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Preface

Water quality aspects of rivers and lakes, especially applications of computational modeling and systems analysis on a variety of problems, have been one of the key topics at IIASA's Water Resources Projects for almost two decades. In fact, a strong tradition in water quality issues has gradually been established around the project. The present paper offers a state-of-the-art view on water quality modeling, including a review and discussion on decision support systems, with the objective of future usage of this disseminated information in the Project. This topic is presently subject to substantial expansion, both in terms of methodological development and importance in water resources studies.

Abstract

Oxygen depletion, eutrophication, acidification, toxic pollution, poor hygienic state, salinity, and excess suspended matter are among the issues usually included in the concept of water quality problems. This report focuses on inland surface waters, namely on rivers, lakes, and reservoirs, to each of which the problem categories listed above are relevant. The variety of problems, the multidisciplinarity among water quality experts, the wide spectrum of societal water needs, together with the high diversity of computational approaches presently available contribute to the present situation in which applicable methodology is developing from a variety of fronts and directions, among which dynamical, partial differential equation models were taken here in focus. Transport, flow and reaction equations for shallow water bodies are reviewed for 1 and 2-dimensional cases, including an introduction to and illustration of a selection of numerical techniques. Four case studies on eutrophication modeling, and a review and discussion on the application of decision support systems on water quality management are presented thereafter.

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WATER QUALITY MODELING OF RIVERS AND LAKES

László Somlyódy[1] and Olli Varis[2]

1 INTRODUCTION

1.1 An overview

The word *model* has several meanings in English. Among adjectives they include ideal, exemplary, and perfected – among nouns, miniature, saint, idol, representation, symbol, prototype, example, and replica – and among verbs, pose and mimic. We think that, among water quality modeling practice, examples can be found of the interpretation of the word model in all these ways. We would like, however, to define a (computational water quality) model to be a case-specific abstraction, bound to be a strong simplification and thus as a description it is a *compromise* in several respects including time, space, focused disciplines, causalities, uncertainty, values, resolution, and many other issues. It can be seen as replica of how we see the problem in the light of data, knowledge, and scopes for the activity.

When a model is being constructed, this problem is most concretely encountered in the phase of defining the structure of the model and the interpretation of parameters. This phase is usually called model *parameterization*, or model *identification*, consisting of structural identification and parameter identification, respectively. Model identification may be an automatic procedure in some cases, but more often it is an iterative process of merging theoretical and empirical information. Target is to arrive at a structure expressing the relative importance of the processes involved in the exercise. In the phase of identification, one may start with a given structure (partial or ordinary differential equations, or algebraic equations) and formulate the hypotheses in this framework. There are some methodologies to be used in this phase (Walter 1982, Beck 1987), though it is in practice still greatly an art of combining theoretical and observed information. In the parameter identification process, calibration and validation phases can often be distinguished.

Terms often used to characterize models and the reasoning underlying them are: analytical vs. empirical models, and causal vs. evidential models. If the model parameters have a physical interpretation, the model is often said to be physically based. Deductive and inductive analysis, or physically / knowledge-based modeling and statistical inference may at first seem to be rather distinct approaches, but in practice these sources of infor-

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mation are usually utilized together. In physically based modeling, the parameters and the model structure are typically given a physical interpretation due to increased efficiency in computation and inference, whereas in statistics this is usually not the case.

Water quality modeling and management is typically a *multidisciplinary* field. Experts with very different educational backgrounds are confronted to solve problems together. Whereas the biologist has generally been educated to use classical statistics in that it provides an objective methodology for inference, the engineer has traditionally been allowed to incorporate prior knowledge into his analysis in the form of mathematical, chemical, and physical formulations or rule bases (Varis 1991*b*). For a physics oriented engineer, it appears natural to focus on the transport part of the basic differential equation model presented later, while a chemistry or process oriented expert would rather concentrate on the reaction part of the equation, and often even omits the transport from the model and ends up with lumped, ordinary differential equation model (Somlyódy 1982*a*).

Extreme, quasi-hypothetical examples of these directions could be, first, a 3D (three-dimensional) flow model with 3D transport description for, say, one constituent, and, second, a completely mixed reactor (ordinary differential equations) with a detailed ecological and chemical description, with tens if not hundreds of state variables, and many more parameters. These pseudo-scientific studies are doomed to have very little scientific and practical importance. The *art* typically lies in the ability to make problem specific compromises between inclusion of physical or ecological details, and producing a model with only the essential in it. Similar compromises are needed, e.g., towards the direction of data analysis.

A further dimension is added to the analysis when management orientation has to be incorporated. Practical management has a man-made subjective, socioeconomic, political, and technical problem setting. It is of great importance when environmental management cases are formulated to arrive at models useful in practice. Often the physical world is no longer the essential dimension of the reality to be described, but instead the focus should be shifted on nested uncertainties of the inference, risk attitudes, costs, benefits, utilities, etc.

1.2 Why to model

The objectives of statistical and computational problem-solving have classically been determined according to the idea that the information available should be represented in a more tractable form, given the problem and its scope. Perhaps the two most profound goals for modeling are either *description* or *prescription* of the system, or a hybrid of those scopes, principally in order to facilitate the control of the system in one way or another. Description implies that priority is given to the comprehension and diagnosis of the information which is typical to scientifically oriented studies, while in prescription the goal is the normative extrapolation of the behavior of the system which is typically helpful in planning and management. With the exception of routine, repetitive operations, a model is typically a tool for thinking, not a substitute for thinking.

It is implicit that the studies conducted using environmental models should yield in decision support in some more or less practical context. We thus allocate less weight to the important use of models in scientific research within water quality studies. The spectrum of the above mentioned practical contexts is of course wide. An attempt to categorize *decision* situations in a rather general level (as "an art of getting things done through people") has been done by Sutherland (1983). He has presented a classification of decisions and consequent modeling approaches into the following four categories. For more perspective, see also Redford (1988) and Greenley (1989).

- *Operational models.* Automated data retrieval from the catchment on focus provide enhanced possibilities for *real-time* decision making on routine and repetitive processes. This data is often being used in real-time operations such as reservoir management and treatment plant operation, and models for short-term predictions and on-line control are needed. It will be increasingly important to be able to filter out the most essential features of this type of data.

- *Tactical models.* Largely the same issues presented within the context of operational decisions apply to tactical decision support, which tackles *finding input-output relationships* between key variables within a system. The time horizon in tactical surface water quality management is restricted inside a couple of days or weeks, up to a season in river management, for instance, by using monitoring data to analyze how the river system is functioning, with a possibility to run short-time what-if scenarios. Finite state approaches such as statistics based control and decision instruments (environmetrics, econometrics, etc.) are typically applicable in tactical modeling.

- *Strategic models.* Advancing to decision problems with a longer time span, such as planning, environmental impact assessment, and prognosis, strategic analysis *projects current situations to states which have a significant probability of occurring.* The approaches used in modeling are typically concentrated on *deductive*, logical analysis tools such as simulation, game models, scenario analysis, and cost-benefit analysis (Sutherland 1988).

- *Directive models.* Problems such as adaptivity, resilience, sustainability, preference analysis, structural analysis, and prescription of a sequence of *possible future events* are included in planning and management of the evolution of a system in the long run. The problems and data sources are essentially more subjective and the focus is on analysis of personal perspectives and opinions.

The categories can be further illustrated by following exemplary, normative statements:

- "Computer takes care of (most of) the routine work" -> operational.

- "What is happening in our system, and how should we react" -> tactical.

- "What if we change the system essentially, would it make sense" -> strategic.

- "What options, due to technologies, preferences, etc., we have open in long term" -> directive.

The time spans related to these categories are proportional to other dimensions of the respective problems, and no absolute time intervals can be provided. In global or continental decisions, one year scale may be very operational, but in local dimension problems such as forecasting the hygienic state of a river a few days' perspective may be maximum for operational decisions. Sutherland emphasizes that in any non-trivial organization, all these classes of decision problems are faced.

Traditionally in water resources management, the two main clusters of management situations have been (1) planning, and (2) operation and control. We think, however, that using the above terminology brings also this field more consistent with other applied fields of operations research and systems analysis. It also is an attempt to clarify the roles of education specific knowledge of methodologies: engineers, for instance, are accepting widely the use of control theory and applied physics. They call the subsequent approaches optimization and simulation, and use widely same tools in operational and strategic decisions. Natural scientists accept inductive tools, and use them to all categories of decisions. Those decision analytic tools that are prone to fall in directive category, are generally poorly known in the field.

1.3 Water quality concerns

When problems of surface water quality are considered, it is a fact that very many *natural phenomena* contribute to the observed situation, and, on the other hand, that there is immense diversity in the *needs and priorities* of societies with respect to the quality of inland waters. Lakes and rivers are used by man for very many purposes including protection, recreation, fisheries, aquaculture, source of water (households, municipalities, industries, irrigation), transport, flood control, hydropower, cooling, and waste recipient. From the management point of view, the greatest motivation for water quality studies derives from the demands on lake water quality set by different uses and the conflicts between them. The water quality requirements are naturally very case specific as well, and so are the ways they are impacted by human activities. The most common problems of river and lake water quality include:

- *Oxygen depletion* caused by degradation of organic matter in the water body. The organic material may be either of external origin i.e. from point source or non-point source loading, or produced in the water body by primary producers able to photosynthesize. The consequences of low dissolved oxygen concentration in freshwater ecosystems include fishkills, increased solubility of phosphorus from sediments leading to enhanced eutrophication, and formation of toxic and non-esthetic gases such as methane and hydrogen sulfide.

- *Eutrophication* caused by the abundance of basic nutrients, such as nitrogen and phosphorus, and other prerequisites of primary production. Apparently the most drastic

outcome of excess abundance of primary producers is blooms of, often, toxic algae, in fresh waters usually blue-green algae (cyanobacteria). Degradation of produced organic material consumes oxygen, and may lead to oxygen depletion. Also discharge of easily biologically degradable organic matter leads to problems of the same kind.

- *Hygienic* problems due to pathogenic organisms such as viruses, bacteria (*Salmonella, Yersinia* etc.), or protozoa (*Schizosomiasis, Plasmidium,* etc.). Household water borne diseases, together with malaria, constitute one of the major global health problems. According to WHO (1978), water resources are involved directly or indirectly in 80% of all human diseases. Water resources management is encountered with a great challenge by the need to eliminate these water quality problems.

- *Acidification* of watersheds including surface waters is caused globally mainly by atmospheric deposition of SO_2 and NO_x. Some industrial and mining activities, and nitrogen fertilization also cause severe regional watershed acidification problems. Acidification enhances several unwished phenomena including chemical changes such as increased mobilization of aluminium and several other substances of soil and rock, and ecological changes, most drastic of them being devastation of forests, and fishkills.

- *Salinization* due to high concentrations of ions such as calcium, sodium, chloride, and sulfate. In arid areas, and especially in connection with irrigation, the accumulation of salts in soils, groundwater, and surface waters leads to degradation of catchments in terms of decrease in fertility of soils and lowering applicability of water in most human uses. An extreme consequence, yet not a rarity, is desertification.

- *Toxic* or *cumulative* compounds such as heavy metals (Hg, Cr, Zn, Co, Cd, etc.), pesticides (DDT, Lindane, etc.) and industrial wastes (PCB, organochlorides, etc.). An ever increasing bulk of substances belonging to this category, with highly varying impacts to aquatic ecosystems and human beings, is known by environmental toxicologists. Yet, the ecotoxicological features of only a minority of all anthropogenic substances is known at any detail.

- High amount of *suspended matter*. Improper land use and water resources management enhances erosion to waters in areas prone to erosion. Also some industrial waste waters contain high amounts of suspended matter. The consequences include filling of reservoirs and river stretches, deterioration of ecosystems, decrease in the applicability of water to human uses such as irrigation, raw water for households and industries, transport, fisheries, and recreation.

1.4 Past trends in modeling approaches

Deterministic water quality modeling

We concentrate on mechanistic, *process* modeling approaches to surface water quality. In the following, a brief history on this, presently ample, field of industry is given. For more

details, see Orlob (1982).

Definitely the classic in surface water quality modeling is the BOD-DO (biological oxygen demand – dissolved oxygen) model for rivers by *Streeter & Phelps* in 1925. A linear dynamic concept developed originally for the Ohio River is still the basis for many river models today (see e.g. Rinaldi et al. 1979).

In the late 1950s, the development of numerical methods for differential equations facilitated the use of more complex equations than those of Streeter and Phelps. However, the Streeter-Phelps concept remained the basis for many models, such as the *Thomann's Delaware Estuary* model in 1963, and even in the 1970s in the QUAL river models of the U.S. Environmental Protection Agency (EPA). The former can take into account multiple waste loads with a varying strengths in an estuary with varying cross-section. It also involves spatially and temporally varying rate coefficients for the Streeter-Phelps processes.

The QUAL models are a series of well-known and widely applied river models distributed on the public domain principle (Ambrose et al. 1989). The first version, published in 1970, simulated the stream temperature in addition to BOD-DO, the biochemical process rates being temperature dependent. The next version also contained the possibility to simulate both steady and unsteady flow and the impacts of nutrient loading on the oxygen regime of a river. Photosynthesis has thereafter been included in these and related river models.

The WRE (Water Resources Engineers, Inc.) models dating from 1968 and the MIT models from 1972 described a reservoir as a 1D system with horizontal slices including the vertical distribution of heat over an annual cycle. Several extensions to these models were presented until 1975, these contained other water quality constituents, such as BOD-DO, nutrients, and even some biota.

Simultaneously, a set of eutrophication models with less emphasis on hydrodynamics and increased emphasis on the ecology and chemistry of lakes were published by, e.g. *O'Melia* and *Imboden*. Those models focused on gross nutrient balances, cause-effect relationships between carbon, nitrogen and phosphorus inputs, and primary production, often separately in the epilimnion and the hypolimnion. Parallelly, *Park* and associates developed the CLEANER model. This model and its extensions constitute an attempt to construct a general water quality model for lakes. It includes several dozen chemical and biotic state variables for each of the several layers. The work on descriptions for toxic substances is still in progress. Nonetheless, however attractive a general lake model would appear, most water quality people have chosen an essentially more case-specific approach.

The late 1970s and early 1980s were an intensive period of development of different descriptions for ecological conceptualizations and unit processes for water quality studies, see Scavia & Robertson (1979), Jørgensen (1982, 1986), Straškraba & Gnauck (1985), and Thomann & Mueller (1987).

As long as lake models have been constructed, there have also been models for

very large lakes. The hydrodynamic framework is usually much more dominant in these models than in models for smaller lakes, owing to the greater importance of flow and transport processes in large basins. *Chen* and associates developed a finite-difference hydrodynamic model, originally for Lake Ontario. *Di Toro* and associates constructed a predator-prey model for primary production with several segments for Lake Erie. *Patterson* and associates developed a 2D finite difference model for Green Bay in Lake Michigan. These all works were published in 1975. Also a number of other large lakes in the world have been subject to hydrodynamically based model studies since the mid-1970s.

The scopes of interest in the development of water quality modeling moved gradually towards the questions of controlling the uncertainty of large, physically based models in the late 1970s (see, e.g. Fedra et al. 1981, Beck & van Straten 1983, Beck 1987). Issues such as the identification of states and parameters, and prediction with models, have been under intensive study in order to provide the mechanistic models with some credibility and reliability in statistical respect (Beck 1987, 1991). The 1980s have brought advancing utilization of statistical and probabilistic (Hornberger & Spear 1981) techniques in the context of physically parameterized models, and on the other hand, increasing use of models in practical management and research.

Other modeling approaches

Besides the advances in physically based approaches, an essential contribution – both from the practical and theoretical points of view – has been also from a number of other directions in the 1980s.

First, the from the direction of data analysis, time series analysis and filtering have recorded a bulk of applications since the work by e.g. Box & Jenkins (1970) in time-series analysis, Young (1974, 1979), Ljung (1979), and Todini (1978) in the use of extended Kalman filtering in state and parameter estimation, and Akaike (1976) in canonical analysis. The term environmetrics has even been launched to describe a.o. this branch of environmental modeling.

The development of knowledge engineering has also been reflected in water quality modeling studies. Rule-based systems and qualitative, linguistic approaches have been introduced to the field (Antunes et al. 1987, Câmara et al. 1987, Recknagel et al. 1991, Seixas et al. 1991). We suppose, that those studies will get a high number of successors.

Bayesian decision analysis has been subject to rapid development already for three decades (von Winterfeldt & Edwards 1986). Even if a very broad use of those techniques in many applied sciences, such as medicine, decision analysis has just taken its first steps in water quality applications (Chapra & Reckhow 1983, Varis et al. 1990). We see no reason for not expecting the number of applications to grow in near future. We dare think so chiefly because of present boom in application software in the field, as is also the case in the other, above mentioned categories of modeling.

Further reading

The supply of textbooks on the topic is today large. As far as mechanistic water quality modeling is concerned, we would recommend to consult the following textbooks: Thomann (1976), Rinaldi et al. (1979), Scavia & Robertson (1979), Orlob (1982), Chapra & Reckhow (1983), Straškraba & Gnauck (1985), Jørgensen (1986), Somlyódy & van Straten (1986), Thomann & Mueller (1987), and Henderson-Sellers (1991). For topics related to uncertainty, see e.g. Beck & van Straten (1983) and Beck (1987), and for management oriented approaches, see Loucks et al. (1981). We provide also to a wide variety of other references, both general methodological as well as specific ones.

Organization of the text

Next chapter presents an introduction to the procedure of constructing physical water quality models for lakes and rivers. Thereafter, the governing equations are presented and discussed. The concepts are being illuminated by four case study examples, two of which concentrate on models with both transport and reaction parts, one focuses totally on substantially detailed reaction descriptions, and one case study illustrates the use of selected, other modeling approaches. A review to decision support systems and software available and the needs for future development are discussed in the last chapter.

2 THE MODEL BUILDING STRATEGY

2.1 On problem solving approaches

Systems analysis and decision theory are rich in tools and approaches to problem solving and modeling. Sage (1981) classifies them into three groups as follows.

- *Wholistic.* The inference is based on previous experience from similar cases. Intuition-based judgment, standardized operation procedures, and analogy-based reasoning are representatives of this class.

- *Heuristic.* Complete alternatives are compared, generally between a restricted set of alternatives and criteria. Minimally acceptable standards may be required as constraints from decision makers.

- *Holistic.* Modeling procedure attempts to break a complex problem into parts for analysis, and then recombine the parts to arrive at a feasible and structured presentation of the problem.

The most natural way to make inference, e.g. in form of a decision, is to rely on intuition (Zajonc 1980). In complex situations, however, intuition can be insufficient, and non-informative to other bodies involved, and analytical methods are required. On heuristic modeling, we give two examples. First, for a given river or lake modeling case, take two or more ready made models, calibrate them, and judge or discriminate (e.g. Kettunen et al. 1988) the best among the models. Second, the so-called multiple criteria/attribute optimization approaches (Chankong & Haimes 1983, Steuer 1986) are based on heuristic evaluation. We have chosen to focus on holistic problem solving approach in this context owing to the objectives stated above in introduction, and present therewith a holistic strategy for systematic modeling and analysis of water quality problems (see also Eykhoff 1974, Young 1979, Beck 1983, Jørgensen 1986).

2.2 The principle of decomposition and aggregation

The procedure of decomposition and aggregation (see Somlyódy 1982*c*, van Straten & Somlyódy 1986) starts with a reasonable decomposition of the system into smaller, more tractable units that are accessible for separate and more detailed studies (e.g. laboratory and *in situ* experiments, mathematical submodeling based on individual in-situ data, literature information, etc.), which form a hierarchical structure. We use the word "reasonable" intentionally because, in reality, processes cannot always be separated completely. For example, it is possible to study detailed hydrodynamic circulation models independently of water quality, but the same is not true for the in-lake water quality processes, because their appearance in the form of data will be influenced by prevailing circulation patterns. On the other hand, a "reasonable" separation is often still possible conceptually, because something is known beforehand about processes in water bodies, and a careful inspection

of data will frequently give clues to which processes are important, irrespective of the disturbances and interrelations with others. It is true, however, that checks on the appropriateness of the decomposition of such interrelated subprocesses can only be made at a higher hierarchical level, unless physical isolation is also possible by performing specially designed experiments (e.g. bottle tests, enclosures, etc.).

The detailed subsystem studies are followed by aggregation process in order to preserve and integrate only the essentials for higher levels of research in the hierarchical structure. A characteristic element of the aggregation procedure is the assessment of the relative importance of the subprocesses in view of the spatial and temporal detail in data, given the objectives of the study. In this way some unimportant processes can be eliminated *a priori* for consideration at higher hierarchical levels. Another characteristic procedure is to achieve aggregation by some form of averaging over space and time or by combining groups of system variables in a way or another (e.g., by putting different algal species into just one group), thus ruling out unnecessary detail. Sometimes aggregation can be performed by reducing the results of more complex detailed models to simple relationships between characteristic features, which can then be parameterized for the use at a higher level.

As a result of decomposition-aggregation process one can avoid the use of one large, fully coupled model which, even today, is difficult to handle, and instead apply a sequence of correspondingly detailed and aggregated models. Only the highest level aggregated models are coupled directly, resulting in a relatively simple model at the top of the model hierarchy where management issues are handled in very many cases. Often preferences, criteria, and decision variables are most essential at this level.

2.3 Model development

The modeling task is often (e.g. Spriet & Vansteenkiste 1982, Young 1983, van Straten & Somlyódy 1986, Kettunen & Varis 1989) presented as that of combining *deductive* and *inductive* analysis within the framework of the *scope* of the model. Given the great variability in all these components, it is apparent that every lake and river modeling case is unique. Fig. 1 shows a set of questions that are crucial in initiating a modeling procedure. It is useful to extend the discussion on the modeling procedure in somewhat more detail. At this step, we follow the outline by Eykhoff (1974) and Beck (1983). Fig. 2 summarizes some of the major activities and the various inputs needed for the activities plus the major products of each step.

At the beginning of each analysis there is a problem to be solved. Usually it is possible to identify which aspects are important, and on which subjects should prior scientific theory be included and on what detail. Next, a conceptualization is made of how the system at hand operates: its basic processes and interrelations, given the scopes. This procedures a conceptual base model, the translation of which into mathematical equations we call here a model structure postulation. It is equivalent in some sense to the selection of a model type, being dictated in practice by a number of constraints due to tools, expertize, data, total time, and other resources available for the study.

The procedure above leads to a model structure. It is important to note that the model structure itself contains parameters, but does not yet contain values for them. They are obtained in the model calibration / parameter estimation phase. Why do we actually need parameter estimation? Parameters can roughly be classified to be primarily theoretical or empirical. The former – such as acceleration of gravity or water density – do not need estimation, the latter do. In mechanistic modeling, the parameters are often somewhere in-between those two asymptotes: they are given physical names but they are empirically calibrated or estimated.

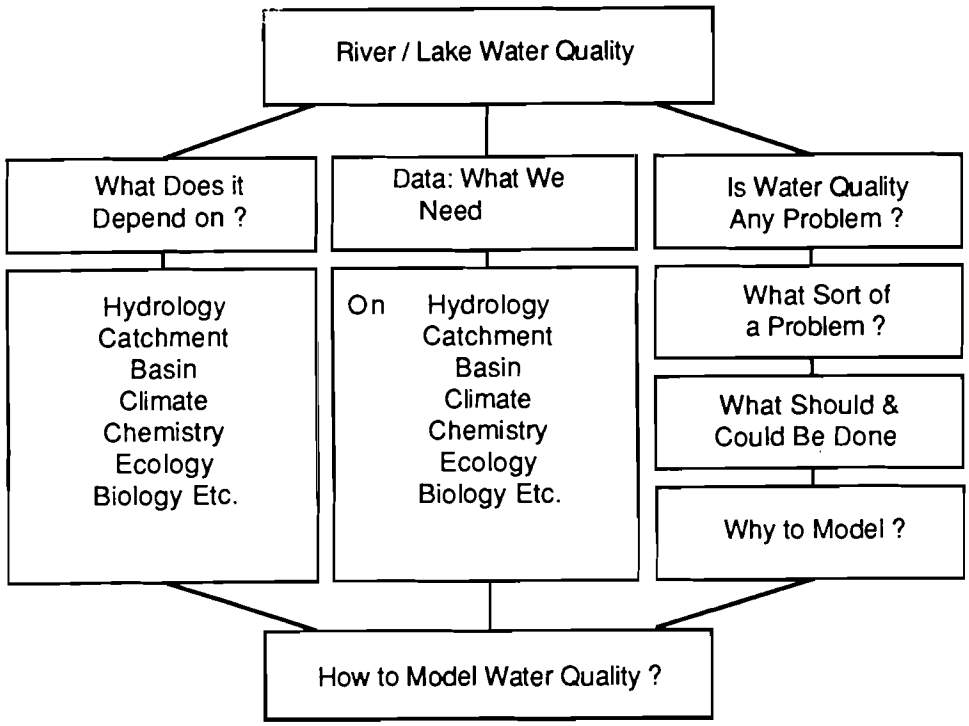

Fig. 1 Structure of questions on water quality modeling: Combining deductive and inductive inference within the framework of goals (Varis 1991*b*).

One of the major reasons to the high level of empirical parameters in aggregated models is that the *model structure postulation* not only *defines* the structure but also the *interpretation of parameters*. We give two examples on hydrobiology. The aggregation of numerous algal species (each with its own growth rate and light optimum parameters) into one community group leads to new community parameters (community average growth rates and light optimum parameters). The relationship between these new parameters and the original, individual ones, if there exists any in reality, are not at all obvious. In fact, even the structure of the aggregated model may be affected. As another example, nutrient uptake rates of phytoplankton may drop with orders of magnitude when considering the physiological time scale, with time constants around microseconds, to microbiological batch culture rates, from seconds to hours, or to whole-lake simulation / management models, where the time step ranges typically between one day and one week (e.g. Varis 1992*b*). Even if the model structure is derived from the same basic concepts and the parameter has the same label, it does not necessarily mean that the parameter has the same interpretation and a comparable value. Thus, the most practical approach is to estimate such overall

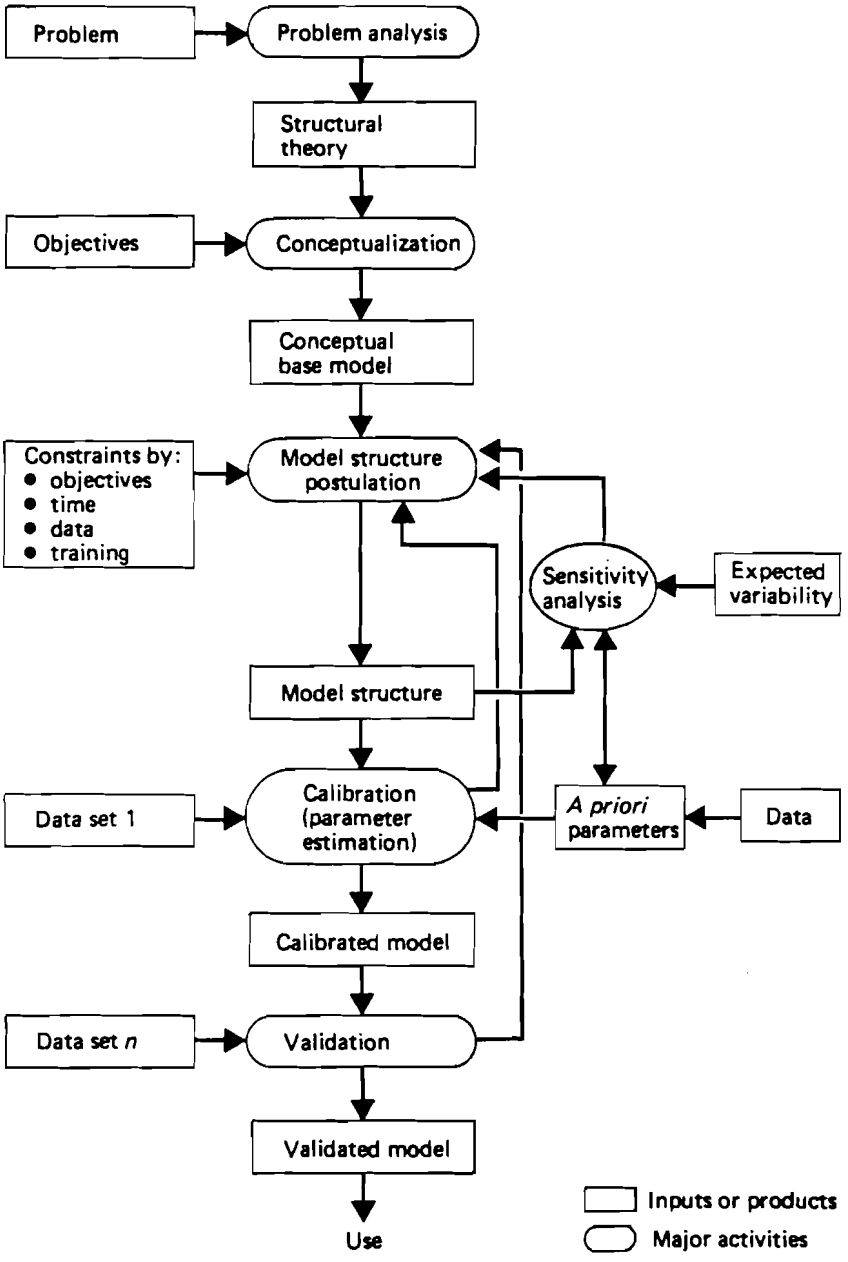

Fig. 2 The procedure for model development (van Straten & Somlyódy 1986).

parameters by comparison with field data. It is apparent that the validity of such parameters is restricted to the given model of the system with the given environmental conditions. Of course, ignoring the concept of aggregated parameters with wider applicability would nor be totally correct, but *aggregated parameters have a strongly empirical character.* Their calibration in a rather ad hoc way has been criticized by e.g. Young (1983), and we admit that there are serious problems. However, owing to the reasons given in introduction, we see good reasons for relying on mechanistic models in appropriate, typically strategic (and sometimes directive) planning cases.

Two aspects that can simplify the task of model calibration must be mentioned. First, sensitivity analysis – an approximative use of partial derivatives of the states with respect to parameters – reveals the parameters to which the model is particularly sensitive, and their sensitive periods, respectively. The calibration procedure can specifically be oriented using this information and, because the model is sensitive, they can usually be reasonably estimated, given a proper model structure. In contrast, it is unlikely that parameters that do not strongly influence the model outcome can be estimated accurately. For such parameters very large confidence bounds appear, in which case it may be better to keep those parameters fixed from the beginning, in case they are not left out of the whole exercise. The inclusion of non-confident, insensitive parameters is debatable and should be avoided unless they are related to future situations and scenarios, which we definitely are not able to validate. Keeping the model as simple as possible has several advantages, the most important of which probably being the fact that the model should be simple to allow its understanding and critique also by other experts. This is, in the Popperian sense, a key to scientific systems analysis (cf. Beck 1987): a scientific analysis should be formulated in a manner in which it can unambiguously be falsified. Sensitivity analyses may also be of good help in design of observations for more exact calibration of the models (see Walter 1982, Godfrey & DiStefano 1987, Kettunen et al. 1989), as well as in more systematic identification of parameter values.

There exists a variety of techniques for the latter purpose such as Marquardt, Newton-Raphson, etc. gradient searches. Perhaps the most used analytical technique in the field for differential equation models is, however, the regionalized sensitivity analysis approach by Young et al. (1978) and Hornberger & Spear (1981). An expert defines acceptable ranges for each of the calibrated model parameters, as well as an acceptable domain for the model outcome trajectory. In a Monte Carlo simulation, the model is run a number of times, giving random values for the parameters from even distributions defined by the acceptable limits. The parameter combinations yielding to the model outcome to stay in the acceptable domain are recorded. Ideally, feasible ranges for each parameters are found. The procedure also may find two or more feasible ranges for a parameter, and thus raising the question if the model structure is correct. Being rather general, it can be used both to partial and ordinary differential equation models. The procedure, together with a selection of other approaches are thoroughly described by Beck (1987).

Second aspect to be pointed out is the fact that in some cases parameters are estimated from more controllable experiments, either in the field or with independent model segments. For example, those for algae can be estimated independently from primary pro-

duction experiments (e.g. van Straten & Herodek 1982), or those for settling and resuspension can be estimated from time series data on suspended solids (Somlyódy 1982*a*, Luettich et al. 1990). The resulting values can ideally be maintained constant, thus reducing the number of parameters to be calibrated. Again, crucial is to take into account the strong dependency of the interpretation of parameters and thus their numerical values on the physical and temporal scale used in the experiment and in the model. When talking about active experiments, one must bear in mind the bulk of theory and experience within classical Fisherian statistics on this subject (e.g. Silvey 1980), and its extensions to dynamic systems (e.g. Fedorov 1972).

Both the calibration and sensitivity analysis may lead to a need to change the model structure. In this *iterative* loop for identification, model structure postulation, calibration, and model update, the different steps of modeling tend to overlap, once the procedure is running efficiently. After all, judgment of whether the model captures the main features of the system and the remaining uncertainty is tolerable depends strongly upon the objectives. Actually, even if the task is to develop a statistical model, a simulation model, a decision analytic model, an expert system, etc., the iterative scheme supported by expert(s) is usually very effective, and it is difficult to replace (formal) trial and error guided with common sense.

A model with calibrated parameters forms the input to the validation phase. The basic idea is to test the performance of the calibrated model against a different data set from the one used for the calibration. In case of failure, again depending on subjective judgment related to the objectives, the model structure requires modification. Note that validation can be understood in several ways, each leading to different "grades" in validation (see Thomann 1982). Irrespective of what validation scheme is being used, we would like to point out the importance of the deductive, more subjective validation of a model. Usually it is sensible to use all the information of the data in the iterative procedure and evaluate the performance of the system against expert knowledge about the system behavior. It is clear, that this judgment should be well reported. This concept and the utilization of sensitivity and perturbation analyses has been discussed by Varis (1988, 1991*b*), ending to the conclusion that if the model identification is based primarily on deduction, then the validation should also be deductive, primarily. If the data is sufficient to inductive model identification (including validation), so why not to use a statistical approach.

Often when constructing models, the marginal benefits of model development are typically subject to decrease after a rather early phase. Therefore, it is often more efficient to study the problem from a couple of different, partly overlapping directions with rather simple models, than to direct efforts to refinement of a complex "all-knowing" model of the system. Here we refer to the case studies on Lake Balaton and Lake Tuusulanjärvi. Also the idea of using multiple, rather simple models is valid within the context of decision support systems (cf. Chapter 5.5).

3 GOVERNING EQUATIONS

3.1 Overview

A deterministic water quality model describes spatial and temporal changes of selected constituents in a river or lake which are due to

- Physical transport such as advection and diffusion (or dispersion).
- Chemical and biological reactions.

If reactions are insignificant we talk about an idealized conservative material, the behavior of which is described by the classical advection-diffusion or transport equation. If we considered, however, a non-conservative material such as BOD or DO, the transport equation should be extended by reaction terms. In both cases the flow field should be known in order to derive a solution, and for this purpose the equations of continuity and momentum can be used. All these mean that a mechanistic water quality model has three components determining its structure:

(1) Equations of motion.

(2) The transport equation.

(3) Process equations for reactions.

This is the case at least in principle. In practice, the relative importance of phenomena affecting water quality changes from case to case and accordingly we find a large number of different approaches in the literature. If, for instance, we treat a lake characterized by intensive mixing, component (1) can be excluded and the linkage of (2) and (3) will lead to a set of ordinary differential equations (ODEs). Quite often, however, the flow pattern is rather complex and the application of a hydrodynamic model and the advective-diffusive equation cannot be avoided as otherwise spatial non-uniformities cannot be matched. This leads to a partial differential equation (PDE) structure even if we considered just a single component, e.g., total phosphorus subjected to sedimentation which is characterized by the so-called apparent settling rate.

The large variety of water quality models is further justified by the nature of spatial changes and simplifications associated. For example, a deep, stratified lake can hardly be treated without describing vertical variations. For a shallow lake, however, the focus should be on horizontal changes, while for a long river we may be interested in longitudinal alterations only (in addition to temporal ones).

The objective of this chapter is to discuss the main equations of the three model components outlined. We will focus on shallow water bodies only. For a more comprehensive treatment, see e.g. Orlob (1982). In harmony with what we said previously, we stress once more that a water quality model has a fourth, often crucial component. This is formed by methodologies to be used for identification, calibration, and validation, as well as

for sensitivity analyses and uncertainty studies.

3.2 Equations of motion

These equations, the continuity equation and the Navier-Stokes equation, are expressing the principle of conservation of material and momentum, respectively. The latter is often called Reynolds equation for turbulent flows, which is the case in rivers and lakes. We assume that these equations are known (see, e.g., Hinze 1959, Abbott 1979, and Orlob 1982) and we will deal with the two- and one-dimensional situations, which are of high practical interest.

Two-dimensional equations

These are obtained by integrating the full equations vertically from the bottom (z_b) to the free surface (z) (the depth is $h = z - z_b$):

$$q_x = \int_{z_b}^{z} v_x \, dz = V_x h, \quad q_y = \int_{z_b}^{z} v_y \, dz = V_y h \tag{1}$$

where V_x and V_y are depth integrated velocities, while x and y are horizontal coordinates. With the usage of expression (1) the depth averaged continuity takes the form

$$\frac{\partial z}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0 \tag{2}$$

where t is time. The corresponding momentum equations in x and y directions can be written as follows (Abbott 1979):

$$\begin{array}{ccccccccc} \dfrac{\partial q_x}{\partial t} & + & \dfrac{\partial}{\partial x}\left(\dfrac{q_x^2}{h}\right) & + & \dfrac{\partial}{\partial y}\left(\dfrac{q_x q_y}{h}\right) & + & gh\dfrac{\partial z}{\partial x} & - & E_x\left(\dfrac{\partial^2 q_x}{\partial x^2} + \dfrac{\partial^2 q_x}{\partial y^2}\right) - fq_y + \dfrac{\tau_{bx}}{\rho} - \dfrac{\tau_{sx}}{\rho} = 0 \\ (1) & & (2) & & (3) & & (4) & & (5)\ (6)\ (7) \\ \dfrac{\partial q_y}{\partial t} & + & \dfrac{\partial}{\partial x}\left(\dfrac{q_x q_y}{h}\right) & + & \dfrac{\partial}{\partial y}\left(\dfrac{q_y^2}{h}\right) & + & gh\dfrac{\partial z}{\partial y} & - & E_y\left(\dfrac{\partial^2 q_y}{\partial x^2} + \dfrac{\partial^2 q_y}{\partial y^2}\right) + fq_x + \dfrac{\tau_{by}}{\rho} - \dfrac{\tau_{sy}}{\rho} = 0 \end{array} \tag{3}$$

where f is the Coriolis parameter, g is the gravitational acceleration, ρ is the water density, E_x and E_y are eddy viscosity coefficients (defined by the Boussinesq assumption for the turbular shear stress), and finally τ_b and τ_s are the shear stresses on the bottom and free surface, respectively. The terms of Equation (3) have the following meanings:

(1) Local acceleration of a fluid at a point.

(2) Convective acceleration caused when fluid is transported with differing velocity.

(3) Horizontal pressure force (by using the hydrostatic approximation).

(4) Horizontal transport of momentum due to turbular shear stresses.

(5) The Coriolis force due to the Earth's rotation.

(6) Dissipation due to bottom shear stress.

(7) Shear stress exerted at the water surface.

The bottom shear stress depends on the character of the flow and on the vertical velocity distribution. The latter is excluded from a velocity integrated model and for this reason the parameterization of τ_b is not a straightforward task. Usually the bottom shear stress is expressed as a non-linear function of the average velocities as follows:

$$\tau_{bx} = c_f \rho V_x \left(V_x^2 + V_y^2\right)^{1/2} = \frac{c_f \rho}{h^2} q_x \left(q_x^2 + q_y^2\right)^{1/2}$$

$$\tau_{by} = c_f \rho V_y \left(V_x^2 + V_y^2\right)^{1/2} = \frac{c_f \rho}{h^2} q_y \left(q_x^2 + q_y^2\right)^{1/2} \qquad (4)$$

where c_f is the resistance coefficient. Several empirical expressions can be used to obtain c_f:

$$c_f = \frac{\lambda}{8}$$

$$c_f = \frac{g}{C^2} \qquad (5)$$

$$c_f = \frac{n^2 g}{h^{1/3}}$$

where λ is the Darcy-Weisbach friction coefficient, C is the Chezy coefficient and n is the Manning's coefficient. The wind-induced surface stresses can be calculated from:

$$\tau_{sx} = \rho_a C_D W_x \left(W_x^2 + W_y^2\right)^{1/2}$$

$$\tau_{sy} = \rho_a C_D W_y \left(W_x^2 + W_y^2\right)^{1/2} \qquad (6)$$

where W_x and W_y are wind velocity components, ρ_a is the density of air and C_D is the drag coefficient which can be calculated from empirical relationships (see e.g. Wu 1969).

Because of the empirical nature of c_f and C_D, they should be calibrated. This can be done for a lake if detailed observations are available at least for the wind velocity components and water levels reflecting properly the dynamic behavior of the system. For details the reader is referred to Shanahan et al. (1986).

The solution of Eqs. (1) to (6) requires the definition of initial and boundary conditions. Possibilities among others include the specification of inflow and outflow velocities for corresponding lake segments or for upstream and downstream river cross-sections studied. At other reaches of the boundary the no-flow condition is applied, although sometimes for lakes the no-slip assumption ($V_x = V_y = 0$) is also used.

The above equations and boundary conditions are rather complex and their (numerical) solution is not an easy task (e.g., the nonlinear convective terms are particularly troublesome). As a consequence, most of the models depend on simplifications by neglecting the less important terms in the equations. For instance, when considering lakes, terms (2) and (4) can be omitted in Eq. (3). However, we stress that such simplifications are meaningful only if they lead to an acceptable compromise of the proper description of the physics of the actual lake considered and the solution of governing mathematical equations. Assumptions made solely to simplify solutions can result in non-realistic model predictions.

One-dimensional equations

For rivers we select x as the longitudinal coordinate, and y as the transversal one. The introduction of curvilinear coordinates following the meandering of rivers is often advisable. In many cases our primary interest is to determine temporal and longitudinal variations which suggest the integration of the previously outlined equations transversally. This procedure can be followed also for lakes of longish shape (Somlyódy 1983). As a result we obtain the classical Saint-Venant equations (e.g. Mahmood & Yevjevich 1975) incorporating cross-sectionally averaged values.

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0 \tag{7}$$

and

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\alpha \frac{Q^2}{A}\right) + gA\frac{\partial z}{\partial x} + \frac{A}{\rho h}\tau_{bx} - \frac{A}{\rho h}\tau_{sx} = 0 \tag{8}$$

where Q is the streamflow rate (no lateral inflow was assumed in Eq. (7)), A is the cross-sectional area, α is the coefficient accounting for non-uniformities of the velocity in the cross-section, and τ_{bx} is the bottom shear stress (cf. Eq. (4)):

$$\tau_{bx} = \frac{C_f \rho}{A^2} Q|Q| \tag{9}$$

where τ_{xx} is unchanged and is expressed by Eq. (6). As boundary conditions, either Q or z, should be given at both ends of the system considered ($x = 0$ and $x = X$, respectively). Alternatively, the relation of Q and z can be employed, which is available in the practice in the form of $Q(h)$ for most of the problems (as initial condition the steady state solution can be utilized). For lakes, the currents due to inflows and outflows are often small in comparison to wind induced flows, and thus $Q(t, 0) = Q(t, X) = 0$ offers a good approximation.

As shown by several studies, water quality is relatively non-sensitive to fast and local changes in the flow. Under such conditions the diffusive wave approximation of Eqs. (7) and (8) can be successfully employed (see Mahmood & Yevjevich 1975):

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0 \tag{10}$$

$$\frac{\partial Q}{\partial t} + C(Q, A)\frac{\partial Q}{\partial x} - D(Q, A)\frac{\partial^2 Q}{\partial x^2} = 0 \tag{11}$$

for the solution of which fast procedures are known. In above equations $C(Q, A)$ is the "propagation" velocity of the wave, while $D(Q, A)$ is "diffusion" coefficient expressing deformation of flood waves. For many water quality studies a critical low flow is selected as a design condition, when the effect of dilution is small. For such purposes the equations of gradually variable, steady flow can be used. They are obtained by introducing

$$\frac{\partial Q}{\partial t} = \frac{\partial A}{\partial t} = 0$$

into equations (7) and (8). The computational effort required for the solution is minimal. The sequential application of the equations may reflect properly also "slow" temporal changes of the flow.

3.3 Transport equation

This expresses the conservation of dissolved, non-reactive materials in the water body considered. The two-dimensional, depth integrated form of the equation is

$$\frac{\partial (hC)}{\partial t} + \frac{\partial (q_x C)}{\partial x} + \frac{\partial (q_y C)}{\partial y} = \frac{\partial}{\partial x}\left(h D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(h D_y \frac{\partial C}{\partial y}\right) \tag{12}$$

where C is the concentration averaged over the depth and the typical time scale of turbulence, and D_x and D_y are the turbulent dispersion coefficients (see e.g. Holley 1971). The first term expresses local change in the concentration at a given point, the second and the third terms the influence of convection, while the right side stands for dispersion. D_x and D_y are lumped parameters expressing the effect of molecular and turbulent diffusion, furthermore of non-uniformities in C, V_x and V_y along the vertical due to the existence of shear flow. As they depend on the flow itself, empirical relationships should be used for their derivation. On the basis of the work by Elder (1959), it is generally assumed that

$$D_x = d_x\, u_* \, h \quad \text{and} \quad D_y = d_y\, u_* \, h \tag{13}$$

where u_* is the bottom shear velocity

$$u_* = \left(\frac{\tau_b}{\rho}\right)^{1/2} \tag{14}$$

For river flows d_y ranges between 0.2 and 2.0, depending on many factors such as roughness, the ratio of depth to width, bed curvature, and several others. For natural rivers, 0.6 can be used as an average, while d_x is larger by an order of magnitude. With respect to details, the reader is referred to Holley (1971), Holly (1975), Fischer et al (1979), Somlyódy (1982*b*), and Shanahan & Gaudet (1990).

The one-dimensional transport equation is obtained by an additional integration of Eq. (12) similarly as it was done for the flow:

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(QC)}{\partial x} = \frac{\partial}{\partial x}\left(A\, D_L \frac{\partial C}{\partial x}\right) \tag{15}$$

where C is now the concentration averaged over the entire cross-section and D_L is the longitudinal dispersion coefficient. Eq. (15) is often called the longitudinal dispersion equation. D_L incorporates the shear over the entire cross section A, not only along the depth h, and therefore $D_L > D_x$. Its value varies strongly from river to river, (see e.g. Fischer et al. 1979), and tracer experiments are often used to determine it in particular situations. The same is also suggested for estimating D_x and D_y. in problems of high importance.

As boundary conditions are considered, concentrations should be given for inflows, while the zero gradient condition is used otherwise, since no mass transport takes place along river banks or shorelines. Because of the parabolic nature of the transport equation, no boundary condition should be specified to outflows corresponding to the downstream cross-section of a river.

Eq. (15) can often be further simplified. If, for instance, complete mixing can be assumed for a lake, integration leads to an input-output relation

$$\frac{d(V\tilde{C})}{dt} = L - Q\tilde{C} \qquad (16)$$

where $\tilde{C}$ is the concentration averaged over the volume V and L is the input load to the system. For rivers, the plug flow assumption may be used as another extreme simplification.

The simplicity, and the resulting attractivity, of Eq. (16) and the corresponding for plug flow leads to the idea to approximate a lake or a reservoir of a rather complex structure as a proper composition of these two types of reactors characterized by full mixing and plug flow, respectively. The approach can be applied quite successfully for water quality studies. This, however, will not happen automatically, and a careful design is needed in each case. First of all, the selection of the size of reactors is a crucial step in order to avoid the introduction of implicit dispersion deviating strongly from the physical one. In details of the methodology, the reader is referred to Shanahan & Harleman (1984). Secondly, the throughflows of the reactors should be estimated. For such a purpose a flow model (chapter 3.1) or field observations of a conservative material can be employed. We would like to stress, that inflow and outflow terms should be estimated independently on rate constants of the water quality model in question (see below). Otherwise, the above procedure should not be applied.

Until now we were handling idealized, conservative materials. However, in reality water quality components are subject to additional changes caused by biodegradation, sedimentation, resuspension, sorption-desorption, mineralization, and so forth. These processes influence both temporal and spatial changes of the concentrations of constituents, and thus also the role of advective and dispersive transport. They can be described by reaction equations which should be incorporated in mass conservation equations. The consequences are at least three-fold:

- We have to handle non-linear equations in most cases owing to the nature of reactions.

- We have to set an equation for each constituent considered. Thus, for instance, the number of equations of the classical Streeter-Phelps model is two, while for the present version of the QUAL model the number is ten. These equations should be solved simultaneously due to the coupling established by the reaction terms.

- Large number of reaction rates and other parameters are introduced. A significant portion of them is subject to model calibration. Moreover, reaction processes can be described using various hypotheses and therewith identification and validation are important issues, too (see above).

All these mean that in contrast to a conservative material, for real water quality problems a more complex set of equations should be handled. They can be written in the two-dimensional case in the subsequent general form:

$$\frac{\partial(h\mathrm{C})}{\partial t} + \frac{\partial(q_x \mathrm{C})}{\partial x} + \frac{\partial(q_y \mathrm{C})}{\partial y} = \frac{\partial}{\partial x}\left(h D_x \frac{\partial \mathrm{C}}{\partial x}\right) + \frac{\partial}{\partial y}\left(h D_y \frac{\partial \mathrm{C}}{\partial y}\right) + \mathbf{r}(\mathbf{p}, \mathrm{C})\, h\, \mathrm{C} \qquad (17)$$

where **C** is the n-dimensional mass concentration vector for the n state variables, **r** is the n-dimensional vector of rates of change of the state variables due to biological, chemical and other reactions as a function of **C**, and **p** is the m-dimensional parameter vector used to characterize the reactions (generally $m > n$). The structure of **r**(**p**, **C**) is often unknown, and this component of the entire model is a special issue in identification.

The latter is a rather complex task which often cannot be treated at all. The situation were much simpler if we used an input-output type of description (see Eq. (16)) leading to ordinary differential equations as follows

$$\frac{d(V\tilde{\mathrm{C}})}{dt} = \mathbf{L} - Q\,\tilde{\mathrm{C}} - \mathbf{R}(\mathbf{P}, \tilde{\mathrm{C}})\, V\tilde{\mathrm{C}} \qquad (18)$$

where the notation $\mathbf{R}(\mathbf{P}, \tilde{\mathrm{C}})$ indicates in comparison to **r**(**p**, **C**) that as a result of integration and aggregation even the structure and parameter set of the reaction submodel can change. This issue is related to the problem of scaling for which little information is available within the domain of water quality studies.

3.4 Process equations of reactions

The last term of Eq. (18) describes changes in water quality due to chemical, biochemical, biological, and physical processes (others than advection and diffusion). These are characterized in most water quality models by aggregated expressions incorporating one or two parameters. One of the most widely used reaction family is given by the equation:

$$\frac{dC}{dt} = K\, C^n \qquad (19)$$

where depending on the value of n we speak about zero-, first-, and second-order processes (with $n = 0, 1, 2$, respectively). For instance, sedimentation and degradation of organic matter (characterized by BOD) is described by first order kinetics when $-K$ is settling rate or decay rate, for instance.

Reaction rates often depend on concentration. This leads to non-linear equations. Among the most used such process equations is the Michaelis-Menten formulation originally set for biochemical enzyme kinetics

$$\frac{dC}{dt} = \frac{K_1}{K_2 + C} C \qquad (20)$$

where K_1 defines the maximum value of dC/dt (i.e. the maximum growth rate) and K_2 is the half-saturation constant. If C is small, Eq. (19) behaves like a first order reaction, while for large C as a zero order one.

Process equations of water quality models are obviously more complex than suggested by Eqs. (19) and (20), as a change in one constituent will automatically influence others due to mass balance conservation. This can be demonstrated by the classical Streeter & Phelps (1925) equation already referred to. Accordingly, bacterial composition of organic wastes discharged to rivers takes place in water, the price of which is oxygen consumption, which in turn is gradually compensated by atmospheric reaeration. The two state variables are C_1 = BOD (the (carbonaceous) biological oxygen demand), and $C_2 = DO_s - DO$, i.e. the oxygen deficit, where DO_s is the saturation concentration at the given water temperature. The process equations (Streeter & Phelps 1925) based on first order kinetic assumptions are

$$\frac{dC_1}{dt} = -K_d C_1$$

$$\frac{dC_2}{dt} = K_d C_1 - K_a C_2 \qquad (21)$$

where K_d is the decay rate and K_a is the reaeration rate. For a river of constant velocity U, t can be interpreted as the travel time ($t = x/U$) and Eq. (21) can be solved analytically (see e.g. Rinaldi et al. 1979, Orlob 1982, Thomann & Mueller 1987) resulting in the so--called dissolved oxygen sag curve. This shows that the DO deficit possesses a maximum at the critical distance downstream from a waste water discharge which is often used to estimate the required level of sewage treatment. In addition to decomposition of organic matter and the atmospheric reaeration considered in the classical Streeter-Phelps model, several other processes take place in natural streams, e.g., the reduction of BOD by sedimentation, and its increase due to stirring-up of earlier deposited organic products. It has also been realized that if organic nitrogen waste sources are significant, their impact on oxygen deficit may be appropriately described by introducing an additional variable, the nitrogenous biochemical oxygen demand, and by using the description of sequential nitrification reactions. This requires the definition of up to four new state variables for the following nitrogen fractions: organic N, ammonium, nitrate, and nitrite, plus the reactions involved. The latter can be handled by using first order kinetics and the result is the reaction component of the first version of the QUAL model family (for details, see Orlob 1982).

Later on, there has been an increasing emphasis on nutrients, algal biomass, and the more detailed description of dissolved oxygen. This required the incorporation of additional state variables such as organic phosphorus, dissolved phosphorus, and chlorophyll-*a* concentration. The latter is used as an approximation for phytoplankton biomass. The model obtained is QUAL2, with several refined versions. The difference in comparison to the Streeter-Phelps model is now manyfold. Not only the number of state variables is

much higher (ten in the last version, QUAL2E, Fig. 3), but simultaneously there is a drastic increase in the number of parameters. Reactions are not based on first-order kinetics any more, but Michaelis-Menten type of expressions are used frequently as well. Nutrient and light limitation are incorporated quite in detail (see Brown & Barnwell 1987).

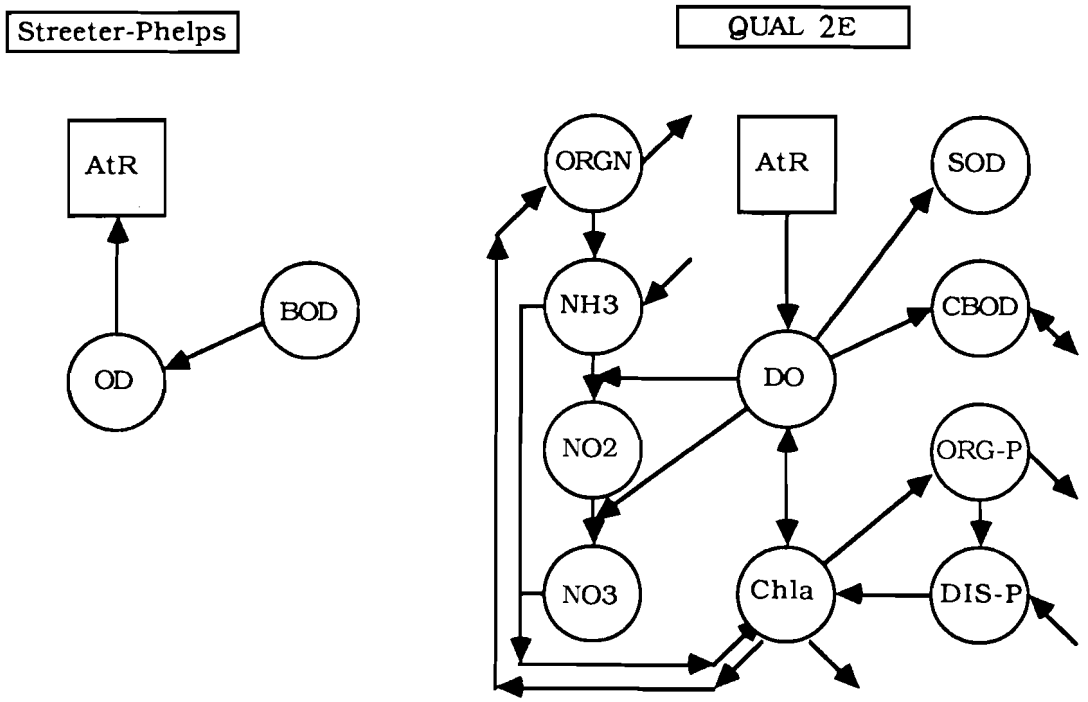

Fig. 3 Flow diagrams of the Streeter-Phelps model and the QUAL2E. DO = dissolved oxygen, OD = oxygen deficit, (C)BOD = biologic oxygen demand, AtR = atmospheric reaeration, SOD = sediment oxygen demand, ORG-P = organic phosphorus, DIS-P = dissolved phosphorus, Chla = chlorophyll-*a*, NO3, NO2 & NH3 are inorganic nitrogen fractions, and ORGN = organic nitrogen. Additionally, QUAL2E can simulate coliforms, one non-conservative, and three conservative constituents.

QUAL2E has 19 temperature coefficients, and 33 other parameters. The latter parameters can be classified as follows with respect to the range of parameter value given: range is within one order of magnitude, range is within two orders of magnitude, range is within three or more orders of magnitude, and no range is given. One half of parameters are river reach specific. Experience has shown that even if QUAL models have been designed generic, their calibration is not a trivial task, even to an expert.

All in all, the approach is widely used. The reaction component of QUAL2E combines the original Streeter-Phelps model with a nitrogen cycle model and a "eutrophication" model. The major difference stems from the latter one. For this reason we subsequently demonstrate process equations of a simple eutrophication model under the assumption that phosphorus (P) is the limiting factor. The model as it will be discussed was developed for Lake Balaton (van Straten 1986*b*). Among a variety of models (Fig. 4) tested for this large shallow water body in Hungary, it is the simplest version. In order to capture seasonal changes in phytoplankton, it distinguishes two algal clusters, the first dominating in winter, and the second in summer.

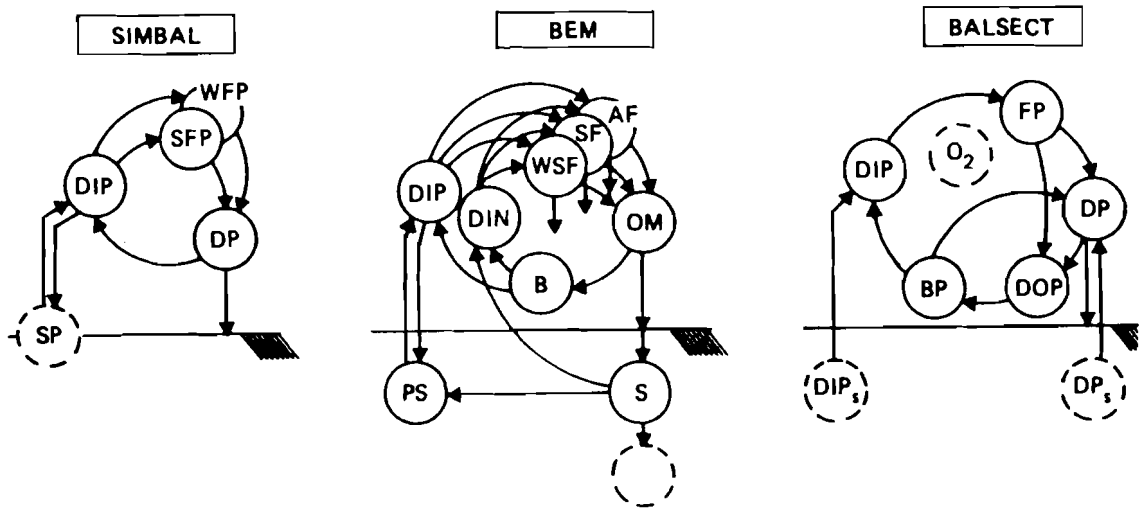

Fig. 4 Three eutrophication models for Lake Balaton: SIMBAL by van Straten (1986*b*), BEM by Kutas & Herodek (1986), and BALSECT by Leonov (1982). WFP & SFP = cold and warm water phytoplankton P, resp., DP = detritus P, DIP & DIN = dissolved inorganic P and N, resp., SP = adsorbed exchangeable P, AF, SF & WSF = autumn, summer, and winter-spring phytoplankton biomass, resp., OM = organic material, B = bacteria biomass, PS = exchangeable P in sediment, FP = phytoplankton P, DOP = dissolved organic P, BP = bacteria P, DP_s = DP in sediment, DIP_s = DIP in sediment.

In what follows, we consider the model as an example, omitting though one of the algal groups in order to keep the example as straightforward as possible. Thus state variables are the P content of algae (C_A), detritus P (C_D), and dissolved inorganic P (C_P). Processes involved are P uptake, growth and death of algae under P, light, and temperature limitation, mineralization, sedimentation, and sorption exchange. State equations are as follows:

$$\frac{dC_A}{dt} = \left(G_A - D_A - \frac{v_{SA}}{h}\right) C_A = G_n C_A \qquad (22a)$$

$$\frac{dC_D}{dt} = D_A C_A - M_D C_D - \frac{v_{SD}(1-\gamma)}{h} C_D \qquad (22b)$$

$$\frac{dC_P}{dt} = -G_A C_A + M_D C_D + k_{ex}\left(C_{P_{eq}} - C_P\right) \qquad (22c)$$

where G_A is the algae growth rate, G_n is the net growth rate, D_A is the death rate, v_{SA} and v_{SD} are settling velocities of algae and detritus, respectively, M_D is the mineralization rate, γ is the dissolved fraction of detritus not subjected to sedimentation, and h is the water depth. The last term of Eq. (22*c*) characterizes the influence of sorption. Suspended solids and the top layer of sediment can serve as sorbents. These two are in interaction with one another in shallow water bodies due to, e.g., wind action. The two parameters are C_{Peq} and k_{ex}, the equilibrium concentration and the transport coefficient of sorption exchange, respectively. The growth rate is obtained from

$$G_A = G_{max}\, G_P\, G_T\, G_I \tag{23}$$

where G_{max} is the maximum rate, G_P is the P limitation factor following the Michaelis-Menten (or Monod) kinetics

$$G_P = \frac{C_P}{C_k + C_P} \tag{24}$$

characterized by the half-saturation constant C_k ($0 \le G_P < 1$). G_T is the temperature reduction factor

$$G_T = \begin{cases} \dfrac{T_{cr} - T}{T_{cr} - T_{op}} \exp\left(1 - \dfrac{T_{cr} - T}{T_{cr} - T_{op}}\right), & \text{if } T \le T_{cr} \\ 0, & \text{if } T > T_{cr} \end{cases} \tag{25}$$

in which T_{cr} is the critical temperature above which no growth takes place, while T_{op} is the optimal temperature (note that G_T is often described as a continuous function of T – e.g., $G_T = \Theta^{T - T_0}$. Θ and T_0 are parameters – but in the referred study Eq. (25) offered a better match of seasonal changes).

Finally, in Eq. (23) G_I is the light attenuation factor averaged over one day and the depth, using the Steele's equation for algae light limitation and the Lambert-Beer law for the vertical penetration of light in water

$$G_I = \frac{2.718\,\lambda}{\varepsilon\, h}\left\{\frac{1}{2L_h}\left[1 - \exp(-2L_h)\right] - \frac{1}{2L_0}\left[1 - \exp(-2L_0)\right]\right\} \tag{26}$$

where $L_0 = R\,/\lambda\, I_s$, and $L_h = L_0\, e^{-\varepsilon h}$. Now I_s is the saturation (or optimal) light intensity of algal growth, R is the daily total global radiation, λ is the length of the photoperiod [–], and ε is the extinction coefficient [m^{-1}] characterizing exponential light penetration along the water depth.

We note that Eq. (26) is a result of double integration according to our interest here which is the description of daily changes in algae biomass in an average along the water column. Obviously, if we looked for diurnal fluctuations and vertical alterations (i.e. changes in smaller scales) integrations outlined above must not be performed.

Eq. (26) is widely used in the literature with the assumption that the extinction coefficient is determined by the color of the water without algae and the self-shading depends linearly on algae biomass. A similar assumption is often used for the effect of suspended solids, the concentration of which is denoted by C_{ss} as will be discussed later in process equations. This yields

$$\varepsilon = \varepsilon_0 + \alpha\, C_A + \beta\, C_{SS} \tag{27}$$

where ε_0 is the background extinction. α and β are proportionality factors.

In Eq. (22) death and mineralization are described classically by first-order kinetics. The corresponding rates are assumed to be temperature dependent

$$D_A = k_d \Theta_d^{T-T_{d_0}} \quad \text{and} \quad M_D = k_m \Theta_m^{T-T_{m_0}} \tag{28}$$

where k, Θ and T_0 are positive constants subject to calibration in both cases.

When comparing reaction equations of such a simple P cycle model to that of a simple BOD-DO model, there are several differences including:

- Equations are much more non-linear. In this respect Eq. (26) is a good example expressing the complex impact of solar radiation, the depth, suspended solids concentration, and algae biomass (cf. Eq. (27)) on the algae biomass itself. The latter feedback is actually determining the highest possible biomass in a lake.

- The role of external forcing functions, i.e., T, R, λ, and C_{SS}, their statistical distributions and cross-correlations, and the coincidence of "extreme" events can play a significant role in the actual water quality.

- The number of parameters is much higher in spite of which the performance of models is still rather poor.

In Eq. (27) we considered C_{SS} *as* a known concentration of suspended solids, e.g., from observations. For many shallow lakes, however, the fast dynamic changes in C_{SS} due to wind induced sediment resuspension can play a significant role from the viewpoint of algal growth and these fluctuations are not captured by routine type of measurements. So, we may need to develop a model for deriving temporal changes in suspended solids concentration. This may lead to process equations aggregating properly various physical processes which should not be handled simultaneously with Eq. (22): the solution of the latter

has no influence on C_{SS}.

As an illustration the structure of models developed for Lake Balaton (see Somlyódy 1982*a*, Luettich et al. 1990, Somlyódy & Koncsos 1991) is shown. Accordingly,

$$h \frac{dC_{SS}}{dt} = \phi_d + \phi_e \tag{29}$$

where ϕ_d and ϕ_e are the flux of deposition and resuspension, respectively. ϕ_d can be approximated as

$$\phi_d = -k_1 (C_{SS} - C_{SS0}) \tag{30}$$

where k_1 is the apparent settling velocity and C_{SS0} is the background concentration. For characterizing ϕ_e several approaches are available, as follows.

$$\phi_e = k_3 (\tau - \tau_{cr})^{n1} \tag{31a}$$

$$\phi_e = k_4 (H - H_{cr})^{n2} \tag{31b}$$

$$\phi_e = k_5 W^{n3} \tag{31c}$$

where τ is the wave induced bottom shear stress, τ_{cr} is the critical shear, H is the significant wave height and H_{cr} is its critical value, while W is the absolute value of wind speed.

All hypotheses incorporate two or three parameters subject to calibration. The use of Eq. (31*a*) would require the application of linear wave theory, while Eq. (31*b*) would need the usage of Sverdrup-Munk-Bretschneider shallow wave hindcasting model. They both use parameters of the wind field as input. The last, empirical assumption directly incorporates the wind velocity. For Lake Balaton it was found that $H(t) \approx W(t)$ and for this reason the last hypothesis worked also quite properly. Since the extinction coefficient and the suspended solids concentration are linearly related to each other, this leads, together with Eqs. (29) and (30) to a direct process equation for the C_{SS} dependent component of the extinction coefficient (ε_{SS}) as follows

$$H \frac{d\varepsilon_{SS}}{dt} = - \dot{k}_1 \varepsilon_{SS} + \dot{k}_2 W^n \tag{32}$$

For further details the reader is referred to Somlyódy & Koncsos (1991). This example further amplifies the complexity of eutrophication and the need for proper combination of processes of quite deviating disciplinary backgrounds.

3.5 Solution methodologies and illustrations

Need for further development of solution techniques

A water quality model is a result of the proper combination of equations discussed in sections 3.1 to 3.4. Having the rather complex nature of governing equations and boundary conditions, it is obvious that classical analytical solutions rarely exist and the application of routine techniques such as the Runge-Kutta method are restricted to cases where reaction processes are "dominating", and thus a set of ordinary differential equations should only be handled.

For the type of partial differential equations outlined here the methods of finite differences, finite elements, or boundary elements can be utilized (see, e.g., Abbott 1979, Mahmood & Yevjevich 1975, Connor & Brebbia 1976, Orlob 1982, Brebbia et al. 1984).

The usage of the techniques of finite differences can be considered as a routine task in engineering practice, but there are also a large number of examples for finite elements. In fact, it was the impression a couple of years back that we possess most of the tools we need to handle intelligently problems related to water pollution and accordingly no further developments were anticipated. The situation was such despite of several existing shortcomings, some of which are listed below:

- The proper approximation of rather irregular boundaries typical for rivers and lakes.

- High numerical dispersion of schemes used widely.

- Relative scarcity of fast (economic) solution methodologies fulfilling basic requirements of convergency, stability, and accuracy.

While all these shortcomings are significant from the hydraulic engineering viewpoint we stress the far most dominating role of the last issue, i.e. the development of more effective solution methods as compared with the routinely used ones, within the field of water quality management. To make the point clear we refer once more to the need of identification, calibration, and validation, mostly related to process equations of reactions (see section 3.4) and to our poor understanding associated: these steps can be made only if "extremely" fast processes are available. In addition to these, we often analyze relatively long periods, i.e. a year or years.

Recent developments are rather promising. As it will be demonstrated, the appearance of some new principles including multigrid techniques and unstructured grids, and refreshing combination of existing methods (Eulerian and Lagrangian treatments, deterministic and stochastic considerations, analytical and numerical techniques, etc.) have led to powerful solution methodologies. In this respect we refer to achievements of the numerical hydraulics group of the Water Resources Research Institute (VITUKI), Budapest, which will serve as basics of our further discussion.

Operator splitting

First we consider the well-known principle of operator splitting (partitioning), the essence of which is that following the temporal discretization each element of the extended water quality-transport equation (convection, dispersion, and reaction, see Eq. (17)) can be solved separately and subsequently for each time step (Δt). As an illustration we consider the 1D longitudinal dispersion equation extended by a reaction term

$$\frac{\partial C}{\partial t} = - U \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2} - rc \tag{33}$$

where we assumed that U, D_L, and r are constants. The use of partitioning is not restricted to these assumptions except that the equation should be linear which may require the linearization of the term $r(C, \mathbf{p})$ within each Δt time increment. Accordingly, Eq. (33) can be written as

$$\frac{\partial C}{\partial t} = A_1 C + A_2 C + A_3 C \tag{34}$$

where A_1, A_2, and A_3 represent operators of convection, dispersion, and reaction, respectively. The solution of the above linear differential equation between time intervals t_n and $t_n + \Delta t$ is

$$C^{n+1} = \exp\left[(A_1 + A_2 + A_3)\Delta t\right] C^n \tag{35}$$

and if the operators A_1, A_2, and A_3 are interchangeable, which is a precondition of applying the method in a strict sense

$$C^{n+1} = \exp(A_1 \Delta t) \exp(A_2 \Delta t) \exp(A_3 \Delta t) C^n. \tag{36}$$

According to this expression, the solution of Eq. (33) can be obtained by the subsequent solution of the pure equations of convection, dispersion, and reaction (and obviously more operators and dimensions can be handled similarly).

$$\frac{\mathbf{C}^{n+1/3} - \mathbf{C}^n}{\Delta t} + U \frac{\partial \mathbf{C}^n}{\partial x} = 0$$

$$\frac{\mathbf{C}^{n+2/3} - \mathbf{C}^{n+1/3}}{\Delta t} - \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} D_L \frac{\partial^2 \mathbf{C}^n}{\partial x^2} dt = 0 \tag{37}$$

$$\frac{\mathbf{C}^{n+1} - \mathbf{C}^{n+2/3}}{\Delta t} - \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} r \mathbf{C}^n dt = 0$$

where the $\mathbf{C}^n$ vector incorporates discretized elements of C on time level t_n .

The obvious advantage of Eq. (37) is that "optimal" schemes can be selected for each operator separately. For instance, the problem of convection can be solved by the method of characteristics, while that of dispersion by the implicit, unconditionally stable Crank-Nicholson scheme (associated with the effective double-sweep matrix inversion, see e.g. Mahmood & Yevjevich 1975). The reaction step can be handled by the Runge-Kutta method or analytically by expressing the matrix exponent with the aid of its Jordan normal transformation (for details, see Bakonyi et al. 1991).

In terms of treating convection, Eq. (37) clearly opens new avenues to combine the Eulerian and Lagrangian description, and to incorporate "stochastic" particle tracking methods (see e.g. Gáspár & Jósza 1991) in traditional numerical solutions.

Fourier approach to advection-diffusion equation

There are certain fields and problems where analytical tools can be utilized surprisingly successfully. As an example, the advective-dispersion equation (see Eqs. (11) and (15)) is mentioned for which Gáspár & Szél (1992) and Szél & Gáspár (1992) developed a new approach using Fourier series and fast Fourier transformation. In comparison to finite differences, the advantages are manyfold:

- Numerical dispersion and stability problems are excluded.

- At any time increment, the solution can be obtained directly from the initial – and boundary condition and no step-by-step procedure is needed.

- No spatial discretization is required, although the number of elements preserved in the Fourier series is roughly equivalent to that of the increments of a finite difference scheme.

As the computational demand is considered, the above procedure is more powerful than a finite difference scheme if we will not need the solution for each regular grid point. Quite often we are not interested in flow parameters in uniformly defined cross-sections and time levels. Particularly the latter aspect makes a significant difference. As it can be shown, the computational effort of the Fourier method depends on the number of consecutive intervals within which the change of the upstream boundary condition can be considered linear, while for a finite difference scheme the much shorter increment (Δt)plays a decisive role.

Multigrid method

In the last decade, a very efficient computational technique has appeared and come into practice, namely, the so-called multigrid method. The essential idea of the approach is following. In the traditional finite difference/finite element methods one applies a – sufficiently fine – single grid (mesh). This procedure results in a discrete (algebraic) system of equations which can be solved in several ways (direct or iterative methods). In contrast to this conventional approach, the multigrid techniques utilize a nested sequence of grids at the same time. It turns out that with the help of the coarser grids it is possible to speed up the familiar iterative methods even with orders of magnitude. In fact, if the number of the gridpoints is N, then the necessary computational cost required by the multigrid method is $O(N)$ only, which is far less than that of the conventional methods.

The multigrid idea has successfully been applied in integral equations and even in Boundary Integral Equation Method (BIEM) as well. As known, one of the greatest advantages of the BIEM is that it reduces the original problem which is a differential equation defined on an n-dimensional domain to an integral equation defined on the boundary of the domain, i.e., an $(n\text{-}1)$-dimensional problem. This makes the discretization procedure much simpler and treats well the singularities arising in the solution. The price to be paid is that the structure of the discretized algebraic system has no advantageous property at all: its matrix is fully populated and non-symmetric. However, this difficulty can be overcame by applying the multigrid technique in the BIEM method. It is also possible to apply this combined method in solving free surface problems, which are essentially non-linear. As to the numerical efficiency, the applied multigrid technique makes the BIEM as economical as the (multigridded) finite differences. See Gáspár (1990*a*, *b*) for details.

In solving partial differential equations of water resources by applying some finite difference method, a common problem arises: This is the proper choice of the cell size of the computational grid. In the majority of practical problems, there are subdomains which require fine discretization (e.g., near the boundaries or in the vicinity of abrupt changes of the input data and/or the solution). On the other hand, there may be other subdomains that allow a considerably coarser grid. Thus by using uniformly fine space discretization the traditional finite difference methods, which introduce the simplest discretization procedure and equations, can often lead to an unnecessarily large discrete system.

A remedy for this problem is the use of finite element method or curvilinear grids. However, in both cases, the discrete schemes become much more complicated. In addition, these methods require a grid (mesh) generation procedure as a more or less difficult and time consuming extra task. Recently, a new approach has appeared which can be considered as a systematic extension of the so-called local refinement techniques. This method is based on the unstructured grid generation. The essential idea is to recursively subdivide a square (or a cube in 3D problems) into four (eight) congruent subsquares (subcubes), if certain predefined subdivision criteria are fulfilled. The structure of the resulting grid can easily be controlled: the procedure results in a nested non-uniform non-equidistant cell system ("grid") which can be supplied with a tree-like graph structure in a natural way.

The above outlined quadtree (octree) algorithm is remarkably cheap in computatio-

nal terms: it is possible, nevertheless, to define locally fine enough subregions in such a way that the total number of cells remains relatively low. The next task is to define proper difference schemes on this non-uniform, non-equidistant grid. In principle, it can be carried out by both the traditional Taylor series expansion technique and other, more sophisticated ways (based on e.g. variational principles or integration over the cells). Note that the construction of an arbitrary scheme needs the neighbors of each selected central cell. The finding of the neighbors is trivial in the case of uniform grid but becomes an extra task in the case of quadtree cell systems. Fortunately, exploiting the graph structure of the quadtree cell systems, it can be carried out in a straightforward way. To create an efficient solution procedure for the discretized problem, the multigrid idea can successfully be applied in this quadtree context. Now the coarser grids can be collected of the larger cells of the cell system. Using this combined (quadtree + multigrid) approach, one obtains a numerical method the efficiency of which can exceed that of even the traditional multigrid methods (used on uniform grids). See Gáspár & Simbierowicz (1992) for details.

Until now this technique has been used for elliptic equations, which facilitates the treatment of simplified shallow water equations (terms (1), (2) and (4) are assumed to be negligible in Eqs. (3) and (4), and $\partial z/\partial t = 0$) after introducing a stream function (Józsa & Gáspár 1992).

The quadtree cell systems can be applied also in completely different problems, e.g., in the evaluation of Monte Carlo simulations (see Gáspár & Szél 1991), where again the "adaptive" non-uniformity of the cell system is exploited. In addition to these, if the generation of the quadtree cell system is controlled by the boundary only, the resulting method exhibits strong similarities with the Boundary Element Method, however, without using explicit boundary integral equations. For more details, see Gáspár (1991).

The above advantageous properties (i.e. that the cell system can be constructed economically, the grid structure can be controlled in a flexible way, the discrete problem can be solved efficiently) make it possible to apply the approach in *Lagrangian* context as well. The Lagrangian systems exhibit a lot of advantages over the Eulerian ones, e.g., they can reduce (or even eliminate) the numerical dispersion arising in most flow simulations. However, they contain dispersion-like (elliptic) subproblems, which can be treated hardly in Lagrangian context since the structure of the moving (Lagrangian) points, if there has been any, is necessarily distorted after a few time steps. A good compromise is the use of the quadtree cell systems: they can be constructed in each time step (controlled by the Lagrangian points themselves) and the elliptic subproblem can be solved in that cell system. The idea can be applied in linear transport problems (see Gáspár et al. 1991) and even non-linear transport problems like the vorticity-stream function formulation of the 2D Navier-Stokes equations.

Illustrations

Subsequently, we illustrate the usage of some of the numerical methodologies outlined above for solving flow and transport problems. All the examples will refer to Lake Balaton, a large, wind affected shallow lake in Hungary with a surface area of 596 km^2 and

average depth of 3.1 m (Somlyódy & van Straten 1986), and the approximately 400 km long Hungarian stretch of the Danube. These will serve also as case study problems for demonstrating the use of water quality modeling concepts in the next chapter.

Fig. 5 shows the application of a 1D hydrodynamic model (Eqs. (7) and (8)) for Lake Balaton. The idea of using such a simplified approach for describing water level fluctuations is justified by the longish shape of the lake (see Fig. 6*c*). Fig. 5 demonstrates that the model captures well the changes in water surface elevation at two ends of the water body during a storm characterized by longitudinal wind conditions (Somlyódy 1983).

As was mentioned earlier, the shallow water equations have two parameters subject to calibration: the bottom friction coefficient and the wind drag coefficient. This step is often considered as a rather straightforward procedure which is a misconception. It is sufficient to note that the friction coefficient as defined in terms of the depth integrated velocity is a strongly (and physically not necessarily correctly) aggregated parameter which cannot be measured directly. In addition to this, rather robust coefficients of friction and drag are counterbalancing one another and thus their several, reasonable combinations can result in similar model performances (i.e. the model is ill-defined from the viewpoint of systems theory). Thus, very often a careful analysis of damping properties of oscillations of the water level are needed for proper calibration (Somlyódy 1983).

The other, frequently overlooked problem stems from uncertainties of the wind velocity vector serving as a forcing function. These are due to turbulent fluctuations, measurement errors and rough resolution of wind recording instruments, as well as errors produced by averaging procedures, and spatial nonuniformities in the wind field.

The impact of these uncertainties can be studied if the flow model is used in a Monte Carlo framework. Fig. 5*b* shows such results for the same event as shown in Fig. 5*a*. Uncertainties were assumed primarily in the wind direction (Somlyódy 1983), according to properties of he actual monitoring. As can be seen, there is not much scatter around the nominal simulation. The situation is quite the opposite if the wind blows perpendicularly to the lake (Fig. 5*c*). Under such conditions a small error in wind direction can reverse the direction of the surface shear stress and thus observed changes in the water level cannot be matched by deterministic simulations. The same was also proven by 2D model calculations.

The first 2D simulations were performed at the early eighties for Lake Balaton (Shanahan et al 1986). Convective and eddy viscosity terms were neglected in Eq. (3) and solution was obtained using a classical, explicit, finite difference scheme with staggered grids. A steady-state flow pattern belonging to the prevailing wind direction is illustrated in Fig. 6*b*.

Due to wind climate and short seiche period the water of Lake Balaton is permanently in an unsteady state. This is well illustrated by Fig. 5*c*. The corresponding 2D flow pattern is shown in Fig. 6*a*: the presence of back and forth motion is evident which may

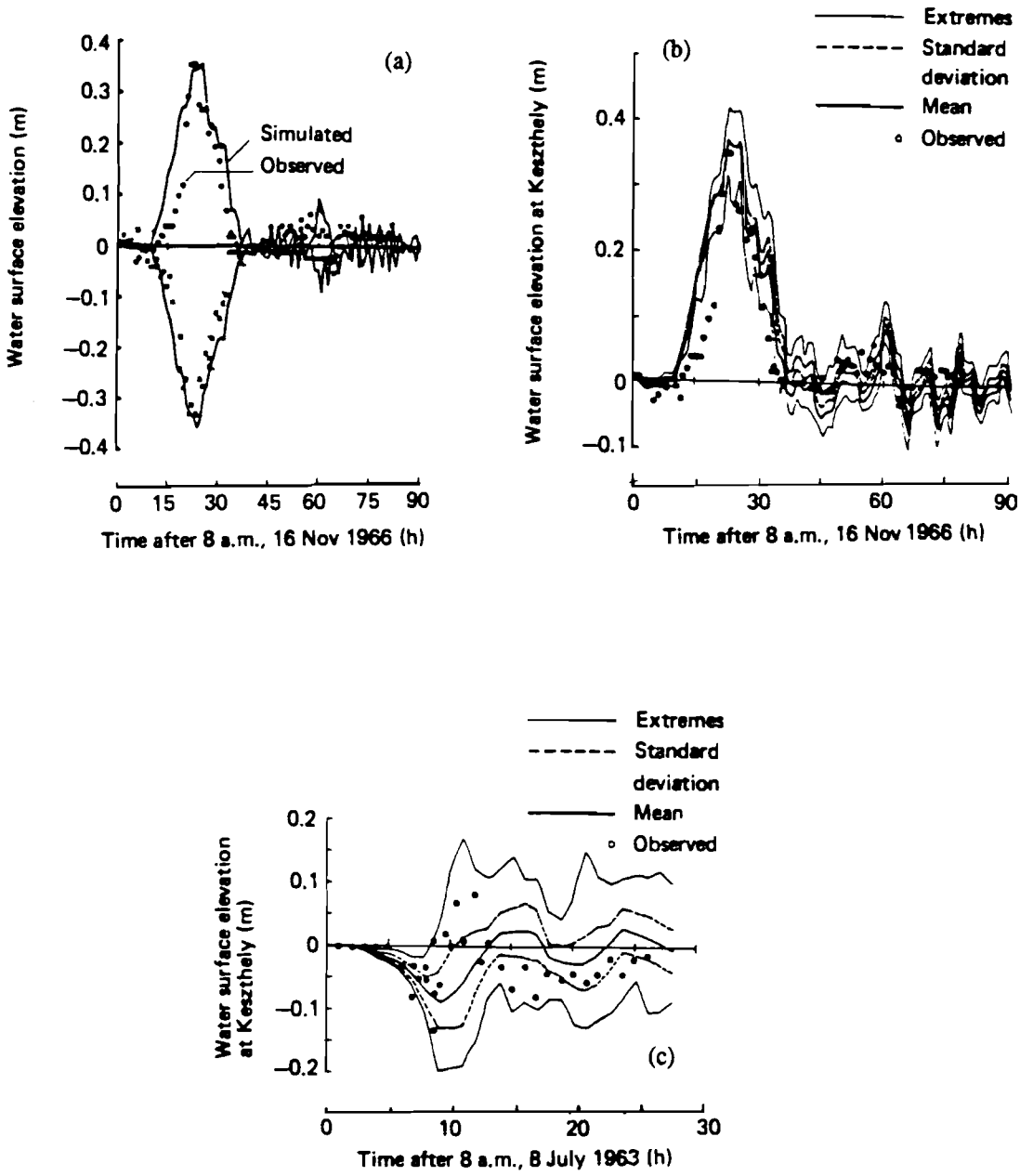

Fig. 5 Simulation of water surface elevations after storm events in respective dates in Lake Balaton. (a) Comparison of simulation results with observations (16 November 1966) in two ends of the lake, Keszthely (Western) and Kenese (Eastern) (a). Monte Carlo simulation results at Keszthely: 16 November 1966 (b) and 8 July 1963 (c) (Somlyódy 1983)

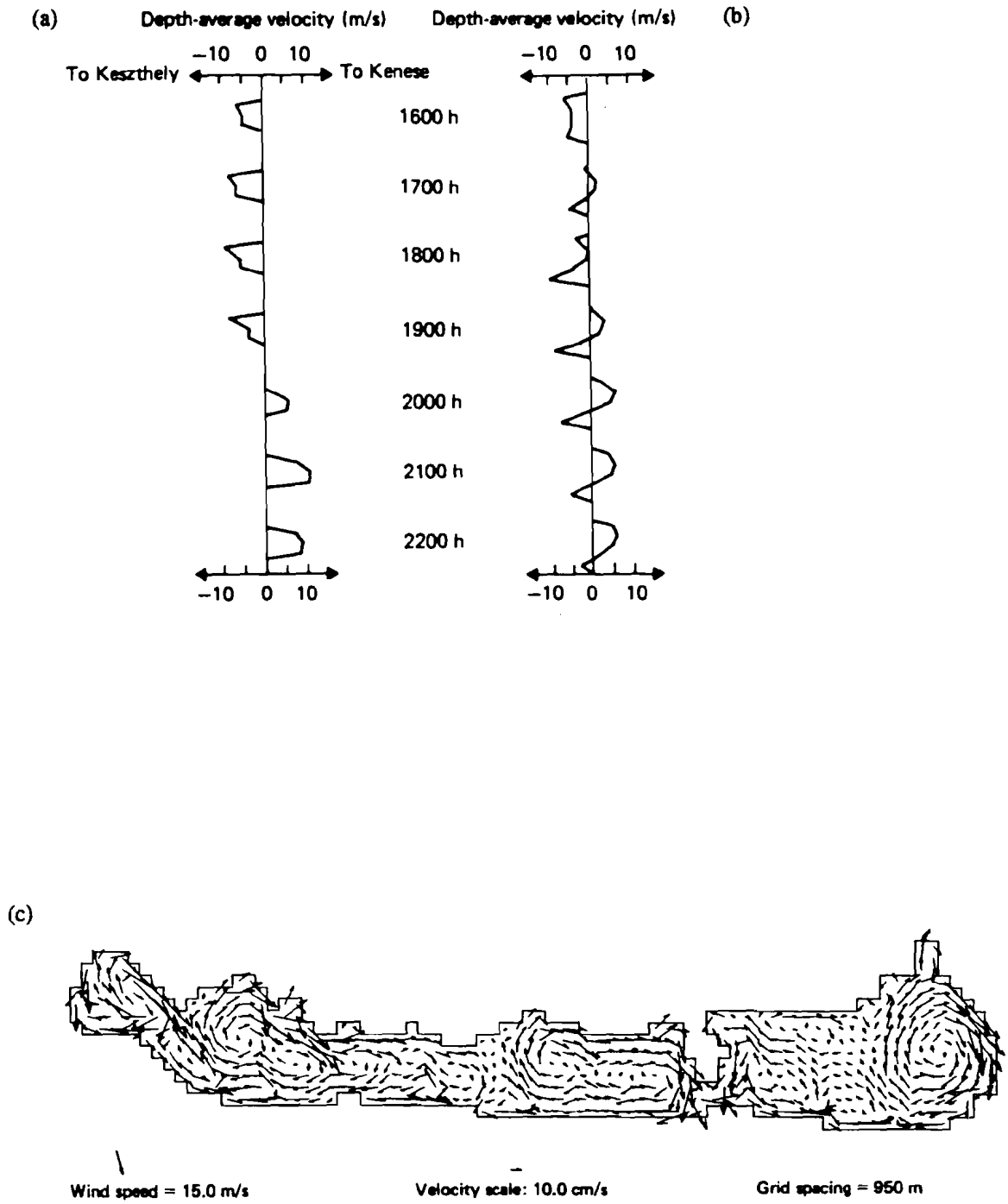

Fig. 6 Simulated lateral velocity distributions on 8-9 July 1963. (a) Middle part of the lake, (b) eastern basin. (c) Simulated steady state circulation in Lake Balaton (Shanahan et al. 1986).

influence water quality significantly, depending on time scales of various processes.

A decade ago computation of flow patterns was strongly limited by the speed and memory of computers available. For this reason the finest grid size used for Lake Balaton was 950 m (for unsteady simulations $\Delta x = \Delta y = 1900$ m was employed). Presently, such a grid is used to obtain a rough impression on the flow, and to derive boundary conditions for certain regions of the lake which are then analyzed by a finer mesh. As an example, Fig. 7 shows the flow for the western half of Lake Balaton ($\Delta x = \Delta y = 333$ m). The overall circulation pattern is similar to that of Fig. 8, but it incorporates much more details. Clearly, the better approximation of the boundary and bottom topography is a major advantage. If additional fine structures of the flow are looked for, in certain domains the grid can further be narrowed down. The smallest grid size used in this case was $\Delta x = \Delta y = 37$ m. For details we refer to Józsa (1990).

Fig 8 illustrates the flow field for the same steady wind condition obtained by the quadtree-based multigrid method (Józsa & Gáspár 1992). The geometry of the lake is approximated nicely, large scale circulations are reproduced well (see also Fig. 7), and currents in the near shore zones are captured perhaps better than by the uniform scheme, despite of the smaller number of computational points.

Fig. 9 shows the joint usage of the flow model and a two-dimensional transport model (see Eq. (12)). The mixing of the water of the Zala River – the major tributary, and major contributor to the external nutrient and pollution loading of the lake – was studied by the particle tracking method. The figure illustrates the distribution of particles after 2 days simulation (10-11 April 1987). Wind direction corresponded approximately to that of previous figures, while the wind speed ranged between 0 and 20 m/s. As is apparent, paths of particles are determined by the large scale eddy observed in Figs. 7 and 8 and by currents along the southern shore (Józsa 1990).

At the end of this chapter we present Figs. 10 and 11, which are analogical to Figs. 7 and 9. This time the full flow model (Eqs. (2) - (4)) and transport model was applied for the Danube to analyze the mixing conditions in the vicinity of the junction of the Váh River, the largest tributary between Bratislava and Budapest. Streamflow rates were 1160 m^3/s for the Danube and 90 m^3/s for the Váh. As is apparent the velocity of the Danube does not show significant spatial changes and the mixing of the water of the Váh River is a rather slow process ($D_y = 0.10$ m^2/s was assumed, see Somlyódy 1977, 1982*b*).

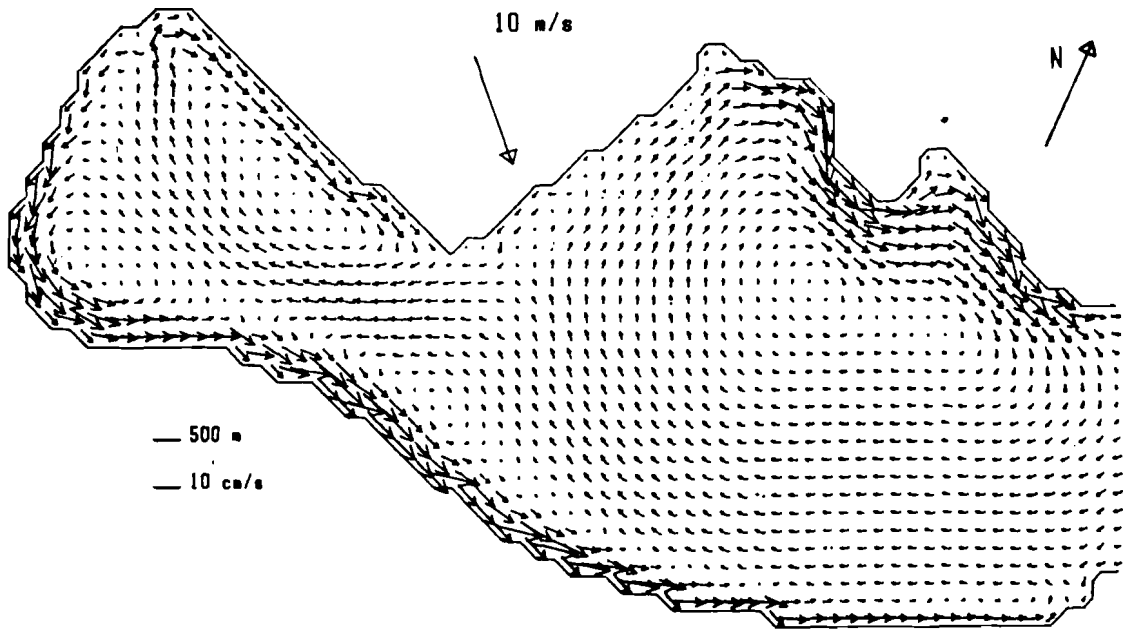

Fig. 7 Simulated steady state flow pattern in the western part of Lake Balaton (Józsa 1990).

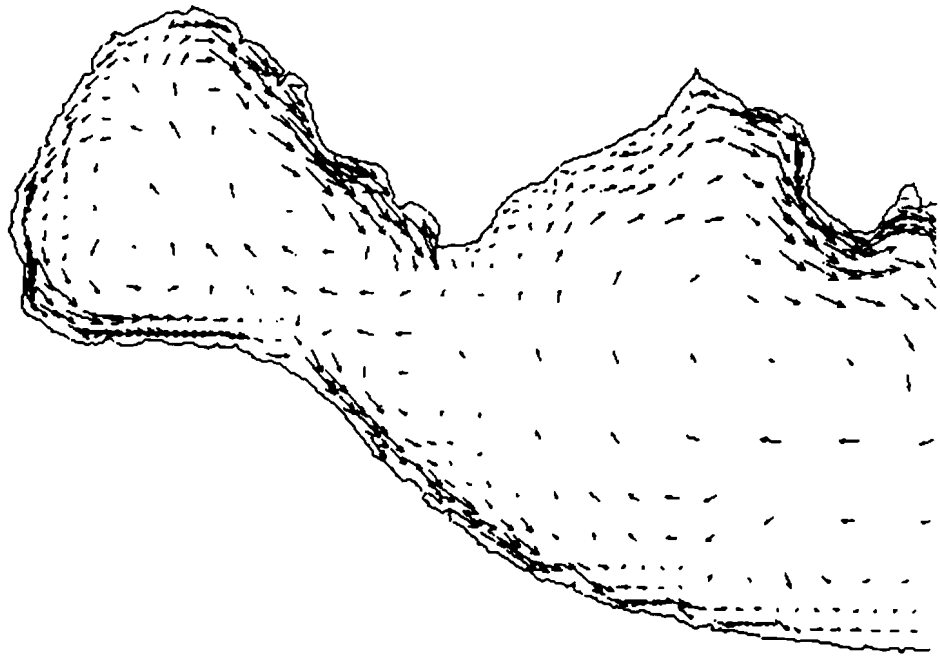

Fig. 8 Simulated steady state flow pattern, multigrid method (Józsa & Gáspár 1992).

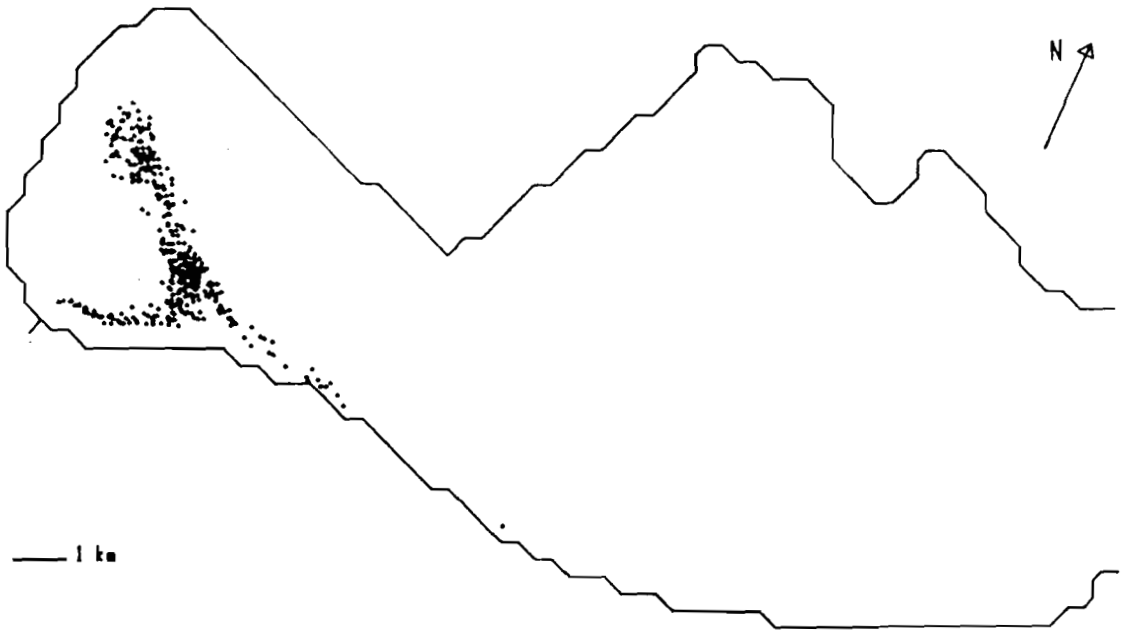

Fig. 9 Simulated mixing of the water of the Zala River in Lake Balaton (Józsa 1990).

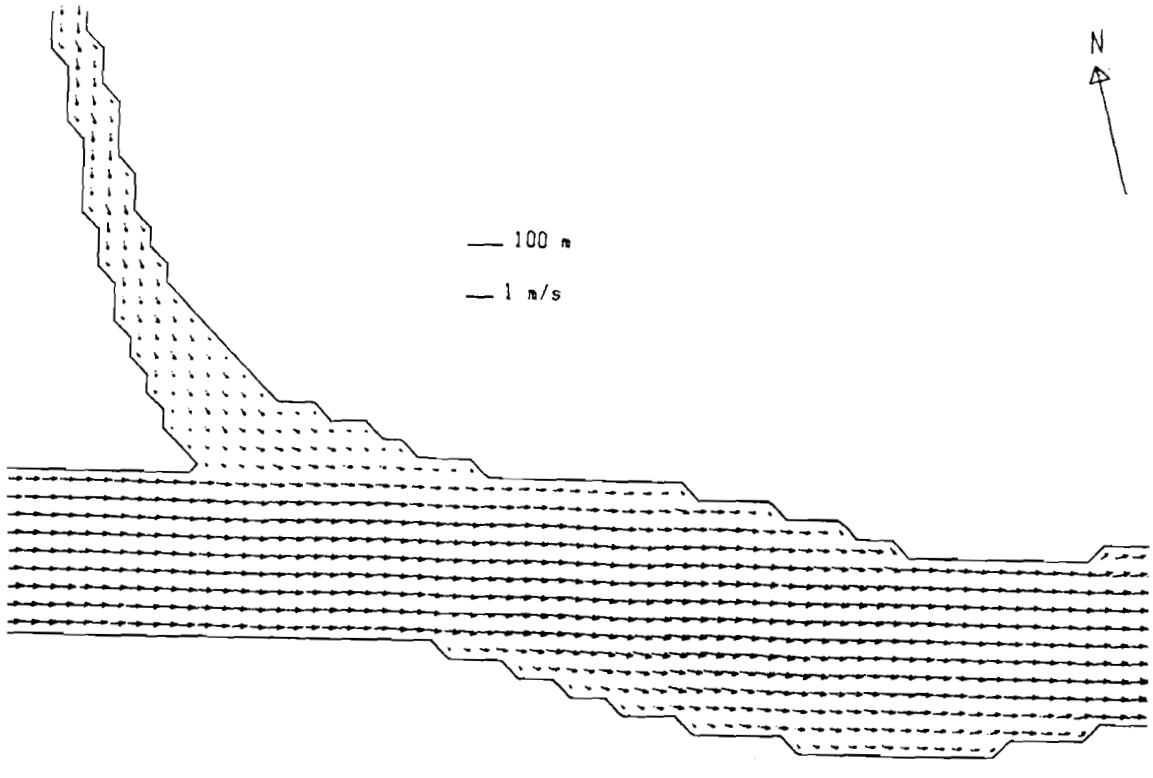

Fig. 10 Simulated steady state flow field at the junction of the Váh River and the Danube.

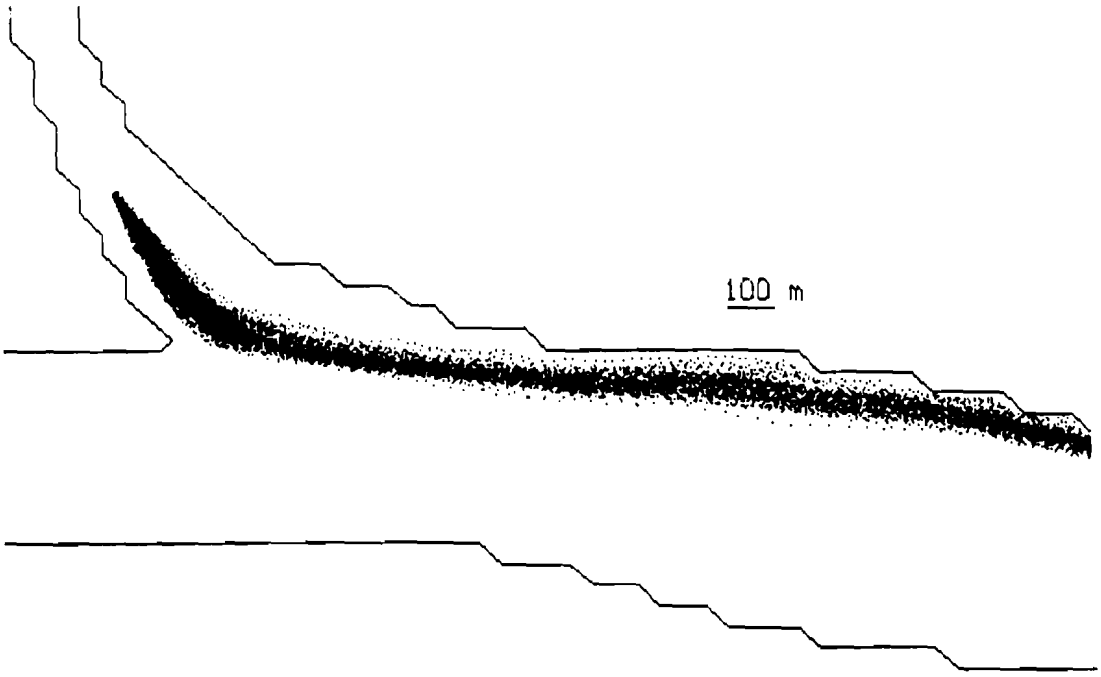

Fig. 11 Simulated mixing conditions at the junction of the Váh River and the Danube.

4 CASE STUDIES

4.1 Why these case studies

As we stated in the beginning, the variety of both water quality problems and surface water bodies is huge. There exists always problems in selecting a finite number of case studies that would provide proper illustration of as many of the most essential features of the modeling work as possible. All of our case studies deal with eutrophication. The reason for this is not that we feel that eutrophication is more important to tackle than the other problems. Instead, our reasons were threefold. First, it is probably worthy to concentrate on one problem domain so as not to label any of the used techniques to a certain problem type. Second, eutrophication is a rather complex problem, and several typical computational features also present in modeling of other water quality problems are encountered. Third, most of our personal experiences are linked to eutrophication modeling and management.

The first study deals with the Danube. It presents the use of flow dynamics based water quality modeling, with strong reference to chapter 3. The second case, Lake Balaton, uses largely the same methodology with a focus on using the descriptive models developed in a management optimization framework. The Lake Kuortaneenjärvi case shows the use of a ordinary differential equation model – without transport equations, but a detailed nutrient and phytoplankton-cyanobacteria description – in ecological sensitivity and scenario analyses in a small, shallow lake. The fourth case, Lake Tuusulanjärvi, concentrates on a variety of other, mainly statistical, modeling techniques besides mechanistic modeling. The case studies proceed from flow dominated water quality models gradually to studies with higher ecological resolution.

4.2 The Hungarian Danube stretch

The motivation for his modeling study was the Gabickovo-Nagymaros barrage system launched in 1977 as a joint project of the ČSSR and Hungary. The scheme was assumed to consist of two barrages: an upstream one close to Bratislava, and the other in the Danube bend in the Hungarian territory. The system was designed for peak operation, with total capacity of 880 MW. A large upstream reservoir with a volume of about $200 \cdot 10^6$ m^3 would also have been necessary.

The construction was stopped by the Hungarian government in several, subsequent steps by the late eighties, and the issue is still a cause of a significant conflict between Hungary and ČSFR (for details, see Somlyódy 1991). Lack of consistent assessments of the impact of the dams on water quality, on the ecosystem, on genetic resources, and on groundwater resources, as well as the growing environmental concern were reasons of the suspension from Hungarian side. The upstream reservoir was considered as a particularly critical element of the system as it could have had a negative influence on surface water quality due to enhanced eutrophication, and subsurface water – a significant potential futu-

re resource for drinking water supply – alike. As a consequence of this a study was proposed to assess eutrophication conditions of the planned reservoir and as a part of this chlorophyll-*a* variations of the entire Hungarian river reach was analyzed. Subsequently, we discuss the latter issue only.

Historical observations show that phosphorus and nitrogen concentrations increased by several times during the past three decades (Somlyódy & Hock 1991) and they are not any longer limiting algal growth. Simultaneously, there was an increase with approximately one order of magnitude in algae biomass leading to chlorophyll-*a* values close or above 150 mg/m^3. This level is typical to hypertrophic lakes. A preliminary analysis has shown that temporal changes in the chlorophyll-*a* concentrations are strongly dependent on how variations in streamflow rate, temperature, and global radiation coincide (Somlyódy 1991). Taking into account the excess supply of nutrients it was decided to develop a model consisting of following elements:

- A diffusive wave model for the flow (with the semi-analytical solution using Fourier series, see section 3.3).

- A water quality model consisting of two state variables, i.e. "winter" and "summer" algae for which Eq. (15) is set by extending it by corresponding reaction terms. These express growth, death, and sedimentation of algae as well as light and temperature limitation (see Eqs. (22*a*) - (28)) formulated for both algal groups, excluding P limitation, i.e. $G_P = 1$). The decision to select two compartments for algae derived again from the analysis of observations, otherwise the description of seasonal changes would not have been possible.

The water quality model was solved on the basis of partitioning (Eq. (37)) using the method of characteristics and the Crank-Nicholson scheme for convection and dispersion, respectively. The reaction step was solved analytically (Bakonyi et al. 1991).

As the boundary condition, observations available at Rajka – the most upstream location of the Hungarian monitoring network – was used. The model was then employed to compute temporal changes at the most downstream cross-section – Baja – close to the southern border, and to derive longitudinal profiles. Weekly observations were available for chlorophyll-*a*, while daily data for the flow, temperature, and global radiation (measured at Budapest) for the period 1980-1985.

Fig. 12*a*. illustrates the calibration of the flow model for 1985. Validation runs have shown similar agreements with observations. Figs. 12*b* & *c* show the comparison of observed and simulated chlorophyll-*a* concentrations (Bakonyi et al. 1991). Calibration was made by simple fine tuning and at the beginning data of 1985 were utilized for this purpose. Agreement was surprisingly good, for both, calibration and verification runs. At a later stage, model parameters were adjusted for each year independently and a small variability – i.e. high stability – was found.

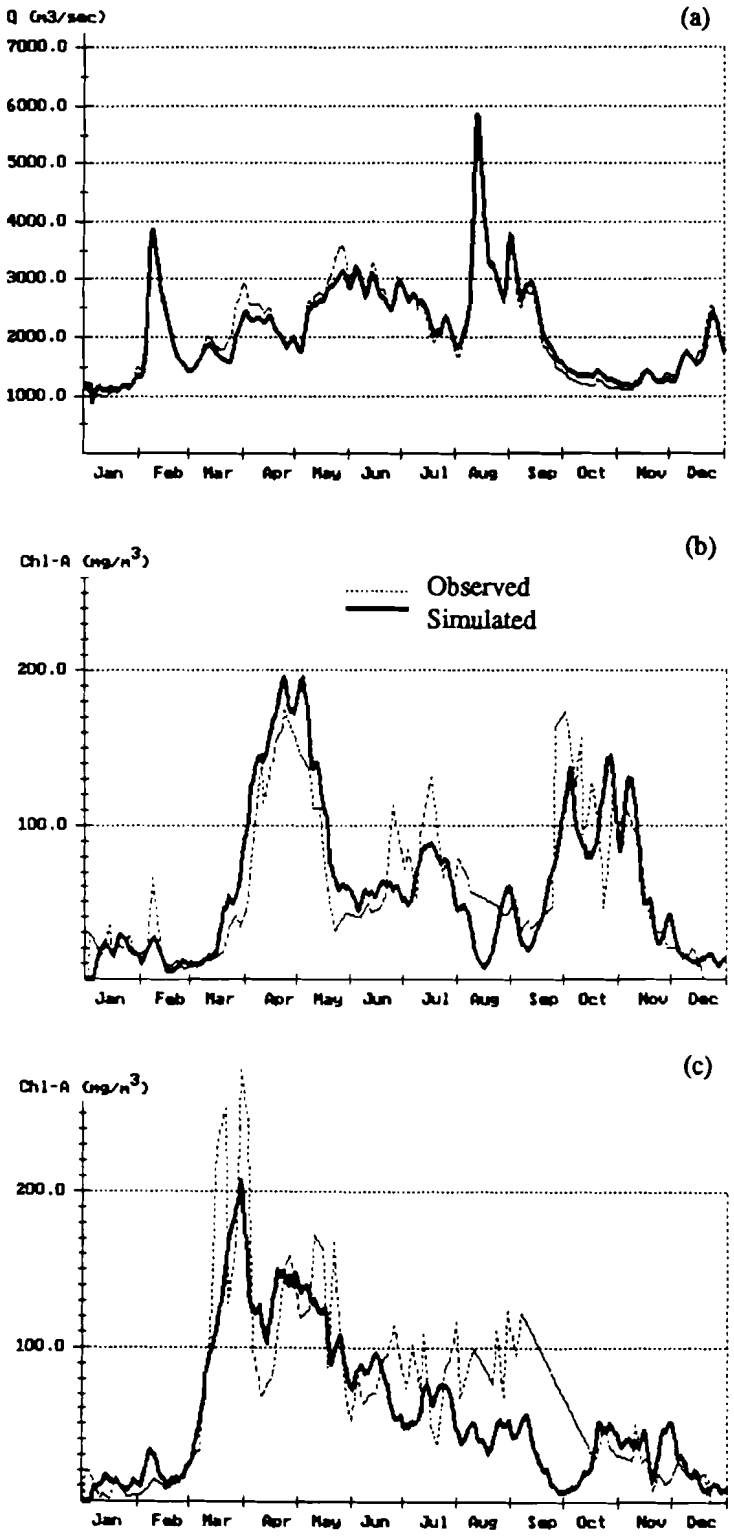

Fig. 12 Danube modeling results at Baja: flow model calibration, 1985 (a), chlorophyll-*a* model calibration, 1985 (b), chlorophyll-*a* model validation, 1984 (c) (Bakonyi et al. 1991).

In spite of the overall good performance of the model, there are changes and peaks which are not captured properly. In this respect we can speculate only on the role of longitudinal variation of temperature, spatial change of climate conditions, suspended solids as influencing light conditions, and finally on all other shortcomings in our knowledge to describe complex processes affecting water quality.

4.3 Lake Balaton

The lake (596 km^2) and its watershed (5776 km^2) are illustrated in Fig. 13. The region is the most famous recreational area of Hungary, also subjected to intensive agricultural cultivation which jointly led to eutrophication of the water body. This is particularly strong in the most western segment of the lake, the Keszthely basin (Fig. 13) to which half of the total catchment area belongs, resulting an order of magnitude higher volume related nutrient loads than in the mesotrophic Siófok basin. Thus water quality varies longitudinally: it is hypertrophic in the western end and gradually improves to the east. The lake was phosphorus limited around the late seventies. For today excess nutrient supply became typical, at least for the western half of the lake (see later).

The study which was undertaken at the late seventies and early eighties had two major objectives (Somlyódy & van Straten 1986):

- To understand major physical, chemical, and biological processes influencing eutrophication and to integrate them into a modeling framework.

- To develop an "optimal" eutrophication control strategy (focusing primarily on the specification of short-term actions needed) on the basis of the descriptive stage of the analysis following the principle of decomposition and aggregation.

To meet the objectives outlined above detailed experimental programs were realized during the study. Among others we mention here the detailed monitoring of the nutrient loads on the Zala watershed (Fig. 13), phytoplankton studies, research on the role of sediment in nutrient cycling, wind induced sediment-water interaction, and wind induced lake circulation.

Here we will consider the first issue mentioned and illustrate step by step various combinations of hydrophysical and biochemical processes, in the modeling framework, from the rather complex treatment to a simple one with the aim to find the relative importance of processes included. As management modeling is concerned, the reader is referred to Somlyódy (1986) and Somlyódy & Wets (1988).

(1) As the first step of analysis, a decision was made on spatial dimensions: a longitudinally 1D treatment was felt appropriate. The argument behind this choice was manyfold:

- On the basis of the longish shape of the lake and the prevailing, "perpendicular" wind direction effective mixing was assumed in cross-sections.

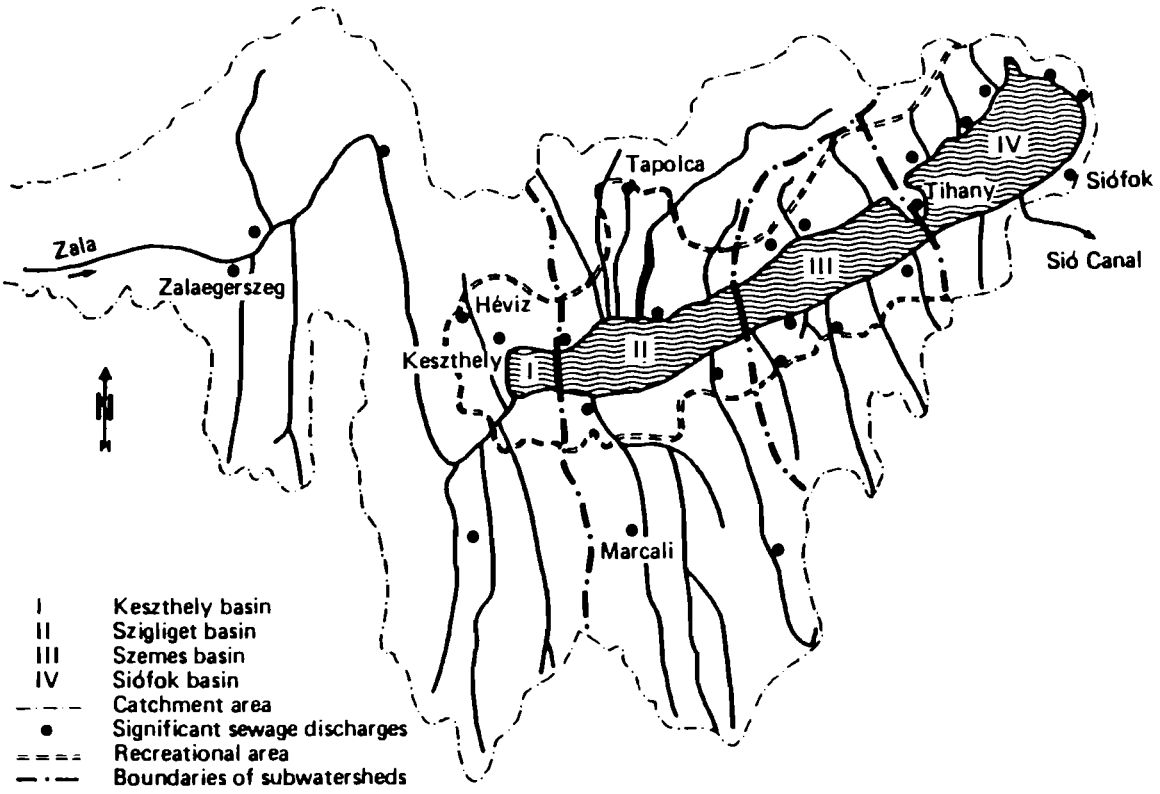

Fig. 13 Lake Balaton and its watershed.

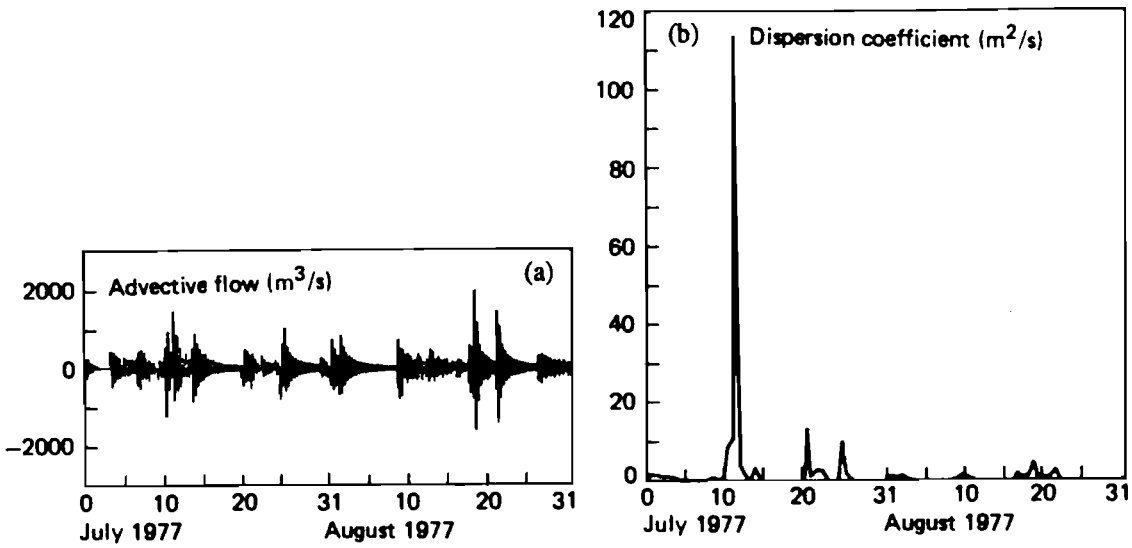

Fig. 14 Advective flow (a) and diffusion coefficient (b) in the middle section of the Siófok basin (Shanahan et al. 1986).

- Available data have shown pronounced longitudinal changes.

- The observational requirement of a 2D model would have been irrealistically high.

Thus the basis of our nutrient cycle model is a classical longitudinal dispersion equation (see Eq. (15)) incorporating the physical characteristics, i.e. the longitudinal velocity $U = Q/A$ and the dispersion coefficient, D_L. Their derivation for a highly variable flow pattern typical for Lake Balaton (see Figs. 5 - 8) is far from being a trivial task.

(2) The computation of the longitudinal advective flow can be done relatively easily. For instance a 1D hydrodynamic model can be employed or results of the 2D model (see Fig. 6*a* and *b*) can be integrated over the width of the lake. Flows obtained this way are shown for two months in Fig. 16*a*. As can be seen, peak values reach 2 000 m^3/s (typical for the Danube at Budapest) but the mean is close to zero due to intensive seiche influence (the situation is similar to a tidal motion).

The dispersion coefficient caused much more difficulties. Eventually the method of Holley et al. (1970) developed for oscillatory flows was extended by assuming that lateral advection due to wind-driven currents dominate (see Shanahan et al. 1986 for details). Results obtained for the middle part of the Siófok basin (see Fig. 6*b*) are shown in Fig. 14*b*. Apparent is the large fluctuation in D_L following the sequence of stormy events. As longitudinal changes are considered alterations in the lake's geometry (see e.g. the Tihany peninsula, Fig. 13) play a significant role (Shanahan et al. 1986). The mean value of the longitudinal dispersion coefficient is about 1 m^2/s (which would be quite acceptable for the Danube).

(3) As we noted in section 3.4 several eutrophication models were developed for Lake Balaton (see Fig. 4). They all assumed that the lake consisted of four completely mixed reactors connected in sequence by hydrologic throughflow. Results obtained by the simplest reaction process description, SIMBAL, which was discussed in section 3.4 (see Eqs. (22*a*) - (22*c*) set for two algal groups as mentioned earlier), are shown in Fig. 15 (a discussion on the model performance will be given later).

(4) In order to test the role of advection and dispersion, process equations of SIMBAL were incorporated into a set of longitudinal dispersion equations by known $U(t, x)$ and $D_L(t, x)$ (see Fig. 14). The numerical solution was obtained as outlined in section 3.5. Such a model is capable now to perform a sequence of sensitivity analyses. For instance, for Lake Balaton it turned out that advective flow plays a negligible role only, the back and forth motion of a couple of hours time scale does not influence daily changes of algal biomass. Similarly, temporal and longitudinal variations of D_L were found unimportant and $D_L(t, x) = 1$ m^2/s gave an acceptable approximation.

The sequence of sensitivity analyses already suggested that significant amount of details of hydrodynamic and transport processes are filtered out by chemical and biological reactions and thus a simplified description for the spatial transport can be quite acceptable.

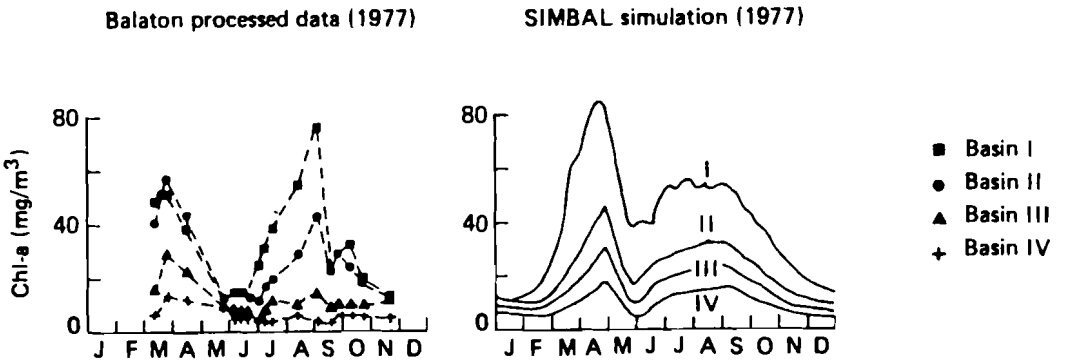

Fig. 15 Phytoplankton simulation for Lake Balaton with a simple P cycle model, SIMBAL (van Straten 1986a).

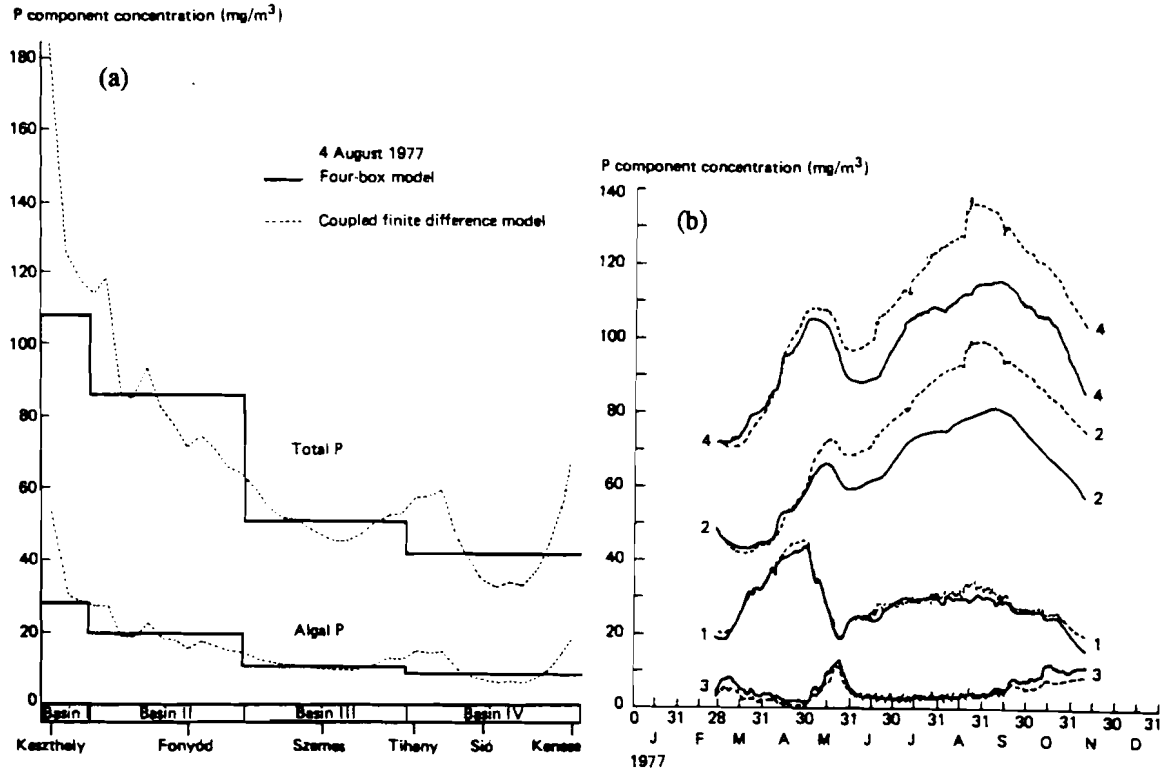

Fig. 16 P distibutions (a) and dynamics (b) predicted by the four-box model and the coupled finite difference model in Keszthely basin (Shanahan & Harleman 1986). 1 = total algal P, 2 = detrital P, 3 = dissolved inorganic P, 4 = total P. Full line = prediction by the four-box model, dashed line = prediction by the coupled model.

(5) Comparison of the four-box model and the "continuous" model is shown in Fig. 16. As can be seen, some of the spatial details are lost when using the ODE model, but temporal changes of algal P, perhaps the most important variable, do not exhibit remarkable deviations in comparison to the detailed model. Thus, the conclusion is that the four-box model is an adequate predictor of the lake's P dynamics (at least on the diagnostic level).

Knowing all the details of the rather complex circulation pattern and irregular temporal changes, the above conclusion may be a surprise at the first glance. A closer look, however, would resolve our doubts (at least after the detailed study was done). First. the compensating role of time scales of various processes is mentioned again. Secondly, the role of implicit dispersion depending on the selection of box sizes is stressed. For Lake Balaton it was close to the physical dispersion (except perhaps the first "reactor") and this was the reason for the "success". The resulting overall conclusion is that the number and volumes of boxes should always be selected very carefully on the basis of the physical dispersion. As details of such a design procedure is considered the reader should consult with Shanahan & Harleman (1984).

After showing that the relative importance of various processes can lead to descriptions deviating significantly from disciplinary precise ones, we return to calibration results of SIMBAL, the simplest P cycle model for the four basins (Fig. 15). Apparent is that the model persistently gives a fairly flat chlorophyll-*a* curve in summer, whereas the actual data are much more peaky. Calibration of other models mentioned earlier shows discrepancies of similar extent and validation runs are perhaps even more "disappointing". This is not an exceptional situation in the field of eutrophication modeling: it is difficult to find an example of a really satisfactory validation of shallow lakes in the literature. Reasons are manyfold, i.e. the "stochastic" behavior of such water bodies depending on hydrologic, meteorologic and climate conditions, improper data collection, and our limited knowledge in the fields of sediment chemistry, mortality processes, algae growth limitation, algal species succession, and the behavior of blue-green algae. The existing shortcomings clearly call for improved description of reaction processes which, however, cannot be done without increasing significantly the effort on data collection and experimental research.

So, there is much to be improved. But the question now is: can such apparently deficient models be utilized for management purposes? If we were asked to make a detailed prediction about future algal dynamics we would certainly be unable to do so. Anyhow, since the models on an annual basis follow the phytoplankton levels from year to year and since this means that the models respond reasonably well to different loads and weather conditions, we may still use them in investigating how indicators of eutrophication management (i.e. the annual chlorophyll-*a* concentration) respond to external load reductions.

Such a load response function is given in Fig. 17 for the four basins of Lake Balaton as derived from the dynamic model (we note that the behavior of other models show remarkable similarities). Two features of the figure are underlined. First, despite quite strong nonlinearities in the models, the response curve is almost linear. Second, the models agree that a full suppression of algal blooms on the short run is not achievable, not even at zero loads if this were even realizable. The reason is the P release from the

sediment, the so-called internal load which was estimated to be roughly equal to the internal load for Lake Balaton. It is clearly a sign of advanced eutrophication and the lack of control program at the right time.

Postponement of launching a lake restoration program will obviously lead to a shift of the load response curve and its saturation nature will become apparent. As an example we refer to Lake Tata, a small hypertrophic shallow lake (~ 2 km^2) close to Budapest (retention time is about a month). The specific load is approximately 50 times higher than that of the Keszthely basin. As a result of this, conditions are favorable practically throughout the entire year to maintain chlorophyll-*a* levels as high as 400 to 500 mg/m^3. This is illustrated in Fig. 18*a*, together with simulation results of a four compartment P cycle model similar to SIMBAL (see Eqs. (22) - (28)). The agreement between observations and model computations is much closer than in the case of Lake Balaton. Actually, the modeling of a highly loaded system with a phytoplankton structure of low diversity is a much simpler task. The load response curve corresponding to Fig. 17 is shown in Fig. 18*b*. It illustrates that a significant load reduction is needed to achieve even a minor change in algae biomass and the internal load in itself will be capable to maintain hypertrophic conditions in the lake. The management of such a degraded lake is an expensive task requiring the direct treatment of the sediment in order to reduce its P release.

Shallow lakes are strongly affected by random changes in hydrologic and weather conditions particularly if non-point source loading plays a significant role. Control actions can influence differently the mean values of chlorophyll-*a* concentration (used as a management indicator) and its variability, and for this reason an evaluation of the statistical distributions is unavoidable. For Lake Balaton synthetic time series generators were developed for nutrient loads (as controllable factors) and climatic parameters. The dynamic P cycle model was then used in a Monte Carlo fashion: the results for the Keszthely basin are summarized in Fig. 19.

The figure shows that the linearity is held as before, not only for the mean, but also for statistical properties (standard deviations and extreme values). When controlling sewage only, the expected chlorophyll-*a* maxima changes, but the variance obviously remains more or less unchanged since most of the stochastic features and uncertainties in loads are associated with tributaries. These can be controlled by pre-reservoirs such as the Small-Balaton system (Somlyódy 1986). The sensitivity of the model and the lake to variations in weather conditions is strikingly large. Taking also into account the "slow" recovery of the sediment, this means that after reducing the external loads, the lake may approach a new equilibrium with considerable fluctuations.

The load response functions as shown in Fig. 19 can now be incorporated into a management optimization framework. The latter obviously requires the definition of major nutrient load components (see Fig. 13) for point and non-point sources, control variables, objective functions, and constraints. With respect to details of the models developed, including a stochastic optimization approach we refer to Somlyódy (1986) and Somlyódy & Wets (1988).

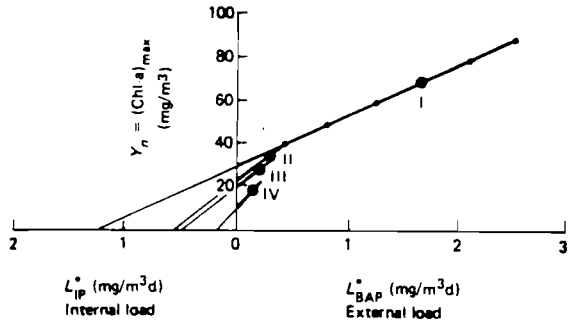

Fig. 17 Load response model for Lake Balaton. L^*_{BAP} = biologically available P load. I...IV = basins as defined in Fig. 15 (Somlyódy 1986).

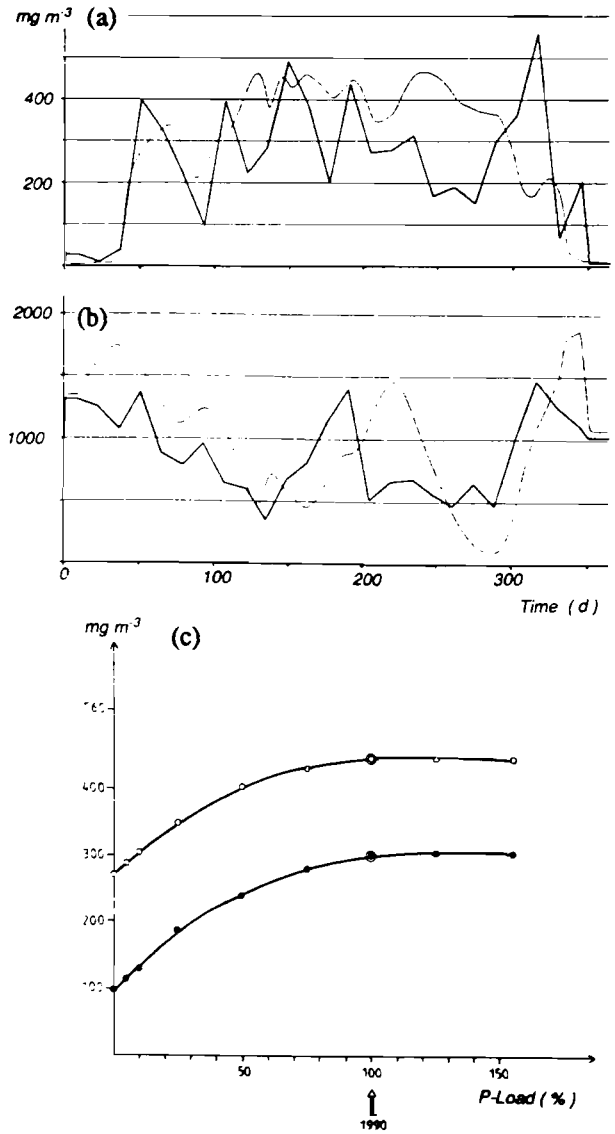

Fig. 18 Lake Tata: Calibration of a P cycle model, 1990 ((a): chlorophyll-*a* [mg/m³], (b): PO_4-P [mg/m³]). Thin line = simulation, thick line = observation. (c): Change in the chlorophyll-*a* concentration as a function of the external P load. Upper line = summer mean, lower line = annual mean chlorophyll-*a*.

The short-term optimal strategy worked out served as the basis of the governmental policy making procedure in 1982 and 1983 (Somlyódy & van Straten 1986). The process had just started, when a striking mass proliferation of N-fixing species, *Anabaenopsis raciborskii*, occurred in August 1982. The chlorophyll-*a* level was roughly doubled for the whole of the lake, in comparison to values observed earlier.

Since 1983 most of the planned control measures were implemented (by P precipitation on waste water treatment plants, sewage diversion, and the construction of the upstream element – ~ 20 km^2 surface area – of the Small-Balaton reservoir system at the mouth of the Zala River, Fig. 13) roughly halving the external P load. As a result, further water quality deterioration was stopped but no spectacular improvement was observed. The reasons were: (a) the significant role of the internal load (see Fig. 17 and Istvánovics 1988), and (b) the dominance of blue-green algae species fixing N from the atmosphere, Thus, at present the trophic state of the lake, in particular in western segments, is determined by sediment-water and water-atmosphere interface processes.

Considerable changes in the phytoplankton structure led to an alteration in the seasonal pattern of the biomass: spring peaks have disappeared and more than 90% of the biomass is governed by *A. raciborskii* in August and September. Simultaneously with this shift, algal dynamics is dominated by light and temperature factors, nutrients having a minor role. A simple phytoplankton model can easily be calibrated and validated as shown in Fig. 20 for the Keszthely basin.

The comparison of Figs. 15 and 20 illustrates major shortcomings in "ecological" modeling: a model can be fitted to given states of the ecosystem (though even this step can be problematic), but our knowledge is not satisfactory enough to predict the transition between two such subsequent states.

4.4 Lake Kuortaneenjärvi

Lake Kuortaneenjärvi (62°45'N, 23°30'E), Finland, is a polyhumic lake with surface area of 16 km^2, mean depth of 3.7 m, and catchment area 1280 km^2. The use of the lake for recreation and fisheries is substantially dteriorated by eutrophication, in terms of excessive cyanobacteria (blue-green algae). This was also the motivation for this study. A model was needed to analyze the competitive ability of N-fixing cyanobacteria, mainly *Aphanizomenon flos-aquae*, against other planktonic algae. The data was collected in one growth season, summer 1980. Due to the character of the lake in terms of shallowness, modest surface area, and unstable sumer stratification, together with the data, and the management problem, the lumped parameter approach with no spatial description was chosen. The model was used as a basis for a number of simulations, reviewed in brief below.

The model

The dynamic model (Varis 1988) consisting of 15 ordinary differential equations, which

are nonlinear with respect to states and parameters. They hence contain only the reaction term. Annual dynamics of P, N, cyanobacteria and other phytoplankton are computed (Fig. 21). When constructing the model, the submodels were first calibrated separately and thereafter iterated to fulfill the mass continuum. This modular, decoupling approach essentially reduced the degree of freedom in identification, since at each step there were only a few parameters to be estimated. This procedure also helps to diminish the drawbacks of uncertainty and reliability, discussed by, e.g. Young (1977) and Beck (1983), which are unavoidably related to the mechanistic modeling approach used.

Simulation studies

In two of the simulation studies (Varis 1988, 1992*a*), the range of application of the model was extended by introducing perturbations to P and N loads (Fig. 22), water temperature and irradiance. In the third simulation study (Varis 1989), outflow was subjected to perturbations.

First, the relative physical limiting roles of the following four growth factors of algae were simulated (Varis 1992a): dissolved inorganic P (DIP), dissolved inorganic N (DIN), water temperature, and irradiance. The importance of the N to P ratio as a driving factor of the formation of the *A. flos-aquae* dominance has been emphasized in numerous studies. The good fit gained in the calibration of the DIN:DIP ratio (Fig. 23*a*) was the key to the analysis of the competition between the N-fixers and other algae. The equal temporal pattern also appeared in the proportional growth limitation scheme (Fig. 23*b*). As summer progressed, N became increasingly dominant over P as the limiting nutrient. Nutrients constituted a notable limitation only during the ice-free period. A set of scenarios on changing nutrient loads to the lake were performed (Fig. 24). Feasible ranges around the nominal input values for 1980 were chosen for the input values considered. For each input variable and each run, a perturbation of a given quantity was introduced to the whole input array of 360 entries.

The increase in N load caused a decline in the biomass of blue-green algae when the N load was low. The competitive ability of N-fixers was diminished by the decreased importance of N as a limiting factor and by the great biomass of other algae competing for the same resources. N-fixing cyanobacteria were favored by the increased P load, since the relative availability of N decreased and a lack of N occurred earlier in the succession procedure. The competition was very sensitive to changes in water temperature but not to changes in irradiance.

The model was not equally sensitive to inputs over the whole year. The temporal sensitivity of the algal competition was analyzed to find out the impact, including lags, of perturbations in the input nutrient loads (Varis 1988) and outflows (Varis 1989) on different dates. The perturbations of 10% were made by changing values of input variables throughout the simulation period so that for each run, a value of only one day and one variable group was perturbed.

The sensitivity of the model to perturbations showed a very rapid increase in

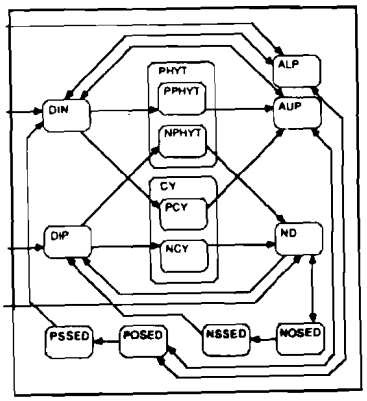

Fig. 21 A flow diagram of the Lake Kuortaneenjärvi model. DIN & DIP = dissolved inorganic N & P, PHYT = eukaryotic phytoplankton, PPHYT = P in PHYT, NPHYT = N in PHYT, CY = cyanobacteria, PCY = P in CY, NCY = N in CY, ALP & AUP = allochtonous & autochtonous detrital P, ND = detrital N, PSSED & POSED = inorganic & organic P in sediment, NSSED & NOSED = inorganic & organic N in sediment.

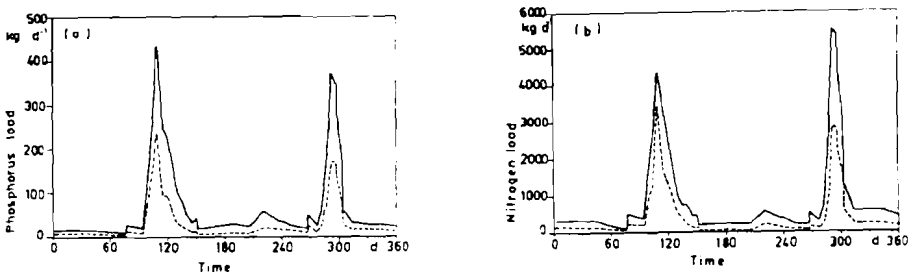

Fig. 22 Nutrient inflow, (a) P, (b) N, in 1980. Solid lines denote total load, broken line dissolved inorganic nutrients.

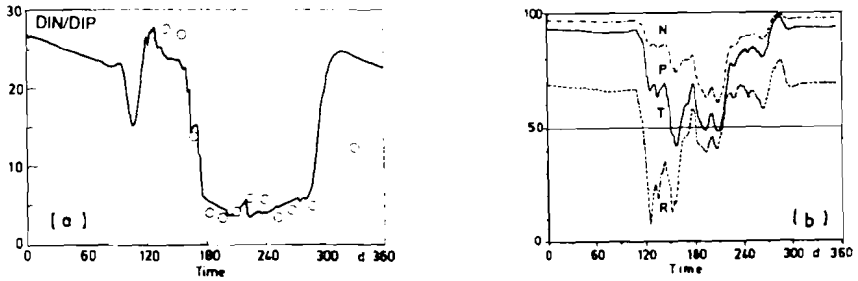

Fig. 23 (a) Model calibration results of the ratio of dissolved inorganic N and P (—— = computed, o = observed). (b) Simulated relative importance of dissolved inorganic N and P, water temperature (T), and irradiance (R) to phytoplankton growth limitation (cyanobacteria excluded).

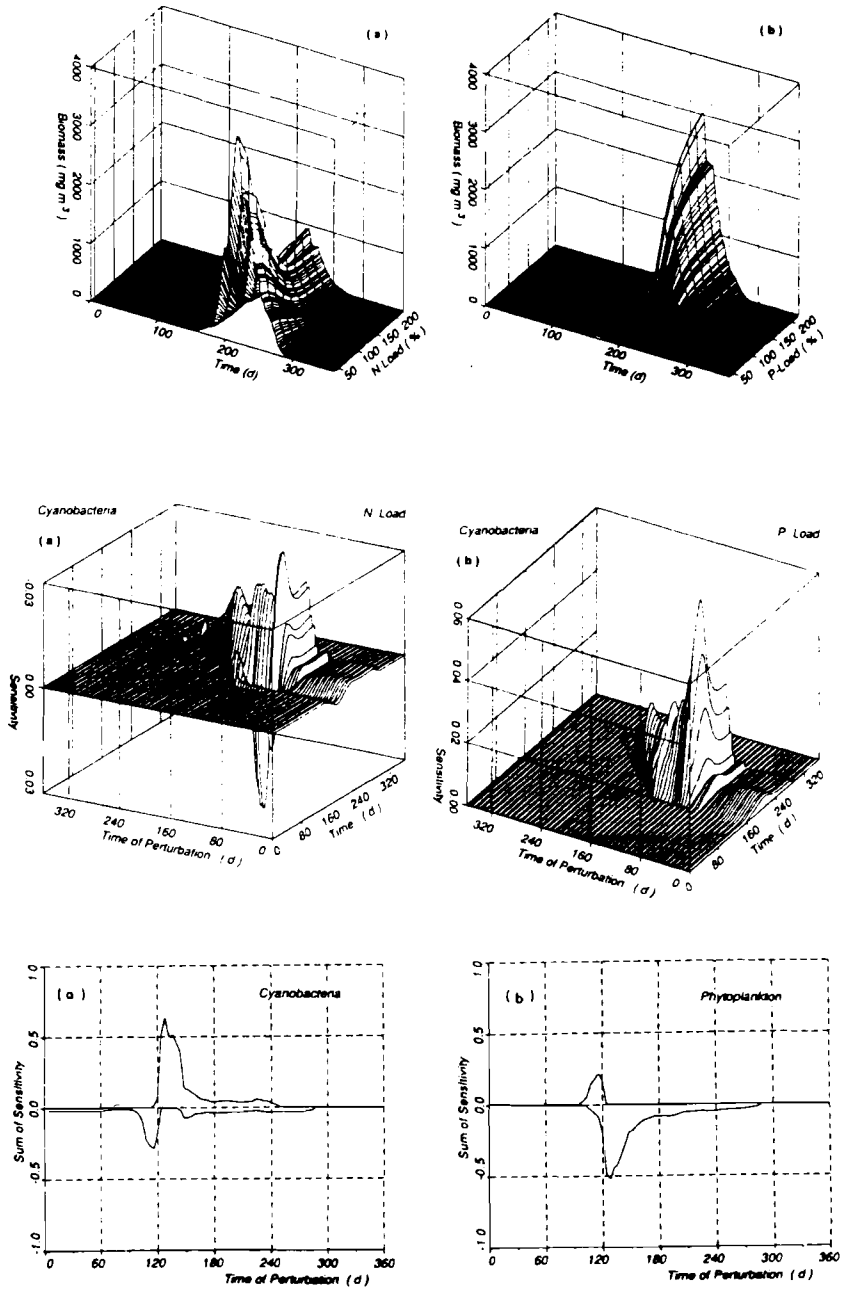

Fig. 24 Selected simulation results from the Lake Kuortaneenjärvi study. *Up:* Simulated fresh biomass of cyanobacteria plotted against (a) N load and (b) P load and time (Julian dates). The 1980 load is used as the nominal (100%) situation. *Middle:* Relative sensitivity of cyanobacteria to time domain perturbation in (a) N load and (b) P load. *Low:* Relative sensitivity of (a) cyanobacteria and (b) eukaryotic phytoplankton to time domain perturbation in water outflow.

spring, between the Julian dates 90 and 100. The sensitivity of algal dynamics to nutrient perturbations was at its maximum in April. The decrease in sensitivity thereafter had a roughly exponential form. Liebigian limiting factors and factors connected with ecological competition differed profoundly in their effect on the periodicity of algae. The response of cyanobacteria to the perturbations was systematically two to five times as great as the response of phytoplankton.

The simulated impacts of the outflow perturbations to the competition between cyanobacteria and phytoplankton can be summarized as follows. If the outflow was increased by 10% during the rising flood – Julian dates 90 to 120 – the cyanobacteria biomass was decreased by a few percent. From the flood peak to the end of the flood season – Julian dates 120 to 150 – the direction of the impact was the opposite: An increased outflow accelerated the growth of cyanobacteria. After the flood, the sensitivity was almost nonexistent. These results imply that the rising flood should not be captured in the lake, but that the lake should rather be filled after the flood peak. The key factor contributing to this phenomenon in Lake Kuortaneenjärvi is apparently the short retention time, in connection to the strong water quality changes, i.e. sharp decrease in the N/P ratio during the spring flood.

Concluding remarks

The model appeared to behave in a logical manner, and the outcome was coherent with theoretical and experimental knowledge on ecology. So the assumptions made during the construction of the model appeared justified. The model appeared adequate for perturbation analyses. The model has additionally been used in methodological studies on the use of D-optimal experimental design approaches to complex nonlinear models (Kettunen et al. 1989, 1992).

The level of adequacy of the results in describing the behavior of the lake ecosystem studied still remained unclear. The results are an outcome of an educated imagination rather than inductively sound evidential inference. If a causal model is validated against observations or prior knowledge, what is then the informativity of the whole exercise? In this case, the answer includes the possibilities to perceive a strict coherence of causal hypotheses, and to extrapolate the observed situation.

The concept of temporal sensitivity is fairly absent from classical limnology. It is, however, often encountered in practice as an important point in practical water quality management, e.g. when designing a regulation or monitoring policy for a watercourse, in non-point source pollution management, or when considering the level and timing of waste water treatment. The perturbation approaches used are suitable for analyses of badly defined systems and their models, since they are easy to apply once a simulation model is available for the lake, and they resulted in an informative outcome at least in this application.

The modeler of a large-scale environmental system is faced with the problem of model aggregation. From the real system with infinite dimensions, a model may contain

only items essential to the problem studied. In this case, the data available also constituted an essential constraint to modeling. The model does not take into account possible changes in dominant algae species nor the control of zooplankton and fish.

In a data-poor case, the approach used here may be recommended and is suitable for application in environmental planning and research. A physically parameterized model can serve to examine the dynamic behavior of the system and interrelationships between the quantities studied. Overparameterization, as was the case in this study, is certainly a problem (Young 1977, Fedra et al. 1981), but if the model is applied with expertise and individually tailored, rather modest data sets can be utilized effectively for management and research purposes, with a type of inference which cannot be obtained through inductive, purely data based analysis. Parameter identifiability studies (Walter 1982, Godfrey & DiStefano 1987) are suggested for further works, although not done in this study. The justification for using physically based models, even with spatial resolution and using partial differential equations, is evidently the greater the more well-established prior descriptions are available for the physical processes studied.

4.5 Lake Tuusulanjärvi

Lake Tuusulanjärvi (60°28'N, 25°03'E), southern Finland, became eutrophicated in the late 1950s. Since then, excessive summertime biomasses of cyanobacteria (blue-green algae) have constituted a great problem to the use of the lake. The lower water layers have been mechanically aerated since 1971 during winter stratification. Before suspension of nearly all point source loading to the lake in February 1979, roughly one half of the nutrient loading came from municipal sewage discharge. In recent years, efforts have been directed to investigations of ecological and socioeconomic impacts of possible extraction of additional water discharge to the basin. The Lake has a surface area of 6.0 km^2, catchment area of 92 km^2, and mean depth of 3.2 m.

Lake Tuusulanjärvi has been a subject to regular water quality monitoring for three decades. Sampling for standard physical and chemical analyses has been running on a monthly basis. Phytoplankton sampling has been concentrated on summer months. This data set has been analyzed using a selection of computerized mathematical and statistical techniques, with both methodological and limnological scopes. Many of the substudies are still in progress, but all the approaches reviewed provide a potential for either practical decision support tools or approaches in the scientific research, or both. Most of the techniques documented below differ intentionally from the outline of the report, in order to give perspectives on other effective approaches besides deterministic modeling. The limnological interest of our studies has been focused on the dynamics of cyanobacteria and nutrients, and on lake restoration.

Data analysis

Due to the complex nature of aquatic ecosystems, statistical data analysis is always to be

included in a basic toolbox of water quality modelers. In this case, studies focusing on both methods of water quality trend detection as well as discovering structural properties of observational series are reviewed.

- *Trend detection* The main goal of the study by Kettunen et al. (1990) was to detect possible changes of the water quality during the years 1960-1988. The software by Cluis (1988), utilizing the properties of inertia plotting and nonparametric statistics, proved to be an applicable tool to study seasonal, strongly autocorrelated, non-normal, sparsely and unevenly distributed data. Volume averaged time-series of various water quality indicators were analysed to detect either linear or step changes. At least one significant change was detected in each of the water quality indicators (Fig. 25), except temperature, oxygen and chlorophyll-*a*. The possible effect of waste water diversion in 1979 from the lake was analysed by comparing the distributions of water quality indicators in the 1970s and 1980s. The reduction of waste water loading had the greatest impact on N compounds in the lake. Also the reduction of algal biomass, chloride concentration and conductivity were significant. On the contrary, turbidity and iron concentrations and color of the water increased after the diversion.

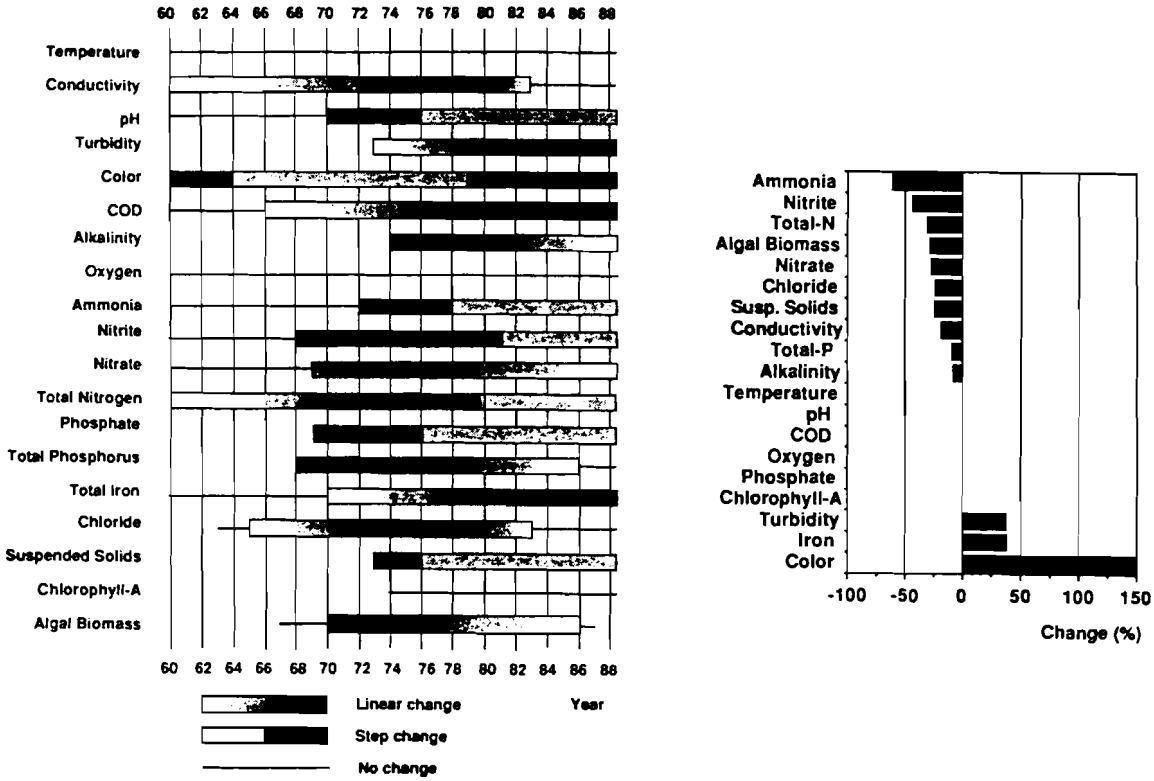

Fig. 25 Significant water quality changes detected in the data of Lake Tuusulanjärvi 1960-1988 (*left*), and relative changes of different water quality indicator mean values in Lake Tuusulanjärvi between 1970s and 1980s (*right*).

- *Multivariate analysis* The phytoplankton community impacts of the restoration measures were studied using multivariate analysis (Varis 1990, 1991*a*), with the focus on cyanobacteria. The monitoring data was used. Most characteristic in the development of the cyanobacteria was the almost complete disappearance of *Oscillatoria* blooms in the lake after the suspension of the sewage input in 1979, and substantial increase in *Aphanizomenon*. Also some slight increase was seen in *Anabaena* and *Microcystis* (Fig. 26). Cyanobacteria are coded from 1 to 10, chlorophyta from 11 to 31, chromophyta from 32 to 47 and cryptophyta with 48.

Seven environmental variables water temperature, pH, total N, NH_4-N, NO-N (NO_3-N + NO_2-N), total P, and PO_4-P, were included in the study. Additionally, the ratio of dissolved inorganic N and P (DIN/DIP) was taken into account since the N to P ratio has very often (e.g. Schindler 1977, Smith 1983) referred to as an important factor driving the formation of cyanobacteria blooms. For the purposes of this study, the monitoring data was not homogenous enough, with respect to methods and timing, until from 1970. The total number of instants to be included was 124.

The above development was studied using canonical correlation analysis, in which the maximum between-set correlation between linear combinations (canonical variates) of variables in two or more sets of variables is found (see e.g. Giri 1977, Gnanadesikan 1977). In this study, two sets, the algae and the growth factors, were used. The main development pattern due to restoration of the lake is the shift from *Oscillatoria* to *Aphanizomenon*. In the correlation diagrams, *A. flos-aquae* is the cyanobacter with the strongest negative correlation with N and the DIN/DIP whereas *Oscillatoria agardhii* (8) is the one with least negative correlation. The analysis was unable to make clear distinction between *Microcystis* and *Anabaena*.

The traditionally diagnostic use of canonical correlation analysis was extended to predictive modeling by Varis (1991*a*). The poweful technique has been applied by Kløve et al. (1992) to constitute the bacteria submodel of an on-line monitoring and prediction system for Kerava River quality, Finland.

- *Resolution of data* The uncertainty of water quality data was studied by Kettunen (1991) using the Kriging technique (Journel & Huibregts 1978). The monthly, volume averaged total P series was interpolated to represent weekly and biweekly observations of water quality with the respective uncertainty estimates. Also, bimonthly, 3-monthly, and annual averages and their variances were constructed by regularization. The uncertainty of the different averagings were compared. Assuming ±15 % standard deviation due to sampling and analyses, it was possible to obtain the approximately 30%, 15%, 10%, 7%, 4% and 2% standard deviations respectively for weekly, 2-weekly, monthly, 2-monthly, 3-monthly and yearly averages of total P concentrations in the lake. The result was suggested as the base of the model identification studies, when temporal or spatial pattern of the data is detectable.

- *Identification and parameter estimation* Traditional time-series analysis and the mechanistic approach are usually considered as being complementary tools for modeling.

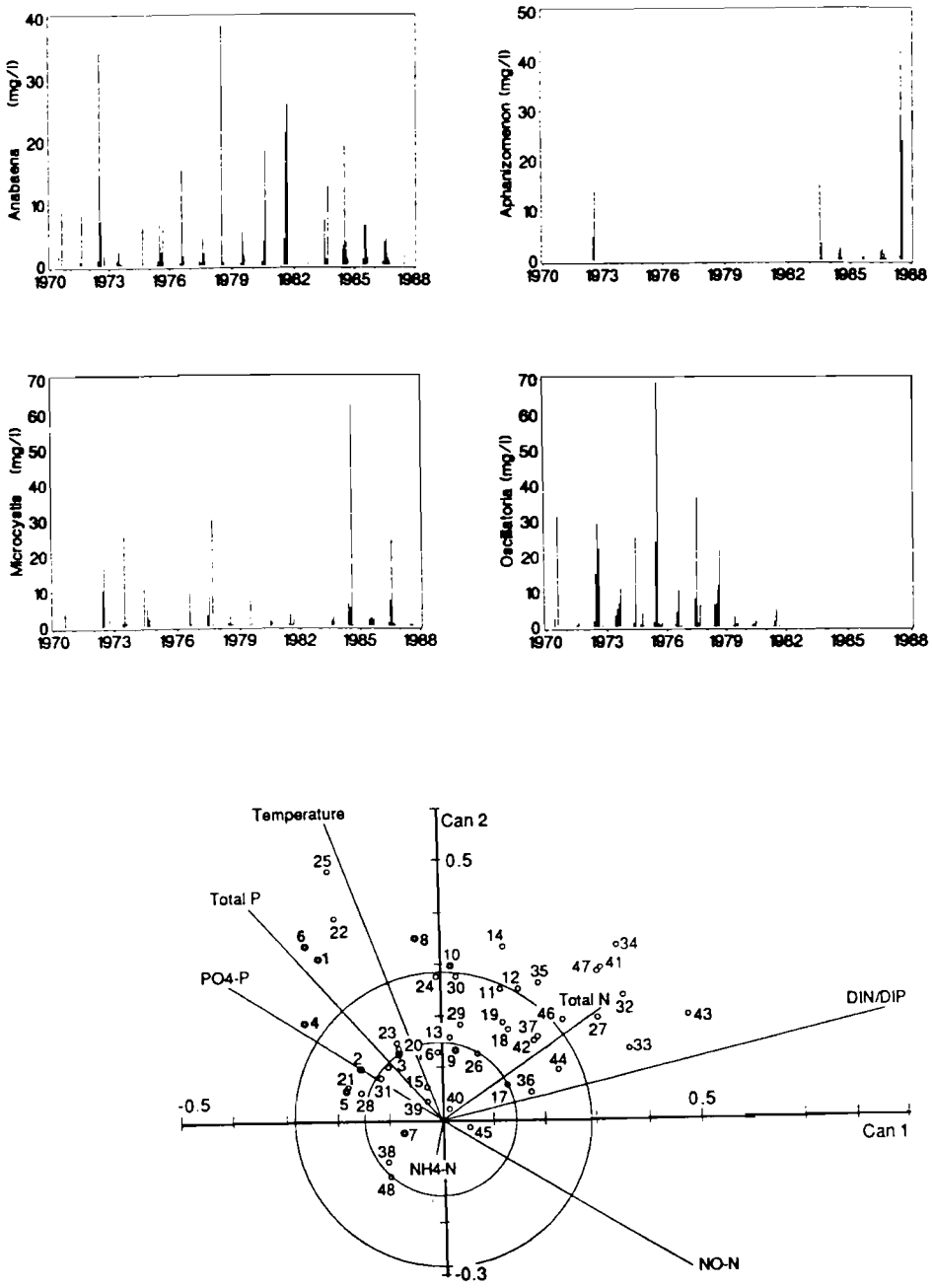

Fig. 26 Canonical correlation analysis. *Up:* The abundance of the four most problematic genera of cyanobacteria (*Anabaena* = 1, 2 & 3, *Aphanizomenon* = 4, *Microcystis* = 6 & 7, *Oscillatoria* = 8, 9 & 10). *Low:* Correlations of the algal taxa and the growth factors with the first two canonical variates. The inner origo-centered circle denotes the projection of the 90 % and the outer the 99.9 % confidence level. The main four bloom-forming cyanobacter species are presented with bold face.

An alternative approach was suggested in a methodological study by Sirviö (1988, 1990). He preferred the construction of models according to a stagewise procedure illustrated in Fig. 27. The modeling exercise is initiated by the data analysis analogical to that of traditional time series approach. Having checked the stationarity and analyzed the correlation structure, an identifiable, deterministic model structure is chosen and the unknown parameter values recursively estimated. Achieving a parameter convergence, the second modeling stage is activated. During it, the structural consistency i.e. logical interpretation of the parameters is checked and depending on the results iteration is continued either from 1st stage or final parameter estimation is performed. Diagnostic checking is formally analogical to that of time series approach.

The main idea behind the suggested procedure is to construct water quality models that are supported by expert prejudice and by existing data. Also the temporal (spatial) uncertainties are included in the modeled system in terms of statistical distribution or respective statistics. In the case of a linear desciption, the mutually interactive state and parameter estimation algorithm described in detail by Todini (1978) can be used. In case data do not adequately support the computation, instrumental variable estimator can be augmented in the algorithm (Sirviö 1988). The procedure suggested above was verified using the P data of Lake Tuusulanjärvi. The models (Fig. 27) were shown to be both identifiable and consistent describtions of the data.

Causal reasoning

The approaches clustered together here have a very crucial point in common. It is the deductive analysis of ecosystems at a phenomenological level defined by practical problem solving objectives. Traditionally, the mathematical formulation of models of this cathegory has been consisting of differential or difference equations, and more recently also on rule-bases.

- *Mechanistic modeling* Presently under study is a phytoplankton-cyanobacteria simulation model consisting of ordinary differential equations (Varis 1992*b*). Among cyanobacteria, three groups: the N-fixers (*Anabaena & Aphanizomenon*), *Microcystis*, and *Oscillatoria* are simulated separately. Additionally, the other phytoplankton is included in the model. Four growth factors, P, N, water temperature, and irradiance are taken into account. 15 years of observations were available for the study. Fig. 28 shows an example of calibration results. In this context, also a set of parameter and state identification procedures will be examined.

- *Rule-based modeling* Rule-based expert systems (see chapter 5) have proved an effective tool in the analysis and control of various processes in industry, and in many cases they have taken the place of complex optimization-simulation models. The applicability of the approach in lake water quality modeling is, however, still highly unknown, and very few studies have so far been published (cf. chapter 1). The objective of this case was to study the applicability of the rule-base approach to lake water quality modeling.

In the preliminary studies (Mészáros et al. 1990), a rule-base is used as a predictive

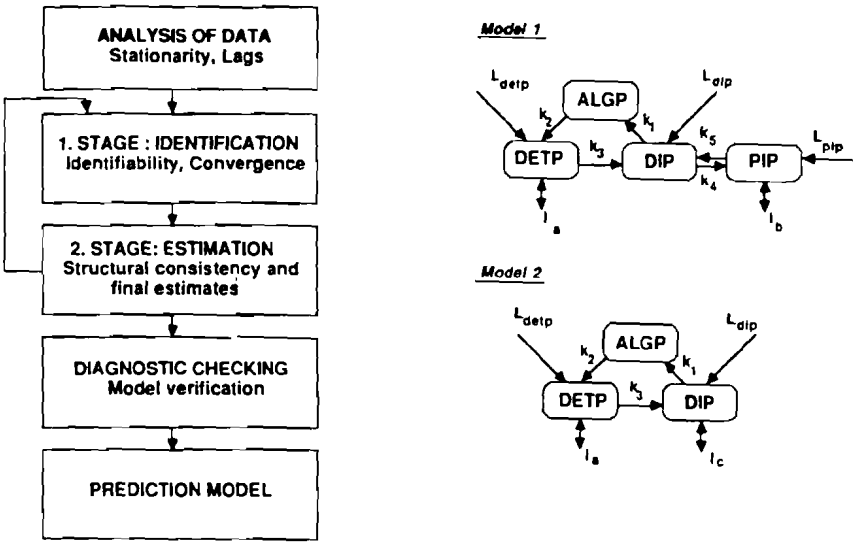

Fig. 27 A procedure by Sirviö (1990) for constructing water quality models (*left*), and submodels used to verify identification and estimation technique (*right*).

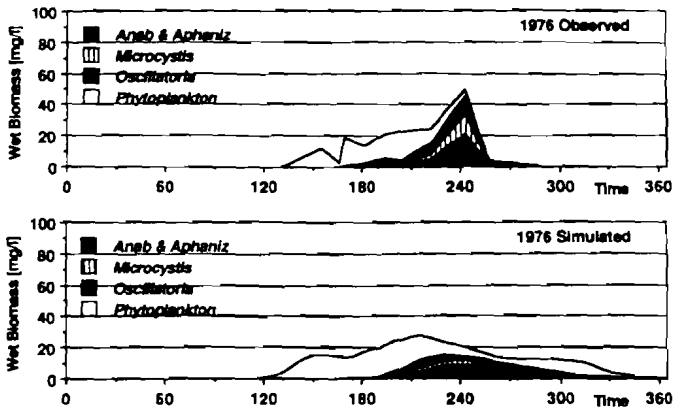

Fig. 28 Example of calibration results of the multispecies cyanobacteria model.

probabilistic model. A prediction of the cyanobacteria biomass in Lake Tuusulanjärvi is updated with the past distribution of observations from the monitoring data, from the calendar month predicted. The expert judgments in formulating the rules can be supported either on observed autocorrelation or cross-correlation between variables included in the model. For instance, the algal biomass in two subsequent months appeared to have a correlation of a certain significance. This phenomenon has taken a form of a rule in the model, with the credibility associated to the rule being relative to the strength of the autocorrelation.

Models for decision support

The common feature in approaches referred to below is the formulation of a model so as to include objectives and decisions, as the analysts see them with respect to the practical management problem to be solved. In other words, a management model focuses on finding the optimal solution to a given management problem, and hence the core of the formulation is bound to be the decison itself, together with the objectives. Around them, the other relevant information is to be formulated. A great deal of information must be acquised from the managers, and in fact the whole formulation of the problem has a subjective setting.

- *Optimal design of observations* Basic idea of the optimal design of observations is to maximize the information gained out of measurements or to minimize the experimental effort. These goals can be achieved by a careful definition of needs for observational activities. The most studied field of the optimal observational design is the design for parameter estimation (Fedorov 1972, Silvey 1980). It is initiated by postulating the model structure *a priori*. The task of the observational work is to facilitate successful parameter estimation. Such designs for water quality studies are given e.g. by Kettunen et al. (1988, 1992), Kettunen (1989, 1992). The studies elaborating such design also for water quality modeling of Lake Tuusulanjärvi are also in progress.

A more general type of designs are those that aim in choosing the best model among the competing candidates. An approach, referred as model discrimination, is to solve this problem by choosing the observations that will minimize the expected *a posteriori* entropy of the system as suggested by Box & Hill (1967). This criterion was applied by Kettunen et al. (1988) to find the better of two P submodels (Fig. 27). Historical data of the lake was utilized in the discrimination process. Results of the analysis are briefly concluded in Fig. 29, where the probability of each of the competing models of being true is given, for each calender year. Model 1 was superior to model 2 during the cold period of the year, whereas model 2 dominated during the production season. Thus neither of the models is universally true one. If such is desired, either new data collection should be initiated or better model structure should be identified.

- *Influence diagrams* An important source of information for a decision making model is the acquisition and merging of expert knowledge. Often several persons with varying backgrounds are to be taken into analysis, e.g. engineers, ecologists, economists, and politicians. Interactive computer graphics provide a possibility to a decision maker or ex-

pert to affect the construction of the model himself. An influence diagram (Shachter 1986) is a probabilistic model with an interactive user interface, focusing on influences of variables to one another (see Varis et al. 1988). Bayesian calculus is used in evaluating the diagrams. The variables (nodes) are connected with directed arcs. The whole diagram is directed, and it may not contain cycles. In case an arc is heading to a decision node, the value of the predecessor is known before the decision can be made. In all other cases it stands for a conditional dependence between the two variables. Depending on the type of the node, it may contain arithmetic functions, IF-THEN-ELSE rules, or probability distributions.

The problem analyzed was to allocate the resources available to lake restoration management between impact assessment studies and restoration measures. Here the resources were a non-fixed quantity with a rational, expected socioeconomic utility to the region. The strategies available involve constant dilution with different volumes, and an adaptive strategy, in which the discharge could be controlled e.g. on a monthly basis owing to the water quality forecasts obtained. An influence diagram model (Varis et al. 1990) with ten nodes (Fig. 30) was constructed to analyze the problem. The influence diagram algorithm by Shachter (1986) was used. The model showed satisfactory robustness in probabilistic sensitivity analysis for the prior distribution and in value of information analysis.

The problem was studied using the risk-benefit sensitivity approach, in the first hand owing to the problemacy in defining a monetary value for benefits due to improved water quality. The risk aversion concept of Pratt (1964) and Arrow (1971) was used. An example of the resulting risk-benefit plots is given in Fig. 30. The risk attitude of the decision makers was not analyzed in this case due to the political character of decisions, but one could assume a modestly risk averse attitude to prevail in an environmental management problem of this character. The risk aversion concept can also be given a frequency analytic interpretation (Varis 1991*b*).

In water quality decisions one can distinguish two major problems: very high uncertainty of measures and the non-commensurability of different attributes used in decison making. These are still made more complex by the intrinsically subjective problem setting of decisions and very high variety of information available. These features make many traditional approaches such as willigness-to-pay in cost-benefit analysis as well as many formal multiple criteria optimization approaches severely handicapped in practice. So, new approaches are needed. The above case study suggested further studies on (a) the Pratt-Arrow approach in coupling the risk attitude and formulation of the objective function to a continuous functional expression, and (b) Bayesian influence diagrams in management of large-scale water resources and environmental problems, in which expert belief, probabilistic inference, knowledge numeric information etc. has to be incorporated in optimization.

- *Decision support system* With the scope of effective information management, a prototype decision support system for Lake Tuusulanjärvi has been constructed (Kylmälä 1992). It includes data display, regression and correlation analysis, and time series analysis

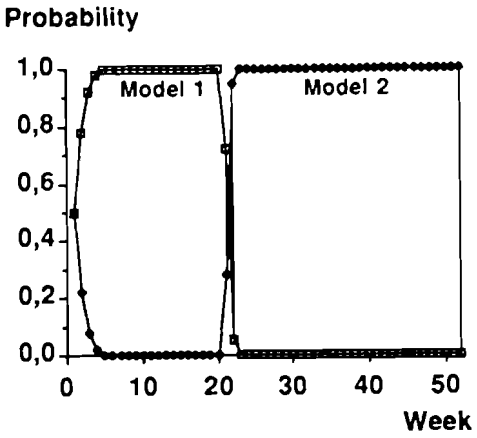

Fig. 29 Probability of the models 1 and 2 of Fig. 27 to be true, when being competing alternatives.

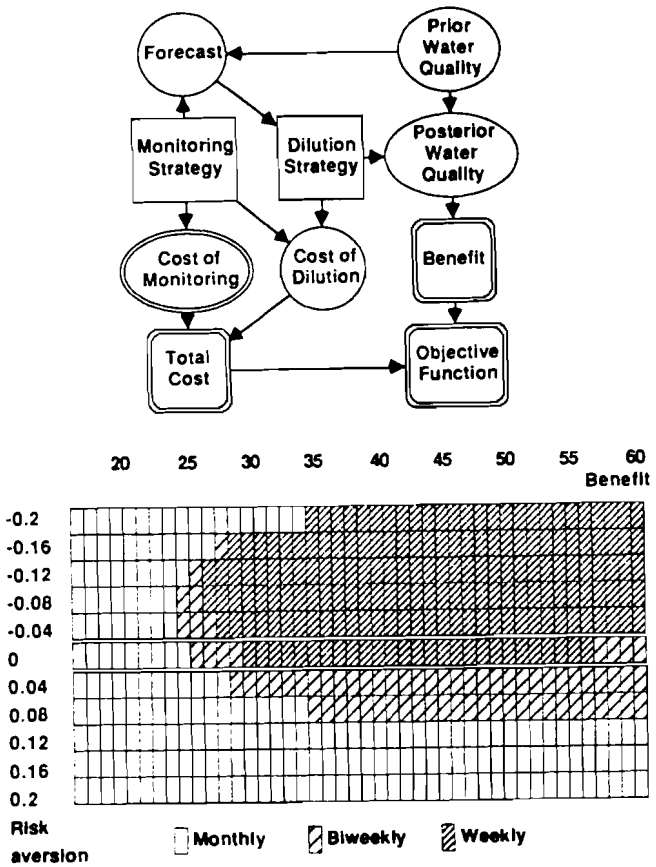

Fig. 30 The influence diagram model. A rectangle stands for a decision node, an oval for a probabilistic, a double oval for a deterministic, and a double rounded rectangle for an expected value node (*up*). The optimal monitoring strategy calculated using the influence diagram model (*low*). The benefits are expressed in 10^5 FIM (spring 1988), and the risk attitude in $(10^5 \text{ FIM})^{-1}$. In the latter, a negative value stands for a risk prone, zero for risk neutral, and a positive value for risk averse attitude.

sections. Also a deterministic simulation model (Varis 1992*b*) will be merged in the packge, with the possibility to change N and P loadings from different subcatchments, and therewith to assess impacts of various land use and restoration options in the catchment.

Concluding remarks

The issue of the applicability of various computer aided modeling approaches available for environmental analysis is a very important field of research. Crucial is the acceptance of and experiences on the methodological plurality, due to the character of environmental problems: scopes data and knowledge vary greatly. Also worth highlighting is the fact, that the methodological excercises should also possess scientific relevance, and vice versa. In the case of lake modeling, this means, that the entire problem setting in modeling should be a realistic reflection of a real world problem.

Even in the case of one lake, it is worth applying a number of complementary approaches illuminating the problems from different settings and at different phenomenological levels. The results of static and dynamic data-analyses serve in this study as the basis of inference, both in ecological and decision making context. Yet, optimization is useful in the stage of evaluation of macro-scale management decisions such as the design of further sampling and monitoring, and studying the socioeconomic acceptability of future lake restoration strategies. Experiences on deductive tools such as mechanistic models and rule-based models are still restricted in this very case. Based on previous experience, however, one can assume that the dynamic behaviour of the lake ecosystem as a whole, including external loading, nutrient cycles, plankton, and hydrodynamics, are the topics in which those approaches are difficult to be replaced by any other.

The study also showed the importance of long, continuous, and rather uniform monitoring data. The intensity of sampling at Lake Tuusulanjärvi has exceeded manyfold the average practise water quality monitoring in Finland and in many other countries as well. The issue of designing of the sampling is evidently just the inverse problem to the question of the applicability of computational methods.

5 DECISION SUPPORT SYSTEMS

5.1 Introduction

The present development in computer technology allows the construction of models which are not just codes of some low level language reading input files and mapping them to output files. This was still the case in the 1970s and in early 1980s. The present supply of application generators, interface software, multimedia, mathematical and statistical packages, etc., has been increasingly put in use also in the field of surface water quality modeling. A model, as understood in previous chapters, is today more and more often a part of a larger set of user friendly inference tools.

The automated support of managerial decision making has been a subject to intensive research since the beginning of the 1970s (Gerrity 1971, Gorry & Scott Morton 1971). In many fields of applied science, the recent years have seen a rapid growth of so called decision support systems (DSS). According to Sprague & Carlson (1982), a DSS is an interactive computer aided system with assists the decision maker(s) to utilize empirical data and mathematical models, in order to solve complex management problems. The following properties are associated to modern decision support systems:

- DSS addresses complex problems.
- DSS couples models and other analytic tools to information management.
- The user interface of a DSS allows easy operation and interaction.
- DSS is flexible and adaptive.

Consequently, there cannot exist a general theory for a DSS. Instead, a DSS tackles a well defined management problem, being either case-specific, or generic for being applicable to an explicit class of decision problems. The concept of DSS has its borders, often very smooth ones, to a couple of directions. They are closely related on one hand to expert systems (ES) and on the other hand to geographic information systems (GIS). Also, models with an interactive user interface approach often problems close to the way a DSS does.

In practice, a DSS is a package, consisting of software and hardware. It should support, in addition to decisions and management, also the process of learning on the problem under concern, through iteration and simulation of different decision alternatives with different initial assumptions and conditions. From the user's perspective, a DSS incorporates the following elements (Johnson 1986, Gray & Lenstra 1988).

- *Data base.* Input, storage, retrieval and updating are often automatized in water resources applications. Also a manual access to these operations is mandatory. The interface to the data should include a possibility for graphics display using diagrams and geographic maps. Also previous strategy profiles and simulation protocols are usually

of high value, if they can be stored and retrieved later on from the data base. The data base often includes a text base, which may include written documentation of the system, forms, tables or graphs to be exported to word processors or for printing, and so on.

- *Model base.* Various statistical tools, such as time series analysis, cross-correlations, regression, and multivariate analysis are often included in the model base. They may be operationally close to the graphical data display, and use same graphics routines. Mechanistic, and socioeconomic models, together with decision analytic tools can be included, taking also the advantage of graphic displays, and moreover, of estimation routines from the statistical analyses. Options for writing new models, and for performing sensitivity analyses, optimization, risk analysis, and preference analysis are useful in many applications. The texture of the model base is naturally case specific. It should support the inference behind decisions in different aspects and spatial and temporal scales relevant to the management.

- *Interface and realization.* The software and hardware chosen for the generation of an application define the framework for the DSS. Toda et al. (1991) present views and a comprehensive application on structuring of information and analytic tools. Andriole (1989) and Wright & Wang (1991) provide a review to contemporary tools to integrated model systems, with emphasis on interfaces. Fedra (1990*b*) discusses integration, simulation and visualization of interactive environmental software. Riedel & Pitz (1986) present an utilization-orineted evaluation of decision support systems.

In addition to those mentioned, several textbooks are available on the topic (Bonczek et al. 1981, Ginzberg et al. 1982, Bennett 1983, Sprague & Watson 1986, Davis 1988, Thierauf 1988, Turban 1988).

5.2 What decisions to be supported

It is clear, that even in the same application, different decision makers appreciate different support. Anyhow, some remarks can be made with regard to decision situations in general. Let us recall the classification by Sutherland (1983) presented in Section 1.1. Here it may serve as a structural guide for a DSS designer in a variety of computational approaches accessible. Sutherland stresses the rationality of the skill of applying methods from different categories to support decisions belonging to either operative, tactical, strategic, or directive category. Like in any modeling, also within the context of decision support systems there is an evident danger for facing the so-called tool of hammer if the repertoire of the tools available is too restricted (Hopple 1986). In decision support systems, often multiple analytical approaches are useful, and if support for decisions in several management time horizons is provided, even mandatory. According to Nunamaker et al. (1988), the early DSS applications were predominantly designed to be operational, and they addressed well structured specific problems. Presently, the trend in decision support systems is to take increasingly also long-term management into account, and handle a wide range of problems, both structured and unstructured.

The scopes of a DSS can also be discussed from the point of view of uncertainty associated with the information available. Uncertainty can further be specified to uncertainty about objectives of actions, and uncertainty about causes and effects of actions (Thompson & Tuden 1959, Earl & Hopwood 1980). The level and type of uncertainty should be reflected in the implementation of the system, of being primarily an answering, dialogue, learning, or idea machine (Fig. 31).

		Uncertainty about objectives	
		Low	*High*
Uncertainty of cause and effect of actions	*Low*	Answer machines	Dialogue machines
	High	Learning machines	Idea machines

Fig. 31 Relationship between information systems and uncertainty (Earl & Hopwood 1980).

5.3 Selected applications

DSS applications have been subject to several recent reviews. Corner & Kirkwood (1991) present a comprehensive review on DSS applications in operations research literature. Eom & Lee (1990) have surveyed 203 specific DSS applications, and they list the most frequent contributors, their institutions, and countries of origin. Loucks et al. (1985) and Loucks & Fedra (1987) discuss the impact of changing computer technology on water resource modeling, with special reference on interactivity of the software.

The DSS approach appears to be in most extensive use in medical and clinical sector. The same applies also to decision analysis and expert systems. But also in water and environmental sector, there exists a rich variety of DSS applications (Johnson 1986, Loucks & da Costa 1991). In fact, decision support systems have become a commonplace in water resources studies.

During recent years, a high number of applications has emerged addressing - or at least taking into account – water quality issues. The number of published works is already too high for any single analysis, but a selection of them is presented below. The reviewed studies serve also as examples of different approaches to the problem.

Generic software for DSS

One basic type of DSS are systems, which have been designed to be applicable to certain types of problems, and are implementable to numerous cases in which the problem domain fulfills the criteria of the applicability of the software. This type of DSS are often called generic.

We have divided the generic DSSs into two groups. The first group includes socio-economic, multicriteria, risk analysis, model integration etc. systems, which have potential applicability in environmental - including water quality - studies. The second group of generic DSS includes packages for lake and river studies. Also a couple of more general environmental systems are mentioned. The first group has some overlap with application generators such as ES generators, simulation packages, statistical software, decision analytic software, add-ins for spreadsheets, etc.

Let us start with the first group. Brill et al. (1990) discuss the MGA (Modeling-to-Generate-Alternatives) approach, and present an implementation including a number of mathematical programming techniques for multiobjective planning and decision making. Mohammed et al. (1988) provide a DSS framework for structuring and diagnosing managerial problems, and Malakooti (1988) for discrete multiple criteria problems.

The DSS application by Kira et al. (1990) is targeted for business administration. However, the work is worth mentioning in this context due to the methodology used, such as risk analysis and multiobjective aspects. Risk analysis has been the object of a couple of other packages as well. those include the REX by Wang & Modarres (1990), the @RISK add-in software for spreadsheets by Palisade Corp. (1990), and the Risk-Disk by Gaver & Omuirchearthaigh (1990). Wu et al. (1989) review the probabilistic risk analysis applications and decision support systems from the point of view of energy production.

Generic, problem specific software for surface waters and the environment

Even if the subsequent packages have been arranged under the title Generic Software, it is noteworthy, that several of them have so far been implemented only to one single case. Their generic applicability is thus not always very clear, and the classification between this and the next section should not be taken all that seriously.

The MASAS program by Ulrich et al. (1991) provides a set of possibilities for evaluation of the behavior of antrophogenic micropollutants in aquatic ecosystems. The first implementation has been for compartmental models for lakes.

The CORMIX expert system by Jirka et al. (1991) assists in the mixing zone analysis of pollutants in streams. The expert system selects between a number of models included in the system, using characteristics such as flow type, river bed width and depth.

The DELAQUA system by Recknagel et al. (1991) addresses lake water quality problems. Support for the following decisions is provided: Recommendations for operational control of undesired impacts of raw water quality classification of raw water quality by means of legal standards analogy conclusions using data and simulations from reference cases and predictions of raw water quality in changing environmental conditions and under different control strategies.

The IMES system by Schreiner et al. (1991) provides support for the selection, validation and uncertainty assessment of a number of models supported by US EPA for envi-

ronmental exposure and risk assessment. There are more than 50 models presently included in the system for a variety of surface water, groundwater, and air quality problems.

The GEnESIS system by Solomon et al. (1991) enables to systematically collect, assess, organize, and improve data and information in the geographic, environmental, economic, and social dimensions. Number of applications from limited to continental scale are available.

Both Okada et al. (1991) and Colas (1991) present packages for basin wide management of water resources including quality aspects. In both systems, also a selection of socioeconomic tools is provided.

The IRIS by Salewicz et al. (1991) and the AQUATOOL by Andreu et al. (1991) are both primarily tools for planning and control of reservoirs in a watershed. Support for water quality simulation is not provided in presently available versions, but for IRIS, a water quality part is in progress.

Schwabl (1988) documents a ES type of DSS named SuSy-EIA, which has been designed to support environmental impact assessment, according to the regulations of the EC.

Håkanson (1989) presents a software for the analysis of environmental consequences in aquatic ecosystems. The system consists of two parts: one describing the scientific framework of the consequences, and the other describing tools available for handling the scientific concepts.

The integrated DSS for environmental planning by Kainuma et al. (1990) consists of eight subsystems. Three of them are for management of relevant data and models, two are for identification of environmental problems, and three are used for their modeling and simulation.

Cluis (1988) has presented an interactive package for detecting trends and changes in water quality data. Various statistical tests are included, as well as graphic displays.

Grobler et al. (1987) have constructed a computerized system to assist the eutrophication control strategy decision making concerning lakes.

Teruggi et al. (1988) have presented a package to support evaluation of stream suitability to various uses. It is based on legislative norms set by authorities for water quality with respect to the uses.

Case specific systems

In contrast to generic decision support systems, case specific systems have been constructed primarily for one single application.

The Hypertejo DSS by Câmara et al. (1991) has been designed to assist in the water quality management of the Tejo estuary, Portugal. The system consists of data bases on dispersion and non-point pollution, and regional water quality management models. Also descriptive statistics and transfer function modeling capabilities are provided.

Lam et al. (1987, 1988) report a comprehensive data management system for acidification and a set of other water quality problems in Canada. The interface makes use of queries through digitized maps. A number of statistical and simulation tools are available for the analyst. An ES is used to give combined predictions based on several models.

The prototype DSS by Davis et al. (1991) will be used to assess the impacts potential land-use and land-management policies in the Mt. Lofty Ranges to the water quality of water supplied to the city of Adelaide, Australia. Also costs can be estimated. The system consists of three parts a policy module, a catchment model including phosphorus, nitrogen, and turbidity simulation, and a query module.

Kylmälä (1992) has constructed a prototype DSS for data analysis and watershed management of Lake Tuusulanjärvi, a Finnish eutrophic lake (cf. case study in 4.5). Data including maps, tools for regression, correlation, and time series analysis are provided. Also deterministic simulation option will be available.

One class of decision support systems is focused on management of large data bases. They are often called information management systems. Law & Moore (1991) document a system permitting retrieval of both spatial and time series data from large environmental data holdings. GIS tools and relational data bases are utilized in a workstation environment.

One of the boundaries of decision support systems faces towards models with user friendly interfaces. Again, the shift from case specific DSSs and case specific model applications with interactive interfaces is very smooth. It is presently even fading. This is due to the developments in generic software and application generators for purposes such as spreadsheets, data base management, statistical packages, macro languages, and hypermedia. On the other hand, also low-level programming languages provide increasing support for generating graphics, and perhaps more importantly, the improving software compatibility contributes to the portability and connectability of codes from different sources.

As examples of case specific models with interactive and animative interfaces let us mention the river basin simulation models by Chen (1991) and Wu & Horng (1991), both including a pollution map interface to a river basin model for water quality and quantity, the wastewater disposal distribution model by Bale & Orlob (1991), and the interactive model system for operating a reservoir by Koncsos & Somlyódy (1991).

DSS as an educational tool

One of the scopes of constructing or applying a DSS in real world management is their function of supporting learning from the problem. In fact, many decision support systems

have been designed to serve also for educational purposes.

Kao et al. (1991) examine discharge permit programs using a microcomputer-based system including an educational program, a water quality model, an optimization package, and an user friendly interface with graphic displays.

Kylmälä (1992) provides support in learning how to use and interpret a menu of statistical analyses including regression, correlation, and time series analyses in the analysis of lake and catchment water quality data, often corrupted by missing observations and uneven sampling intervals.

Wood et al. (1989) have applied a DSS to educate students to multiresource management. The scopes have been primarily in forestry management, but the system has apparently a potential in water resources and environmental studies.

DSS and Expert Systems

The terms DSS and expert system (ES) appear often together. This does not mean, however, that those terms were synonyms. They have a certain overlap in decision support applications. Above, a number of applications studied are primarily named as ESs. In our opinion, those studies belong to the before mentioned overlapping domain.

Also more profound analyses exist on the differentiation of DSS and ES approaches. Connell & Powell (1990) compare the possibilities of the DSS and ES in general level. They present a number of criteria of differentiating between them, the most crucial being the idea that a DSS is primarily a data based construction, while an ES is knowledge based. Most realized systems, however, make use of both information.

Greathouse et al. (1989) review the use of expert systems in environmental control. White (1990) presents a review on applications of decision analytic tools and expert systems in decision support. Page (1990) has reviewed 24 environmental ES applications in Canada and Germany. Graham & Jones (1986) discuss the methods of handling uncertainty in decision support and knowledge based systems.

GIS as DSS

Applications of geographic information systems (GIS) are often – but definitely not always – rather close to what we understand with a decision support system. A GIS is primarily based on a map interface, using typically remote sensing data from satellites. Very rapidly increasing number of applications is also true within the GIS field. Fedra (1990*a*) has discussed the decision support function of geographic information systems.

Lee & Terstriep (1991) have integrated GIS databases and a set of water quality models for agricultural and urban watersheds. Rudra et al. (1991) have accomplished a watershed management model focusing on modeling the non-point source loading within a GIS framework. In the GIS by Myhre & Shih (1991) a water quality section using remote

sensing data is included. Ruland et al. (1991) have studied pollutant transport processes in lakes and river basins using the GIS approach. Corbin & Dirdal (1991) discuss the possibilities and applicability of utilizing geographic information systems in surface water quality management. Olivier et al. (1990) document experience in choosing GIS for the use by national water management authorities.

5.4 Concluding remarks

The above, selected studies indicate quite clearly, that the application of decision support systems to management of lacustrine and riverine water quality problems is a very rapidly expanding field of industry. In very many present cases, water quality aspects have reached a status of being essential to take into consideration, and they are increasingly included into water management models. The same applies to decision support systems. More and more often lakes and rivers are modeled as a part of a watershed, or even as a part of a larger regional system, and starting from management objectives.

In the studies reviewed, both operational, tactical, strategic, and directive systems, and hybrids of these were present. Probably the highest number of applications was scored by strategic planning and management systems. When discussing DSSs for water quantity management, the applications of operational and tactical management appear today essentially more frequent than in water quality management.

The variety of used software in the studies reviewed is substantial, as expected. Also the range of hardware used includes all what one could suppose: personal computers (DOS & Macintosh), UNIX system, other workstations and mainframes, and supercomputers. In terms of both software and hardware, there exists an excessive menu of options for a body initiating a process of constructing a decision support system.

It is clear, that with the present rate of evolution in both software and hardware, as well as in skills in using them, we more often face a situation that an efficient DSS is less and less a black box which provides a selection of buttons as an access to predefined operations. It will probably evolve towards a a symbiosis of user and a variety of generic software, which can be made compatible and put behind an user-friendly interface more and more easily. The same will most probably apply to the future of computational models for riverine and lacustrine water quality.

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