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SIMULATION OF WATER QUALITY IN LAKES

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This paper summarizes the work carried out for developing a water quality simulation model that would be suitable for lakes in Finland and other northern temperate regions. The work was started by applying the EPAECO model to lake Päijänne. On the basis of the experience gained from this application a new model entitled the FINNECO model was developed. This model is a typical water quality simulation model: it includes numerous state variables and is deterministic, one-dimensional and applicable to lakes and reservoirs. Special features of the model are its ability to take into account the mixing effect of wind and to simulate ice covered conditions in the winter. The model was applied to lakes Päijänne and Pyhäjärvi with the data sets of four and two years, respectively. In lake Päijänne the model gave reasonably good results, particularly in the case of chemical state variables. In lake Pyhäjärvi, however the results were less accurate. Because phytoplankton is an important variable in water quality models the factors affecting the growth of phytoplankton and the mechanisms used in the simulation were investigated more closely. A suggestion for the potential division of phytoplankton into functional groups that can be used in models is presented in that paper. The results and experience obtained in this work are discussed with reference to the theoretical background of water quality models.

Index words: Mathematical models, water quality models, simulation, the FINNECO model, the EPAECO model, lake Päijänne, lake Pyhäjärvi

1. INTRODUCTION

Mathematical models have traditionally been used as a research method in several branches of science, especially in physics and chemistry. Natural laws such as the law of gravitation or the relationship between the pressure,volume and temperature of ideal gas are examples of mathematical models. Models are commonly used in hydrology,meteorology and geology for predicting movements of water, the phenomena of the atmosphere and earthquakes, respectively. The use of models is also well advanced in the fields of economics and social science, for example socio-economic problems are typically treated using global models (Meadows et al. 1982). In recent years the growth of systems analysis has stimulated the development of mathematical models (Miser and Quade 1985). Regardless of the branch of science in which models are used, their strength lies in a fact that they simplify to some degree the reality which they represent and express in a concise form the essential features of the system. The procedure used is to construct a model for making a prediction of real phenomena. The output of the model is then compared in a simulation experiment with the actual behaviour of

reality. According to the results of this experiment, the model may be considered to simulate reality with sufficient accuracy or to be faulty, in which case a better model must be built. The objectives of modeling are generally a synthesis of existing knowledge, basic research of the phenomena of the system, quantitative calculations and prediction.

The development of water quality models has been rapid during the past twenty years in limnology and related fields. The objective of modeling has been a quantitative synthesis of the information available concerning aquatic ecosystems. Streeter and Phelps (1925) developed probably the first water quality model, an oxygen model of rivers, which has been used as such or with only minor modifications until the present day. During the period from 1940 to 1970 mainly phytoplankton models were developed (e.g. Fleming 1939, Riley 1946, Talling 1957, Steele 1962, Vollenweider 1965, Patten 1968). These models calculated plankton productivity and represented an effort to quantify the processes observed in the field. Since 1970, the field of water quality models has become wider and it now includes various types of models e.g. empirical models, dissolved oxygen models, eutrophication models and models that simulate the whole aquatic ecosystem. The models may be analytical models or simulation models, stochastic or deterministic. The broad field of water quality modeling has been discussed e.g. by Middlebrooks et al. (1974),Russel (1975),Hall and Day (1977), Jørgensen (1979), Orlob (1983) and Beck and van Straten (1983). Niemi (1981, 1984) presented the development of water quality models in Finland, particularly in the National Board of Waters.

Empirical models represent one group of water quality models. They are built on the basis of a large number of observations but the mechanisms giving rise to the observed reactions are not considered, i.e. they are black-box models. Most empirical models are built for predicting total phosphorus or chlorophyll-a in lakes (e.g. Sakamoto 1966, Vollenweider 1969, 1975, Dillon and Rigler 1974a, 1974b, Jones and Bachman 1976, Lappalainen et al. 1979, Frisk et al. 1980, OECD 1982). These models are relatively simple and can be solved rapidly.

More complex models simulating the whole aquatic ecosystem became increasingly common along with the development of computers (e.g. DiToro et al. 1971, Orlob 1972, Gaume and Duke 1975, Kelly 1975, Park et al. 1975, O'Connor et al. 1975, Bierman 1976, Jørgensen 1976, Jansson and Wulff 1977, Nixon and Kremer 1977, DiToro and Conolly 1980, Benndorf and Recknagel 1982). These models include mathematical equations describing the processes occurring between the state variables. They have many state variables, forcing functions and parameters and therefore require detailed data of the case study area and considerable computer resources. Most of them can be divided into hydrological and water quality modules. The emphasis laid on the two modules varies from model to model. Generally, however, models simulating the whole ecosystem tend to have detailed water quality module and relatively simple hydrological module.

The objective of the work summarized here was to develop a water quality model that would be suitable for lakes in Finland and in other northern temperate regions. The work was started by carrying out a rather extensive literature survey (Niemi 1977). On the basis of this survey the EPAECO model (Gaume and Duke 1975) was selected for further examination. After some minor modifications the model was applied to lake Päijänne (Niemi 1979). In the course of this application it was found that the model had some incompatibilities with Finnish conditions. The model was therefore modified so that it could simulate the whole annual cycle in a water body and take into account the freeze-up and break-up of ice. Furthermore a mechanism for taking into account the mixing effect of wind was introduced. Other modifications included changes in the nutrient cycles and state variables. The new model, entitled the FINNECO model, was applied to two Finnish lakes, to lake Päijänne (Kinnunen et al. 1982) and to lake Pyhäjärvi (Niemi and Eloranta 1984). Niemi (1985a) summarized the results and experience of these two applications. The computer program and users' manual of the FINNECO model are available (Kauranne 1983). Most of the factors active in the aquatic ecosystem affect the growth of phytoplankton. The theoretical background and practices of simulating phytoplankton biomass were therefore discussed in some detail (Niemi 1986). The experience obtained in developing and applying these models is summarized and the general principles and theory behind the model building are discussed with special emphasis on the modeling of phytoplankton.

2. THE MODELING APPROACH

Predictions are often made on the basis of mental models, existing only in the mind. These models

incorporate the assumptions and intuition of the person who developed them. They may include a lot of information and be suitable for many purposes, but their exact structure and logic are not necessarily clear even to the holder and are even less so to other persons. Communication with other people using these models may be difficult and the models cannot give quantitative answers.

Mathematical models contain a synthesis of the available information in the relevant field. Mathematical models are therefore thought to have advantages over mental models, because they must be defined explicitly, can process more information than the human mind, function logically, can be applied to different situations and give quantitative results. If science is considered as a body of knowledge or as a collection of facts, mathematical models represent one method for processing this data into such a form that it can be more effectively used.

Water quality simulation models are constructed on the basis of the data and knowledge available concerning aquatic ecosystems. The factors that are considered to be most important in the ecosystem are included in the model as state variables and the factors affecting the ecosystem from outside, e.g. light, are included as exogenous variables often called driving variables or forcing functions. The model is a group of mathematical equations that describe the processes occurring between variables. These equations include a number of parameters that must be estimated for every application. Typical features of water quality simulation models are: simplification and aggregation of the real ecosystem, modular-hierarchical structure and great numbers of state variables, forcing functions and parameters. Because of this the number of equations increase and the computer programs necessary for solving these equations become rather complex. The principles of the construction of water quality models have been discussed by Niemi (1977, 1986).

Construction of a model can be divided into phases, such as defining the objective of the model, identification of its structure, calibration, verification, documentation and application. Definition of the objective of the model largely determines its structure. In the papers summarized here, the term calibration is understood to mean the fitting of the model to a set of real data by adjusting the model parameters. Verification is understood to mean the application of the calibrated model to another set of data, different from the calibration data, with the aim of testing the applicability of the model. These terms are often used with somewhat different meanings in the literature. Estimation of the values of parameters is based on actual measurements made in the laboratory or in the field, or the parameters are estimated by calibration. Sensitivity analysis can be carried out by changing the value of one parameter at a time, several parameters at a time or by Monte Carlo simulation. In large models the number of calibrated parameters is so high that full sensitivity analysis cannot be carried out. Documentation of the model is necessary so that it can be applied by other investigators. Without documentation mathematical models tend to be disregarded along with mental models.

Despite the limitations and problems encountered with mathematical models their use is encouraged as it is felt that imperfect calculations e.g. of water quality are better than none and that alternative measures can be compared with a model even if it is not entirely accurate.

3. STRUCTURE AND DEVELOPMENT OF THE MODELS

3.1 The EPAECO model

Chen (1970) and Chen and Orlob (1972) developed a model for Lake Washington. Later Gaume and Duke (1975) further developed this model, when it was first entitled the EPAECO model. This model is a typical water quality simulation model. It has about twenty physical, chemical and biological state variables which is rather a high number when compared with most models of that time. The model includes several biological state variables, e.g. three groups of phytoplankton, zooplankton, benthic animals and three species of fish. The model solves the advection-diffusion mass transport equation for all biotic and abiotic state variables. This equation includes the effects of advection, diffusion, decay, growth and external sources and sinks for all the state variables. It is assumed in the model that mass and energy are transferred only along the vertical axis of the lake. In the model the lake is considered as a one-dimensional system of horizontal elements with uniform thickness. Advection and diffusion transport water and state variables from one element to another across the horizontal plane. The basic principles of the model are the law of conservation of mass and the kinetic principle. According to the kinetic principle the rate of change in the mass of a state variable is equal to the product of a coefficient and the concentrations of one or more state variables that interact to cause

the change. The model is suitable for the simulation of water quality of lakes and reservoirs during the open water season. The detailed structure of the model was presented by Gaume and Duke (1975) and Niemi (1979).

3.2. The FINNECO model

The FINNECO model was constructed according to the experience obtained in applying the EPAECO model. The objective of the work was to develop a model that would simulate more accurately the water quality of Finnish lakes and also be applicable in the winter when lakes are frozen over. It was assumed that the model should also be applicable to other lakes of the northern temperate regions. The number of state variables of the original model was decreased by omitting some of the biological state variables, e.g. benthic animals and fish, partly because it was realized that sufficient data concerning these state variables are seldom available and partly because these state variables were simulated in a relatively simple manner. Some new state variables, e.g. sodium lignosulphonate, were added. Simulation of nutrient cycles was modified and the mechanisms for simulating ice cover and taking into account the effect of wind in mixing water were added. The simulation of phytoplankton was also modified. Up to ten phytoplankton groups can be modeled with the new model if there is sufficient data. A new correction factor for taking into account the dependence of the chemical and biological reaction rates on temperature was added.

The basic structure and principles of both models are the same. The FINNECO model, however because of the changes described above, was assumed to be capable of simulating aquatic ecosystems more realistically and therefore to be more broadly applicable than the EPAECO model. Kinnunen et al. (1982) presented the structure of the FINNECO model in detail.

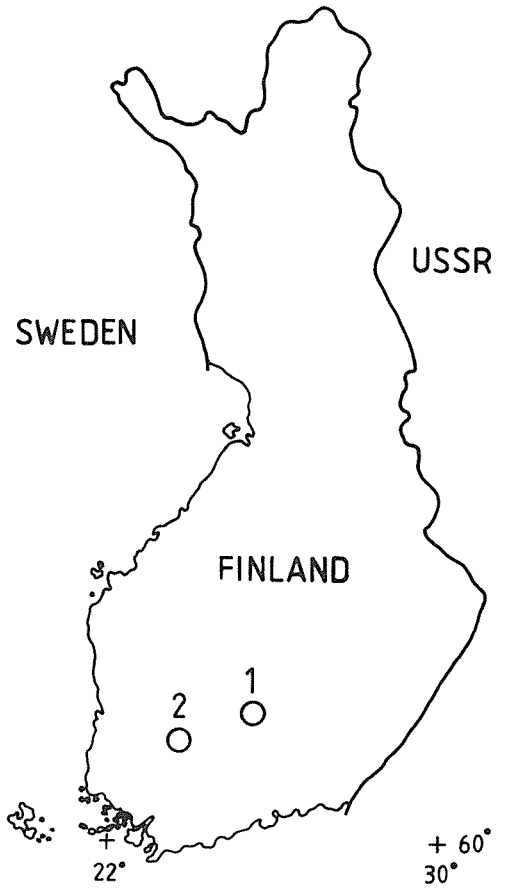

Fig. 1. The case study lakes: lake Päijänne (1) and lake Pyhäjärvi (2).

4. CASE STUDY

4.1 Case study lakes

After construction of a water quality model it must be calibrated and verified by comparison with data from a real water body. The requirements of such a water body are among others: sufficient available information for running the model and the existence of a water quality problem suitable for investigation with a model. The two lakes selected for the application were lakes Päijänne and Pyhäjärvi, both situated in southern Finland (Fig. 1). The models were actually applied only to parts of these lakes; to the northern sub-basin of lake Päijänne and to the major part of lake Pyhäjärvi from the Tammerkoski rapids to the bridge of Rajasaari.

Lake Päijänne is one of the most extensively studied Finnish lakes and therefore a good set of historical data concerning its water quality is available. The investigation of the lake was started by the water authorities in the beginning of the nineteen-sixties. Granberg (1973) described the eutrophication process of the lake. Hydrobiological Research Centre of the University of Jyväskylä has actively investigated the water quality of lake Päijänne. Material balances of the lake have been

calculated and the lake was included in a eutrophication research project conducted by the OECD (OECD 1982). Lake Päijänne is polluted by waste waters of the wood processing industry and several municipalities. The city of Helsinki and its neighbouring municipalities use the lake as a raw water supply. Water is conducted from the lake to the city of Helsinki along a 120 km underground tunnel. At the time of the application of the model the tunnel was still under construction and one objective was to use the model for calculating the water quality of the lake under different loading alternatives. Since the application of the model the loadings to the sub-basin have decreased as some older factories have been shut down and a new wood processing plant upstream has modern purification facilities. The characteristics of lake Päijänne were presented in more detail by Niemi (1979) and Kinnunen et al. (1982).

Lake Pyhäjärvi, situated close to the city of Tampere, is more severely polluted by both municipal and industrial wastes than lake Päijänne. It has a short detention time and resembles a slowly flowing river. The hypolimnion is at times anoxic and nutrients are released to the overlying water. This lake was considered to be a difficult test area for any model.However,it was thought that application of the model to this lake would give some idea of the suitability of the model. The set of data concerning the lake was unfortunately not as complete as that of lake Päijänne. A description of lake Pyhäjärvi was given by Niemi and Eloranta (1984). Table 1 shows the main characteristics of both lakes.

4.2 Application of the models

The application of a water quality simulation model to a lake consists of several different stages. These stages include gathering the necessary data, e.g. the quality and quantity of all the waters inflowing to the lake from diffuse loading, precipitation, industry and waste treatment plants. The meteorological data and the historical data of the water quality of the lake must also be obtained. The extensive data requirements of complex models are treated to some extent in various papers on modeling but a more detailed consideration has been presented by Niemi (1979) and Kinnunen et al. (1982). Optimal material for application purposes consists of detailed data from several years, one set of data for calibration and the others for verification. However, in most cases the application has to be carried out only with a limited amount of data, typically with the data of two years, one for calibration and the other for verification. Application of the model to several independent sets of data naturally provides better information concerning the suitability of the model. In addition to the data discussed above the model requires values for the parameters, the number of which may be large in this type of model. Estimation of parameters is carried out on the basis of laboratory measurements, field measurements or literature data, or they are estimated by calibration. An example of the data file used in models is that of the EPAECO-model (Niemi 1979).

Application of the EPAECO model was presented by Niemi (1979). Calibration was carried out with the data of summer 1974 and verification with the corresponding data of 1975 and 1976. The data of chemical state variables were relatively complete but insufficient observed data on the biological state variables hampered the calibration. The agreement between the simulated and observed results of chemical variables, e.g. temperature, dissolved oxygen, alkalinity, pH and carbon dioxide was rather good. Simulation of ammonia and nitrate nitrogen was also good, whereas the simulation of nitrite nitrogen was less accurate. The results of phosphate phosphorus were poor: the model calculated much higher concentrations in the hypolimnion than were observed. The model simulated correctly the total mean phytoplankton biomass but was unable to calculate the maximum values observed. This may be due to the fact that only total phytoplankton was simulated in this application. Some of the observed values of phytoplankton were calculated on the basis of observed chlorophyll-a values which naturally represent less accurate data for calibration than the original phytoplankton measurements. No observed data was available concerning BOD, coliform bacteria, detritus, total dissolved solids, organic sediment, zooplankton, benthic animals and fish biomass. The calibration of these state variables must therefore be considered only as tentative.

Table 1. Morphological data of the case study lakes; the northern sub-basin of lake Päijänne and lake Pyhäjärvi (the area from the Tammerkoski rapids to the bridge of Rajasaari).

	Northern sub-basin of lake Päijänne	Sub-basin of lake Pyhäjärvi
Surface area (km^2)	142	22.1
Volume (km^3)	2.53	0.19
Average depth (m)	18	8.7
Maximum depth (m)	76	46
Detention time (d)	140	27

The potential of the model in making predictions was tested (Niemi 1979). The phosphorus load from the wastewater treatment plant discharging to the case study area was first increased and then decreased by 30 percent in comparison with the reference situation and simulation runs were carried out. It was found that these changes produced a slight increase and decrease in the concentration of the phytoplankton biomass, respectively.

The same experiment was carried out with the BOD load entering the lake from the tributary. The BOD load was increased and decreased by 30 percent and a computer run was made. In comparison with the reference run the concentration of dissolved oxygen increased or decreased slightly near the thermocline due to the respective decrease or increase in the BOD load.

It was pointed out that the loading alternatives applied only very slightly affected the concentration of dissolved oxygen. However, the model seemed to react correctly to the changes in loading, although not necessarily quantitatively. The experimental nature of these test runs with alternative loadings must be stressed as the results cannot be verified in nature.

As a summary of the application of the EPAECO-model the following conclusions could be drawn (Niemi 1979): Firstly, by using the model the aquatic ecosystem could be examined as a whole. Secondly, the model seemed to be suitable to a certain extent for use as a management tool, as long as the accuracy of the simulated results was taken into consideration and that they were not necessarily regarded as strictly quantitative. It was also concluded that the data available for running the model should have been more extensive. The results of the chemical state variables were better than those of the biological variables. In discussing the results of this application it was proposed that the following modifications of the model would be likely to improve its simulation capacity: Firstly, the effect of wind in mixing water should be included, secondly a version of the model that could be applied also in the winter when lakes freeze over would be convenient for Finnish conditions and thirdly, division of phytoplankton into functional groups would possibly improve the simulation of phytoplankton. Modifications of the nutrient cycles should be carried out so that the simulated results of e.g. phosphorus could be improved. These modifications, together with a more accurate data base were felt to result in a more realistic simulation of the aquatic ecosystem.

The FINNECO model was developed on the basis of this experience and was first applied to the northern sub-basin of lake Päijänne (Kinnunen et al. 1982), i.e. to the same basin where the EPAECO model had been tested so that comparisons between the results obtained with the two models could be made.

The model was calibrated with the data of one year starting from May 1977 and continuing to April 1978 and verification was carried out with three additional sets of data, namely 1974—1975, 1975—1976 and 1976—1977. The model simulated temperature rather well, the results being more accurate during the summer than in the winter. In the winter the model could not produce exact temperature profile, thus causing an error which was reflected in the values of other variables. Dissolved oxygen and BOD were also simulated satisfactorily in the summer whereas in the winter the agreement was less exact. The modifications made to the nutrient cycles of the original model were apparently improvements, as the simulations of phosphorus, ammonia and nitrate were relatively good. In this application the phytoplankton was divided into three groups, namely *Chrysophyta, Pyrrophyta* and the unspecified group "other phytoplankton". The calibrated model produced the dynamics of phytoplankton and the level of phytoplankton biomass rather well. The dynamics of the total phytoplankton could also be calculated with the model. In the verification runs, however, the results obtained with the data of 1976 were better than those with the data of 1975. Calculated and observed results of phytoplankton in 1977 could not be compared because of the lack of observations.

The FINNECO model was also applied to lake Pyhäjärvi (Niemi and Eloranta 1984). In this application only the open water season was simulated. The lake is normally artificially aerated in the winter, which makes the simulation of winter difficult as the estimation of the amount of air pumped under the ice to the lake could not be measured exactly. The calibration was carried out with the data of 1980 and verification was attempted with the corresponding data of 1981. Calibration gave satisfactory results but the model could not be verified. The data of 1981 was used by changing the values of five parameters of the calibration run of 1980. This gave relatively good agreement between the simulated and observed results. The model was therefore in fact calibrated with two data sets.

The sensitivity of the model to the input data was tested with this material (Niemi and Eloranta 1984). The test was made by making six computer runs with different sets of input data (the quality and quantity of the waters of the tributaries,

wastewater treatment plants, diffuse load and precipitation and the meteorological data), which were given to the model in various combinations of weekly or monthly averages. The results showed that giving the input data as weekly or monthly averages gave nearly as good results as giving them at eight hour intervals. The simulation of phytoplankton, however, was an exception in this respect and its simulation in the test was poorer than in the reference run.

The results of applying the FINNECO model to these two lakes were summarized by Niemi (1985a).

5. SIMULATION OF PHYTOPLANKTON

Phytoplankton is the main primary producer in aquatic ecosystems. The extensive mass growth of phytoplankton produces odours in the water, causes off flavours in fish and may even produce toxic chemicals in the water and thus restrict the utilizability of a water body as a water supply or for recreation. Decaying masses of phytoplankton can decrease the concentration of dissolved oxygen and inhibit aerobic aquatic life. Knowledge of the concentrations of phytoplankton is therefore important in practical water quality management. Niemi (1985b) used statistical methods in an attempt to find relationships between the chemical water quality variables and groups of phytoplankton and pointed out that modeling could perhaps give better results. In the prediction of water quality the simulation of phytoplankton is therefore particularly important. Phytoplankton, together with the main factors affecting its growth, are included as state variables in most models. In both the models applied, phytoplankton was modeled either as total phytoplankton or as separate functional groups. On the basis of the experience of simulating phytoplankton in these models a detailed investigation of the aspects of phytoplankton modeling was carried out (Niemi 1986).

In nature the growth conditions of phytoplankton, e.g. concentrations of nutrients, light intensity and temperature are seldom optimal and the prevailing growth rate in the water body is lower than the maximal growth rate. Modeling of phytoplankton consists of measuring the optimum growth rate and identifying the factors and the mechanisms which decrease the rate. The growth rate of phytoplankton is considered to be a function of nutrients, light intensity and temperature.

Of the nutrients phosphorus, nitrogen and silicon are typically included in the models. The nutrient cycles, including various processes such as e.g. uptake of nutrients by phytoplankton, mineralization, excretion, release of nutrients from sediments, must then be constructed. The main mechanisms used in the uptake of nutrients are based on Michaelis-Menten kinetics. Michaels-Menten -type expressions written for the nutrients considered in the model are either multiplied by each other or the smallest of them is used in the calculation of the growth rate of phytoplankton. In the third mechanism the growth of phytoplankton is considered as a two-phase process, the uptake of nutrients and the growth of phytoplankton are treated separately.

Investigations of the effects of light intensity on the growth of phytoplankton have a long tradition. Some of the equations used were reviewed by Niemi (1986). Increasing light levels stimulate the growth of phytoplankton up to a certain optimum, above which the growth rate decreases because of photoinhibition. Some of the equations written for the effect of light on phytoplankton calculate only the linear part of the curve, whereas others also take into consideration the photoinhibition.

Temperature affects most chemical and biological reactions. This effect must be included in all models. The development of the equations used for this purpose are based on the Arrhenius' equation, developed for the chemical reactions and the equation presented by Streeter and Phelps (1925) and to their modifications. One of these is the equation developed by Frisk and Nyholm (1980) that was used in the FINNECO-model. Besides developing the correct equation for taking into account the effect of temperature, the maximum, minimum and optimum temperatures for certain processes, e.g. for growth, must be defined. This may cause problems in some cases e.g. in simulating large heterogenous phytoplankton groups.

Phytoplankton respiration rates are calculated in the models in a relatively simple manner. Typically, the rate is assumed to be a function of temperature. Sometimes an equation defining the respiration rate as a function of the weight of an organism is used. As well as temperature there are several other factors which affect the respiration rate, e.g. the size of an organism, its physiological state, activity and degree of acclimatization. In order to take these factors at least, partly into consideration, two different respiration rates for organisms are defined: an active respiration rate for growing cells and a passive respiration rate for non-

growing cells, both rates being functions of temperature.

There are several factors which affect the sedimentation of phytoplankton, such as species composition, vertical turbulence, vertical density distribution, nutrient depletion and the physiological state of phytoplankton. Sedimentation rate is typically simulated in a simple manner by assuming it to be constant, although sometimes it is determined by calibration.

Grazing of phytoplankton by herbivorous zooplankton is an important reaction in most models and was therefore discussed at some length by Niemi (1986). This requires the simulation of zooplankton, which is basically carried out with the same type of equations as the simulation of phytoplankton. The grazing equations written for the uptake of phytoplankton are based on laboratory experiments carried out with different species of zooplankton and algal or bacterial cells. Decisive questions in zooplankton modeling are e.g. determination of the digestive efficiency, the preference of zooplankton for certain phytoplankton species, the possible existence of a feeding threshold, i.e. a certain phytoplankton concentration below which zooplankton ceases to prey, dependence of the feeding rate on phytoplankton concentration etc. The equations often used for describing the ingestion rate of zooplankton preying on phytoplankton are based on Michaelis-Menten kinetics or on Ivlev's (1966) equation.

The number of toxic chemicals in water may be very large, especially in wastewaters of industrial plants discharging into water bodies. Simulation of the effects of these chemicals on the growth of aquatic organisms requires extensive research. Presently, the effects of toxic compounds are taken into account in models in a relatively simple manner. It is assumed that they increase the normal mortality rate and this is taken into account with specific toxicity coefficients and the concentrations of different toxic compounds. Often the effects of these compounds are included in models e.g. by increasing the death rate or sedimentation rate of phytoplankton.

Attempts to simulate phytoplankton accurately lead to the question of dividing the total phytoplankton into functional groups. If total phytoplankton is simulated the estimation of the growth rate, temperature optimum, sedimentation, respiration rate etc. becomes difficult for such a large heterogenous group of different phytoplankton species. The ideal case would be to specify the groups on the lowest possible taxonomical level, even to have one group for each phytoplankton species. This would naturally introduce a prohibitively large number of groups. The best compromise therefore lies somewhere between these two extremes. Division of phytoplankton into groups should be carried out on the basis of their ecology in order to obtain natural groups, containing species behaving to a certain extent in the same manner so that the estimation of parameters would be possible. A proposal for a division that would be suitable for Finnish lakes was presented by Niemi (1986). The suitability of this division should be tested in practical modeling e.g. by using the FINNECO model and the phytoplankton data bank. It must be pointed out that the division is always a compromise between small concise groups, for which exact values for parameters are likely to exist, and larger groups that are less homogenous and for which parameters are difficult to estimate.

6. DISCUSSION

The work carried out here is a typical example of attempting to synthesize the mass of information relating to the aquatic ecosystem into the form of a model. The use of models in limnology and ecology originates from physical sciences, computer science and systems analysis. The terminology used is borrowed from these sciences and does not always fit the problems dealt with in life sciences. These problems became evident e.g. in the verification of the models.

Models can be divided in different ways depending on the objectives of modeling. Loehle (1983) proposed that simulation models should be classified into three groups: logical models, theoretical models and predictive models. A logical simulation model does not necessarily simulate reality, but may be based on a conceptual model or algorithm. A program written to simulate the topological process of turning a sphere inside out is an example of a logical model (Loehle 1983). This group of models does not in practice include ecological models. Theoretical models are based on the theories of ecosystems and they cannot be universally verified by comparing them with observations. Predictive models have two extreme cases: Application models are based on the laws and theories which are applied to solve a certain problem and calculation tools which are methods of obtaining a solution to a particular problem and are not necessarily based on any laws. Examples of application models are the models applied in this work. An

example of a calculation tool is a regression model. Many of the empirical models in limnology are of this type (e.g. Frisk et al. 1980). In practice several types of models can be constructed between these two extremes.

Modeling consists of phases such as aggregation and simplification of the real system, gathering of data, data reduction, testing of the model and judgement of the agreement between the observed and simulated results. All these phases affect the functionality of the model. The models applied here aggregate some of the reactions of the ecosystem and on the other hand simplify others. Relatively speaking the hydrological parts of the models applied are quite simple, as both models are one-dimensional. The chemical parts are comparatively detailed, whereas only phytoplankton and zooplankton in the FINNECO model and phytoplankton, zooplankton, benthic animals and fish in the EPAECO model represent the biological state variables. Aggregation of real phenomena is carried out e.g. in simulating phytoplankton and zooplankton. Simplifications are made by omitting something that is not considered to be important or because of a lack of observed data. The result is a model that should, despite its simplifications, retain the essential features of the original system.

Both the FINNECO and EPAECO models have a modular structure and are hierarchically constructed. The relative complexity of modeling state variables increases from temperature, oxygen and biological oxygen demand to conservative substances and further to phytoplankton and zooplankton. The models are suitable for lakes and reservoirs, typically those with eutrophication problems. The change between e.g. aerobic and anaerobic phases in the water mass of the lake are included in the FINNECO model but this mechanism has not turned out to be sufficiently sensitive to produce realistic simulations in practice, as the application of the model to lake Pyhäjärvi showed. It should be further investigated whether the balance between sufficient resolution and sufficient simplicity in the structure of the models is correct. The time span of prediction with the EPAECO is the open water period. With the FINNECO model, simulation of several successive complete 12-month periods is possible. However, the cumulation of errors e.g. in predicting the formation and break-up of ice cover may limit the accuracy of the simulation. If the objective is to simulate e.g. phytoplankton biomass during the open water period, simulation should be started during the spring turnover. Normally the concentration of phytoplankton under the ice-cover during winter is not of interest. More often the development of the concentration of dissolved oxygen is examined which can be taken into account with the FINNECO model. The structure of the model in simulating the winter period should be developed further for more realistic results. Many different factors affect the functionality of the model in the winter, e.g. the location of incoming waters to the correct depth in the lake.

Many of the reactions of the aquatic ecosystem, when presented mathematically, show the same type of relationship. For example the relationship between light intensity and the growth of a phytoplankton species first increases with increasing light intensity, reaching a plateau at saturation level, and then decreases with higher light intensities due to photoinhibition. Similar curves are also obtained for temperature and pH. The growth of phytoplankton as a function of nutrient uptake and the growth of zooplankton as a function of phytoplankton follow similar curves but without the decreasing part. Other typical mechanisms in these models are the sedimentation rate of phytoplankton, the decay rates of many reactions and the death rates of organisms, which follow the first order decay reaction. All these sub-processes of the ecosystem include a certain amount of error because they cannot represent the real phenomena absolutely correctly. When a chain of these reactions is formulated into a mathematical model, the model necessarily includes more internal uncertainty or inherent noise, which must be minimized as much as possible in preparing the model.

The data base required for the running of large models has been treated in previous articles (Niemi 1979,Kinnunen et al. 1982, Niemi and Eloranta 1984). Usually, the data base must be large in order to be sufficient for a simulation model. A problem which often becomes evident is that although an extensive set of data is available it has not been collected in the way required by the model. In particular water quality data is seldom temporally and spatially large enough. Interpolation and extrapolation of input data often introduces errors to the driving variables. Although the modeler would normally like to have more data than is available, this is perhaps not at present the main problem in modeling. Earlier, the potential of models was thought to be limited by the calculation capacity of computers, whereas now the limiting factors seem to be firstly the lack of understanding of natural phenomena and secondly the lack of data.

In some previous articles of this author (e.g. Niemi 1979), calibration was defined as a process of

tuning the model to fit observational data and verification as a test of the applicability of the calibrated model to a new set of data. However, these terms are often used with different meanings. Quade (1985) defined verification as a test of the functionality of the computer program of the model and validation as the process of determining whether the model output agrees with the observations, i.e. the same as verification above. He defined calibration in the same way as Niemi (1979). Validation (verification) criteria of the models have been discussed widely in the literature (Miller 1974, Caswell 1976, Schaffer 1981, Beck and van Straten 1983). These questions bear a close relationship to the philosophy of science, especially to the investigation of scientific methodology (e.g. Reckhow and Chapra 1983). Opinions presented on this issue in the literature are varied, but the general conclusion seems to be that validation of the models is normally insufficient. Validation should be made bearing in mind the purpose for which the model was constructed and sufficient data should be available for the validation. Of course absolute validation of the model is impossible. In connection with the theoretical models the term corroboration would perhaps be more suitable than validation. If a theoretical model seems to react correctly after stringent tests the level of confidence in the model increases and it is considered to be corroborated. Results of the two applications made here show that from the practical point of view the FINNECO model seems valid for the calculation of water quality in lake Päijänne but not in lake Pyhäjärvi. The criteria of agreement are based on subjective judgement. The method used for improving the model is to change its structure, modify the mathematical equations and estimate the parameters. This cycle can be repeated until a model meeting the criteria given is obtained.

It may be asked whether the simulation technique is appropriate for water quality models. Simulation as a modeling technique requires much effort: the phases of constructing and analysing the model are long and expensive, as are the phases of application when much time is spent in gathering the data and in parameter estimation and calibration. Furthermore the model does not explain theories or provide answers to the question why the output is such as it is. However, simulation will undoubtedly remain in use in water quality modeling until new techniques are developed.

How should water quality simulation models be further developed? This question can be divided into two parts, firstly to the fundamental question of the construction of models, their structure, validation and other theoretical problems and secondly to the technical improvement of the models e.g. by development of data banks for estimation of parameters and by improving graphical output.

In the theory of modeling the following aspects should be considered: The model should be selected according to the problem at hand. The domain of applicability of the model must be specified and the validation should be carried out with sufficient historical data so that the model can be used with confidence within its domain. This approach stresses the idea that models should be rather specific, thus guaranteeing more compact structure and facilitating validation. Sub-models should be validated independently. In practical work, consideration should also be given to other modeling alternatives besides simulation. Certain specific problems could perhaps be better approached with other methods, e.g. with regression models.

There are several technical aspects of the models that could be developed further. For example data banks should be developed to include information for the parameter estimation, calibration and meteorological data. Computer programs for processing the data to the form required by models should be made available. Graphical output from the models would facilitate the comparison of calculated and observed results. Furthermore, automatic calibration techniques for the sub-models would assist the analysis of the model structure and the construction of larger models. If models are planned to be used as an aid in decision making, the development of interactive programs with graphical output would be useful. Some of these points are already taken into account in modern models. More emphasis should however be placed on the development of these characteristics.

A water quality simulation model, by its very nature, is a simplification of the real ecosystem and thus the output of the model must be treated with caution. If the limitations of the models, such as the domain of applicability and the time scale at prediction, are taken into account the models will be useful in limnology for advancing the theoretical investigation of the phenomena occurring in lakes.

TIIVISTELMÄ

Artikkelissa esitellään työtä, jossa kehitettiin suomalaisille järville sekä muille vastaavan tyyppisille

järville soveltuva veden laatua simuloiva malli ja sitä sovellettiin kahteen järveen. Työ aloitettiin laatimalla laaja kirjallisuusselvitys olemassa olevista malleista. Näistä valittiin EPAECO-malli Pohjois-Päijänteelle sovellettavaksi. Soveltamisessa saatujen kokemusten perusteella ryhdyttiin kehittämään uutta mallia, joka soveltuisi paremmin Suomen olosuhteisiin. Kehitetty FINNECO malli on yksidimensioinen, deterministinen veden laatua simuloiva malli. Mallissa on kahdeksantoista tilamuuttujaa, se simuloi tuulen vettä sekoittavaa vaikutusta ja jääpeitteen syntyä ja sulamista energiataseeseen perustuen. Mallia sovellettiin Pohjois-Päijänteelle ja Tampereen Pyhäjärveen. Päijänteelle malli soveltui hyvin, erityisesti kemiallisten tilamuuttujien lasketut arvot vastasivat hyvin havaittuja arvoja. Pyhäjärvelle malli soveltui huonommin. Kasviplanktonin simuloinnilla on tärkeä osuus tällaisissa malleissa. Tämän vuoksi on erityisesti tarkasteltu kasviplanktonin kasvuun vaikuttavia tekijöitä sekä niiden simulointia. Mallien laatimiseen liittyy joukko kysymyksiä, esimerkiksi mallien validisointi, jotka ovat lähellä tieteen filosofiaa. Näitä mallien rakentamiseen, validisointiin ja käyttöön liittyviä teoreettisia perusteita tarkastellaan lyhyesti.

Koska malli on aina yksinkertaistus todellisuudesta on sen antamia tuloksia tarkasteltava kriittisesti. Jos mallien rajoitukset kuten sen soveltuvuusalue, ennustettavan aikajakson pituus ja tulosten tarkkuus otetaan huomioon on malleilla käyttöä limnologisen tiedon kokoamisessa ja laskentavälineinä. Malleilla saatava kvantitatiivinen tieto on tarkempaa kuin arvioimalla saatava. Edelleen malleilla laskettavat vaihtoehtoiset laskelmat ovat keskenään vertailukelpoisia vaikka ne eivät olisikaan absoluuttisesti oikeita.

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