Mathematical Modeling of Water Quality

Summary Report of a IIASA Workshop
September 13-16, 1977

M. B. Beck

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International Institute for Applied Systems Analysis
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Preface

In many countries the use of water is increasingly restricted by its quality. The improvement and control of water quality in a water body can be achieved by regulation of municipal, industrial, and agricultural waste discharges. Waste treatment techniques by chemical and biological processes are highly developed, and while it is technically possible to approach "zero discharge" of wastes from point sources, in most cases it is neither necessary nor economically feasible. The important management decisions in water quality control relate to determining the degree and level of waste treatment consistent with the multiple uses of natural and man-made water bodies. This implies the ability to forecast or predict the response of the waste-receiving water to future investments in waste treatment facilities. Therefore, the planning of regional development and the management of water resources systems requires an analysis of the interaction of waste discharges with the hydrophysical and ecological processes taking place in the aquatic environment.

The organization of an IIASA Workshop on Mathematical Modeling of Water Quality thus fulfilled two objectives: it provided an opportunity for intensive discussion of future research needs in developing hydrophysical and ecological models for water quality; and it allowed some assessment of the present state of scientific knowledge in this subject. It was hoped in particular that the Workshop would promote the establishment of a collaborative international network of research groups interested in the advancement of water quality modeling.

As a basis for discussion, it was suggested that the workshop participants focus their attention on a number of key issues, for example:

- the modeling of eutrophication in water bodies with significant nonpoint nutrient loading, i.e. agricultural runoff;
- the impact of toxic pollutants on aquatic ecosystems;
- problems of model dimensionality and complexity;
- the relationship between models and the objectives for model application;

- consideration of stochastic phenomena in water quality modeling; and

- interfacing the models with planning and management-oriented studies.

All of these topics, among others, can be found in this report on the Workshop.

Moreover, it will be evident to the reader that the workshop participants offered many suggestions for future possible directions of the Institute's involvement in water quality modeling activities. We are indeed gratified by this encouraging response and we look forward to a continuing fruitful collaboration and exchange of ideas.

O. Vasiliev
Chairman
Resources and
Environment Area

Foreword

The current Task 2 of IIASA's Resources and Environment Area (REN) —Models for Environmental Quality Control and Management—is concerned with hydrophysical and ecological models for water quality. The emphasis in this work is at present identifying, developing, and communicating the state of the art in water quality modeling. In September, 1977, a Workshop on Mathematical Modeling of Water Quality was therefore organized as one of the initial activities of the Task. This paper is a summary report of that Workshop written by M.B. Beck; it is not an edited collection of formally presented papers.

The principal objective of the Workshop was to obtain a comprehensive picture of trends and ongoing studies in the broad field of mathematical modeling of water quality. In this sense the Workshop complements Task 2's (REN) state-of-the-art survey, which aims both to clarify the capabilities of water quality models, especially as they will eventually relate to management applications, and to accelerate the exchange of existing modeling technologies.

This report on the Workshop proceedings attempts to capture the essence of the key themes emerging from the discussion. It also shows how these themes are related to the future directions of IIASA's studies in water quality modeling.

Summary

This report summarizes the proceedings of an IIASA Workshop on Water Quality Modeling held at Laxenburg, Austria, September 13-16, 1977. The Workshop was held as an initial activity within IIASA's research Task on Models for Environmental Quality Control and Management.

In convening the Workshop, the organizers invited participants to express their views on the current state of mathematical modeling of water quality. They were also encouraged to speculate on future directions for the subject and to make recommendations for the ways in which such research could be organized in collaboration with IIASA. The report on the Workshop divides broadly into two sections: the first deals with key themes and salient problems of water quality modeling; the second reproduces the concluding statements of nine ad hoc working groups established during the Workshop. These working groups considered a number of specific areas such as deep lakes and reservoirs, the impact of toxic pollutants, systems methods in model development and analysis, and so forth.

An intermediate section of the report looks briefly at future perspectives in water quality modeling, and in the final section particular reference is made to the Institute's plans for water quality model development and application in particular case studies.

Contents

Mathematical Modeling of Water Quality

Summary report of a Workshop held at IIASA, Laxenburg, Austria, September 13 to 16, 1977

1. INTRODUCTION

This report summarizes the key points of the discussion from the Workshop on Mathematical Modeling of Water Quality, held at Laxenburg September 13-16, 1977. The principal reason for convening the Workshop was to obtain a comprehensive picture of trends and ongoing studies in the mathematical modeling of water quality. It was intended that such a picture would be instrumental in clarifying, to some extent, future directions for IIASA's research Task on "Hydrophysical and Ecological Models for Water Quality". Further, it was hoped that, with the assistance of the Workshop participants, suggestions could be made for ways in which collaborative working groups (external to IIASA) might be established as complements of the Institute's in-house research activities. The Workshop was, therefore, very much a planning workshop. This report on the proceedings is accordingly a reflection of the conclusions from discussion groups--it is not an edited collection of formally presented papers.

An agenda for the Workshop and a list of participants are given in Appendixes A and B, respectively. The report here starts with an editorial view of some of the salient features of the informal presentations at the Workshop. The intention is that such a summary will capture those aspects of water quality modeling that the participants considered either controversial or critical to future progress of the subject. In section 3 we have attempted to summarize some possible future perspectives for water quality modeling. These are statements that, though they draw upon the discussion of the Workshop reported in section 2, are essentially independent in their outlook. From the Agenda (Appendix A) it can be seen that one afternoon of the Workshop program was devoted to informal discussion. Nine ad hoc working groups were established and their concluding reports are given in section 4. Finally, section 5 describes how various themes emerging from the Workshop are being incorporated into the Institute's research plans for the development and application of water quality models.

2. SOME SALIENT PROBLEMS

While the Workshop was very broad, it did not cover all aspects of the development and application of water quality models --for instance, very little work in marine systems was presented. The distillation of the current status and salient problems of water quality modeling presented here is organized along the following lines. Where possible, general themes occurring in one or more of the informal presentations are listed in section 2.1; reference is given to those presentations that dealt with each theme. (We have, in fact, selected for discussion those presentations that were not intended primarily as statements from the national member organizations of IIASA.) Subsequent subsections deal respectively with the approximate division of the detailed technical proceedings into "overview" papers (2.2), reports on the modeling of water quality in rivers and estuaries (2.3), thermal discharge problems (2.4), and lake systems (2.5). In some instances, principally in sections 2.4 and 2.5, further discussion of the same or similar topics has been reported for the November 1977 Workshop on Models for Waste Heat Management in Rivers (Harleman, 1977), and for the December 1977 Workshop on Hydrophysical and Ecological Modelling of Deep Lakes and Reservoirs (Jørgensen and Harleman, 1978). Both Workshops originated as proposals from the ad hoc working groups (see sections 4.1 and 4.5).

A selected bibliography supporting some of the presentations is given in Appendix C; Appendix D provides some definitions of terminology in water quality modeling.

2.1 General Themes

Insomuch as it is possible to classify and separate themes, the following can be identified and listed approximately in the order of the modeling procedure itself (names in parentheses refer to principal speakers and discussants):

Models and Modeling Objectives (Orlob, Beck, Whitehead)

The nature of the model should match the nature of the problem and the intended application of the model; this is, therefore, a distinctly different standpoint from the view that a general model can be developed for solving, in general, any given problem.

Distributed-Parameter or Lumped-Parameter Models (Aggregation) (Orlob, Bierman, Rinaldi, Thomann)

There are several different aspects of the choice between distributed-parameter and lumped-parameter models, for example:

- The questionable reliability of increasing model complexity to two- and three-dimensional spatial representations in view of severe data-base restrictions for verification (Orlob, Bierman).

- The improvement in model performance for more highly aggregated representations, i.e., large spatial segments, for simulation of lake-wide or basin-wide responses; in other words, averaging field observations over large areas increases the ability to perceive deterministic (as opposed to random) patterns of behavior (Thomann).

- The systematic aggregation of model compartments, or state variables, for the reduction of model order (Rinaldi).

Parameter Estimation and Sensitivity Analysis (Harleman, Whitehead, Rinaldi, Jørgensen)

The arguments here centered upon two problems, the first being a dilemma:

- Should we substitute laboratory chemostat-determined rate constants into models of the field system, with the assumption that the chemostat environment parallels the field situation? Or should we determine parameter values from the in situ field data, with the risk of hidden identifiability problems whereby unique values for parameters cannot be estimated? (Harleman, Whitehead).

- An analysis of the sensitivity of the model responses and predictions to uncertainties in the parameter values (Rinaldi, Jørgensen).

The Determination of Sufficient Model Complexity (Harleman, Jørgensen, Thomann, Grenney, Bierman, Whitehead, Orlob, Beck)

Of all the matters raised at the Workshop this attracted most attention. A determination of sufficient model complexity enters the modeling process at two stages:

- During the initial phases, where the analyst must choose a certain level of model complexity before attempting to verify this a priori model against field data (Grenney, Bierman)--for example, one may choose to neglect benthic demand for oxygen, or one may choose to differentiate between species of phytoplankton.

- During the final phases, where the analyst must decide whether his model has been verified and has sufficient complexity for its intended application (Harleman, Jørgensen).

Although there was no consensus, some of the participants felt that in spite of all attempts to the contrary, these two choices were essentially subjective (Beck, Grenney, Bierman). Between the a priori and a posteriori models there may be:

- A gradual increase in model complexity, whereby additional complexity is included only if a simpler model is demonstrably inadequate as a formal representation of the behavior observed in the field data (Whitehead, Beck).

This last attitude is consistent with another view that:

- The complexity of the ecological part of the model should be built upwards from the stronger a priori foundations of the hydrodynamic part of the model--a view that implies confidence in the understanding of the hydrodynamic properties of the given water body (Orlob, Harleman).

And yet, while we might expect "progress" to mean increasing sophistication, there was a very strong plea that:

- Model complexity should be reduced, not simply for reasons of computational economy, but primarily for reasons of preserving the ability to comprehend model forecasts (Thomann).

<u>Model Verification and Validation</u> (Rinaldi, Jørgensen, Beck, Thomann)

Thomann's second key comment was that more detailed verification of existing water quality models was needed. Others agreed and it will become evident from the concluding statements of the ad hoc working groups that it is thought generally desirable to see different models verified and compared against the same field data set.

<u>Models for Management Applications</u> (Stehfest, Harleman, Rinaldi, Thomann)

The discussion was not limited by the title of the Workshop and the following subsections mention many model applications to the solution of management problems. There was, nevertheless, some debate over the justification for accepting the applied results if the prior verification of the model cannot be demonstrated (Stehfest, Thomann).

2.2 Surveys and Critical Reviews

G.T. Orlob: State-of-the-Art Review of Mathematical Modeling of Surface Water Impoundments

This was both an appropriate speaker and topic with which to begin the proceedings; Professor Orlob is Chairman of IIASA's Task Group on the State-of-the-Art Survey of Water Quality Modeling. Other members of the group are:

M.J. Gromiec
J. Jacquet
S.E. Jørgensen
D.P. Loucks
P. Mauersberger
O. Vasiliev
M.B. Beck (Secretary)

The general objective of the Survey Task is to enhance the exchange of scientific and technological information on mathematical modeling between research and development people, and potential users. Among the reasons for initiating such a task, Orlob noted a desire to avoid duplication of effort in modeling; and he observed further that, in his experience, models appearing in the refereed literature frequently do not prove to be either the most useful models or the models best documented or most easily transferable from one case study to another. Thus, because reports and documentation on the more useful models tend to receive only limited circulation among the profession, IIASA would seem to be well placed to act as a clearing house, or central registry, for information.

From a review of the current models for water quality in lakes and reservoirs, two weaknesses in particular can be identified:

- The lack of adequate characterizations of sediment/water column interaction--clearly in shallow lakes the exchange of nutrients between the benthos and water column, the resuspension of sediments, and the recirculation of phosphorus, are important factors.

- The "primitive" state of two- and three- spatial dimension models as attempts at describing the extremely complex hydrodynamic circulation mechanisms in large impoundments.

The one-dimensional models for temperature profiles in small reservoirs, developed principally by Harleman and Orlob and their coworkers during the 1960s, are the models now receiving the widest application in the solution of management problems. (These management problems are frequently concerned with selective reservoir withdrawal policies and with the impact of reservoir construction on downstream water quality.) The application of the models is, however, restricted in the sense that they deal with reservoirs having long detention times with a tendency to become strongly stratified. Despite this restriction, such models have been the basis for extensions into water quality/ecology modeling--and a natural progression in complexity--so that at present we are facing the fundamental problem of whether a sufficiently comprehensive data base can be found to verify the two- and three-dimensional model forms. With respect to the high cost of data collection (and some perhaps remarkable figures are quoted later in section 2.5) the question arises whether models can themselves be used to define economic data collection programs. This indeed they can, especially in terms of desired sampling frequency and experiment duration; unfortunately, however, good experimental design is strongly dependent upon good a priori knowledge (model) of the system's behavior.

S. Rinaldi: An Overview of Modeling and Control of River Quality

Professor Rinaldi and his colleagues have approached the subject of the Workshop with a rather different perspective from that of Orlob. A major objective of his group's work has been to assess the usefulness of control and systems theory applications in the modeling and management of river water quality. As one of the first of several subsequently suggested modeling procedures, Rinaldi identifies three basic steps:

- Conceptualizing the problem--wherein "reality" is idealized as a set of simple conceptual models, such as, for example, tanks in series and in parallel, as in a conceptual hydrological model.

- Parameter estimation--a step that follows the correct determination of model structure; parameter values must be estimated from in situ field data and estimation of more than about ten simultaneously is an almost intractable problem.

- Model validation--a step rarely attempted either because of insufficient independent data sets or because models so rarely perform adequately other than with the data for which they have been verified.

On the intractability of parameter estimation in large, complex models the existence of systematic methods of model aggregation --what we might also call model-order reduction techniques-- should be noted. Such techniques permit a sensible treatment of the parameter estimation problem given fewer parameters to be evaluated. This desire for simpler models implies, in the case of inland river systems, the use of models that are in lumped-parameter, ordinary differential equation forms. Models of this kind facilitate the application, inter alia, of recursive parameter estimation, state estimation, and state reconstruction algorithms--all topics that are familiar to the control engineer but perhaps unfamiliar to the water resources or sanitary engineer. Lumped-parameter models also allow a consideration of such management problems as the optimal allocation of wastewater treatment and in-stream aeration facilities, and on-line (or real-time) control of water quality. This is because the vast majority of control system synthesis procedures are designed for process models that have time (or some transform thereof) as the single independent variable.

The distinctive theme of Rinaldi's presentation was, then, one of seeking rather simple models, but not oversimplifications, strongly coupled to the application of the model in resolving issues of management and decisionmaking.

R.V. Thomann: The Need for New Directions in Water Quality Modeling: The Hazardous Substances Example

Here the "need for new directions" was interpreted by Professor Thomann in two ways:

- The requirement for more detailed verification of already existing models.
- The need to begin to reduce the complexity of models.

To illustrate the first point, the historical development of compartmental models for lakes and estuaries may be sketched. An earlier model for phytoplankton in the Potomac estuary divided the estuary into 23 segments giving approximately 200 simultaneous, nonlinear differential equations to be solved. That number of equations represents merely the biogeochemical portion of the simulation and does not include any modeling of the estuary's hydrodynamic and mixing properties. By the late 1960s/early 1970s, with the transition to the study of lake systems, came the development of a model for Lake Ontario containing some 700 equations. Hence there seems, in principle, no limit to the number of either ecological compartments or spatial segments that can be accounted for in a model. The only restraint on further increases in model complexity, according to Thomann, is the quite fundamental matter of being able to comprehend the information generated by the model: imagine plotting the yearly variations of ten variables at 67 spatial locations. An analysis of the statistics for verification studies indicate that only by aggregation and reduction in the order of the a priori model (700 equations) can a figure of "50% verification" be increased to a figure of "between 80% and 90% verification".

For the hazardous substances example, in which again the role of sediment behavior is identified as particularly important (cf. Orlob), the size of the model can expand very rapidly. Apart from the ever smaller discrete elements into which the spatial (and temporal) continuum is divided, the size of the model is also governed by more and more precise (species-specific) ecological compartments. It is the converse of this latter that brings us to Thomann's appealing concept of an ecological continuum. In other words, by introducing a further independent variable, say trophic length, where this term means the physical length of an organism, instead of further (time, space) dependent compartmental variables, there is the potential for significantly reducing model complexity. Each compartment of an ecological model represents, as it were, a discrete segment of the ecological continuum; and trophic length, the independent variable, is interpreted as that continuum with minimum and maximum bounds given approximately by small particles and large fish respectively.

The central debate of Thomann's proposal hinged primarily upon some evaluation of the functional forms of a food-chain transfer velocity. That is to say, at what rates are the hazardous substances transferred from one point in the trophic length to another, and how are these rates expressed as functions of trophic length? A secondary debate followed from questions on the matter of field data for model verification and on the extensive data probably required as input information for the model as a predictive planning tool. Since standards on permissible hazardous substance concentrations are about to be made more stringent--the striped bass in Lake Ontario are already excluded from commercial fishing--any insights afforded by the model on concentration in the ecological food chain are nevertheless likely to be of considerable importance in a management context.

2.3 Rivers and Estuaries

M.B. Beck: Mathematical Modeling of Water Quality: A Case Study in the UK

The purpose of the case study (the River Cam in eastern England) is that it illustrates a certain viewpoint on the modeling process. The modeling process can be separated into the following (cf. Rinaldi, section 2.2):

- Design and implementation of specialized experimentation;
- Choice of a priori model;
- Model structure identification;
- Parameter estimation;
- Verification; and
- Validation.

If the problem of organizing a suitable field data base has been overcome, model structure identification remains a fundamental technical problem. This partly concerns the choice of the number of state variables in the model, and partly with identifying the correct form of the mathematical expressions in the state equations. The view adopted here is that model structure identification can be interpreted as repeated hypothesis testing and decision making. There are two points about this view that are of some importance: firstly, it reinforces the notion that modeling is to some extent subjective--it depends on the analyst's decision to accept or reject a hypothesis (model); secondly, it emphasizes the fact that the ultimate problem of modeling is the generation of a subsequent hypothesis given that the existing one is inadequate.

The example of the Cam shows how a simple a priori water quality model, based essentially upon the assumptions of Streeter and Phelps, evolves within the above framework into a rather more complex model for the dynamic interaction of an algal population with the river's biochemical oxygen demand (BOD) and dissolved oxygen (DO) concentrations. In spite of the author's strong reservations about further increases in model complexity, especially when the problem is circumscribed by the high level of uncertainty and inaccuracy in the field data base, a major criticism of the a posteriori model has been its lack of sophistication.

H. Stehfest: Systems Analysis Studies on the Rhine River Quality

Continuing along a similar theme, Stehfest addressed the question of whether one should use a complex or a simple model in an applied management context. For the Rhine it is found that the performance of a six compartment ecological model is marginally better than a Streeter-Phelps model in its predictions of steady-state spatial profiles of material concentrations in the German section of the river. Such a marginal difference is not a justification in itself for the exclusive use of the ecological model in the design of, say, a sanitation program for the Rhine. How sensitive, then, is any investment decision to the choice between alternative models as (conflicting) predictive tools of future conditions?

Although Stehfest chose to tackle a specifically management-oriented problem, it was the technical details of his modeling approach that attracted most argument. Since the problem focuses upon the regulation of levels of in-stream oxygen-demanding matter, it is necessary to explain why nitrification and bottom sediments are not included in either model as sinks for oxygen. The explanation is that trace pollutants substantially inhibit the development of nitrifying organisms and that the velocity of river flow rarely permits significant formation of bottom deposits. The counter to the explanation is that, although substantial nitrification may not be a problem at present, it might possibly become one depending upon the particular combination (or sequence) of treatment plants specified by the design sanitation program. For instance, the installation of a partially nitrifying plant, whose discharge would "seed" the river with nitrifiers, upstream of an ammonia-rich discharge that receives no secondary biological treatment may create deoxygenating conditions in the river. If this kind of future possibility exists, then a consideration of nitrification (as an example) should be included in the model, even though we may recognize that such a part of the model cannot be verified against historical data.

D.R.F. Harleman: A Real-Time Model of the Nitrogen Cycle in Estuaries

The first of Professor Harleman's two presentations dealt with a subject closely allied with Stehfest's. Harleman viewed the role of the predictive water quality model as one of supplying information to decision makers on the type and degree of treatment to be provided for waste discharges to receiving water bodies. Yet, while this design problem has been traditionally based on the concept of DO-BOD interaction, it is now widely acknowledged that decisions regarding secondary and tertiary treatment processes require a rather broader interpretation of water quality. In particular, there is concern for the removal of not only oxygen-demanding matter, but also for the removal of nutrients such as nitrogen, phosphorus, and carbon. The focus of attention on the nitrogen cycle signifies the general agreement that in a majority of river and estuarine situations, nitrogen is the rate-limiting nutrient for phytoplankton growth. As examples of applications, a model of an estuary with idealized (constant) geometry and two wastewater discharges, and a model for an analogous situation on the Potomac estuary were quoted.

The following are three of Harleman's conclusions:

- The equivalence between models and parameter values for laboratory chemostat experiments and the field situation--although the assumption of equivalence may provide valuable insights and order-of-magnitude estimates for the multiplicity of parameters, the validity of the assumption is still elusive and difficult to prove.

- Coupling the biochemistry with the correct hydrodynamical model--an averaged form of the system's hydrodynamics should not be substituted into an essentially biochemical model; if any averaging is required then it should be carried out in an a posteriori fashion on the output of a combined hydrodynamic/biochemical model for water quality.

- Field data collection is a most critical problem--given limited financial support and facilities it is better, at least for an estuarine system, to channel efforts into measuring temporal variations at a few field spatial locations, than to attempt boat cruises covering a large number of spatial locations for very short periods of time.

2.4 Hydrothermal Problems and Waste Heat Discharges

D.R.F. Harleman: Hydrothermal Studies on Reservoirs Used for Power Station Cooling

We can draw upon the first of Harleman's three earlier conclusions (section 2.3) to introduce this, his second presentation. The essence of the modeling approach adopted is that a physical laboratory model of the reservoir is constructed and by reference to this a mathematical model is developed, which is then evaluated with field data from the actual reservoir. The objective for the application of the model, specifically a model for Lake Anna in Virginia, is to predict vertical temperature profiles and to assess the effectiveness of the reservoir as a cooling pond. The given basis for verification is three year's of field data describing conditions before the sequential installation of four 1100 megawatt units of electrical capacity.

The analysis of the laboratory reservoir model reveals two salient features: that for reservoirs with an appreciable inflow and outflow (short detention times) temperature profiles are relatively insensitive to vertical diffusion; and that since surface temperatures are also insensitive to assumptions about vertical diffusivity, it makes little sense to test vertical diffusion models on the basis of surface temperature data. In the case of Lake Anna, which has low inflows and outflows, the surface temperature behavior can be adequately modeled by incorporating an algorithm for the simulation of wind-mixing effects, thus relaxing the sensitivity of the model to assumptions about constant or variable vertical diffusion coefficients.

The solution of the waste heat management problem, which itself involves further development of some basic thermal circulation models, suggests that a small isolated (or nearly isolated) "hot pond" section of the reservoir can effect the major portion of the heat dissipation without undue elevation of the main reservoir temperatures.

O. Vasiliev: Numerical Models for Hydrothermal Analysis of Water Bodies

One of the primary purposes of Professor Vasiliev's presentation was to review the developments leading to current investigations of three- and two-dimensional models for analysis of the hydrothermal behavior of water bodies. In this, Vasiliev paid particular attention to the contributions of the Institute of Hydrodynamics in Novosibirsk on the prediction of hydrodynamic and thermal phenomena in cooling water bodies.

For many practical applications there has been, and continues to be, a widespread use of (physical) laboratory models (cf. Harleman) for examination both of the water body to be used as a cooling pond and of the more detailed behavior to be expected in the vicinity of intake and outlet structures. There are, however, certain notable limitations to such models: they do not simulate all the interactions of the hydrodynamic and hydrothermal processes; and they cannot take into account the effects of wind action on the water body, which determine the two important features of free surface evaporation rates and convective heat exchange through the surface.

A three-dimensional transient (mathematical) model was thus proposed for the characterization of unsteady hydrothermal processes wherein stratification is described via a Boussinesq approximation. One variant of the model includes horizontal turbulent exchange and the other does not. The representation of salinity variations, and their effects on the density distribution, may be adjoined to the basic model if necessary. The coefficients of turbulent exchange are determined by using the turbulence energy balance equation. The problem is numerically solved by the method of fractional steps with the aid of an implicit difference scheme. A method of numerical realization of the latter variant was briefly described and some results of practical computations for cooling water bodies were reported.

There are possibilities for reducing the three-dimensional model to a two-dimensional approximation either by depth averaging or width averaging. Preliminary results are available for the application of such an approximate three-dimensional model to the Ekibastuz No. 1 Thermal Power Plant cooling reservoir, in Kazahstan (USSR), for the prediction of velocity and temperature distributions.

J. Jacquet: Studies in France on Water Quality Modeling

The guiding principles of the water quality modeling studies reported by Jacquet are those concerned with the siting of power plants and with evaluating the effects of temperature changes on an ecosystem. A major objective is to predict, as in Harleman's second presentation, the differences in behavior between the natural and the man-modified system. To meet this objective, models have been developed for prediction of both the near-field and far-field temperature distributions that result from a waste heat discharge. An additional desirable function of these models is to predict statistical distributions of temperatures. In other words, given historical distributions and sequences of hydrometeorological data, the models are employed to generate time-series of stream temperature in much the same way as hydrologists have been concerned with stream flow forecasting. Both the Seine and Rhone rivers are examples of where this latter kind of modeling has been applied.

A more intensive investigation of water/atmosphere exchanges and the development of thermoclines and reservoir stratification has been initiated. By chance, a lake which had been formed in an extinct volcano--and therefore has no watershed--provided an excellent experimental facility for these purposes. Elsewhere water quality modeling activities are being extended from the basis of temperature models to a consideration of dissolved oxygen models, with special reference to the impact of artificially elevated stream temperatures on increased photosynthetic production. This line of approach thus reflects the historical progression of water quality models reviewed by Orlob (see section 2.2).

2.5 Lakes and Reservoirs

S.E. Jørgensen: Water Quality Modeling of Lakes

In this presentation, Dr. Jørgensen offered the third, and perhaps most detailed strategy for water quality modeling (cf. Rinaldi, section 2.2; and Beck, section 2.3). This strategy for modeling is composed of:

- Definition of the goal for model development and application;
- Selection of the state variables;
- Development of conceptual flow diagrams;
- Development of system state equations;
- Parameter sensitivity analysis;
- Calibration of model with field data; and
- Validation of model with a second and further independent set(s) of field data.

The key question is determining "sufficient complexity" of the model to meet the stated goal for model application. Broadly speaking, complexity is interpreted as the number of state variables and the goal is the response of the ecological system--e.g., phytoplankton growth--to a change in nutrient input loadings. In order to confer a quantitative value to "sufficient complexity", the concept of ecological buffer capacity is introduced. We can intuitively relate such a concept to the stated goal of the modeling exercise, and formally ecological buffer capacity can be expressed and computed in terms of the exergy of the ecological system. More precisely, exergy, the mechanical energy equivalent of distance from thermodynamic equilibrium, is found to be correlated with ecological buffer capacity. The contribution of each state variable to the total exergy is calculated from given field observations and selection may be made between those variables that make a significant contribution and those that do not. For example, from this kind of analysis of a eutrophication model one concludes that sediment is significant but the division of zooplankton into two classes is not significant. Notice here, however, that the analyst is once again involved in a subjective judgment on the required level of model complexity: he must make a decision on what is and what is not significant.

P.G. Whitehead: Designing the Model to Suit the Nature of the Problem and the Field Data

Dr. Whitehead's discussion focused upon two Australian case studies:

- The modeling and management of estuarine systems--Western Port Bay, Victoria.
- Analysis of effluent disposal and eutrophication problems in the Murrumbidgee--Burrinjuck Lake System, Canberra.

The title is an adequate statement of Whitehead's attitude to water quality modeling. The question of sufficient complexity of the model is clearly related to the objective for model application: otherwise, from the basis of an essentially simple a priori model, the approach is to increase model complexity only when additional dominant modes of behavior can be identified from the given field data. An important feature of this approach is its recognition of the difficulties of distinguishing "deterministic" properties of the system from the substantial uncertainty in the observed system behavior.

As an illustration of the fundamental relationship between models and modeling objectives the Western Port Bay Study demonstrates a certain inconsistency. A simple steady-state water quality model for the inland catchment area, which would describe generally the long-term effects of urban and industrial development, was connected to a three-dimensional dynamic water quality model for the bay. The considerable computational effort of solving the latter does not appear to be justified either in terms of the study's objectives, i.e., to determine average, long-term impacts of development, or in terms of the input information originating from the steady-state catchment water quality model. A better alternative formulation, according to Whitehead, is the development of a highly aggregated, lumped-parameter, input/output model for salinity distribution in the estuary/bay area.

Mention of an input/output model and its usual association with black box models gives an opportunity of pointing out a common misunderstanding. A black box model of system behavior does not necessarily imply a completely stochastic model for there is as much determinism about the relationship between measured (input) disturbance and measured (output) response in a black box model as there is in an internally descriptive, or mechanistic model. Equally so, an internally descriptive model should not preclude some account of the random processes inevitably a part of any system's behavior.

V.J. Bierman: Comments on Water Quality Modeling: Saginaw Bay, Lake Huron, as an Example

The emphasis in Bierman's presentation was:

- That close cooperation is necessary between modelers and experimentalists; and

- That data requirements place a practical upper limit on the complexity of water quality models.

Perhaps data requirements may be interpreted as financial requirements: during the period 1974-76, more than 250,000 data points were obtained from Saginaw Bay at a cost of approximately one million dollars.

A single segment model for the inner portion of Saginaw Bay differentiates the representation of the Bay's ecological system into five phytoplankton types, two zooplankton types, higher predators, and the three nutrients--phosphorus, nitrogen, and silicon. Two of the primary reasons for choosing this level of (a priori) complexity are that different classes of algae have very different nutrient requirements and that not all of these classes have the same nuisance characteristics. In the course of testing the model against field data interaction between experimental work and model evaluation occurred in a number of forms:

- Since conventional chlorophyll measurements would not provide adequate field data for model calibration, an experimental program for measuring phytoplankton cell volumes was initiated; this permits the resolution of field data into the required categories of phytoplankton species.

- A notably poor correspondence between model response and field measurements was identified as unrepresentative sampling caused by thick mats of blue-green algae on the water surface.

- Sixteen laboratory chemostat experiments were conducted that explored phytoplankton growth-rate limitation as control was progressively transferred from nitrogen to phosphorus; this permits acceptance of the hypothesis that a (single substrate) *threshold* growth kinetics function be employed in the lake model in preference to the use of a (multiple substrate) *multiplicative* growth kinetics function.

Two of the above points illustrate problems of a more general character. Firstly, verification of the model against field observations must sometimes take account of the fact that all elements of the model state vector, e.g., phytoplankton species, are not linearly observed, or are only observed in an aggregative fashion, e.g., by chlorophyll-a measurements. And secondly, although Bierman uses the threshold growth hypothesis, he admits that the number of parameter values to be estimated in the model will allow the multiplicative growth hypothesis to be suitably fitted to the data. In other words, the number of parameters in a model are equivalent to the degrees of freedom available for matching the model to the data.

Finally, the differentiation between phytoplankton species is most important in this case for distinguishing the behavior of diatoms from the behavior of all other species.

3. FUTURE PERSPECTIVES

Is it possible then, to draw any conclusions about the state of the art of water quality modeling? Since the title of the preceding section mentioned only salient problems, it might be thought that the current status of the subject is more one of problems than one of solutions. This is perhaps a misleading view for the following reason. The present state of a subject can only be properly judged on the basis of its historical development. Also it is necessary to judge how the present will determine the likely future of water quality modeling. These are indeed difficult judgments to make. The history of water quality modeling is relatively easy to trace within one particular scientific or engineering discipline, for example, from the sanitary engineering viewpoint. The difficulty, however, is that besides a sanitary/public health engineering background, the history of water quality modeling has been shaped by almost quite separate and independent contributions from the limnological, microbiological, ecological, and hydrological sciences. A part of the present problem, therefore, even in so basic a matter as the rather confused terminology, is the multidisciplinary nature of water quality modeling, and it is this that in some ways has obscured the historical perspective.

Although we might still expect a unification of the subject's literature, a primary conflict for the future, as gauged by this Workshop, may be one of reaching for accuracy through further model complexity, yet striving for applicability through simplification of already existing models. The well documented case study would seem to be the most desirable kind of model development exercise since it indicates that water quality modeling tends to be problem oriented and that some form of experimental data collection program will be undertaken. Hitherto, field data in the form of time series, and the application of techniques of time-series analysis and system identification have not been a principal feature of water quality modeling. It might further be expected that future studies will concentrate on integrating water quality models with hydrological models for rainfall-runoff/river-flow prediction as the application of models moves towards problems of regional river basin management. In the past there has also been a distinct lack of overlap between models describing those water quality characteristics affected by waste disposal and models describing those water quality characteristics that affect the suitability of river water for industrial, municipal, and domestic consumption. A particularly good example of this is dissolved oxygen concentration, so often quoted as the central index of water quality with respect to the effects of effluent discharges, yet a variable that is not in itself a vitally important characteristic in establishing whether river water is fit for human consumption. Models not possessing this required combination of waste assimilation and public health considerations are inadequate in the sense that they do not allow the problems and opportunities of water reuse in a river basin to be properly explored.

4. REPORTS FROM THE AD HOC WORKING GROUPS

This section gives the concluding reports and recommendations from the nine ad hoc working groups that appraised water quality modeling activities under the following classifications:

- Deep Lakes and Reservoirs;
- Shallow Lakes and Reservoirs;
- Application of Systems Analysis to Eutrophication Problems of Rivers, Lakes, and Reservoirs;
- River Systems;
- Hydrothermal Processes and Thermal Pollution;
- Estuaries, Coastal Waters, and Inland Seas;
- Water Quality Planning and Management;
- Impact of Toxic Pollutants;
- Systems Methods in Model Development and Analysis.

4.1 Deep Lakes and Reservoirs (G.T. Orlob)

During the discussion two major topics were treated:

- Objectives of IIASA's program of in-house research for the next several years, and
- Topics for discussion at a special IIASA workshop on Hydrothermal Processes of Deep Lakes and Reservoirs--subsequently held at IIASA in December 1977 (see Jørgensen and Harleman, 1978).

The setting up of possible task force groups was also considered. The results of these discussions were the following tentative recommendations:

In-house Research at IIASA

Research into the modeling of deep lakes and reservoirs should emphasize the resolution of such problems as:

- Identification of internal mixing processes and estimation of mixing in terms of measurable in situ properties of the limnological system--e.g., temperature, salinity, and suspended solids--affecting density or velocities (water and wind) and water levels.

- Effects of hydrodynamic behavior on biological (ecological) behavior--e.g., effects of thermal stratification in limiting exchange of nutrients in the water column--and effects of internal mixing on nutrient exchange between deposited sediments and the overlying water column.

- Characterization of stratified flows in deep, narrow (two-dimensional) lakes, i.e., problems where hydromechanical behavior and water quality (density influences) are closely coupled. An example of interest is destratification.

- Influence of major inflows (or outflows) on vertical and longitudinal (or lateral) distribution of water quality in a lake or reservoir.

- Formation of ice cover--both freezing and thawing processes--and its influence on hydromechanical and ecological processes within the impoundment.

- Transfer (or diffusion) of nutrients between sediment in suspension or at rest near the bottom of a deep impoundment and the overlying water column.

- Type of model best suited to simulation of water quality processes, i.e., single versus multiparameter models.

<u>The Workshop on Hydrophysical and Ecological Modeling of Deep Lakes and Reservoirs, December 12-15, 1977, (specification by M. Markofsky)</u>

The workshop, as proposed, should address the following topics:

- Boundary conditions--surface (O_2, CO_2, heat transfer, benthal, runoff);

- Thermal stratification--winter regime;

- Numerical methods;

- Water quality--limiting parameter versus total cycle description--theory and application;

- Retention time in stratified lakes;

- Field data collection techniques for model verification and their limitations;

- Pumped storage reservoirs;

- Construction of reservoirs--water quality constraints;
- Reservoir systems;
- Reservoir management (selective withdrawal, artificial mixing and oxygenation, pre- and in-reservoir treatment);
- Artificial destratification;
- Lake description and model choice.

A Possible Task Force Group

This would consider education of decision makers in the form of "guidelines" for the use of ecological models. Thus, the titles "Are BOD-DO Models Enough for Water Quality Prediction in Lakes and Reservoirs", or "Beyond Streeter Phelps--Water Quality Models of Lakes and Reservoirs" were suggested for the Task Force Seminars.

Group Members: G.T. Orlob, USA (Chairman)
M. Markofsky, FRG (Vice Chairman)
E. Bogdanov, Bulgaria
G. Dinelli, Italy
B. Georgiev, Bulgaria
K. Kinnuen, Finland

4.2 Shallow Lakes and Reservoirs (P. Mauersberger)

Some Characteristic Features of Shallow Lakes

- They are strongly affected by wind and wave action. In spite of this, they may be stratified at least for short periods. This has significant consequences for the ecological system.
- Wind is a stochastic "impact" and a primary forcing function. Wave action is also a stochastic process and has an important influence on mixing.
- Mass transport processes along the vertical axis are of great importance, especially for the exchange of nutrients between the water body and the sediments.
- Binding and movement of nutrients in the sediments plays an important role in the cycling of matter and in bioproduction. The release of nutrients from sediments has (significantly through fish at the bottom) direct influence on the entire water column.

- The water body and type of sediments may also show horizontal gradients.

Research Problems

Hydrodynamics of transport and diffusion processes:

- Vertical transport in the water column and across the water-sediment interface (IIASA is asked if it can contribute to this research).

Ecological modeling:

- Evaluation of available data by simple models including sensitivity analysis;
- Improvement of measuring methods and improvement in the volume and quality of data, e.g., data concerning the binding and movement of phosphorus (research external to IIASA); and
- Further development of ecological models of (shallow) lakes taking into account the binding and movement of nutrients in the sediments.

Case Studies

Representatives of the NMOs of Czechoslovakia, the GDR, Hungary, the Netherlands, and the UK propose:

- to intensify the exchange of preprints, reprints, and reports;
- to improve the availability of data;
- to organize collaboration through IIASA.

IIASA and its NMOs are encouraged to take part in these activities.

Group Members: P. Mauersberger, GDR (Chairman)
J. Davis, UK
J. Fischer, Hungary
L. Lijklema, Netherlands

4.3 Application of Systems Analysis to Eutrophication Problems of Rivers, Lakes, and Reservoirs (S.E. Jørgensen)

The group proposes that IIASA should conduct a study of lake and river ecology using well documented case studies for comparison of different types of eutrophication models. These case studies need therefore to establish comprehensive data bases at IIASA for testing the models.

The data base must be broad enough to ensure adequate verification and validation of the models for each case study and should, if possible, contain a major perturbation of the system --e.g. a major effluent discharge--so that the predictive capability of the models can be assessed.

The models must be transferred to IIASA as working versions of various documented models.

The project should be carried out by a working group at IIASA with additional assistance from those Institutes or organizations that provide either data for case studies or working versions of models. Such assistance could be realized by short-term visits to IIASA.

The aims of this project are:

- To assess the role that system analysis methods can have in the study of eutrophication;
- To identify the structure of a eutrophication model;
- To assess the degree of model complexity required to describe the system adequately;
- To assess which methods of systems analysis are most suitable to identify the model mechanisms and to estimate model parameters;
- To provide understanding of the ecological mechanisms of importance for the eutrophication process;
- To examine the transferability of models: although a general model does not exist, it might be possible to transfer parts of models from one case to another.

Several members of the working group expressed a willingness to contribute comprehensive data bases as well as documented models.

The selected case studies should include alpine lakes, rivers, shallow lakes, and reservoirs; and at least some of the case studies should not contain spatial variability, since the available methods of analysis can more easily be developed in the context of lumped-parameter models.

This program was considered to be of great interest and could be implemented under UNESCO's Man and Biosphere Project 5--Inland Waters. Consequently, it was suggested that the International Coordinating Council of "Man and Biosphere" be informed of this project. (The next session of this Council was planned for October 26 - November 1, 1977, in Vienna.)

Group Members: S.E. Jørgensen, Denmark (Chairman)
V.J. Bierman, US
J. Davis, UK
H. Löffler, Austria
P. Mauersberger, GDR
S. Rinaldi, Italy
H. Stehfest, FRG
P.G. Whitehead, Australia

4.4 River Systems (M.B. Beck)

The group found it difficult to establish how its interests and IIASA's position could be made compatible within the scope of collaborative studies. The interests expressed are catalogued below, and the summary concludes with some suggestions for unifying themes.

Interests

- The discussion began with a stressing of the similarities between lakes and river systems, particularly in certain respects of nutrient and phytoplankton behavior.

- Part of the group agreed that methods of system identification and parameter estimation should be applied to well documented case studies.

- Others felt that there was a pressing need to clarify the performances of the various river water quality models before proceeding with increased model complexity. Indeed there was the possibility that this could be done with data made available at the Institute.

- A fourth interest, expressed by more than one individual, was the suggestion that the "systems" approach could be used to analyze the impact of large civil engineering construction on river basin water quality (specific examples, such as the successive impoundment of parts of the Rhine and Danube, were given).

- Several participants thought that real-time operations, i.e., on-line forecasting and control, were an important facet of potential collaborative projects to be undertaken in Task 2.

- Although with limited resources only a minimal effort could be expended in this direction, two participants remarked upon the lack of general discussion of the relationships between wastewater treatment and river water quality.

- Lastly, but by no means the least significant comment, we felt that consideration of "philosophical" aspects of modeling should not be ignored. For example, we suspect that a trade-off exists between model complexity and model accuracy; we disagreed about the transferability of models from one system to another; and the opinion was expressed that stochastic features of modeling should receive much more attention in the future.

Suggestions

Many of the seven above points fall naturally within the scheme of in-house IIASA studies. However, for collaborative undertakings the most easily accommodated themes are those relating to model comparisons against the same field data set (the third point), and the exchange of ideas about fundamental problems of modeling.

Group Members: M.B. Beck, UK (Co-Chairman)
S. Rinaldi, Italy (Co-Chairman)
W.J. Grenney, USA
G. Huthmann, FRG
M. Kozak, Hungary
R. Krasnodebski, Poland
N. Matsche, Austria
G. Pinter, Hungary
H. Stehfest, FRG
P.G. Whitehead, Australia

4.5 Hydrothermal Processes and Thermal Pollution (D.R.F. Harleman)

The following topics were suggested by representatives of National Member Organizations as areas for future cooperative research with IIASA.

Condenser Water Discharges into a River

Specifically, these are river bank discharges (at various angles to the axis of the river) in relatively shallow water in which the thermal plume is expected to be attached to the near river bank. Specific problems and possible case studies mentioned were on the Vistula River in Poland and on rivers in Czechoslovakia and Bulgaria (where additional problems will arise due to future increase in river depth and reduction of velocity as a consequence of downstream dam construction).

From the conclusions of the Workshop discussions, there are two potentially useful models under development by other members of IIASA; namely, VINTRI and TRIMI--models reported by Dinelli, ENEL (Italy) and Sündermann and Fischer (Hannover, FRG). These are three-dimensional models, incorporating buoyancy effects, but must be considered as far-field models because of difficulties with the turbulence closure problem related to momentum jet entrainment. Near-field effects may be treated by experimental and analytical studies conducted at MIT (Harleman) and Karlsruhe (Naudascher).

A specific proposal was that a meeting at IIASA be organized in November 1977 [subsequently held during November, and reported by D.R.F. Harleman] for interested individuals to initiate cooperative research, possibly involving periods of residence at IIASA by representatives of both model developers and users.

Use of Lakes and Reservoirs in Conjunction with Electric Energy Production

To review the state of the art of prediction of the hydrothermal effects of waste heat addition to ponds, lakes, and impoundments. This includes criteria for stratification, effects of wind and internal dikes, surface heat exchange with elevated temperatures, and consumptive water use. To make a comparison of models developed at MIT, Novosibirsk, and others with field data (e.g., from Commonwealth Edison cooling ponds and Lake Anna).

To study the effect of pumped-storage operations with daily cycling of large inflows and outflows on temperature distribution and water quality.

An Italian group is interested in eutrophication due to the accumulation of nutrients in two artificial lakes (upper and lower reservoirs) receiving make-up water (to replace evaporation) from an adjacent river. Otherwise, long-term data on pumped storage reservoirs, as mentioned by J. Davis (UK), may be of interest.

Group Members: D.R.F. Harleman, USA (Chairman)
G. Abraham, Netherlands
E. Bogdanov, Bulgaria
W. Czernuszenko, Poland
G. Dinelli, Italy
K. Fischer, FRG
B. Georgiev, Bulgaria
J. Sündermann, FRG
L. Zahrer, Austria

4.6 Estuaries, Coastal Waters, and Inland Seas (R.V. Thomann)

Recommendations for Further IIASA Activities

- Sediment transport and water quality, including such topics as transport of nutrients, toxics attached to sediments, bed-sediment interactions, turbidity motions (provided the sediment transport itself is sufficiently well described).

- Effect of treatment on model coefficients; should the parameters be changed during the investigation?

- Mixing behavior of stratified flows, including the proper modeling of turbulence and dispersion phenomena.

- Optimization of total system treatment (including receiving water).

- Interaction of water quality and fishery resources, e.g., the question of migrating species in transition zones.

- Hydrodynamic and water quality models operate normally within different scales. Thus how do we convert the fine grid information on the hydrodynamics to the coarse grid of quality models?

- Case studies. These should have a sufficient, well documented data base (including the inputs); they should be not too complicated (from the point of view of geometry), and should study a well posed problem where collaboration is possible with some chance of success. Possible areas are the Odra entrance, the near shore zones in the Baltic, the Black Sea, and the Mediterranean. A data base should be constructed at IIASA(?).

Other questions to be discussed (but not as subjects for recommendation) are:

- Review of water quality management decisions already made (post audit);

- Objective measures for the quality of models;

- Which constituents in water quality modeling and why?

Group Members: R.V. Thomann, USA (Chairman)
G. Abraham, Netherlands
K. Cederwall, Sweden
N. Chlubek, Poland

G. Dinelli, Italy
K. Fischer, FRG
J. Sündermann, FRG

4.7 Water Quality Planning and Management (D.P. Loucks)

There seem to be two general types of water quality models. One results from a desire to achieve a more comprehensive understanding of the physical, biochemical, and ecological processes that take place in water bodies receiving potential pollutants or nutrients. IIASA should not attempt to undertake a major program of this type of model development.

The second type is oriented toward planning, management, and/or real-time control. The core of such models are derived from the first type of water quality predictive model, but are usually simplified versions of them. In planning models there are variables representing various management alternatives and their economic and other impacts. For water quality planning and control, the simplest model that provides the information needed seems to be the best. (It is no accident that most consultants use some form of the Streeter-Phelps model for DO and BOD prediction, or the rational formula for runoff prediction, since they are easily understood and do not require extremely expensive data collection and analysis exercises.) Can decision makers appreciate, for example, the difference between a minimum dissolved oxygen concentration of 4.5 or 3.5 mg/1 or a reliability of 90 or 95%? We suspect not, especially given the impact that institutional or bureaucratic objectives and future economic and technologic uncertainties have on the planning process.

IIASA is in an excellent position to make a contribution in water quality management and control modeling--specifically towards developing experience in assessing the appropriateness of various models to various planning problems or situations. The best model will depend on the information needed, which will differ for different water bodies, on management alternatives, and on possible institutional objectives and constraints. Only through case studies can we learn more about how to predict the appropriate model complexity and how to improve the quality of information derived from models for the planning process. IIASA has made contacts with some organizations in NMO countries who need help in using models to evaluate water quality management alternatives of actual river systems. We strongly urge IIASA to pursue these contacts and become involved in case studies in water quality planning.

Another significant improvement in the state of the art of water quality management modeling could come from the development of models that can be used when planning objectives are unknown at the beginning of the planning process, and change during the process. Research is also needed in the combined interactive use of optimization models for preliminary definition and evaluation of alternatives, and more complex simulation models for more detailed and precise evaluation. IIASA could contribute to this needed systems methodology.

Group Members: P. Loucks, USA (Chairman)
L. de Mare, Sweden
M.J. Gromiec, Poland.

4.8 Impact of Toxic Pollutants (M.J. Gromiec)

Many water quality constituents are toxic at certain concentrations and interact directly with living components of the ecological system causing death or severe stress and limiting the use of water resources.

Water quality models for toxic pollutants are in a preliminary state of development, but a few are available for various toxicants. In addition, a body of literature exists for modeling the fate of radioactive substances in the environment. Functions relating toxic pollutant concentration, type of exposure, and survival or effect are available from literature on toxicity and may be incorporated into water quality models.

With growing industrialization and an increasing number of new toxic compounds, there is a great need for development of water quality/ecological system models that can be used for prediction of safety levels and for establishment of water quality criteria. The investigations should include:

- heavy metals;
- chlorinated hydrocarbons, oils;
- pesticides, herbicides, and insecticides;
- new toxic organic compounds together with their biodegradability; and
- radionucleides.

A small working group should be established to clarify and refine the necessary directions for toxic substance model development at IIASA. This group would

- review the present state of modeling and related models in water areas;
- determine case studies and data bases;
- suggest a specific program of model development to IIASA.

This group should complete its work within six months.

Group Members: M.J. Gromiec, Poland (Chairman)
S.E. Jørgensen, Denmark
C. von Stempel, FRG
R.V. Thomann, USA

4.9 Systems Methods in Model Development and Analysis (E. Halfon)

Objective

If one or more case studies are agreed upon and a data set is available, then the members of this group will provide their expertise in model development and its verification.

Methods

- Identification of a black box nonlinear model by the GMDH (Group Method of Data Handling); this will provide information on the relative influence of the state variables and thus an estimation of the model order and structure.

- Identification of model structure by stability analysis and modeling in state space.

- Estimation of model parameters; definition of an ecologically valid objective function and the weights to be used--a corollary of this research might be the verification of a model in the sense of a set of tests made to establish that the developed model works as expected.

- Other identification methods.

- Coordination of research so that the results are ecologically valid; comparison of results of many methods on one set of data can produce insight on the system and help other researchers in model development.

- These techniques can also be used in model verification and thus the group can contribute to the standardization of methods for model verification and validation.

Rationale

The fact that the group can work on the same data set implies that the results can be compared. Also, each investigator will be able to contribute to the project from his own institute without loss of continuity. Further individual or group visits to IIASA will result in productive research.

If a test case is agreed upon, and provided scientists will be working on this case at IIASA, then collaboration with other groups could be significant. In addition, since this group is interested in methodological (systems) problems, then collaboration with several groups (research projects) can be initiated.

Group Members: E. Halfon (Chairman)
N. Adachi, Japan
J. de Graan, Netherlands
R. Krasnodebski, Poland
H. Tamura, Japan

5. CONCLUSIONS

I will now try and illustrate how the recommendations of the working group discussions are being, or can be, accommodated within the research activities of the Institute. When the Workshop was originally conceived, it was seen as an opportunity for gathering interest and participation in the development and application of water quality models. Where participation is possible it should clearly be understood to be *collaborative research* that both encompasses and stimulates those studies conducted at IIASA by the in-house, core, research staff. An oft-quoted criticism of our research plans is that they address too big a problem (or problems) with too little manpower. If we were to respond to all the suggestions listed in this report we should indeed be attempting once again to spread our resources too widely over too large an area of activity. It is true that global or universal problems are the subjects of our research plan; yet we recognize that what can be achieved is no more than the sum total of the efforts of a few individuals. It is also true that we are not insensitive to the carefully reasoned counsel of the Workshop discussion and working group reports. How, therefore, are the future plans for the Task a response to this advice? The number of directions in which the Task, "Models for Environmental Quality Control and Management (Hydrophysical and Ecological Models for Water Quality)", could proceed is in fact remarkable for its size and great variety. A sample of the additional and modified foci of attention currently being drafted into a longer-term (five-year) research plan follows.

Perhaps most significantly, the Hungarian delegation to the Institute's Council Meeting of November, 1977, proposed Lake Balaton as a specific water quality case study in which the objectives would be to manage the problems of eutrophication through the appplication of systems analysis (cf. section 4.3). The agreement reached between the Hungarian institutions and IIASA delineates the following areas for cooperation:

- Comparison of existing eutrophication models against field data for Lake Balaton (cf. section 4.3).

- Development and application of improved models with special reference to phosphorus exchange between water and bottom sediments, to stochastic nonpoint nutrient loading, and to wind-induced mixing mechanisms (cf. section 4.2).

Two case studies from Task 1 of IIASA's Resources and the Environment Area, "Regional Water Management", overlap with the topic of water quality management (cf. section 4.7). It is hoped that a study in Sweden will permit the exploitation of water quality models at the planning/design phase of management, while a joint project with the Ohre River Board in Czechoslovakia may call upon the use of water quality models in a real-time operational forecasting and control situation (cf. section 4.4).

Elsewhere, time-series field data available from experimental programs in the UK will facilitate the realistic application of system identification and parameter estimation techniques in model development (cf. section 4.9).

For the intermediate future a need can be identified for work to be initiated in the area of estuaries and coastal waters (cf. section 4.6), if the Task is to achieve its objectives for a balanced and comprehensive coverage of case studies in water quality modeling. And lastly, as a topic arising naturally from studies of the impact of waste discharges on the environment, a significant reorientation of the Task might be provided by the problem of modeling the movement of toxic substances through aquatic ecosystems (cf. section 4.8). In any event, it is IIASA's intention to seek advice and participation in those matters. We expect that the ad hoc working groups, though not formally constituted, will be equally responsive.

References

Harleman, D.R.F. (1977), *Models for Waste Heat Management in Rivers*, Summary Report on a Working Group Meeting, International Institute for Applied Systems Analysis, Laxenburg, Austria (internal publication).

Jørgensen, S.E., and D.R.F. Harleman (1978), *Hydrophysical and Ecological Modeling of Deep Lakes and Reservoirs*, CP-78-11, International Institute for Applied Systems Analysis, Laxenburg, Austria.

APPENDIX A: WORKSHOP AGENDA

Tuesday, September 13	10:00	OPENING ADDRESS by Dr. R. Levien, Director of IIASA.
	10:30	Overview of IIASA's research on Resources and Environment, by Prof. O. Vasiliev, IIASA.
	11:30	State-of-the-Art Review of Mathematical Modeling of Surface Water Impoundments, by G.T. Orlob.
	14:30	A Real-Time Model of the Nitrogen-Cycle in Estuaries, by D.R.F. Harleman.
	15:30	An Overview of Modeling and Control of River Quality, by S. Rinaldi.
	16:30	Informal Presentations by Workshop Participants representing IIASA National Member Organizations.
Wednesday, September 14	09:00	Numerical Models for Hydrothermal Analysis of Water Bodies, by O. Vasiliev.
	09:45	The Need for New Directions in Water Quality Modeling: The Hazardous Substances Example, by R.V. Thomann.
	11:00	Studies in France on Water Quality Modeling, by J. Jacquet.
	11:45	Informal Presentations by Workshop Participants representing IIASA National Member Organizations.
	14:30	Ad hoc Working Group Discussions
Thursday September 15	09:00	Information on IIASA's State-of-the-Art Survey of Water Quality Modeling, by G.T. Orlob.
	09:45	Mathematical Modelling of Water Quality; A Case Study in the U.K., by M.B. Beck.
	10:45	Water Quality Model of Lake Biwa and the Yodo River System, by N. Adachi.

	11:15	Modeling Activities in Canada, by E. Halfon.
		Water Quality Modeling in Hungary, by G. Pinter.
		Application of Water Quality Models, by M. Kozak.
		Water Quality Modeling in Finland, by K. Kinnuen.
		Work in Italy on Water Quality Problems Arising from Industrial Plant Effluents, by G. Dinelli.
	15:45	Review of the Activities in Water Quality Modeling in FRG, by G. Huthmann.
		Water Quality Modeling in Czechoslovakia, by J. Habrovski.
		Mathematical Modeling Case Studies in Utah, by W.J. Grenney.
		A Scheme for Optimal Water Quality Control in a River System, by R. Krasnodebski.
		Modeling and Identification of River Quality Systems Using Distributed Lag Models, by H. Tamura.
Friday, September 16	09:00	Water Quality Modeling of Lakes, by S.E. Jørgensen.
	09:30	Examples of Water Quality Modeling in the GDR, by P. Mauersberger.
		Water Quality Modeling of Lake Balaton, by J. Fisher.
		Comments on Water Quality Modeling: Saginaw Bay, Lake Huron, as an Example Study, by V.J. Bierman.
		Hydrothermal Studies on Reservoirs Used for Power Station Cooling, by D.R.F. Harleman.
		Water Quality Problems and Recent Studies in Bulgaria, by B.V. Georgiev.

Solving the Convection Diffusion Equation by Means of a Monte Carlo Method, by J. Sündermann.

Water Quality Modeling in Austria, by N. Matsche.

Designing the Model to Suit the Nature of the Problem and the Field Data, by P.G. Whitehead.

14:30 Closing Session: formulation of conclusions and reports from ad hoc Working Groups.

APPENDIX B: LIST OF PARTICIPANTS

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APPENDIX D: GLOSSARY

With so many different scientific and engineering disciplines represented at the Workshop it is not surprising that there was some confusion over the terminology used in (water quality) modeling. The following list of terms and their definitions is given as clarification of that generally adhered to in this report. Where more than one term is employed for roughly the same concept this is indicated by additional words or phrases in parentheses.

Black Box (Input/Output, Time-Series) Model

A black box model of a system assumes no a priori knowledge of the internal physical, chemical, or biological phenomena that govern the system's behavior. For the input/output situation the model accounts only for *what* the input disturbance is observed to do to the output response (compare with *internally-descriptive model*); as an example, we can imagine a black box model which relates a time-series of in-lake chlorophyll-a measurements to a time-series of point-source phosphorus loadings. A black box model is rarely a general description of process behavior and its validity is usually restricted to the range and conditions of the experimental data set from which it is derived.

Internally Descriptive (Mechanistic) Model

As its name suggests, an internally descriptive model exploits much more, if not all, of the a priori information on the physical, chemical, or biological mechanisms that govern process behavior. An internally descriptive model is capable of describing *how* the input forcing functions (disturbances) are related to the state and output responses of a system (see also *state variable* and *linear observations*). Such a model is generally capable of universal applicability and has an apparent grounding in theory or the "laws of nature".

Linear Observations

It is mostly assumed that the state of water quality in a system can be directly, or linearly, measured (in the presence of an additive kind of random measurement error). That is to say, we can measure DO concentration and temperature as the state of a reach of river; by the same token, this implies that the output response of the system is, straightforwardly, the measured variations in the system's state. A more complex situation for model verification arises, however, when the state of the system is not linearly observed. For instance, if the state of the system includes blue-green algae and diatoms as separate states, and if output response is measured as chlorophyll-a concentration, then the model predictions of blue-green algae and diatom concentrations will have to be added together and this sum prediction compared with the chlorophyll-a measurement. To some extent, therefore, model verification (against field data) is required to distinguish between the way that a system behaves and the way in which that behavior is observed.

Model Order

Not to be confused with the order of a differential equation, model order is the number of elements (variables) in the system's state vector.

Model Structure Identification

A broad definition of model structure identification is the problem of establishing how the measured system inputs are related (mathematically) to the system's state variables and how these latter are in turn related both to themselves and to the measured system outputs. Implicit in this definition is the assumption that these relationships are to be identified by reference to a set of field data. Model structure identification is partly concerned with the selection of the number of state variables and partly concerned with the selection of appropriate forms for the mathematical expressions included in the model. An example of the latter is discussed in the text (section 2.5, Bierman): choosing between the expressions for the multiplicative growth hypothesis and the threshold growth hypothesis is precisely the problem of model structure identification. In short, model structure identification as a concept is akin to the problem of deciding whether to draw a straight line or a curve through a set of data.

Parameter (Coefficient)

Model parameters are those constants--e.g., reaeration coefficient, maximum specific growth-rate constant--appearing in the model equations.

Parameter Estimation

Parameter estimation is the use of algorithms for estimating the model parameter values given a set of in situ field data for the measured model inputs and outputs.

State (Compartment) Variable

These are quantities--usually functions of both time and space, such as salinity concentration or temperature--that characterize the essential properties and behavior of a system.

State Estimation

Since all measurements are subject to chance error and since a system may be disturbed in an unknown or uncertain fashion, state estimation is the use of algorithms for the provision of some "best" estimate of the system's state variables. As well as a best estimate, the algorithms also compute a measure of expected error in that estimate.

State Reconstruction

Suppose we have a model for nitrification in a river that includes mass balances (state equations) for *nitrosomonas* and *nitrobacter* bacteria. State reconstruction is the use of algorithms whereby estimates of *nitrosomonas* and *nitrobacter* concentrations can be reconstructed from field measurements of ammonia, nitrite, and nitrate concentrations. In other words, it is the reconstruction of information about state variables that cannot be measured.

System Identification

This is not really a term but a subject in its own right. System identification covers all matters relating to the derivation of mathematical models from field data, where field data are usually assumed to be available in the form of time-series measurements. System identification thus embraces *model structure identification*, *parameter estimation*, *verification*, and *validation*, among other topics.

Validation

Validation is the testing of a model's performance, adequate or otherwise, against two or more independent sets of field data.

Verification (Calibration)

After the model structure identification and the parameter estimation phases of analysis, comes verification. The analyst sets out to check that the statistical properties of the model fitting errors are such that there is no further "information" in these errors not attributable to chance or random behavior. This is, perhaps, a rather narrow interpretation of verification. Section 4.9, however, gives a slightly broader definition whereby verification is understood as a set of tests made to establish that the model works as expected. Calibration, on the other hand, might best be described as a process that includes both *parameter estimation* and verification.

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