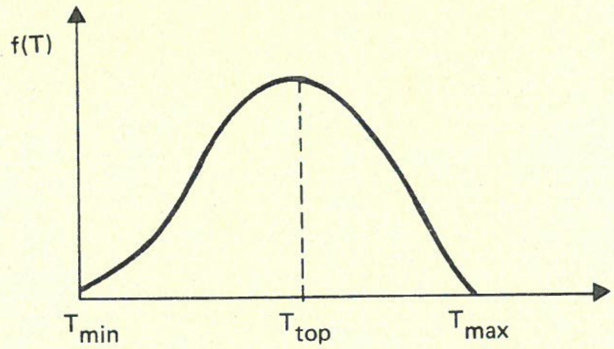


Figure A1

For this type of function it is recommended that a look-up table is employed in order to minimise computer time.

It is recommended to use these expressions in situations discussed in conjunction with question A(1). The Michaelis-Menten expression, which is often used, shows however, little difference from the more detailed description referred to above when short-term batch culture experiments are interpreted.

It has been suggested that regression analysis can be used to lump together unknown parameter values when long term data are available. However, this method can only be recommended for simple cases. It was also stated that when combining a number of limiting terms (N, P, T, light, Si) a minimum or threshold approach is superior to a multiplicative equation, see above.

However, the whole process of nutrient uptake and growth is more complicated and fraught with difficulties; it seems necessary to assume that parameters change with the temperature. The same is true for the "Michaelis-Menten Constants", since they change with light intensity. Unfortunately, there are at present insufficient data for constructing a response function for phytoplankton growth as a function of temperature, nitrogen, phosphorus, silica etc. It would be interesting to print out the values of the various rate limiting terms throughout an annual cycle to illustrate their relative importance under different conditions. The question, how do we take adaption of phytoplankton into account? merits further discussion.

3. Which equation is relevant for describing the grazing rate? Should more than one species of zooplankton be included?

Reported by D.O. Logofet.

There are several types of predator function response to an increasing prey density; these include the prey-predator system phytoplankton/zooplankton of particular interest here.

There is a possibility to select a model type by means of statistical procedures of hypothesis testing. In the simplest case of distinguishing between two analytical expressions f_1 and f_2 the dichotomy problem has a form as follows:

$$f = \theta f_1 + (1 - \theta) f_2 \quad ,$$

the hypothesis being:

$$H_1 : \theta = 1, \; H_2 : \theta = 0 \quad .$$

However, in complex simulation models with more than one phyto- and zooplankton species the results appear often to be insensitive to variations of the grazing rate parameters. From a theoretical point of view this insensitivity is caused by the fact that the data are insufficient to distinguish between two or more hypotheses. From an ecological point of view it is worth while to investigate the means for applying a few classes of phytoplankton and at least two classes of zooplankton. But in a management situation we are often only interested in some average situation and in this case the modified Michaelis-Menten expression might suffice. In this expression, however, the influence of temperature and the threshold effect of low phytoplankton concentration must be included.

4. Should fish and benthos be included in a eutrophication model? How?

Reported by P. Mauersberger.

Theoretical considerations as well as recent limnological observations suggest that fish should be included in some way in a eutrophication model. It was, for instance, observed in a 60 ha reservoir in Czechoslovakia that the algal concentration was significantly reduced by a controlled low stock of predatory fish. This may even be used as a management tool in situations where it is impossible or too expensive to reduce the input of the limiting nutrient. (H.R. Baček, Čsav, presented at the XXI Congress of Limnology, to be published in "Verhandlugen IVL").

Fish can sometimes be included in the eutrophication model simply by modifying the mortality coefficient in the zooplankton equation. But for a more detailed model it appears necessary to include explicitly fish as an additional state variable. In this case the balance equation(s) for the fish component(s) may be similar to those for other consumer groups. While the biomass for the fish components may be high, the energy or mass fluxes between the higher trophic levels are small. It may be reasonable to distinguish in some instances between juvenile and adult parts of the fish population and to take time variations into consideration. Of course, it is not easy to get the basic information about fish biomass which is required when fish are included as a state variable in a eutrophication model.

The complete model of a shallow lake must most often include benthic components and the exchange processes between sediment and the water body in order to obtain the correct nutrient balances. In many eutrophic lakes the primary production by the phytobenthos is small compared with the phytoplankton production. Therefore, we can assume that only the superior nonshaded parts of the submerged plants assimilate. Thus the growth of phytobenthos does not depend upon the biomass of the phytobenthos, but upon the optical properties of the overlying water body. Some observations suggest that the decrease of phytobenthos in eutrophic lakes is combined with an increase of phytoplankton.

5. How to model the exchange of nutrient between sediment and water. How much detail would be needed in the description of biological, chemical and physical processes within the bottom sediment? Should the description be different for aerobic and anaerobic conditions?

Reported by M.W. Lorenzen.

The exchange of nutrients between sediment and water is a key process in simulating eutrophication. Unfortunately, available knowledge shows that the rate of exchange varies considerably from lake to lake and is a function of time.

A model was presented which includes a "reactive" sediment layer, oxidised and reduced conditions, sorbed phosphorus, chemically fixed phosphorus, dissolved phosphorus in interstitial waters and iron compounds. The processes considered in this model are sedimentation and decay of organic material; desorption, reduction and oxidation of iron; adsorption of phosphorus to iron compounds; chemical reactions and different redox conditions; transport between water and sediment and into deeper sediments; and oxygen transport also. All the reactions were of first order and the adsorption followed Langmuir's isotherm.

In general it was apparent that sediment-water exchange processes should be considered in more detail. However, there has not yet been sufficient field experience to determine the most appropriate formulations.

6. Which parameters in the exchange process description are general and which are specific? Is it possible to set up a relation between these parameters and some sediment characteristics? What will be the relevance of laboratory experiments with substracted (disturbed or undisturbed) bottom sediment samples with respect to modelling the exchange of nutrients?

Reported by G. van Straten.

From the discussion in conjunction with question (A5) it is clear that some fundamental models have been developed for the sediment sub-system, but they have not yet been examined sufficiently in relation to any available data. Therefore, the alternative is to conduct laboratory experiments-preferably with undisturbed sediment samples. By changing pH, oxygen and nutrient content in the overlying water, it should be possible to provide the information needed for the derivation of parameters in a schematic submodel. An example of such a submodel was presented see [1]. In its original form it contains only interstitial phosphorus, and exchangeable and non-exchangeable forms of phosphorus in the solid phase. The non-exchangeable portion is determined from the P-content in older sections of the sediment by applying the argument that this phosphorus must be non-exchangeable since it is still present in the sediment. Such an argument can be questioned, for it is known that bioturbation may be responsible for mixing the sediment as deep as up to 10-15 cm.

The model presented is at the same time an example of the problems that may arise in such an empirical approach. Simulation results were not satisfactory with the original version and thus it was necessary to expand the model by adding other phosphorus components, thereby introducing more and more parameters. One may conclude that although empirical models are of value today, the ultimate answer can only come from a better understanding of the real chemical-biological behaviour of the sediment.

In the case of simultaneous diffusion and chemical reaction, which is a characteristic feature of undisturbed sediment layers, some insight may be obtained from classical chemical engineering. The analysis of such engineering systems stems from the 1950's. The enhancement of material flux towards or from the sediment due to reaction, can be characterized by two dimensionless parameters, the Hatta number and the infinite enhancement rate, which can both be derived from measurable factors of the sediment. Such a theory explains the observed relationship of oxygen uptake rates according to the square root of the oxygen concentration in the overlying water. It also clearly demonstrates the decrease in uptake or release rates as time proceeds, which may be of significance in the interpretation of laboratory experiments for parameter estimation.

8. How could the settling of phytoplankton and detritus be included in the model?

Reported by Janos Fischer.

Vertical transport results from a settling velocity of about 5-10 m/day and a vertical mixing. When considering the problem of reduction by diffusion in order to avoid contradiction one has to suppose for the velocity that

$$V = f(D, \text{physical state}) \quad . \qquad (D = \text{diffusion coefficient})$$

In some investigations in the Netherlands it has been found that there is a better correlation with settling rate and light than with settling rate and wind speed. It seems certain that density gradients play an important role. Hvpolimnion diffusion is much greater than epilimnion diffusion.

Since algae can change density it might be necessary to include this phenomenon in the model to get a good description of the settling rate. There is no doubt that the physiological condition of the algae plays an important role in determining the settling rate. Typically the settling rate is greater when the phytoplankton concentration is decreasing than when it is increasing. It is still an open question whether anyone has measured such settling velocities realistically. Settling velocity does not appear to be a fundamental physical quantity, and there is little confidence in trap methods, although a rough estimate can be obtained by this kind of direct measurement.

9. How do we model the following chain of processes: organic N $\rightarrow NH_4^- \rightarrow NO_2^- \rightarrow NO_3^-$? What about stable dissolved organic nitrogen such as humus?

Reported by L. Lijklema.

Since phytoplankton show little preference for either ammonia or nitrate as a nutrient, it was felt unnecessary to give a detailed description of the nitrogen conversions: organic nitrogen $\rightarrow$ ammonium $\rightarrow$ nitrite $\rightarrow$ nitrate in most ecological models, unless substantial oxygen consumption is involved. Also in many situations nitrate is predominantly present in the water.

In chemostat experiments strongly fluctuating concentrations of nitrifying organisms may occur but in the field such variations are generally slow. Therefore a temperature dependent first-order conversion process for available nitrogen will be sufficiently accurate for most practical purposes.

10. How do we model the process organic $\rightarrow$ ortho-P?

Reported by V.J. Bierman, Jr.

It was recognised that the transformation of phosphorus in the natural environment is the result of many complicated and simultaneous chemical and biological processes. The net process can be very detailed multi-compartment kinetic models. In practice, the choice of the approach will depend on the particular objectives and the available data. The accompanying Table 1A includes a representative sample of various approaches that have been proposed for phosphorus transformations. The schemes presented range from the very simple to the very complex models.

Recent experimental evidence has emphasised the importance of protozoa and zooplankton types in the transformation of organic phosphorus. It was also reported that the bacterial uptake of inorganic phosphorus may increase the bacterial consumption of organic phosphorus under certain conditions and that the presence of predators relative to bacteria can greatly accelerate the bacterial transformation of organic phosphorus.

<u>11. How can algal succession be included in the model? As blue green algal blooms are an important problem, how could we at least distinguish between "other algae" and blue green algae?</u>

Reported by V.J. Bierman, Jr.

Algal succession should be included in a model according to the particular circumstances in the system of interest. In Lake Balaton for example, it was reported that non-grazed Pyrrophyto are outcompeting other grazed species in the summer and that accurate results cannot be obtained for zooplankton concentrations by using only a single algal group in the model. It is suggested that at least five phytoplankton types by included in the Lake Balaton model:

1. Bacillariophyta,
2. Pyrrophyta,
3. Cyanophya,
4. Chlorophyta,
5. Others.

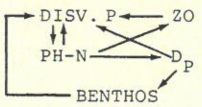
Another aspect to algal succession was discussed, although it does not bear a direct relation with algal production rates. In Lake Balaton, it was reported that substantial increases in blue-greens from the sediment layer, where they apparently grow

NN SCHEMES AUTHORS

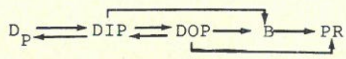
1 $DOP \rightarrow DIP$ — Skopintsev (1938), Maksimova (1972)

2 $DIP \rightarrow B \rightarrow DIP$ — Grill, Richards (1964)

3 $DIP \rightleftharpoons PP \rightleftharpoons DOP$ — Watt, Hayes (1963)

4


Corner (1973)

5


Barsdate, Prentki (1974)

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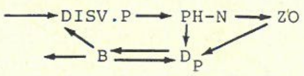
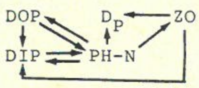


Porter, et al. (1975)

7


Richey et al. (1975)

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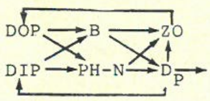

Richey (1977)

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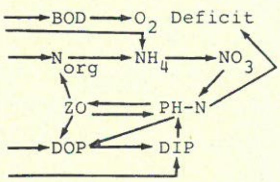
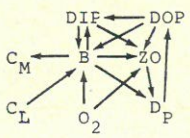


Thomann et al. (1973)

10


Aijzatullin, Leonov (1975)

List of symbols used in above table:

DOP, DIP	-	dissolved organic and inorganic phosphorus
DISV.P	-	sum of dissolved organic and inorganic phosphorus
PP	-	sum of particulate phosphorus
D_P	-	detrite phosphorus
B	-	bacterial phosphorus
PR	-	protozoan phosphorus
PH-N	-	phytoplankton phosphorus
ZO	-	zooplankton phosphorus
BOD	-	biochemical oxygen demand
O_2	-	oxygen
N_{org}	-	organic nitrogen
NH_4	-	ammonium nitrogen
NO_2	-	nitrite nitrogen
NO_3	-	nitrate nitrogen
C_L	-	labil carbonous organic matter
C_M	-	organic matter transformated by bacteria

TABLE A1

in large quantities. The opinion was expressed that ecological models will never be able to describe this phenomenon adequately.

In one attempt to describe the buoyancy phenomenon in another lake, it was reported that the apparent settling velocities of 1 m/day to 20 m/day were required to fit the data. In this case the total blue-green biomass in the first 2 cm of sedimented material was approximately the same as the total blue-green biomass in the water column.

There was a suggestion that, in general, algal succession should be included in the model when:

1. Silica is limiting - this will cause a succession in species from diatoms to non-diatoms.
2. There is a substantial blue-green bloom - these species have different characteristics from other types of species.
3. Fixation of nitrogen is shown to occur - this frequently occurs in lakes, where the ratio N/P is relatively low.

Criteria for selecting algal species with functional characteristics best suited to a given set of circumstances were presented using a self-optimising (self-organising) principle with maximisation of a specified goal function for the algae. For complete information refer to Radtke et al [2].

The characterisation of blue-green algae with regard to temperature preferences was discussed. Blue-greens are usually observed to be dominant when temperature exceeds 20°C. However, it was pointed out that there are certain blue-green species, for example, Oscillatoria, which grow well at lower temperatures.

It was pointed out that the microclimate around blue-green algae may lead to certain functional differences as compared to other types of algae. Blue-greens are known to maintain a close relationship with symbiotic bacteria. This characteristic may be responsible for influencing the pH-value and uptake kinetics for phosphorus and carbon dioxide.

Reference was made to results by Shapiro, which apparently indicates that blue-greens are more efficient than other species for CO_2 uptake. This conclusion was challenged because the experiments performed did not measure independently the effect of the change in pH on the carbon and the phosphorus uptake kinetic. The distribution of the dissolved forms of both nutrients changes as a function of pH.

There was discussion of the point that commonly accepted notions of blue-green settling and freedom from grazing pressures may not be correct in all cases. Apparent settling velocities for blue-greens may not be slower than the settling velocity for other species, but may be faster due to clumping and colony formation. Recent experimental work by McNaught on Lake Huron has indicated that blue-green species may actually be preferred by the zooplankton when compared to certain non-blue-green species. It is not clear whether the zooplankton assimilate the blue-greens or merely ingest them in these cases.

Local blue-green algae problems are not primarily caused by their rapid mass growth, but rather by their buoyant rising to the surface, where they form clumps. The well-known disadvantage of biomass decay which is highly concentrated in a relatively small part of the lake will appear. This phenomenon is very difficult to include in the model.

12. Do we need to include anaerobic conditions, denitrification and nitrogen fixation in the model, and if so, how?

Reported by G. van Straten.

One approach for taking into account the effects of nitrogen fixation upon the nitrogen budget is to set up the rate of nitrogen fixation proportional to the difference in soluble phosphorus and soluble nitrogen and by multiplying the soluble phosphorus with some factor (about 5) which is related to the P/N uptake ratio. It has been stated that there seems to be no sharp threshold concentration for nitrogen fixation - some 300 μg N/1 of soluble nitrogen has been mentioned as a suitable figure. A simple solution then is to set the fixation rate at zero for 300 μg N/1 and account for a linear increase if soluble N drops to zero. This is a more elaborate case of the simple approach whereby nitrogen is not allowed to become limiting to the nitrogen fixing blue-green algae; one merely traces the changes of nitrogen during their growth. To prevent problems with regard to the ratio of N-fixing to non-N-fixing algae, the introduction of a separate state-variable for N-fixing algae might be envisaged.

General agreement was obtained regarding the occurrence of denitrification in the sediment. The theoretical possibility of denitrification in the oxygen depleted core of clumps of algae does not seem to be of importance in practice. For denitrification to occur it does not seem to be of great significance that the sediment is entirely anaerobic, because there will also be nitrate in the anaerobic portions due to the fact that nitrate penetrates much deeper than does oxygen. A simple first order reaction has been applied as a reasonable approximation, although the results of analysis of the simultaneous diffusion and reaction system would suggest a square root dependence (a half order dependence). Of course a more detailed model would require incorporation of the denitrifying bacteria.

13. 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 out the balancing point? What is the role of chemical data?

Reported by M. Straskraba.

Three methods were suggested for how to select the number of state variables to be included in the model:

a) The ecological buffer capacity, β, expressed as the ratio between change in loading and change in the state variables in focus, e.g., $\beta = \frac{\Delta \text{ loading}}{\Delta \text{ PS}}$, where PS is the state variable soluble phosphorus. For further details, see Jorgensen et al. [3]. It was stated that β cannot be used for comparing several models.

It is noticeable that β is time dependent, if such external factors as temperature and irradiance are functions of time.

b) The variance of the property which the model is intended to predict is affected by the number of state variables or parameters. This is a method for deciding which degree of model complexity is sufficient for the purpose at hand. We assume:

1) That the purpose of the model is to predict the consequences of some changes to the system under study, such as increased loading.

2) That the change can be quantified by some numerical quantity P (such as the maximum concentration of phytoplankton). A model based on N_1 parameters α_{N_1} will yield an estimate $\hat{P}(N_1)$ of P, and this estimate will have a sampling distribution because its parameters are calculated from observed data, which can be regarded as random variables. Similarly, a more complex model with N_2 parameters α_{N_2} ($N_2 > N_1$) will yield a second estimate $\hat{P}(N_2)$ of P; the closer $\hat{P}(N_i)$ is to P, the better is the model. It is suggested that the root mean square error could be taken as a measure of the model "goodness". However, P is never known, so that some less satisfactory alternative has to be used, such as var $\hat{P}(N_i)$.

Now var $\hat{P}(N_i)$ is a function of the sampling variances of the

$$\text{var } \hat{P}(N_i) = \sum_{j=1}^{N_i} \left(\frac{\partial \hat{P}}{\partial \alpha_j}\right)^2 \text{var } \hat{\alpha}_j + 2 \sum_{j=1}^{N_i} \sum_{k=1}^{N_i} \left(\frac{\partial \hat{P}}{\partial \alpha_j}\right)\left(\frac{\partial \hat{P}}{\partial \alpha_k}\right) \text{var } (\hat{\alpha}_j, \hat{\alpha}_k) \quad . \qquad j \leq k$$

This quantity will have more terms, whether the model is complex (N_i large) or simple (N_i small). We could therefore plot var $\hat{P}(N_i)$ as ordinate against N_i as abscissa, and choose that value of N_i beyond which an increase in the number of parameters gives little or no reduction in var $\hat{P}(N_i)$.

The approach could be adapted to include consideration of the greater cost associated with more complex models; if the cost were taken as a linear function of N_i, the number of parameters show that

$$\text{Cost} = A + BN_i$$

then the following picture would be obtained:

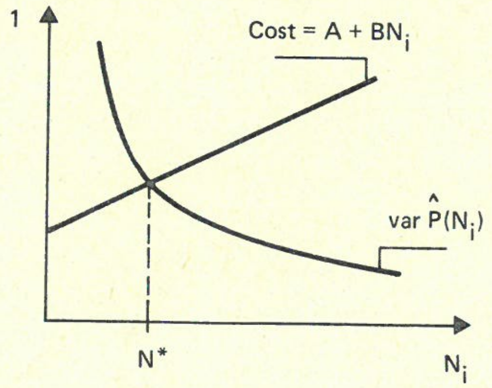


Figure A2

The model with N^* parameters would then be adequate for the given purpose.

c) The development of some statistical indexes similar to the indexes of diversity where instead of the number of species the number of variables would be used. This is merely a suggestion, but it has not yet been tested in practice.

Generally it is felt that we need more systems analytical methods directed towards the complexity and validation problems of complex models.

Other aspects of the validation problem were raised, particularly the impossibility in most instances of validating the model during different loadings. Even when loadings are changed, the response will in most cases be delayed and thus several years will need to elapse before a good validation can be undertaken. One suggestion is to substitute this validation by a validation of the same model when it is applied to a number of lakes with different loadings. Finally, in conjunction with the complexity of the model, it may be noted that the level of model error increases with an increase in the number of parameters.

14. What is the reliability of present-day ecological models? To what extent is it possible to predict the response to changed loading?

Reported by P. Mauersberger and K. Bauer.

From the mathematical point of view the equations characterizing a microscopic, deterministic water quality model form a system of non-linear differential equations with boundary conditions and initial values. It is very difficult to investigate the existence and uniqueness of the solution to these equations. From the thermodynamic point of view the aquatic ecosystem is a non-linear open system, (exchanging energy and matter with the environment) which is far from thermodynamic equilibrium. Completing this system of basic equations by adding entropy it becomes possible to apply the methods and results of the modern theory of thermodynamics of irreversible processes [4] to aquatic ecosystems. This theory offers local and global evolution and stability criteria. The mutual effect of entropy producing and entropy reducing processes inside the water body and across its boundaries essentially regulate the structure, state and further development of the aquatic ecosystem. Since the non-linear basic equations are shown to have, in general, more than one solution if the system is far enough from thermodynamic equilibrium, fluctuations (generated by the system itself or excited by external factors) play an important role in the transition of the ecosystem to a new structure. The succession of structures characterizes the anthropogenically influenced processes of self adaptation and self organisation of the ecosystem. This theory is not yet completely elaborated; in particular, the regulating mechanisms of living sub-systems should be included. Thermodynamical considerations must be combined with cybernetics and stochastic elements should be incorporated. In spite of these factors it seems that such a theory may offer precisely that "comprehensive" (or "condensed") approach to water-equality modelling which was asked for in the introduction to this workshop.

Many problems in the range of this question remain open for discussion. For example, is the influence of microconcentrations (MbO_2, Glycin, etc.) taken into account in such a way that the model correctly reacts to changes of the content of these substances.

15. It is possible to develop models for predicting the rate of eutrophication? Should simple or complex models be used? What are the possibilities and limitations of the models? Are the analytical expressions of the relationship between phytoplankton biomass and total loading of nutrients, average depth, retention time of water etc., valid (Vollenweider index)?

Reported by V.A. Vavilin.

If a modification of Vollenweider's approach is used then,

$$
\begin{aligned}
dB/dt &= \frac{1}{T} B + \mu(X,t,I)B \\
dX/dt &= \frac{1}{T} (X_o - X) - \gamma\mu(X,t,I)B
\end{aligned}
\tag{1}
$$

where B is the phytoplankton concentration and X is the limiting nutrient concentration, $T = V/q$ is mean retention time (V = volume of the water body, q = flow), γ is a stoichiometric coefficient, $\mu(X,t,I)$ is the phytoplankton growth rate as a function of the limiting nutrient concentration (X), temperature (t) and light intensity, I. X_o is the nutrient concentration of the influent.

Let us now assume

$$\mu = \mu_m(t)f(I)\phi(X) \tag{2}$$

where

$$f(I) = \begin{cases} 1 & I > I_m \\ I/I_m & I < I_m \end{cases} \tag{3}$$

and where I_m is a saturation constant. Then

$$\phi(X) = \frac{X}{K_x + X} \tag{4}$$

in which K_x is a half saturation coefficient.

The intensity of light at depth h is

$$I_h = I_o \cdot e^{-(n_o+nB)h} \quad , \tag{5}$$

where I_o is the light intensity at the surface, n_o is the light absorption coefficient for water, n is the specific extinction absorption coefficient for phytoplankton. Thus, if light intensity is a limiting factor at depth

$$h_m = \frac{1}{n_o + nB} \ln \frac{I_o}{I_m} \tag{6}$$

then

$$I_m \leq I_o \leq I_m e^{-(n_o+nB)H} \quad , \tag{7}$$

where H is the maximum depth.

The mean value $\bar{\mu}$ is given by

$$\bar{\mu} = \frac{1}{H} \left(\int_0^{h_m} \mu dh + \int_{h_m}^{H} \mu dn \right) - \mu_m(t) \frac{1}{(n_o + nB)H}$$

$$\{1 + \ln \frac{I_o}{I_m} - \frac{I_o}{I_m} \cdot e^{-(n_o+nB)H}\} \frac{X}{K_x + X} , \tag{8}$$

and instead of the influent concentration of limiting nutrient X_o let us now consider the mean nutrient loading X_ε

$$X_\varepsilon = \frac{X_o \cdot q}{S} \tag{9}$$

in which S is a surface of water body.

Under a steady state condition these equations are transformed into:

$$\begin{cases} -\frac{1}{T} + \tilde{\mu} = 0 \\ \frac{1}{T} \left(\frac{X_\varepsilon \cdot S}{q} - X\right) - \gamma\bar{\mu}B = 0 \end{cases} . \tag{10}$$

In the linear case $K_x >> X$. If

$$1 + \ln \frac{I_o}{I_m} >> \frac{I_o}{I_m} \cdot e^{-(n_o+nB)H} \tag{11}$$

then

$$B \approx \frac{\frac{X_\varepsilon \cdot S}{qK_x} \cdot \alpha - \frac{n_o}{n}}{1 + \gamma \frac{1}{K_x} \cdot \alpha} \tag{12}$$

where

$$\alpha = \frac{\mu_m(t) \cdot T}{nH} \left(1 + \ln \frac{I_o}{I_m}\right) . \tag{13}$$

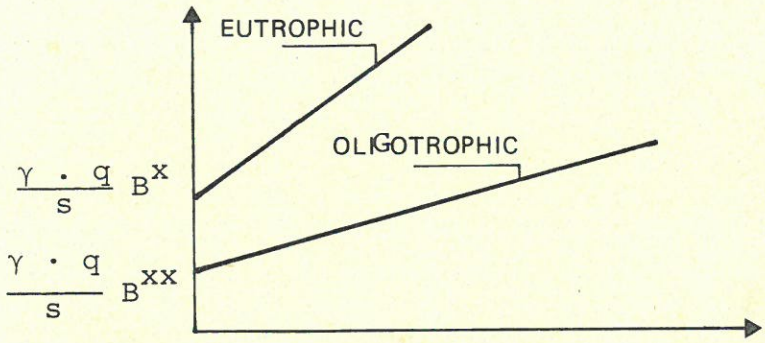
From the equation (12) it is easy to obtain:

$$X_{\varepsilon} = \frac{\gamma \cdot q}{s} \cdot B + \frac{q}{s} K_x (B + \frac{n_o}{n}) \frac{1}{\alpha} \quad . \qquad (14)$$

We can distinguish between the following three cases:

$$\begin{aligned} &B < B^{+} \text{ - oligotrophic state} \\ &B^{+} < B < B^{++} \text{ - mesotrophic state} \\ &B > B^{++} \text{ - eutrophic state.} \end{aligned} \qquad (15)$$

From this can be deduced the following graph:



$$K_x \frac{1}{\alpha} = \frac{K_x \cdot nH}{\mu_m(t) \cdot T} (1 + \ln \frac{I_o}{I_m})$$

Figure A3

with the parameters γ, $\frac{q}{s}$, $\frac{n_o}{n}$ being constants in a given case.

In a more general case when equation (7) is valid, the following expression can be obtained:

$$X_{\varepsilon} = \frac{\gamma \cdot q}{\delta} \cdot B + \frac{q}{\delta} K_x \frac{{}^{1}/_{\alpha}}{\frac{1}{{}^{n_o}/_{n} + B} - \frac{1}{\alpha}} \quad . \qquad (16)$$

The plot of equation (16) is shown in the following figure:

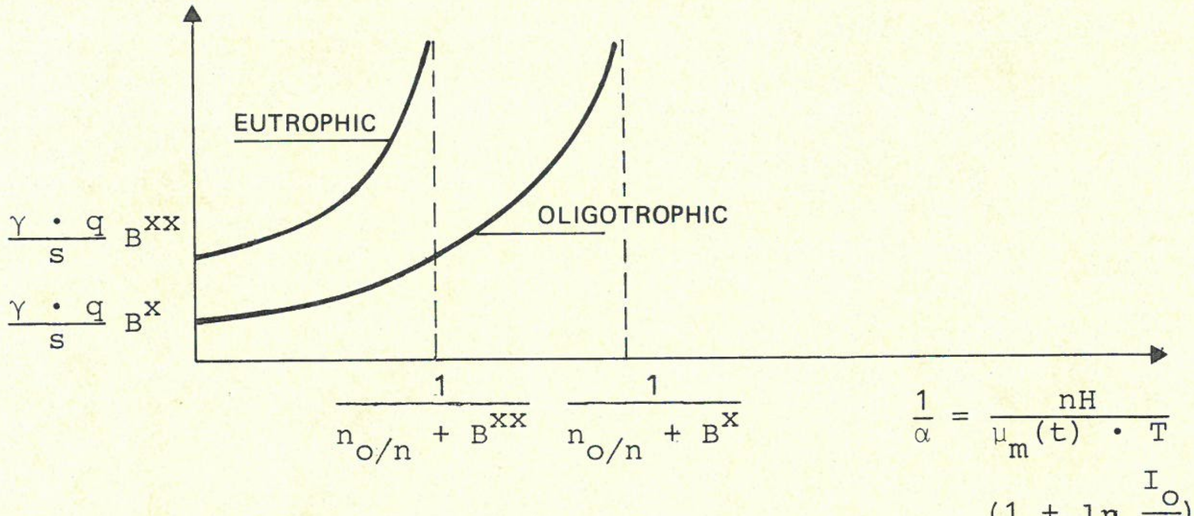


Figure A4

It is possible to consider some modifications of equation (1). As given the model permits good estimation of the trophic state, when the limiting nutrient loading is changed. The classification of lakes by deduction from Vollenweider's diagram, is not suitable for some instances. Dillon improved this approach, considering the dilution rate as an important parameter.

The approach which was presented above depends on retention time, depth and intensity of light, maximum growth rate etc. The important question is the validity of the steady state approach, both for the model and for the real lake system. In systems analysis it is important to establish whether the local stability conditions are indicative of globally stable dynamic behaviour. The validity of steady state approach first of all depends on seasonal variations of nutrient loading.

Vollenweider's approach is attractive, because it is rather simple and demands no large scale amount of experimental work. However, from a decision making point of view, it seems that the necessary procedure is to construct and investigate *dynamic* models.

<u>16. What parameters and processes should be considered for the lake subject to acidic deposition?</u>

Reported by M.W. Lorenzen.

A survey of lake susceptibility to acid precipitation would be very useful.

It was noted that literature from Norway and Sweden has reported on studies in those countries although a final conclusion about how to solve this problem could not be taken.

17. A suggestion for an IIASA publication: should IIASA publish a list of parameters?

Reported by L.J. Hajdu.

The value of model parameters is of great interest for all scientists within the field of ecological modelling. Many data can be found in the literature e.g. in Lehmann et al. (1975) are several parameter values listed.

It is of some importance to produce a publication (a handbook) containing the most important parameters, such as half saturation constants, death, sinking, grazing -rates, min. phosphorus concentrations in algae etc.

Concurrently with the development of the field, revision of these parameters values must of course take place. It is recommended that a list of parameters be completed according to standard units, SI, and with the necessary conversion tables included. It might also be of interest to standardize techniques of parameter measurement, such as for the phosphorus half saturation constant, since it is not a constant parameter, but changes with ecological and hydrological factors. The methodology of parameter measurement may appear to be of marginal interest for IIASA, but undoubtedly the reality of a model is to a great extent dependent on the reliability of the basic parameters.

Modern limnology textbooks reflect this attitude of modelling but may be of limited value to the practical model builder, as they usually contain few, if any actual model parameters. The general validity of these parameters is not fully understood. A collection of widely distributed literature data gives the possibility of studying the generality of the parameter values suggested by a number of authors. It would also be advisable to include a list of the recommended literature and the addresses of authors and contributors in the above suggested handbook.

It was announced that the suggested handbook was actually under preparation in Denmark and would be ready for publication in the autumn of 1978. The data are available on tapes. Approximately 50 international journals and 500 books have been reviewed and the handbook will probably cover as much as 75% or more of the total relevant literature. Parameter values only are compiled *without* critical evaluation, but all data are accompanied by appropriate references and the given measuring conditions. In this handbook no average values or standard deviations are calculated; the reader should evaluate the reliability of the parameter values for himself. An EPA report will soon be ready in the U.S.A. which will contain a review of equations and expressions used in water-quality models. A list of parameter values will also be included in this report although the review of the literature is limited.

It was pointed out that confusion may arise by comparing different parameter values such as half saturation constants, since they might have different physiological meanings from one case to another.

<u>18. How and when should quick phosphorus recycling due to phosphate excretion by phytoplankton be considered in the model?</u>

Reported by F. Chahuneau.

In the literature inverse relationships between alkaline phosphatase activity and phosphorus cell concentration has often been reported. It is not well established whether the enzymes are located at the cell surface or are released to the environment. Under the first assumption the algae will behave exactly as if they were able to assimilate dissolved organic phosphorus directly--a factor which is not usually accounted for in models. However the rate of dissolved organic phosphorus hydrolysis is at least one order of magnitude lower than average phosphorus uptake rate. The conclusion is that this phenomenon can usually be neglected in the model.

B. HYDROPHYSICS

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

Reported by M. Markofsky.

No definitive answer can be given to the question raised. In general most of the comments suggested that the degree to which the hydrodynamics needs to be modelled depends on the problem being investigated and the time scales of the relevant phenomena.

Two case studies were presented. The first required the prediction of the likelihood of entrainment by a 3200 megawatt power station in the western basin of Lake Erie, where the mean depth is approximately 6 m. Here a three dimensional description of the wind induced velocity field was found necessary for use as input to the transport equation describing larval transport. [5].

In the second case study, which concerned a drinking water intake on Saginaw Bay, it was felt that the primary current patterns could be sufficiently well deduced by intuition so that no mathematical description of the wind induced circulation was required. In this example it had been observed that strong odours were associated with a rapid increase in intake temperature. The increase in intake temperature was judged to be associated with a change of wind direction as shown on the accompanying figure. Since the intake is near the bottom, cooler lake water is withdrawn for the situation in Figure B1A and warmer bay water for the situation in Figure B1B. The suggested solution to the water quality problem is to construct an addition to the intake in order to allow it to draw surface water during the wind condition of Figure B1B.

It was proposed that the degree of hydrodynamical description depends upon the relative time scales of the biological and hydrodynamical processes. For example, if the biological processes occur on a time scale considerably larger than the circulation

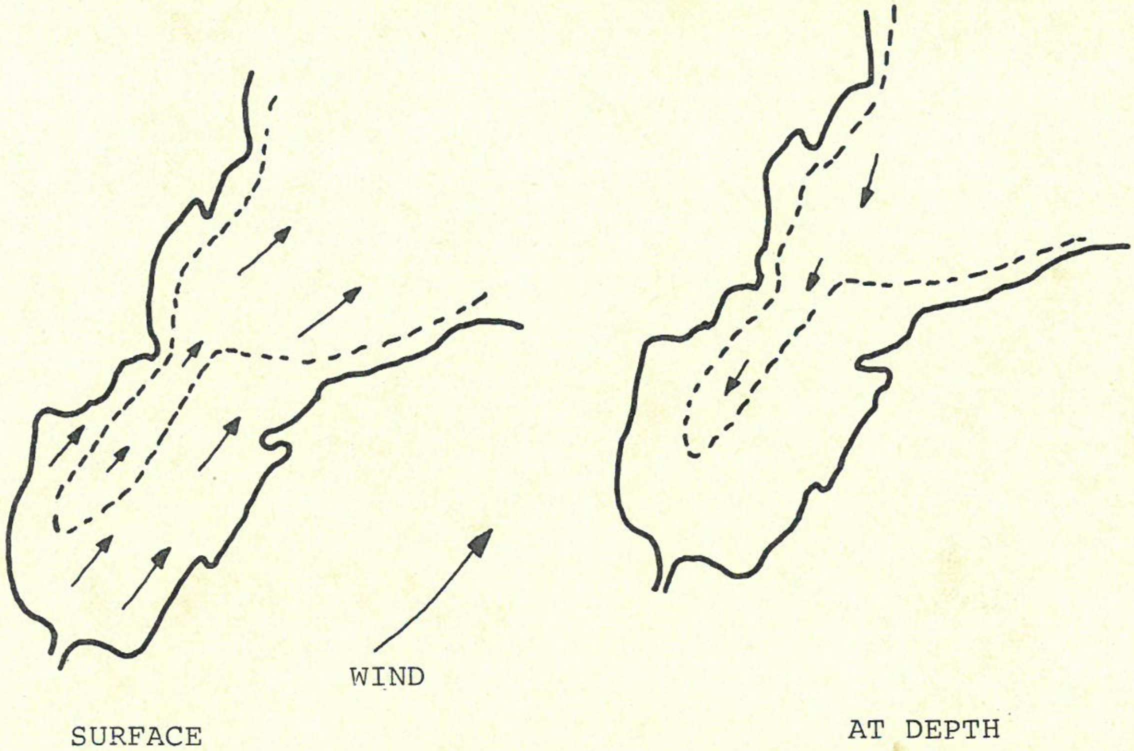


FIGURE B1A

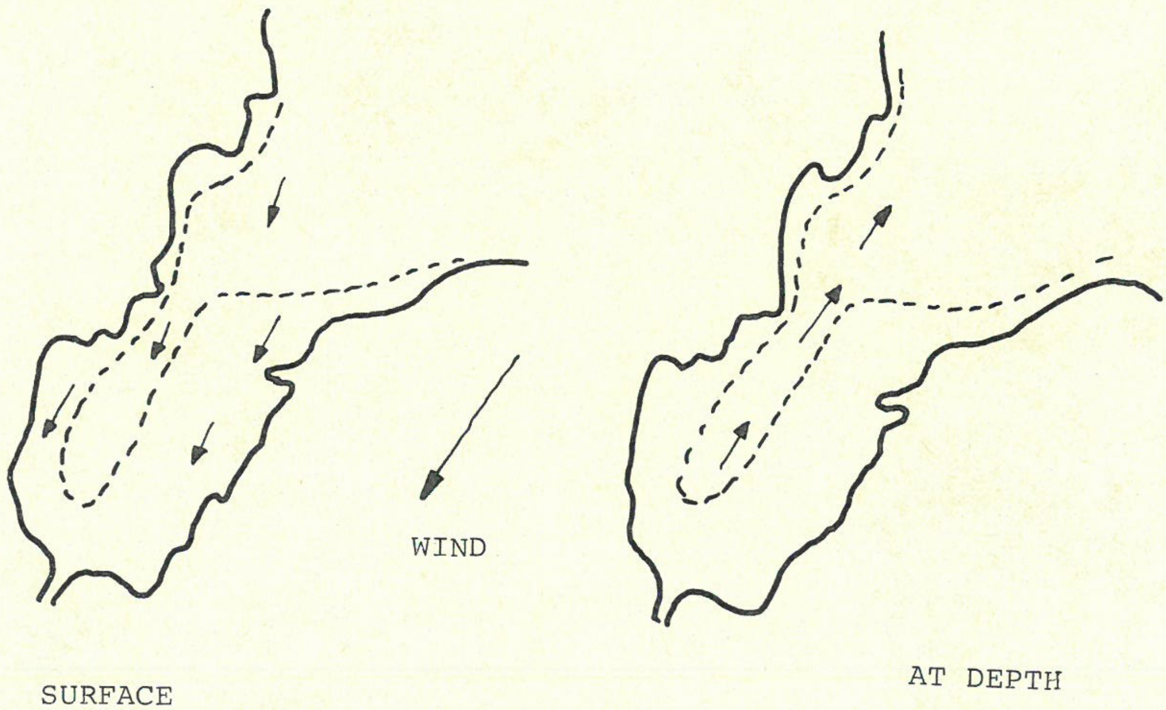


FIGURE B1B

and wind induced mixing time of the water body, the details of the hydrodynamics can probably be neglected.

In any case, hydrodynamical and water quality models are very often solved in quite different time steps, Δt, and space steps, Δx, since Δt and Δx for the hydrodynamical resolution are generally considerably smaller than those required for the water quality description. This is increasingly important when considering an ecosystem description in many state variables.

2. What is the relative importance of lake or reservoir inflows and outflows in the vertical and horizontal exchange as opposed to vertical and horizontal mixing by diffusion or wind?

Reported by M. Markofsky.

Case studies in reservoirs which experience thermal stratification were reported.

The varying input elevation of the inflowing water is a functions of both the inflow temperature and the thermal structure of the reservoir. Neglecting vertical advection results in vertical dispersion coefficients which are a function of depth and time.

A sensitivity analysis for a reservoir with a retention time of the order of one year was presented. The governing equation for temperature prediction is

$$\frac{\partial T}{\partial t} + V\frac{\partial T}{\partial y} = \frac{1}{A(y)}\frac{\partial}{\partial y}\left[AE\ \frac{\partial T}{\partial y}\right] + q_i\ \frac{(T_i - T)}{A} - \frac{1}{A\rho C_p}\ \frac{\partial(\phi_b A)}{\partial y}$$

and for mass $(J = 1 \rightarrow n)$

$$\frac{\partial C_j}{\partial t} + V\frac{\partial C_j}{\partial y} = \frac{1}{A(y)}\frac{\partial}{\partial y}\left[AE_M\ \frac{\partial C_j}{\partial y}\right] + q_i\ \frac{C_{inj} - C_j}{A}$$

$$+ \frac{\text{sources}_j}{\rho} - \frac{\text{sinks}_j}{\rho}$$

T = temperature; y = depth; v = vertical velocity (function of depth and time); E and E_m the dispersion coefficients for temperature and heat, respectively; A = horizontal cross sectional area; q_i = inflow rate/height; ϕ_b = solar radiation penetrating the surface; T_{in} and C_{in} = inflow temperature and concentration, respectively.

The vertical velocity field, v(y,t) may be calculated from the inflow and outflow rates and density considerations. Varying E_m from 0 to 100 x molecular value produces no changes in the concentration profiles indicating that for the reservoir of the above stated order of magnitude, or retention time, a good description of the velocity field is supposed which allows the neglection of a dispersion term.

For shallow reservoirs it is to be expected that wind mixing plays a dominant role in the vertical and horizontal exchange processes. The shorter the residence time the greater the role of inflow and outflow on the horizontal exchange phenomenon. However, the better the mathematical description of the flow and wind induced current fields, the less is the reliability of the dispersion coefficient as a fitting parameter. The extent to which one attempts a detailed formulation of the velocity field, however, is related to the discussion associated with question B1.

3. What are the factors effecting the concentration of suspended sediment in lakes and how do we model the resuspension of bottom sediment?

Reported by G. van Straten.

The main factor determining the resuspension of sediment particles from the lake bottom is turbulence in the region of the sediment bed.

Turbulence may originate from two possible sources. The first is the shear at the bottom surface caused by a return flow along the bottom in the case of a wind driven circulation, or by a transition flow in a narrow part of the lake. The effects are quite similar to sediment transport in rivers, although the range of velocities that might occur is less. The second mechanism is the turbulence generated by waves and more notably by breaking waves.

From the point of view of mathematical modelling of ecosystems it might be imagined that the time for which a particle remains in suspension is a governing factor. With regard to this aspect attention was drawn to the so-called *saltation* theory as opposed to the diffusion theory for resuspension. According to this theory particles are whirled up and then settled again after some time. It would be a great help, if an age distribution of particles in suspension could be established. However, among other matters, effects such as cohesion forces--due to potential differences stemming from the electro-chemical properties of the sediment flocs--are a serious barrier towards reliable modelling.

Another factor to be borne in mind is that in many cases no clean/sharp interface between water and sediment exists. The concept of the "liquid sediments" strongly suggests an analogy with the erosion of the thermocline due to waves induced by wind.

A practical example was given for a Scottish lake where a striking coincidence was observed between the change in the sediment composition and the line where the wave length due to wind reached half depth.

In a Dutch shallow lake turbidity seemed to have more relation to inlet water solids concentration than to resuspension. Although some resuspension had to be expected during a severe storm in the more shallow part of the lake, almost no increase in turbidity was observed. A possible explanation might be that the deeper parts of the lake acted as an effective "dust-binder", since more quiet conditions may be expected there, thus favouring sedimentation.

C. GENERAL QUESTIONS

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

Reported by John Paul.

The following question was raised: How will it be possible to calculate hydrodynamic currents for basic wind conditions (Steady state currents)?

The answer to this question was given along the following lines:

> Process the hydrodynamics results so that they can be used in ecological models. When they are used in ecological models the speed and direction of the wind should be picked, in some stochastic manner which is changed at every time step. Over a time-scale of weeks, which is in most cases the smallest time-scale of interest in ecological models, the wind pattern can then be considered as this steady wind condition.
>
> For prediction, it is necessary to look at past wind histories in order to obtain a proper stochastic model of wind behaviour. Major events will occur at different times and in different numbers but over several years these fluctuations would be averaged out to give typical wind conditions. For calibration and validation, wind data for the given specific year should be used; in this fashion particular events, which could produce major effects will be included in the calibration and validation.
>
> At any rate the above suggestions would seem to be an efficient way of coupling hydrodynamic and ecological models in order to make hydrodynamic calculations once only for each lake.

Generally three approaches were suggested for taking meteorological factors into consideration in lake models:

1. Time varying inputs of wind or other external factors are used in the hydrodynamic model.
2. A correlation analysis between meteorological data and influenced variables or parameters is carried out.
3. A correlation analysis between calculated or estimated variables and parameters and meteorological data is carried out.

It was stated that the method of time averaging wind as an input forcing function may cause a strong interaction with the response of the system. In a network of small lakes interconnected by canals a detailed description of the wind function was reported to cause a high frequency variation in output flows and water level, due to the interaction with natural frequencies of the system itself. By averaging wind data over a longer period, these high frequencies can be filtered out and the more important low frequency response associated with the major flows are illuminated more clearly.

In averaging of wind velocity, however, care should be taken with respect to the effect that the wind velocity is squared in the equation of motion.

2. How do we distinguish between point and non-point sources and how do we consider them in the model?

Reported by D.O. Logofet.

This problem is rather complex and probably all non-point sources of nutrients such as land run-off, urban run-off, precipitation, surface infiltration of ground waters etc. must be treated in a stochastic manner. One way of solving the problem is to carry out a correlation analysis by use of the data available. But if the correlation coefficient appears to be too small, should we then conclude that there is no correlation at all? It was mentioned for example that the correlation between the phosphorus concentration in Lake Balaton and the entire discharge into the lake appeared to be rather small $r = 0.007$, although we know that there must be a correlation between these two variables. However, the correlation might be better if the land run-off, the flow input and the rainfall are considered separately. The correlation might also be better if the discharge is measured directly at the source point, but this approach requires a great deal of careful treatment of each source and adds considerable complication to the model.

Another question in conjunction with this problem was raised: what values of time-lags should be selected, when we consider a correlation analysis? This is not an easy question to answer, because of the time variability of loading in different sources.

Under all circumstances it seems necessary to take into account in the model the distribution pattern of non-point sources. To do so it is required to conduct measurements and excercises with hydrological sub-models.

3. Which parameter estimation procedure do you suggest to apply?

Reported by M.B. Beck.

One of the suggested procedures can be summarised as follows: since the calibration problem for a system with, let us say, 10-15 parameters to be estimated can be likened to the situation of "a blind man searching for a hole in a 10-15 dimensional room" it is required to limit the problem in some fashion in order to obtain tractable solutions. Suitable maximum and minimum bounds can be imposed on the permissible values of the parameters, where these bounds are derived from parameter estimates previously published in the literature. An automatic calibration can, however, be carried out for fine-tuning of perhaps some 3-5 parameters given reasonable a priori estimates of these parameters. A third solution is to use the submodels containing a relatively small number of parameters which may be calibrated against data collected from an intensive field experiment--an experiment which might measure more variables at a higher sampling frequency than the routine monitoring programme. The objective of this last option would essentially be to calibrate those parts of the model which exhibit relatively fast dynamic behaviour and which can be isolated, to some extent, from variations in the other parts of the eco-lake system. There is also a possibility of examining individual process mechanisms by laboratory studies or by field studies in which it might be possible to isolate such process mechanisms.

The automatic calibration mentioned above is based on a sensitivity analysis, which provides a matrix of partial derivaties for the ratio of changes in the state variable responses to changes in the parameter values. This matrix determines the directions of a search routine which then attempts to locate a minimum value for the squared prediction error loss function.

Some improvement in the efficiency of this procedure might be offered by the use of Rosenbrock's search-algorithms. It is further of importance to notice that the automatic calibration procedure, as expected, cannot prevent some of the parameter values reaching and being constrained at their maximum or minimum permissible limits. In this context it must also be underlined that several of the parameters may be time-varying; thus the automatic calibration is actually finding an average parameter value and does not take into account the possibility of seasonal variations.

Clearly, many difficulties prevail in this area of ecological modelling. Not the least of these difficulties is that of credibility of the results; thus the following cautionary messages are appended:

Automatic calibration may be dismissed as a meaningless curve fitting exercise; a predominantly hydrodynamic event might be erroneously calibrated within the ecological portion of the model; there are few cases where such a degree of detail is warranted by the overall objective of the modelling programme.

4. 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 calibrating and validating the model.

Reported by M.B. Beck.

Two presentations in response to this question were given.

The first presentation was an outline of a procedure for modelling:

1. Definition of the problem (model application objectives).

2. Development of conceptual flow diagrams.

3. Selection of the state variables--based on the preceding two steps and the concept of ecological buffer capacity (see also question A13).

4. Calibration of *submodels* against *intensive* sampling programmes.

   - notice at this stage that the model, or submodel, can be used as a scientific tool for evaluation of which description gives the best characterization of observed behaviour.

5. Fine-tuning, or polishing, of the total model against intensive and other available data.

6. Validation of the model, preferably by reference to an independent set of measurements taken during a period with changed conditions (e.g. changed loadings).

The second presentation developed a more detailed discussion of the problem of model structure identification and parameter estimation. Both problems can be considered as parts of the overall calibration problem. In some ways this presentation deals with topics which did not arise in the "Procedings of the Workshop on Geophysical and Ecological Modelling of Deep Lakes and Reservoirs". [6]

It is worth noting that a number of parameter estimation procedures have been applied successfully for modelling purposes in other fields of study. Each estimation procedure can be classified approximately according to whether it is applicable to black box models or internally descriptive (mechanistic) models and according to whether it is "off-line" or "recursive"--these terms will be defined below:

<u>For black box models</u>--the following procedures can be applied:

1. Least squares (R) (O)
2. Instrumental variable (R) (O)
3. Maximum likelihood (O)
4. Group Method of Data Handling--a self-organisation method.

For internally descriptive models--the following procedures can be applied:

1. Maximum likelihood (O)
2. Extended Kalman Filter (R)

The symbol (R) denotes a recursive procedure and the symbol (O) denotes an off-line procedure. Figure C1 gives a pictorial representation of the essential differences between the two types of algorithm.

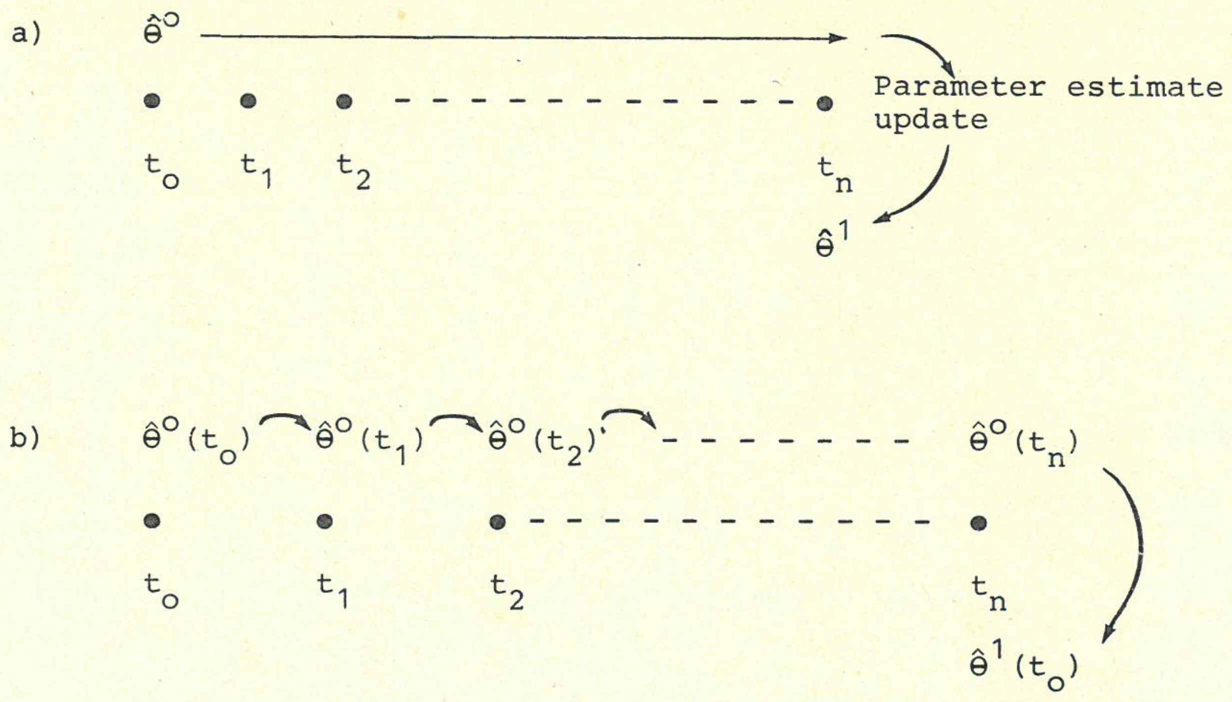


Figure C1. Methods of Parameter Estimation:
a) off-line; b) recursive.

An *off-line* procedure keeps the parameter estimates constant at their a priori values ($\hat{\Theta}^o$), while the complete block of time-series field data (from $t_o \rightarrow t_n$) is processed. A loss function, generally based on the errors between observed and model responses, is computed and an optimisation algorithm for minimising the loss function over the parameter space then computes updated parameter values ($\hat{\Theta}^1$) for substitution into the next iteration through the data (i.e. from $t_o \rightarrow t_n$). It is this form of parameter estimation procedure that was discussed in response to Question C3. A *recursive* parameter estimation algorithm, in contrast, computes updated parameter estimates $\hat{\theta}^o(t_k)$ at each sampling instant t_k of the field data; the minimisation of the error function is implicitly, rather than explicitly, included in the algorithms. At the end of the block of data, the estimates $\hat{\theta}^o(t_n)$ are substituted for the a priori parameter values $\hat{\theta}^1(t_o)$ of the next iteration through the data. An example of each approach to parameter estimation can be found in the papers of Di Cola et al (1976)[7]--an off-line estimation scheme--and of Gnauck et al. (1976)[8]--a recursive procedure.

One advantage of a recursive estimation algorithm is the possibility of estimating time-varying parameter values--see Young (1974)[9] and Young and Whitehead (1977)[10] for a more complete discussion with special reference to hydrological and water quality modelling problems. In fact this particular aspect of recursive techniques lends itself to the solution of the model structure identification problem and may also lead to an interpretation of the self-organisation problem mentioned elsewhere by Straskraba. Figure C2 attempts to represent the essence of the model structure identification problem. Suppose that the state variations are represented by the nodes of Figure C2(a) and the parameter values represent "elastic" connections between the state variables, e.g. as in growth-rate, grazing rate functions etc. If the assumption is made that all the parameters have values that are constant with time, and yet the recursive algorithm yields an estimate for Θ_4, say, which is significantly time-varying, one may question the correctness of the chosen model structure. The

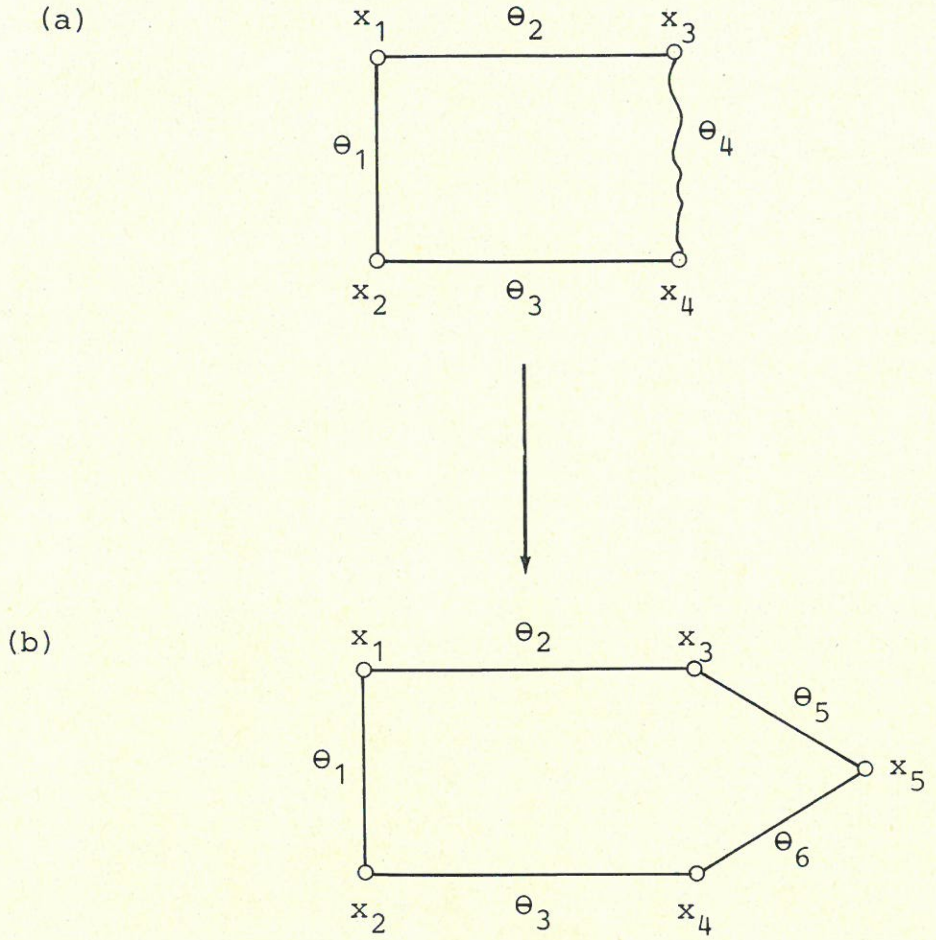


Figure C2. A Conceptual Picture of Model Structure Identification

reason is as follows: the general nature of the estimation procedure is to fit the state variable predictions to the field observations; thus if any structural discrepancy is detected between the model and "reality" this will manifest itself as an attempt by the estimation procedure to adapt the model, i.e. the parameter values, towards "reality". Such time-variations of the parameter values can, of course, occur for different reasons. For instance, the parameter may be truly time-variant in some seasonal fashion or there may be hidden problems of identifiability associated with the given model structure. For the purposes of our example in Figure C2(a), however, we might suppose that the actual structure of the relationships underlying the observed behaviour are better represented by the introduction of a new state variable and two new parameters, Figure C2(b). These kinds of argument form the basis of an approach to model structure identification illustrated with the Extended Kalman Filter in Beck and Young (1976)[11] and Beck (1978)[12]. Two further comments are pertinent. The approach suggested here clearly parallels the proposal made earlier in the response to question A5. Model structure identification also addresses questions similar to whether a multiplicative or a threshold growth hypothesis should be employed for the description of phytoplankton growth.

The problem described above with respect to Figure C2 is closely related to one interpretation of the notion of self-organisation depicted in Figure C3, where in fact we have reduced the self-organisation problem to a self-adaptation problem. A six state variable system is visualised. At time t_o the structure of the system is given by the connections indicated in Figure C3(a). Some time later, at t_i, recursive estimation of the parameter values, which here are assumed to be time-varying, reveals an apparently different structure: a number of the parameters are now estimated as being not significantly non-zero, while other parameters previously zero at t_o, have assumed significantly non-zero values (Figure C3(b)). Further changes can follow at time t_j, Figure C3(c), so that apparent structural changes in the ecosystem are accounted for by time-varying changes of the parameter values between essentially negligible and substantially significant magnitudes.

Stripped of any sophistication, model structure identification is analogous to the problem of choosing to fit a straight line or a curve (quadratic, cubic, quartic, etc.) to a set of field data, Figure C4(a). And while on the subject of simple regression analysis such as this it might be useful to try and dispel one illusion about parameter estimation. The illusion is that, say, twenty observations allow the determination of twenty pieces of information, i.e. parameter values. In principle there is no illusion, but in practice there is. Suppose that the true relationship between u and y in Figure C4(b). is the continuous straight line drawn through the two observations denoted by x's. Now suppose that a second

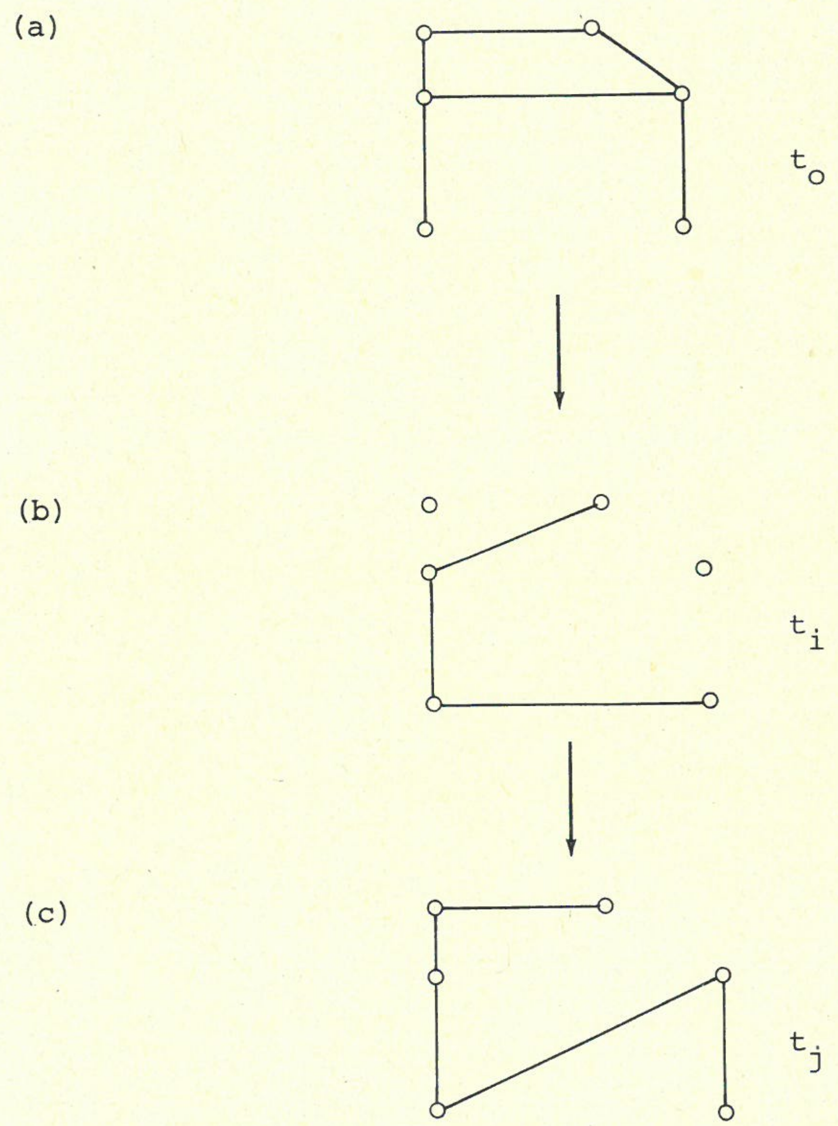


Figure 3. A Conceptual Picture of Self-adaptation (self-organisation

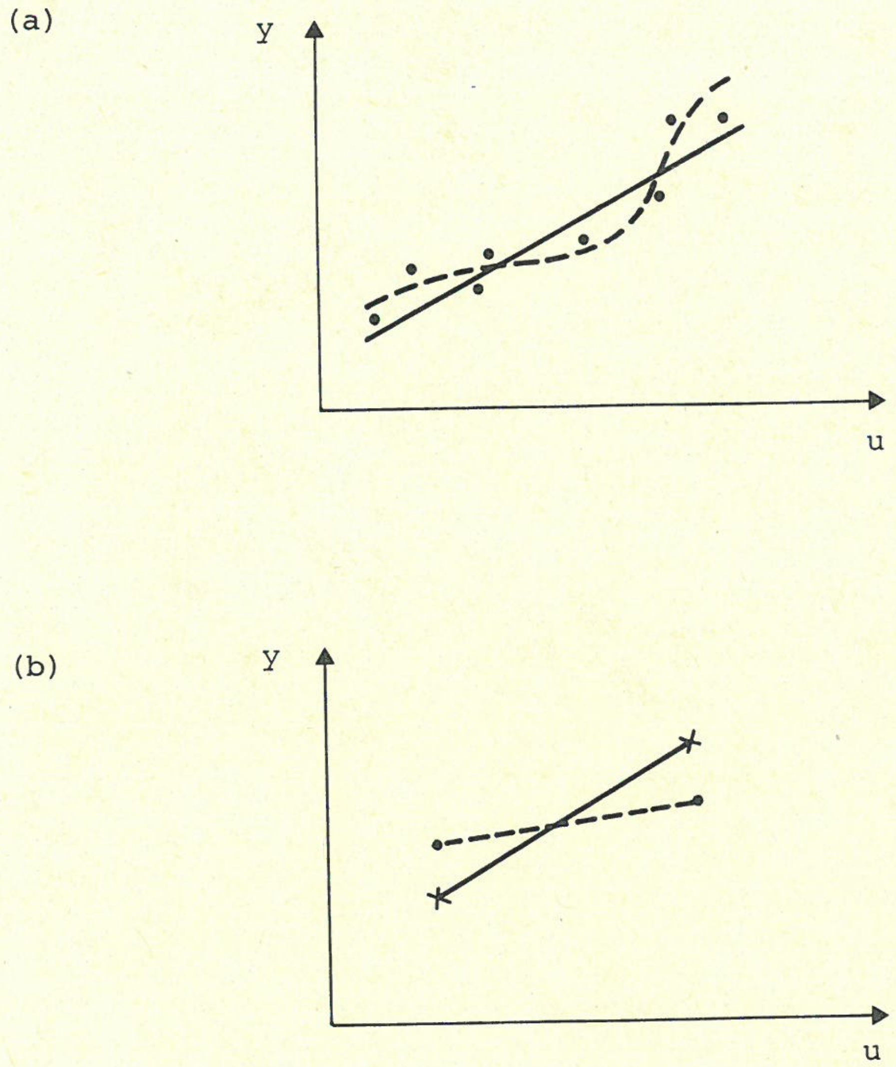


Figure 4. Curve-fitting: (a) the Analagous Problem of Model Structure Identification; (b) the effects of Measurement Error

set of observations for y is given by the o's, in which the observations contain a small amount of measurement error, and through which an equally feasible straight line could be drawn. Comparing the two sets of measurements it is clear that quite different values would be obtained for the gradient and intercept (the parameters) of the two straight-line fits. The solution of twenty simultaneous (deterministic) algebraic equations to obtain twenty parameter values is the same problem, and it ignores a primary unwritten rule of parameter estimation: namely, that it is necessary to obtain many more observations than there are parameters to be estimated in order that the analysis can discriminate effectively against the ever-present errors in the measurements.

The final point of the discussion of this question concerned the role of black box modelling approaches, since these have received little attention and were perhaps not thought to be very useful. A black box model identifies *what* the input disturbances (forcing functions, loadings) are observed to change in the output responses of an ecosystem. An internally descriptive model expresses *how* the inputs are related to the state variables, how the state variables are connected among themselves, and in turn how the state variables are translated into output observations. Both types of models tackle the problem of formalizing the relationship between cause and effect. So at the stage of model structure identification, when the analyst's understanding of observed behaviour is incomplete, a black box analysis of cause/effect relationships--for instance, the speed, type and magnitude of responses to changes--may well yield some initial clues about corresponding possible internally descriptive model forms (Beck (1978a)[13]. Some benefit to the subject of ecological modelling seems likely from a cross-breeding of the two approaches.

It might be expected that black box models, with their associated computational simplicity, would be especially useful in a real-time forecasting and control situation. On the other hand, as a response to a question by Markofsky it was admitted that in general the validity of a black box model does not extend beyond the conditions covered by the sample data set from which the model is derived.

5. Which lakes or reservoirs should be considered for case studies in cooperation with IIASA? Would it be desirable to compare various models with the same data set? (Answers should include a short summary of available data--parameters measured, duration, physical characteristics, etc.).

Reported by Janos Fischer.

The following case studies were suggested:

Straśkraba: A considerable number of data are available for Slapy and Kličava reservoirs. The model CLEANER has been applied to these data and cooperation was extended to any participant interested in using the data. Data already used by IBP are also available. Meteorological data are partly taken into account in an MIT model used for description of thermal stratification.

Bierman: A comprehensive measurement programme has been carried out over several years to assess the quality of water in Saginaw Bay, Lake Huron. Reports have been published on this case study from time to time and the data will be transferred to the IIASA data base shortly. (Shortly after the workship this transfer was completed.)

A simple hydrodynamic model was offered for use by Paul. The model works on a steady equations solution basis--it requires only topographic and wind data as input information. It is available at IIASA and might also be used for the Lake Balaton case study.

Jørgensen's Lake Model has already been transferred to the IIASA computer in December 1977.

Lastly, it was pointed out that any inter-comparison of models should take place ideally with the authors of the model present for such a study.

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