Lecture Notes in Engineering

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PREFACE

During 1978–1982 the International Institute for Applied Systems Analysis (IIASA) was responsible for a research project on Environmental Quality Control and Management. The project was begun under the direction of Professor O.F. Vasiliev (from the Institute of Hydrodynamics of the Siberian Branch of the USSR Academy of Sciences) and was subsequently led by myself. This review is very much a reflection of that IIASA project.

The major themes of the IIASA project were:

(i) research into the methodological aspects of modeling river and lake systems [some of the principal results of this research appear in M.B. Beck and G. van Straten (eds.) (1983), Uncertainty and Forecasting of Water Quality (Springer, Berlin (West)), and in K. Fedra (1983), Environmental Modeling Under Uncertainty: Monte Carlo Simulation (IIASA Research Report RR-83-28)];

(ii) case studies in the application of mathematical models to lake eutrophication control [results of which are summarized in L. Somlyody, S. Herodek, and J. Fischer (eds.) (1983), Eutrophication of Shallow Lakes: Modeling and Management (The Lake Balaton Case Study) (IIASA Collaborative Proceedings CP-83-S3), and in K. Fedra (1983), A Modular Approach to Comprehensive System Simulation: A Case Study of Lakes and Watersheds (in W.K. Lauenroth, G.V. Skogerboe, and M. Flug (eds.), Analysis of Ecological Systems: State-of-the-Art in Ecological Modelling, pp. 195–204. Elsevier, Amsterdam)];

(iii) a policy study of operational water quality management [M.B. Beck (1981), Operational Water Quality Management: Beyond Planning and Design (IIASA Executive Report ER-7)].

The project was also responsible for an international survey of the subject of water quality modeling, the results of which have been published in G.T. Orlob (ed.) (1983), Mathematical Modeling of Water Quality: Streams, Lakes, and Reservoirs (Wiley, Chichester).

In the latter part of 1981 I was invited by UNESCO to prepare an introductory paper for an International Workshop on The Comparison of Application of Mathematical Models for the Assessment of Changes in Water Quality in River Basins, both Surface Water and Groundwater (La Coruña, Spain, April 1982), and this review is a substantially revised version of that paper.

My intention in preparing this review has been to provide a context for the development and application of models for water quality management over the past two decades, and then to place some of the IIASA studies in that context. Because of its several disciplinary origins the subject of water quality modeling is rather amorphous. In this review I have therefore been concerned to categorize the problems of water pollution, to assess how one might use models to address these problems, to examine the philosophical basis for developing such models, and thence to survey the application of models for the purposes of management. It was not my intention here to provide a text on how to use models for managing water pollution problems; nor was it my intention merely to provide a catalogue of who has done what in this subject area. I hope rather that I have provided a historical account, a view of the current state, and a sketch of the possible future of water quality modeling.

The stimulus to prepare this review came from UNESCO. I am sure that I would not have attempted such a task without their invitation to do so, and I acknowledge my debt to UNESCO both for this invitation and for their permission to publish the review in its present form. I am also deeply indebted to IIASA, to the experience it provided, and to the many colleagues and persons who collaborated in the project on Environmental Quality Control and Management. I am particularly grateful to Oleg Vasiliev, Janusz Kindler, Kurt Fedra, Alexander Leonov, Laszlo Somlyody, and Gerrit van Straten. I am grateful to M. Straskraba and D. Scavia for their comments on an earlier draft of this paper, and to R.B. Ambrose, Jr., D. Imboden, D.C.L. Lam, G.T. Orlob, and R.V. Thomann for the provision of papers and technical reports. I have also an apology to make. The more one tries to include in a review, the more one is embarrassed by having to put aside relevant contributions, simply in the interests of finishing the task.

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CONTENTS

1 INTRODUCTION

As for many other subjects, the 1960s and early 1970s were a period in which mathematical modeling became firmly associated with studies in the science and management of water quality. It was (presumably) an exhilarating time when the boundaries of what was possible, in terms of computer simulation, advanced with the ever increasing capacity and speed of the digital computer. This period of accelerating development was also characterized by the generalization and amalgamation of previously particular models for specific case studies into what might be called "all-purpose, off-the-shelf" models intended to be adaptable and applicable to any water body (e.g. Water Resources Engineers, Inc., 1973, 1975; Hydrologic Engineering Center, 1974; Park *et al.*, 1975). The papers collected by Russell (1975) are representative of the most advanced studies conducted up to that date. But already by the late 1970s the concentration of effort on the development of large, complex simulation models – models not necessarily intended for management – had passed its zenith. Serious questions had been raised about the problem of "verifying" the models against field data (e.g. Thomann and Winfield, 1976). It was clear that what could be simulated in principle was quite incompatible with what could be observed in practice in the field. The lack of adequate field data was, and still is, a major constraint on progress in water quality modeling. From the mid-1970s an element of uncertainty in water quality modeling began to be formally recognized (Burges and Lettenmaier, 1975; Tiwari *et al.*, 1978; O'Neill and Gardner, 1979), the outgrowth of which is the current focus of studies in "uncertainty analysis" and the analysis of prediction error propagation (e.g. Beck and van Straten, 1983). No doubt it would be claimed for the application of models to management issues that there were some notable successes during the past decade (Biswas, 1981a). But in certain instances, where earlier the advantages of modeling had been confidently embraced (Newsome, 1981), a retrospective appraisal has shown clearly a less positive attitude toward the benefits of using models for water quality management (Woodward, 1980). After twenty years of intensive research and development there is still "considerable reluctance", as one author has put it (Holmes, 1982), to use models for the purpose of water quality management. There are certainly those who believe that regression models are adequate until proved inadequate, or that common practical experience cannot be substituted by models in any form.

To summarize, then, a personal view of the current state of water quality modeling, one sees that the initial enthusiasm and promise, which typify any new subject, have given way latterly to more realistic and dispassionate considerations. Different types of models are appropriate for solving different kinds of problems; there is no universal model for solving all manner of problems; comprehensiveness and complexity in a simulation are no longer equated with accuracy; and there is a healthy mood of critical questioning of the validity and credibility of water quality models. There is evidence, too, of a pragmatic skepticism about the virtues of using anything but the simplest of models for management. Whether this skepticism is justified is not clear, however. Probably the most that can be expected is that the process of modeling and its results may significantly influence the debate about how best to manage water pollution problems. It is difficult, if not impossible, to state categorically that a specific decision was determined by a particular result of any modeling exercise. The evolution of water quality management and of the models whereby some of the issues of management are resolved are two distinct, but interacting, trains of development. The one (modeling) is both a distillate of past experience and a stimulus to the possible future development of the other.

The purpose of this paper is to review the development, extent, and relevance of mathematical models in understanding and managing various classes of water pollution problems. The balance of emphasis in the review is weighted toward the application of models for management purposes, and it is principally for this reason that we have chosen not to classify and categorize the subject according to whether a certain model is deterministic or stochastic, dynamic or steady-state, and so forth. There is, nevertheless, adequate discussion of both the procedure for model development and the more methodological questions of the role of uncertainty in water quality modeling. These topics, however, are dealt with in more detail elsewhere (Beck, 1983a, b, 1984). In spite of its length, the review is no more than a rapid sweep across the contours of an extensive, and often fragmented, field of research. There are omissions, and this is inevitable. The primary focus is on lake and stream water quality models, with notably less attention given to problems of estuarine and groundwater quality. The matter of thermal pollution will only be occasionally mentioned in passing, and in general the review does not enter into a discussion of process kinetic expressions or the mathematical aspects of streamflow, transport, hydrodynamics, and lake circulation. Again, these are topics adequately reviewed elsewhere (Orlob, 1983a).

Section 2 of the paper deals with approaches, methods, and making predictions in water quality modeling; it is essentially concerned with analytical techniques. We shall, however, begin this discussion with a brief statement of the long-term temporal succession of pollution problems, since this is a natural preface to the review. Assuming, then, that many problems of water quality management are large-scale, complex, and not necessarily well defined, we discuss intuitive approaches to decomposition of the overall problem into more tractable subproblems. This is followed by the examination of a procedure for model development bearing in mind the relationship between models and modeling objectives, questions of scale (or detail), and the balance between theory and observation (Section 2.3). Section 2.4 discusses the analysis of field data, its relevance to management, and the design of experiments and monitoring programs. In the last part of Section 2 (Section 2.5) we look at matters concerning validation, prediction, and uncertainty.

Section 3 begins with an examination of standard-setting and monitoring procedures and a classification of management into the three phases of planning, design, and operation. It also considers several important questions that might be asked of any proposed solution to a problem, including the role of determining optimal solutions. We then review successively the development and application of models for the management of easily degradable organic wastes, eutrophication, the nitrate problem, and toxic substances. Throughout this succession of problems a primary objective is to assess critically the usefulness of modeling to management.

Section 4 is concerned with the kind of management issues likely to succeed the pollution problems reviewed in Section 3 and with the outstanding methodological problems arising from the review in Section 2. It covers, therefore, topics such as the consequences of multiple, interacting pollution problems, strategic changes in the character of these problems, and potentially new approaches to the analysis of acceptable future behavior.

Finally, while the review is quite clearly about mathematical modeling, it inevitably touches upon matters of policy, particularly in Section 3.1 on water quality standards and monitoring programs, and more generally in speculating about the problems of the future in Section 4.

2 APPROACHES, METHODS, AND MAKING PREDICTIONS

Before reviewing the development and application of water quality models it is helpful to describe their context by classifying the historical development of water pollution problems themselves.

2.1 SUCCESSION OF POLLUTION PROBLEMS

It has been said that there are three eras of pollution, beginning with pathogenic pollution, followed by gross pollution, and then chemical pollution (Newsome, 1975). Pathogenic pollution, arising from the largely untreated discharge of sewage, animal wastes, and domestic refuse, is the principal problem of concern in the earliest stages of river basin development. Gross pollution, characterized by high levels of biochemical oxygen demand (BOD) and suspended solids (SS) concentrations, accompanies the process of industrialization in the river basin. The era of chemical pollution is already implied by this same process. Appreciation of the fact that one has actually entered it, with a decreasing concern for the macroscopic variables, BOD and SS, and an increasing concern for more specific pollutants (especially micropollutants), depends partly upon having solved the problems of gross pollution and partly upon an improving level of resolution in the monitoring of water quality.

No classification is unique, however useful it may be as an organizing principle. The individual's, society's, or the scientist's ***perception*** of how the problems arise, and which of them requires the most urgent attention, determines the allocation of resources for their solution; hence the level of funding given to different areas of research, and hence the number of publications dealing with the development and application of water quality models. For instance, one might loosely trace a succession of pollution problem "groups" reflected in the literature on water quality modeling as follows: from "easily degradable organic wastes" (models of dissolved oxygen (DO) and biochemical oxygen demand (BOD)); from "point-source discharges" to "nonpoint-source discharges"; to "eutrophication" (nutrient cycle, phytoplankton, and ecological models); to "the nitrate problem" (nitrogen cycle models); and so to "toxics" (food chain and ecological models). These four categories of problems and models (in parentheses) will be used to organize the discussion of this review and, in particular, of Section 3. Figure 1 sketches a scenario for the levels of effort devoted historically to research activities under these categories.

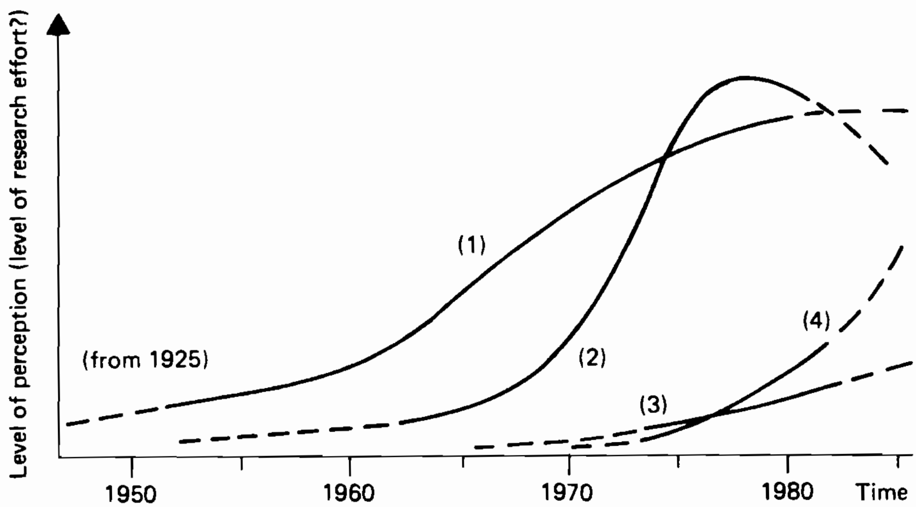

FIGURE 1 An approximate scenario for the level of research effort applied to model development in association with the problems of: (1) easily degradable organic wastes; (2) eutrophication; (3) nitrates; and (4) toxics.

But again, this classification is not unique and requires qualification. First, it is more refined than Newsome's classification of three eras. It suggests, too, that pathogenic pollution has been largely overlooked as a subject for modeling, perhaps because the emphasis on modeling began in specific countries at a time when the local problems of major incidences of water-borne diseases had been effectively solved. Second, the development of models for assessing the expected disturbances of large civil engineering projects, although not given prominence here as a separate issue, could be interpreted as an important theme underlying more than one of the four problem groups. Third, the speculation that the levels of activity in DO–BOD and eutrophication modeling might decline in the immediate future does not at all imply that the associated problems have been completely overcome. The critics of modeling will be quick to point out, and rightly so, that solution of the problems in practice is not synonymous with the level of research activity. Fourth, sketching four distinct lines of development does not mean either that the problem groups occur separately or consecutively, or that there are no models covering two or more problems. It might be argued, for example as follows, that the DO–BOD models are the progenitors of all the subsequent models: interest in photosynthetic/respiratory DO variations led to a more detailed interest in phytoplankton growth; accounting for a nitrogenous BOD leads naturally to considerations of the nitrogen cycle; and accounting for benthic BOD calls for an understanding of sediment–water interactions, which in turn may be seen as a focal point of several toxic substance models. In fact, such an evolutionary process is clearly displayed in the development of a sequence of models for the Neckar River in the Federal Republic of Germany (Hahn and Cembrowicz, 1981). But whether the above argument is justified is not important. What is more important is that it illustrates the natural process of separating the original macroscopic understanding (of BOD variations and of gross pollution) into ever more detailed component parts. Such a process is coupled inextricably with developments in monitoring and the evolving perception and "discovery" of new problems (such as those typical of the chemical pollution era). Finally, with respect to Figure 1 we note that water quality management is not merely a matter of solving one problem and then turning attention entirely to another problem, although it may sometimes appear to be so. In Section 4 we shall argue, on the contrary, that the problems exist in various combinations together and interact significantly with each other.

2.2 PROBLEM DECOMPOSITION

Let us consider the control of lake eutrophication as a typical problem of water quality management. The general features of such a problem are that the physical system is large and complex, comprising both the water body and its surrounding watershed. At the detailed (*microscopic*) level of analysis there are strong interactions among the biological, chemical, and hydrophysical processes governing the behavior of the lake. At the *macroscopic* level answers to questions of management involve economic considerations of the most efficient allocation of resources to sewerage, sewage treatment, and other control projects. How, then, should the analyst begin the modeling exercise for such problems? At least two basically distinct approaches might be adopted:

(1) The adaptation, or direct application, of a previously developed general-purpose model, where this single, comprehensive model is intended to address the overall problem as a whole. Further specialized field or laboratory experimentation is assumed implicitly not to be an integral part of the program for problem solving.

(2) Prior conceptual decomposition of the overall problem into its natural component parts and the development of either *independent* models or a *linked* set of models relevant only to the solution of the individual subproblems. Specific experimental work related to these subproblems is regarded as an integral part of model development.

To clarify the differences between these approaches it is instructive to take the particular example of controlling eutrophication in Lake Balaton, a large, shallow lake in Hungary (van Straten *et al.*, 1979; van Straten and Somlyody, 1980; Somlyody, 1982a). Figure 2 shows an intuitively natural decomposition of the overall problem into a hierarchically arranged set of subproblems (Somlyody, 1982a). An approach along the lines of (1) above would attempt to tackle the (overall) problem using a single model, let us say, at a

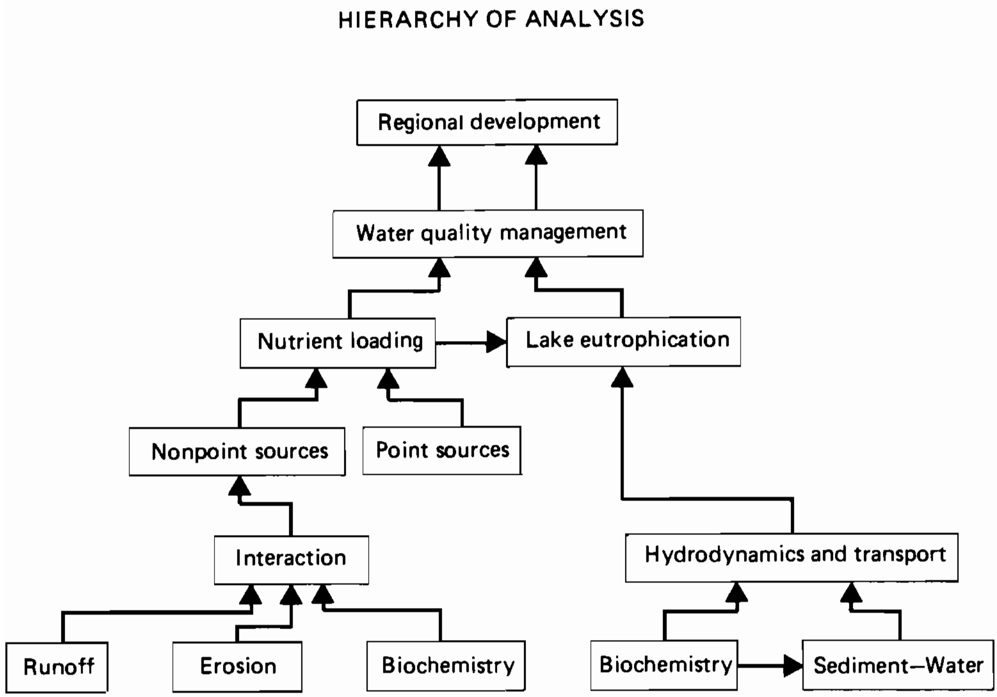

FIGURE 2 Natural decomposition of the overall problem of lake eutrophication control (Somlyody, 1982a).

certain level, a "lake eutrophication" model, which would subsume detailed submodels for "hydrodynamics and transport", "biochemistry", and "sediment–water" interactions (according to Figure 2). The adaptation by Kinnunen *et al.* (1978) of the United States EPAECO model (Gaume and Duke, 1975) to study a lake in central Finland is one of few reported cases typifying approach (1). Indeed, it is questionable whether such an approach, as defined (and obviously stylized) above, has ever been fully implemented. It stands now as a point for comparative discussion – a marker, as it were, of a goal toward which research in water quality modeling might well have been moving during the early and mid-1970s. In retrospect, one can clearly question, for example, how comprehensive a "comprehensive" model can possibly be, for it no longer seems reasonable to contemplate a single, comprehensive model for water-body–watershed interactions. There is, however, an implicit basic assumption of this now dormant approach that has contemporary relevance. It is that there is sufficient confidence in *a priori* theory to state that all lakes behave according to a common set of basic principles. Universal applicability of the comprehensive model is bestowed by making the model sufficiently complex and detailed in order to encapsulate all these basic principles. But whether the status of water quality modeling justifies this assumption is a suitable point for debate, as is evident both in the introduction to this review and elsewhere (Young, 1978; Beck, 1981a, 1983b). It is also a point to which the review will return frequently, in discussing questions of scale (or detail) in Section 2.3.2, the balance between *a priori* theory and observation (Section 2.3.3), model structure identification (Section 2.4), and again in Section 3.4 on the problem of eutrophication.

A quite different approach, which might equally lay claim to being "universally applicable", is that of the Organization for Economic Cooperation and Development's cooperative program on eutrophication (Vollenweider and Kerekes, 1980). It could be argued that a simple regression-type relationship for the "lake eutrophication" model (of Figure 2) is generally valid on the grounds that it has been derived from (macroscopic) data aggregated over a respectably large number of lakes. For this approach the model and its development make virtually no reference to the more detailed (microscopic) analyses of "hydrodynamics and transport" and the other lower-level blocks in Figure 2. Here generality is sought, not from the inclusion of details, but from the specification of an extremely simple rule (model) of average, or aggregate, behavior. It is an approach, with specific reference to the problem of eutrophication, endorsed in a notably exhaustive discussion of the detailed and specific aspects of phytoplankton ecology (Harris, 1980).

There are two variations on the theme of approach (2), depending upon whether (according to the definition) the models relevant to each subproblem are considered to be "independent" or "linked". To clarify this distinction it is convenient to compare two case studies of the eutrophication problem (Somlyody, 1982a; Fedra, 1983a).

The first variation on approach (2), in which the models developed are treated as essentially *independent*, is, naturally enough, the approach

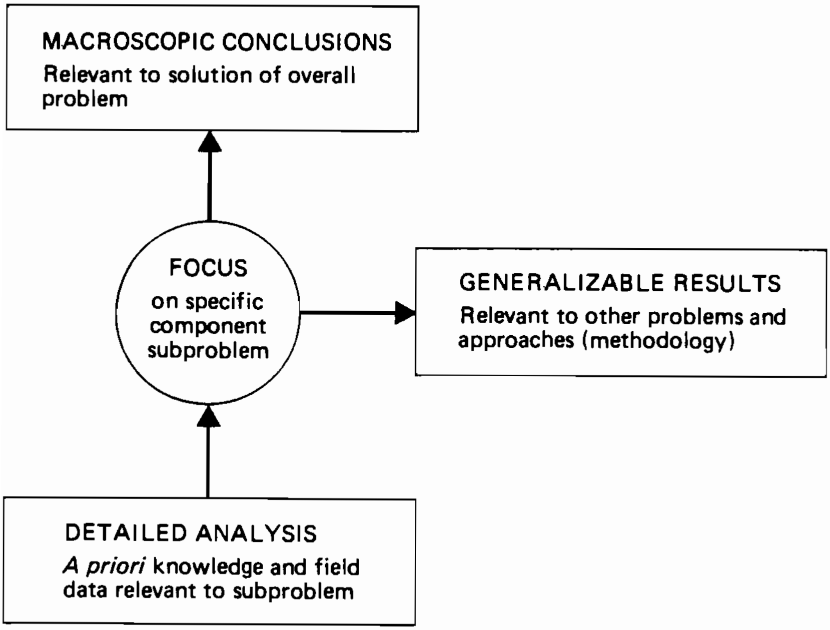

FIGURE 3 Problem decomposition in detail: focusing analysis on the individual subproblems.

adopted for the case study of eutrophication management in Lake Balaton (Somlyody, 1982a). It is, in many ways, a common-sense approach. It has the typical advantages of applied systems analysis in encouraging a clear focus on the detailed (microscopic) component subproblems without losing sight of the (macroscopic, whole) overall problem. Figure 3 illustrates how, in principle, the approach is implemented. The focus of analysis on the specific component problem demands the marshaling of all relevant field data and *a priori* theory and yields, in return, not only the more macroscopic conclusions pertinent to a higher-level problem (in the hierarchy of analysis in Figure 2) but also methodological results that can be generalized as being relevant to other problems and approaches. For example, a characteristic feature of the Lake Balaton problem is the pronounced and stable longitudinal gradient in the observed state of eutrophication, with basin I in Figure 4 being the most polluted sector of the lake. A conceptual representation of the lake as four fully

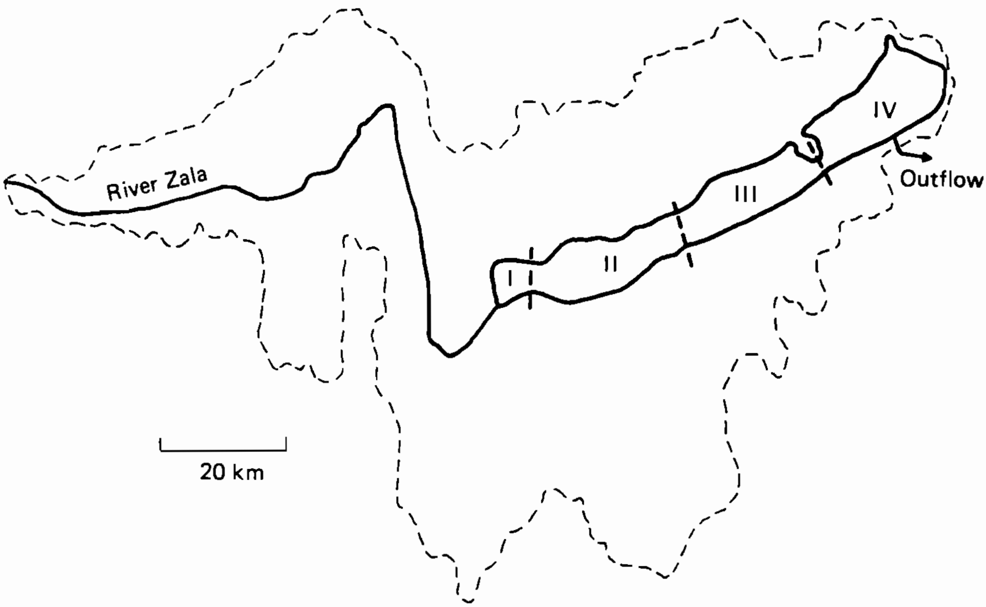

FIGURE 4 Lake Balaton (Hungary), its watershed, and its principal tributary (the River Zala); the conceptual division of the lake into four segments (basins I to IV) is indicated.

mixed segments (basins I to IV) offers considerable simplification of the model that would be required for analysis of the "lake eutrophication" problem of Figure 2. The most pertinent questions for the definition of "hydrodynamics and transport" are therefore: do the lake water circulation patterns deny the justification for the simplifying assumptions above; and are hydrodynamics and transport mechanisms more important than biochemical process interactions in determining the observed state of eutrophication? Interpreted in terms of Figure 3, the analysis conducted with respect to this specific problem (Somlyody, 1982a; Somlyody and Virtanen, 1982) is summarized by Figure 5, where analysis of the role of uncertainty in hydrodynamic models is cited as an important, more generalizable facet of the study (Somlyody, 1983a).

A *linked* set of models for water quality management first appears to have been suggested, though not implemented, by Fleming (1979) with regard

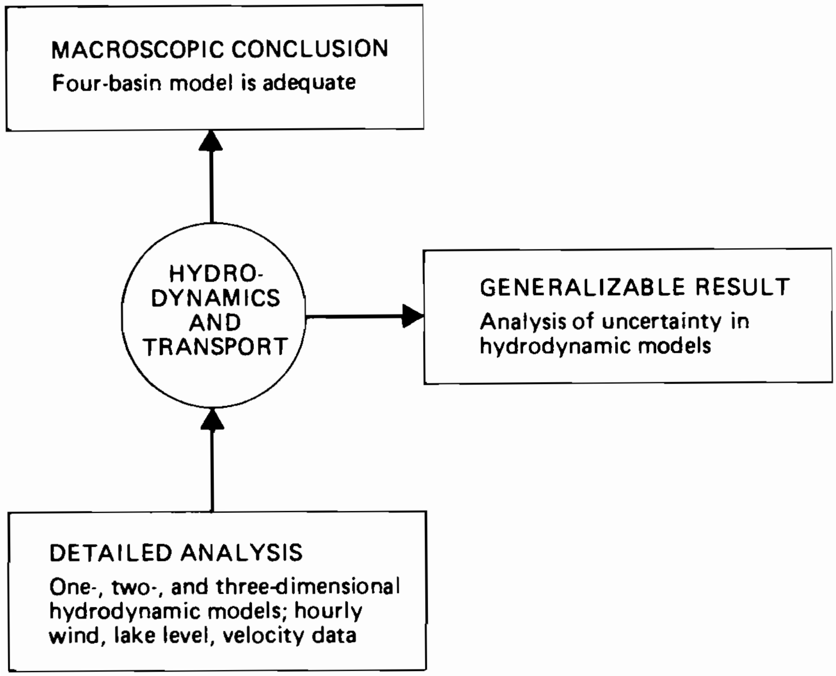

FIGURE 5 Subproblem analysis in practice, for the Lake Balaton case study.

to pollution and sediment transport in the Danube River basin. Fedra's (1983a) studies of the Neusiedlersee and four of the Salzkammergut lakes in Austria can therefore be said to be prototype exercises in the development of a linked-model system. It is with respect to the problems of the Neusiedlersee, a large, shallow lake in eastern Austria (with characteristics similar, therefore, to those of Lake Balaton), that Fedra's approach has been more fully developed. His conceptual decomposition of the overall problem is essentially identical with that of Figure 2, although the notion of a hierarchical structure requires a slightly different interpretation. Indeed, it is in the preparation of output information (as the linked set of simulations proceeds) that aggregation and disaggregation in a hierarchical context play an important role. For instance, the temporal evolution of the overall simulated system behavior is summarized in effect at the level of the "regional development" block in Figure 2; only on demand – as in response to the occurrence of peculiar conditions – is the output information disaggregated to a lower level in order to identify the origin of the "peculiarity". The approach exploits to the full the availability of the computer and computer graphics. It derives its flexibility from the ability to substitute different models for the different blocks (or "modules" in Fedra's terms) of Figure 2; and it comes remarkably close to the idea of an interactive decision support system.

Certainly, prior conceptual decomposition of the overall problem in the manner illustrated by Figure 2, provided that it does not obscure possible changes in problem perception as the study proceeds (Majone and Quade, 1980), is intuitively a good organizing principle. Yet, in accordance with Figure 3, the macroscopic conclusions expected from analysis of the individual problems more or less imply the prior definition of objectives for such analysis, and hence the objectives of modeling. The relationship between modeling objectives and the type of model developed will be an important consideration of the next section.

2.3 A PROCEDURE FOR MODEL DEVELOPMENT

This review does not claim that there is a universal, systematic procedure for model development, although in the following a particular sequence for this procedure will be suggested. The primary advantage of being specific is that the proposed procedure covers most of the problems encountered in model development except, notably, aspects of the numerical solution of differential equations. What is given is a distillate of procedures suggested by several authors (Orlob, 1975; Jørgensen, 1978; Young, 1978, 1983; Beck, 1979, 1983a; Rinaldi *et al.*, 1979); it represents a current consensus.

Two questions provide the motivation for this discussion of a model development procedure:

(1) How is a set of relationships, i.e. the model, derived from the ensemble of general prior theory for a specific water body?

(2) How does one demonstrate the good or poor approximation of that model's behavior to the observed behavior of reality?

These two questions define the natural division of the modeling procedure into those steps related to the use of *a priori theoretical knowledge* and those related to *a posteriori measurement knowledge*. Figure 6, adapted from Eykhoff (1974), gives an example of the relationship between these two types of knowledge. Loosely speaking, for this review the term "*a posteriori*", in relation to model development, will be used to indicate "after having analyzed the field data". Figure 7, as a companion diagram to Figure 6, defines the procedure for model development.

Rather than discuss each step of the procedure of Figure 7 in sequence, especially those steps associated with the *a priori* stages of modeling, we shall examine here just three issues:

(i) the relationship between models and modeling objectives;

(ii) questions of scale (or detail) in the spatial, temporal, and ecological dimensions;

(iii) the balance in model development between the use of *a priori* theory and observations.

In fact, Figure 7 is something of a straitjacket – it is not really possible to restrict the logic of model development to any one sequence of procedural steps.

A separate section (2.4) is given to the discussion of the *a posteriori* stages of modeling, since they are concerned with the particularly important subject of field data analysis. The subjects of validation and sensitivity analysis will also be considered separately in Section 2.5. A more complete discussion of model types can be found in Rinaldi *et al.* (1979).

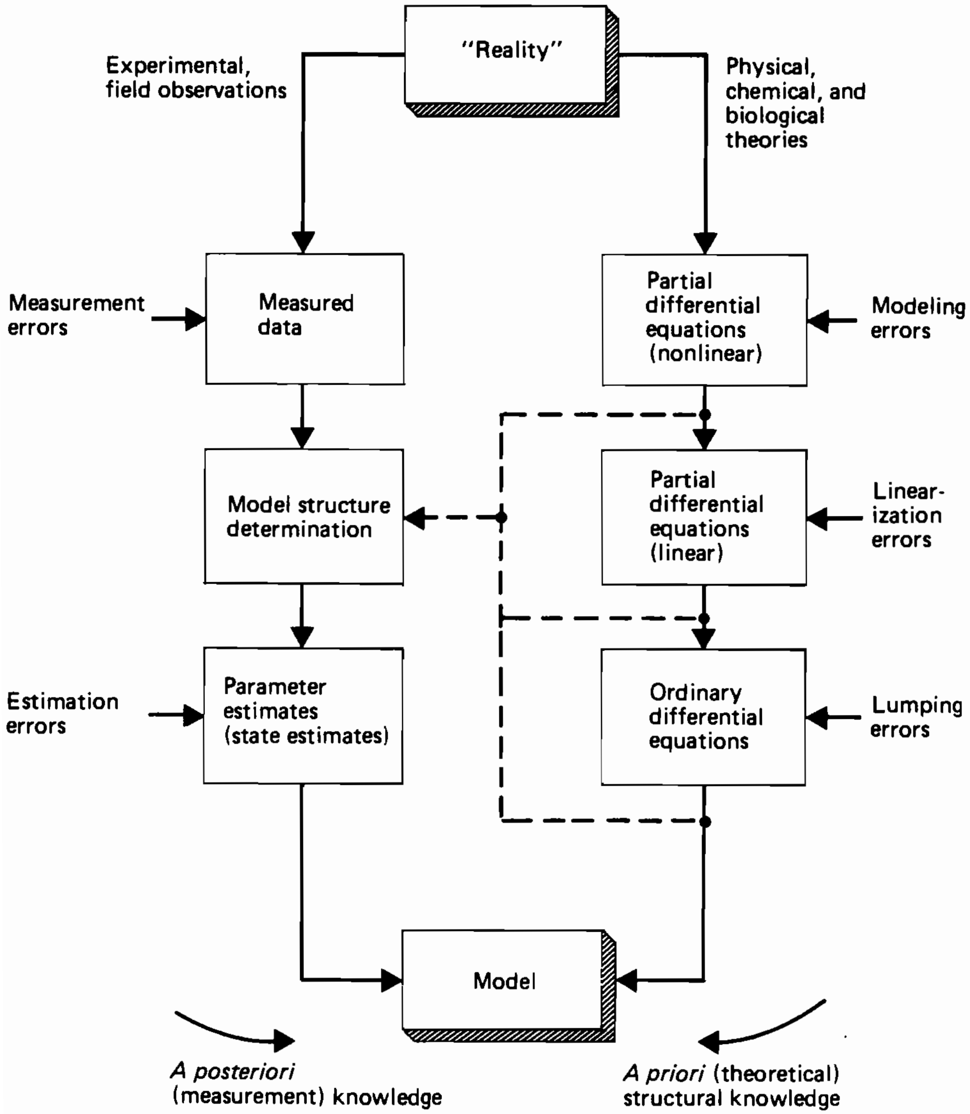

FIGURE 6 Combining *a priori* and *a posteriori* knowledge in the modeling procedure (adapted from Eykhoff, 1974).

2.3.1 Models and Modeling Objectives

Today's student of water quality modeling would find it a curious statement that models are to be related to the objectives of modeling; it is to him trivially obvious. But in retrospect this would not have been self-evident when

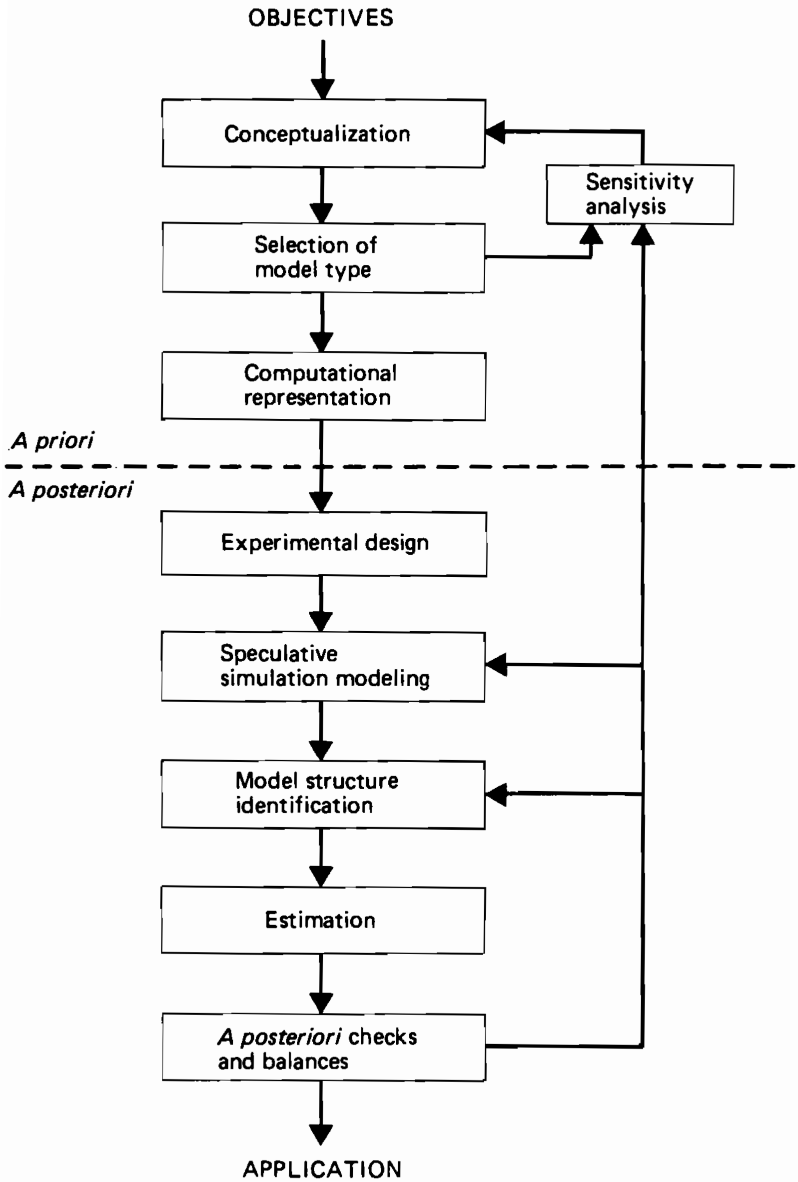

FIGURE 7 A procedure for model development.

the "movement" from particularization to the synthesis of general-purpose models was at its peak. (The strong implication here was that, irrespective of the purpose of modeling, one would ultimately have employed the same detailed, general-purpose model.) Nevertheless, lest it be forgotten, the word "objectives" is given prominence at the beginning of the modeling procedure in Figure 7. The fact that in a number of major case studies of water quality management conducted during the past decade several different types of models have been constructed as a means for solving an overall problem is unmistakably apparent: in the Saint John River (USA) study (deLucia and McBain, 1981); for a study of the Neckar River in the Federal Republic of Germany (Hahn and Cembrowicz, 1981); and in a case study of the Bedford Ouse River in central-eastern England (Bedford Ouse Study, 1979). There is, of course, a broad distinction in objectives between addressing *management issues*, which was largely the motivation for the above-mentioned case studies, and developing a model for the purpose of *improving understanding*. Bierman *et al.* (1980), for instance, have viewed model development "as providing a quantitative framework for organizing and interpreting experimental data". Let us note, however, that improving understanding does not necessarily set the modeling exercise on a course toward comprehensive and highly complex models. It may well be that insight and understanding derive, and probably more dramatically so, from simplification and the rudimentary theory that captures much of the essence of many empirical observations (this spirit of simplification can be seen, for example, in some of Thomann's (1981) work on modeling the fate of toxic substances).

There is thus a wide variety of ways in which different types of models can be developed to serve different purposes (to solve different types of problems). Such variety is an intrinsic part of the approach to problem decomposition that underpins Figure 2 and that was adopted as an organizing principle for the case study of eutrophication management in Lake Balaton (Somlyody, 1982a). The case study itself illustrates well the richness of this variety. The development and application of one-, two-, and three-dimensional partial differential equations to represent "hydrodynamics and transport" (Figure 2) have already been mentioned in connection with Figures 3, 4, and 5. One reason for the relatively detailed spatial representation of the physical system was to evaluate the level of error likely to be introduced into a "lake eutrophication" model that approximated observed behavior by assuming merely four spatially uniform segments for the lake. Elsewhere, for instance for analysis of the "nutrient loading" problem (Figure 2), very simple input—output (black-box) models were employed. The purpose of the analysis, as largely defined by the requirements of the "water quality management" and "lake eutrophication" problems, was to analyze relatively detailed daily time-series data records for the principal tributary – the Zala River as indicated in Figure 4 – to determine (at a more macroscopic level) the average balance of nutrient loadings between point- and nonpoint-source discharges and between available and unavailable forms of the nutrients (Beck, 1982a). In the case of the "water quality management" problem, a set of coupled simultaneous linear algebraic equations describing the change in the lake's water quality as a function of changes in nutrient loadings was embedded, as a model for the lake, into an optimization routine for the allocation of investments in sewerage and sewage treatment alternatives (Hughes, 1982). It is a logical extension of this macroscopic analysis to take the preferred management options as input scenarios for more detailed evaluation with the nonlinear, ordinary differential equation models developed for the "lake eutrophication" problem (e.g. van Straten and Somlyody, 1980; Somlyody, 1983b).

2.3.2 Questions of Scale (or Detail)

It is clear from the foregoing discussion that questions of scale (spatial, temporal, and ecological) are decisive factors in the type of model chosen for a particular purpose. It is also apparent that these questions of scale are tied closely to the evolving capacity of the computer, on the one hand, and of monitoring and data collection, on the other. Normally, the analyst would first address these questions at the stage of "conceptualization" in the procedure of Figure 7.

We have already alluded to the early DO–BOD models (deriving from the now classical studies of Streeter and Phelps (1925)) as progenitors of many water quality models. It is useful to start this discussion of scale from the same point of departure. The Streeter–Phelps model is a *steady-state* characterization that describes changes in two *aggregate* state variables of water quality (DO and BOD concentrations) along the longitudinal axis of a river. The degree of spatial resolution afforded by the model is relatively high in comparison with its resolution of microbiological (or ecological) detail and the complete absence of resolution on a temporal scale. But then the resolution of water quality monitoring at that time was almost certainly not of a sufficiently high sampling frequency for temporal (i.e. dynamic) variations to be distinguishable. Moreover, the purpose of modeling was to formulate a hypothesis for the *aggregate* self-purifying behavior of river systems subjected to steady and, usually, heavy loadings of degradable organic matter. The management options available would only have been capable of restoring a good *average* level of water quality to a heavily polluted stream. In short, the model was compatible with the contemporary monitoring and management capabilities. It has certainly stood the test of time, as Cembrowicz *et al.* (1978) point out.

The general progression in water quality modeling since the original work of Streeter and Phelps has been one of almost monotonic increase in the degree of resolution in describing spatial, temporal, and ecological variations (see also Thomann, 1982). Such development is arguably the natural course of scientific endeavor. It is apparent, for the ecological dimension, in the rapid succession of refinements of the Streeter–Phelps model (see Section 3.3) leading ultimately to truly ecological models (e.g. Boes, 1978; see also Hahn and Cembrowicz, 1981).

Considering the temporal dimension, there has been a gradual refinement, from models developed initially for long-term, year-by-year trends, to modeling of within-year seasonal differences and subsequently of short-term, daily and even hourly variations. The models developed for the Bedford Ouse River in the UK illustrate well this spectrum of time scales. A steady-state model has been used for predicting yearly changes of water quality over the period 1973–1991 that would result from the projected development of a major new point-source discharge in the upper part of the river basin (Bedford Ouse Study, 1979). The steady-state model was also used to assess the significance of *average* differences in the seasonal patterns of water quality across the whole river basin. Complementary to the steady-state model, a dynamic model was developed for part of the basin in order to assess the effects of the same point-source discharge in terms of the ***variability*** of water quality for a downstream potable water abstraction (Bedford Ouse Study, 1979; Whitehead and Young, 1975, 1979). The dynamic model accounts for day-to-day changes in water quality, was originally calibrated against daily data for a summer season, and was subsequently modified to accommodate seasonal variations across a summer, autumn, and winter period (Whitehead, 1979). More recently, and notably with the introduction of a telemetered monitoring network (and possibly with a changing perception of the most urgent pollution problems), a dynamic model characterizing hourly variations in water quality has been developed for the same stretch of river (Whitehead, 1980).

Finally, with respect to the spatial scale, Somlyody's (1977) two-dimensional model for solute transport in the Danube River and Orlob's (1981) brief chronology of the development of models for stratified impoundments are indicative of the increasing degree of resolution in the representation of spatial variations (the pattern of this development is charted further still by Orlob (1983b) and Watanabe *et al.* (1983)).

Given the increasing capacity and decreasing costs of digital computing facilities, it is logical, some would argue, to expect the development of models with ever more detailed representation of spatial, temporal, and ecological characteristics. But it overlooks certain *pragmatic considerations*:

(C1) that such detail is not compatible with current monitoring and data retrieval capabilities;

(C2) that the results produced from a highly refined (disaggregated) model would be so copious as to be not comprehensible to the analyst without some form of aggregation (we have already encountered this in discussion of Fedra's (1983a) set of linked simulation models); and

(C3) that such complexity is not consistent with the relatively crudely effective policy options that are either available to management or perceived by management to be practical.

It is these kinds of considerations – a fourth, of potential future significance, will be added later – that have stimulated the current critique of the trend of the past decade toward large-scale simulation models (e.g. Thomann and Winfield, 1976; Young, 1978; Fedra, 1980a, b; Beck, 1981a).

One of the most thorough studies of these questions of scale has been presented by Thomann *et al.* (1979) for a verification analysis of models for Lake Ontario. Significantly, they concluded that:

> as one progresses to smaller scales ... hydrodynamic transport and local phenomena become more and more significant. Often, however, data are not available to specifically quantify these phenomena. At the larger spatial scales, system kinetics dominate and the importance of hydrodynamic structure is decreased. Increased kinetic complexity did not appear to materially affect model [verification] status over the simpler kinetic structure.

A comparative review of models for freshwater wetland and shallow-water ecosystems has been recently conducted in a similar vein (Costanza and Sklar, 1983). It introduces a property denoted as "articulation" as a scalar aggregate measure of model complexity, where complexity is roughly equated with the degree of resolution along the spatial, temporal, and ecological dimensions. The review concludes with the provocative speculation that increasing articulation is associated with decreasing accuracy (although this presupposes a suitably universal measure of "accuracy").

Undoubtedly, the pragmatic considerations above stimulated, at least in part, Thomann's (1978) innovative discussion of trophic length as an independent variable (equivalent to time and space) for representation of the continuum of an ecological "dimension". The role of an ecological scale, alongside the conventional spatial and temporal scales, becomes particularly clear in his discussion. However, while Thomann's model for the transfer of hazardous substances along an aquatic food chain provides insights that other approaches might obscure, it would in principle seem to suffer from limitations that are symptomatic of more general current constraints. Notably, first, the parameters (coefficients) of the model are likely to be variable functions of trophic length, which leads to an awkward parameter estimation problem. And, second, the inherent transformation of a finite set of ordinary differential equations (representing the dynamics of discrete elements or compartments of the ecological continuum) into a partial differential equation will, if other simplifying assumptions are not made, require a reversion to some form of discretization in order to implement a numerical solution This is, as it were, one of those familiar situations in which the state of analysis has reached a barely perceivable but definite boundary at which gains in one direction are traded against losses elsewhere.

The present status can thus be summarized as follows. The essential questions of scale are ones of distinguishing those variables that can be considered to be effectively constant or uniform across discrete intervals of space, time, and the ecological dimension, and those that cannot. Since straightforward, brute computing power is no longer an overriding constraint, the analyst has great flexibility in making these choices. Such freedom can be interpreted as analogous to the choices involved in problem decomposition. Hence, for example, the separation of a near-shore spatial zone from the remainder of the water body (as in Thomann *et al.*, 1979), and the separation of nuisance-species algae from a lumped representation of all other algae (as in Bierman *et al.*, 1980) are distinctions directly equivalent to the notion of focusing on the individual subproblem without losing sight of the whole.

There are certainly still constraints, as we have already indicated, and generally they can be seen in terms of the sacrifice of detail in one dimension for a gain in detail in another dimension. In the past these trade-offs, and the resulting nonuniformity of detail, have been most evident in the interplay between (in the spatial dimension) characterizing the physical movement of water and (in the ecological dimension) specifying trophic relationships and chemical-element cycling. Yet this reflects also the disciplinary heterogeneity of water quality modeling as clearly identified by Somlyody (1982b). The significance of this point, in following the modeling procedure of Figure 7, is especially important. It is concerned with the relative degree of confidence in *a priori* theory and, in effect, with the confidence placed in *a posteriori* measurement knowledge (see also Figure 6).

2.3.3 The Balance between Theory and Observation

Karplus (1976) has introduced a spectrum of modeling problems ranging between the two extremes of analyzing socioeconomic systems (black-box modeling) and electrical network analysis (white-box modeling). One might also associate with these two polar positions, as does Vemuri (1978), respectively, an inductive reasoning process (from a specific set of experimental observations to more general conclusions), and a deductive reasoning process (from general theory to a model of a specific situation). And these two complementary processes reflect, respectively, in the extremes, a complete reliance upon *a posteriori* measurement knowledge and a complete reliance upon *a priori* theoretical knowledge. Somlyody (1982b) has argued, in effect, that water quality modeling occupies a fairly broad arc – at the center of Karplus's spectrum (see also Beck, 1981a, 1982b) – across the range of hydrodynamic, chemical, and biological theory. Bound to this arc is the intuitive idea that hydrodynamic behavior is more "predictable" than biological behavior; that one can place greater confidence in the *a priori* theory of hydrodynamics.

Using Figures 6 and 7 as frames of reference, Somlyody asserts that both the transport-oriented and ecology-oriented approaches to modeling, while they may differ significantly in other respects, have hitherto exhibited a much stronger dependence on *a priori* theory than on experimental observations (Somlyody, 1982b). That there has been this imbalance in the utilization of *a priori* and *a posteriori* knowledge is not surprising in view of the introductory comments and the preceding discussion. As we shall see in the following section, it is in part consistent with the very considerable difficulties in analyzing field data on water quality. In general, too, there will always be a gap in any area of study between the leading edge of the theories postulated and the experiments subsequently designed to evaluate and test these theories. Such a gap is only unacceptable if it becomes too large, which, in fact, can be argued to be the case at present with water quality modeling (Beck, 1983b). The predominant use of *a priori* theoretical knowledge, at the expense of ignoring *a posteriori* measurement knowledge, will be especially limiting to real progress and debate if it engenders an arguably unjustified overconfidence in conventional, classical assumptions (e.g. Young, 1983) and a lack of critical questioning that should accompany model calibration exercises and field data analysis.

2.4 UNCERTAINTY AND THE ANALYSIS OF FIELD DATA

One can sense, therefore, that the review is approaching the nub of the issue of uncertainty and its analysis in the development and application of water quality models; it will be the subject of the present section and the following section on prediction error propagation. But the treatment here will be qualitative, with a view to disentangling a discussion of the issues, and their relevance ultimately to matters of management, from the particulars and complications of method. The methodological aspects of the analysis of uncertainty in system identification and prediction are in any case discussed fully elsewhere (Beck, 1983b, 1984).

Some preliminaries are necessary. Let us suppose that the model of the system's behavior can be represented by a set of ordinary differential equations for the state variable dynamics, as summarized in Table 1 for the accompanying system definition of Figure 8. Admittedly, this is a restrictive form of model, being a lumped-parameter representation; but then most models will eventually be solved by making some kind of lumping, or discretization, assumption leading either to equation (1a) (in Table 1) or to its integrated discrete-time equivalent. Variability in the spatial and ecological dimensions is assumed in equations (1) to be subsumed under the definition of $\boldsymbol{x}$, which may, for example, include elements representing the same property at different points in space. The definition of the model in Table 1 is

TABLE 1 Summary definition of a model for the system's state-variable dynamics with discretely sampled output response observations.

The variations with time of the system state vector are given by

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}\{\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\alpha}(t), \boldsymbol{\xi}(t)\} \tag{1a}$$

with sampled discrete-time output observations

$$\boldsymbol{y}(t_k) = \boldsymbol{h}\{\boldsymbol{x}(t_k), \boldsymbol{\alpha}(t_k)\} + \boldsymbol{\eta}(t_k) \tag{1b}$$

where

$\boldsymbol{x}$ = n-dimensional vector of state variables,

$\boldsymbol{u}$ = m-dimensional vector of measured input disturbances,

$\boldsymbol{y}$ = l-dimensional vector of (discretely sampled) measured output variables,

$\boldsymbol{\alpha}$ = p-dimensional vector of model parameters,

$\boldsymbol{\xi}$ = s-dimensional vector of random unmeasured (unknown) input disturbances,

$\boldsymbol{\eta}$ = l-dimensional vector of random output measurement errors,

and $\boldsymbol{f}$ and $\boldsymbol{h}$ are nonlinear, vector-valued functions; t is the independent variable of time, t_k is the kth discrete sampling instant in time, and $\dot{\boldsymbol{x}}$ denotes the derivative of $\boldsymbol{x}$ with respect to t.

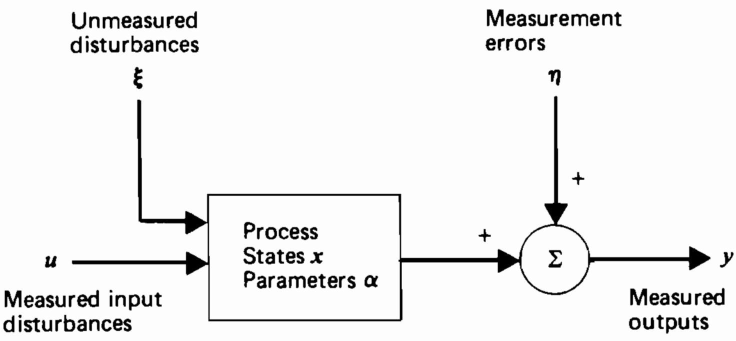

FIGURE 8 Definition of the system and associated variables.

simply convenient for the purposes of illustration. Perhaps surprisingly, it will be the only model to be discussed in mathematical terms in this review.

2.4.1 A Change of Perspective

The shift of emphasis in water quality modeling toward considerations of uncertainty is probably both part of a natural process of maturation and a reflection of the attitude that the behavior of river and lake systems, for instance, is somehow not as predictable as was once thought. It can be seen, too, as a reaction to the absence of such considerations in the mainstream developments of the subject during the 1960s and 1970s; a reaction, moreover, to the trend toward ever larger and more complex models; and as an acknowledgment of the serious difficulties of evaluating rigorously against field observations the ensemble of hypotheses in all but the simplest of models (Young, 1978; Beck, 1981a). What is really being brought into question by these reactions is the way in which the entire subject of developing water quality models is to be viewed (Beck, 1982b).

For the sake of argument, therefore, let us caricature the limitations in a generally accepted approach to water quality modeling as follows. According to this approach it is assumed that one can (conceptually) divide the field system into smaller, individual components, whose (conceptual) behavior can usually be approximated by laboratory-scale replicas (for example, chemostat and open-channel flow experiments). Submodels for these components are assumed to be "verifiable" against experimental observations of the behavior of the replica; and the model for the field system can be assembled by linking together the submodels. Thus, the content of the model is supported by arguments that admit extrapolations from laboratory systems and equivalent or similar field systems. At the stage of model calibration the tendency is to assume that *a priori* theory is correct unless *demonstrably* inadequate. It is especially difficult to demonstrate inadequacy, and the need to question the validity of the original extrapolations is thus all too easily likely to remain obscured.

The argument that the extrapolations inherent in the above approach are legitimate would appear to remain in doubt unless one can develop and apply a complementary approach that provides a more direct evaluation of the prior hypotheses about observed system behavior, without dividing the system into its component parts. ***Model structure identification***, which we shall define more fully below, is a fundamental part of that complementary approach: it has to do with the questioning so easily set aside because of the imperfections of the available field data; it is a problem for which seemingly few systematic methods of solution have been developed; and, possibly most significant, it requires a subtle but important change of attitude toward modeling. In spite of very many laboratory-scale experiments and a number of major field studies, current knowledge of the structure of the relationships among the mineral, organic, and microbiological components of an aquatic ecosystem is still quite uncertain. This, it will be argued in Section 3.4, is very much the case in characterizing phytoplankton growth for the purposes of eutrophication control. Too much confidence has been placed in *a priori* theory. Perhaps, in Popper's terms, environmental systems have been modeled as though they were "clocks", being "regular, orderly, and highly predictable", whereas they may well be more like the "irregular, disorderly, and more or less unpredictable clouds" (Popper, 1972). This reflects simply a change of attitude, because, as is evident in the earlier references to Somlyody's papers (1982a, b), there is clearly a spectrum of regularity and orderliness associated with the prior knowledge relevant to water quality modeling (ranging from hydrodynamics to biology). In short, central to the problem of model structure identification is the question: how are theories developed about the behavior of large, complex systems, given the assumption that observations can be obtained (and subsequently interpreted) from experiments broadly similar in form to the classical experimentation in laboratory science?

This change of attitude, from an underlying assumption of determinism to a concern with indeterminism, may be merely a swing of the pendulum that others have suggested is a characteristic of oscillating attitudes toward science more generally (e.g. Brush, 1980). It has certainly given rise to a pause for reflection on the role of large-scale models in the subject of water quality. It also implies that a conscious effort should be made to redress the underutilization of *a posteriori* measurement knowledge; and, much more narrowly, it implies that the use of the single concept of model calibration unwittingly obscures the important procedural distinction (as indicated in Figure 7) between the two steps of *model structure identification* and (state-parameter) *estimation*.

2.4.2 Speculative Simulation Modeling

Much of the preceding discussion hinges upon the strong assumption that *adequate* field data would be available, or could be made available, for analysis. But *a posteriori* measurement knowledge may come in several forms, and usually not in the form of even reasonably complete records of time-series observations. It is much more common that a few quantitative observations (probably sampled irregularly and infrequently) are available together with less quantitative, more qualitative, empirical experience of the system's behavior. In these circumstances the procedural steps of model structure identification and estimation, as discussed below, are quite irrelevant. The need for an approach by which to tackle these situations is obvious. The surprising point is that such an approach, couched significantly in the terms of the associated gross uncertainties, had until recently not been proposed. It is due collectively to Hornberger, Spear, and Young (Young *et al.*, 1978; Hornberger and Spear, 1980, 1981; Spear and Hornberger, 1980; Young, 1983); their preference would not be to refer to their approach as "speculative simulation modeling", as here, but to call it a "generalized sensitivity analysis" or a "procedure for hypothesis generation". This is a matter of semantics: labels are not important; what *is* important is that the approach is understood as uniquely appropriate to the preliminary analysis of a system's behavior under the (all too familiar) conditions of sparse and qualitative field "data".

The customary view of the problem of estimation is that shown by Figures 9(a) and (b): in essence one tries to fit the curve to the data (Figure 9(a)), and there exists an optimal solution, usually the minimum of a

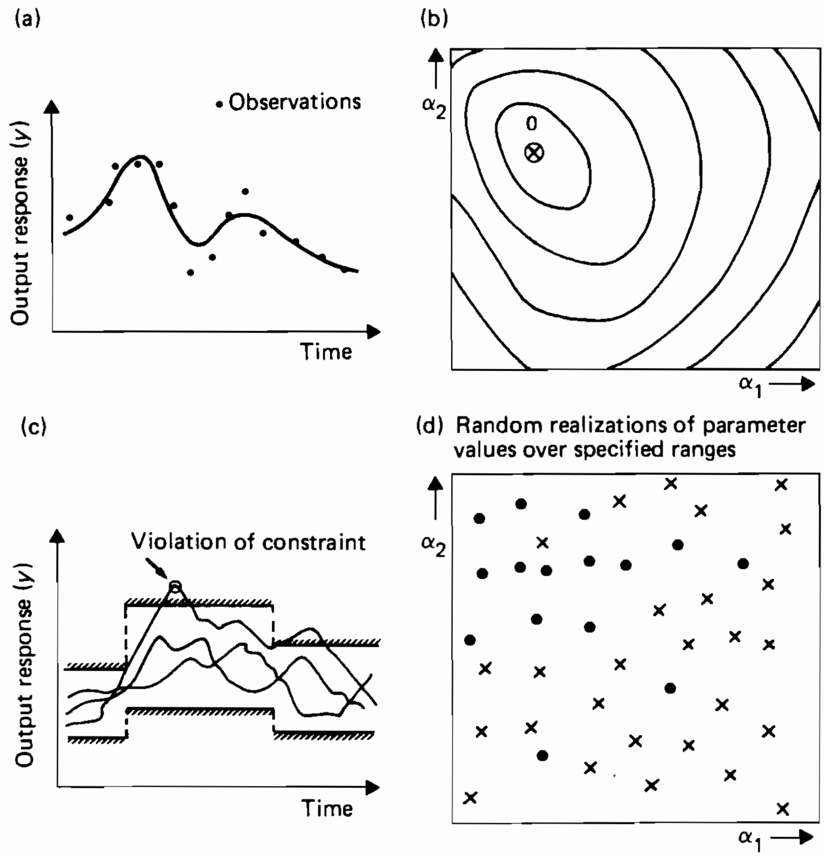

FIGURE 9 A comparison of the concepts of estimation (a and b) and speculative simulation modeling (c and d): (a) fitting the model response to the data; (b) contours of the fitting-function surface in the parameter space; (c) specification of constraints on acceptable model responses; (d) analysis of model parameter values (dots indicate values giving rise to acceptable behavior and crosses indicate values giving rise to unacceptable behavior).

squared-error criterion (such as at point 0 in Figure 9(b)), which yields the "best" estimates of the model parameter values, α_1 and α_2, say. Both facets of this customary use of *a posteriori* measurement knowledge are discarded and replaced by the following two cardinal points behind the idea of speculative simulation modeling:

(1) The trajectories of the time-series observations ($y(t_0)$, $y(t_1), \ldots, y(t_N)$), against which the performance of the model is to be evaluated, are replaced by a definition of (past) behavior (B) in terms of less detailed (more qualitative) constraints derived from the limited available observations (thresholds, topological constraints, and logical constraints, among others, are permissible).

(2) The "fitting" function for locating best estimates $\hat{\alpha}$ of the parameter vector is replaced by a criterion that *either* accepts *or* rejects a sample vector α^* as giving rise to the past behavior (B) defined according to (1).

In other words, the model is required, as it were, to pass through a "corridor" of constraints with "hurdles" to be overcome (as in the most simple form of Figure 9(c)), and it either succeeds or fails.

For example, to quote from the original study of a problem of agricultural eutrophication in Peel Inlet, Western Australia (Hornberger and Spear, 1980; Spear and Hornberger, 1980), one item of the behavior definition (B) was chosen from empirical observation to constrain the estimated yearly peak biomass of the nuisance alga *Cladophora* to be greater than 1.5 times and less than 10.0 times its initial biomass at April 1 (defined as time t_0), i.e.

$$1.5x(t_0) \leq x_{\max}(t) \leq 10.0x(t_0) \tag{2}$$

In addition, the ranges of permissible values from which the sample model parameter vectors are to be drawn were specified as rectangular distributions with upper and lower bounds, i.e.

$$\boldsymbol{\alpha}_l \leq \boldsymbol{\alpha}^* \leq \boldsymbol{\alpha}_u \tag{3}$$

The two types of inequalities (2) and (3) reflect, respectively, the uncertainty of the empirical evidence and the uncertainty of the prior hypotheses.

The procedure of the analysis is a form of Monte Carlo simulation. A sample vector $\boldsymbol{\alpha}^*$ is drawn at random from its parent probability distribution, such as that of inequality (3), and substituted in the model of Table 1 to obtain a sample realization of the trajectory $\boldsymbol{x}(t)$ (Figure 9(c)), which is then assessed for its satisfaction, or otherwise, of the set of constraints defined in the form of inequality (2). Repeated sampling of $\boldsymbol{\alpha}^*$, for a sufficiently large number of times, allows the derivation of an ensemble of parameter vectors that give rise to the behavior (B) and a complementary ensemble associated with not-the-behavior ($\overline{\mathrm{B}}$). For this analysis, therefore, there is no meaningful interpretation of a degree of closeness to a uniquely best set of parameter estimates. Each sample vector $\boldsymbol{\alpha}^*$ giving rise to the behavior is equally as "good" or as "probable" as any other. The crux of the analysis is the identification of which among the hypotheses parameterized by $\boldsymbol{\alpha}$ *are those that are significant determinants of observed past behavior*, however limited or qualitative such empirical evidence may be. "Significance" is indicated here by the degree to which the central tendencies of the marginal and joint distributions of the (*a posteriori*) ensembles of the "behavior-giving" parameter values $\boldsymbol{\alpha}^*(\mathrm{B})$ and their complement $\boldsymbol{\alpha}^*(\overline{\mathrm{B}})$ are distinctly separated. Thus, for example, the distinct *clustering* of parameter combinations that give the behavior, toward high values of α_2 and low values of α_1 in Figure 9(d), suggests that the hypotheses associated with α_1 and α_2 are likely to be fruitful speculations in understanding the observed system behavior.

The speculative character of the analysis should be apparent. The objective is to generate a preliminary set of promising hypotheses about a system's behavior. It is also possible to see the origins of the term *generalized* sensitivity analysis, as opposed to the *local* sensitivity analyses illustrated, for instance, by Jørgensen *et al.* (1978), Rinaldi and Soncini-Sessa (1978), and van Straten and de Boer (1979). A local sensitivity analysis is usually concerned with determining the changes in the state-variable trajectories (in the neighborhood of a set of nominal reference trajectories) that would result from small changes in the values of the parameters. The generalized aspect of the approach outlined above is its evaluation of the sensitivity of a broad range of possible realizations of the state trajectories to (nonlocal) ranges of values for the parameters. For example, had there been no clustering effects discernible in Figure 9(d), an intuitive conclusion would have been to say that the behavior definition is not sensitive to any particular values for α_1 and α_2.

The significance and appeal of speculative simulation modeling, in occupying an important niche in the procedure of model development, can be measured by its rapid propagation to other case studies (e.g. van Straten, 1981; Fedra, 1981, 1983b; Fedra *et al.*, 1981; see also Beck and van Straten, 1983). Notable among these later studies are extensions of the approach to cover problems of prediction (Fedra *et al.*, 1981; see also Section 2.5) and model structure identification (Fedra, 1983b). It is to a brief discussion of this latter problem that we now turn, although the notion of speculative simulation modeling will be encountered again toward the end of this review.

2.4.3 Model Structure Identification and Estimation

The distinguishing definitions of model structure identification and estimation can now be summarily dealt with; the foregoing discussion has in any case covered some of the concepts involved. Thus:

(1) *Model structure identification* is concerned with establishing unambiguously, by reference to the *in situ* field data, how the measured input disturbances $\boldsymbol{u}$ are related to the state variables $\boldsymbol{x}$, and how these latter are in turn related among themselves and to the measured output responses $\boldsymbol{y}$ of the system under study.

(2) *Estimation* consists of the following problem: given a set of (time-series) field data comprising the measured inputs $\boldsymbol{u}(t_k)$ and the measured outputs $\boldsymbol{y}(t_k)$ of the system, and given the model structure, determine values for the model parameters $\boldsymbol{\alpha}$ and state

variables $\boldsymbol{x}$ such that some (loss) function of the differences between the estimated ($\hat{\boldsymbol{y}}$) and observed ($\boldsymbol{y}$) output responses is minimized.

Clearly, model structure identification is a much broader problem than that of estimation. It amounts to the problem of drawing inferences about $\boldsymbol{f}$ and $\boldsymbol{h}$ in the model of Table 1, which implies discriminating among choices for $\boldsymbol{x}$ and $\boldsymbol{\alpha}$. It is, quite deliberately (as the discussion of a change of perspective should suggest), addressed to the evaluation of models based, as the saying goes, on "the physics, chemistry, and biology of the system under study". Logically, model structure identification must precede the more specific problem of estimation. But both problems are essentially ones in which the analysis of what is measurable ($\boldsymbol{u}$,$\boldsymbol{y}$), the "external" description of the system, is used to infer the characteristics of $\boldsymbol{f}$, $\boldsymbol{h}$, $\boldsymbol{x}$, and $\boldsymbol{\alpha}$, i.e. the "internal" description of the system.

The determination, or choice, of model structure is an item of analysis that occurs in almost every instance of model development. It is also very probable that a satisfactory choice of structure is not made at one attempt alone. The distinguishing feature in our definition of model structure identification is that the solution of this general problem proceeds specifically by reference to a set of *in situ* field data. Yet this distinctive feature still leaves the problem definition very broad – so broad, in fact, that there is the danger of sculpting all problems such that they fit the particular problem of interest to this reviewer. This danger, then, is openly acknowledged.

One must be careful, therefore, in citing case studies that are clearly illustrative of a systematic attack on the problem of model structure identification (Beck and Young, 1976; Beck, 1978, 1983b; Whitehead, 1979, 1983; Scavia, 1980a; Fedra, 1981, 1983b; Cosby and Hornberger, 1984; Cosby *et al.*, 1984) and in referring to others (e.g. Canada Centre for Inland Waters, 1979; van Straten and Herodek, 1982; Ambrose and Roesch, 1982) that have been concerned with the same problem, though less formally and less consciously. Without doubt, however, this is an area of analysis ripe in its need for methodological advances (Beck, 1984), and some of these advances can be expected to emerge from an approach based on recursive estimation algorithms (Young, 1974; Beck, 1979, 1982b, 1983b). Progress so far with this approach has been modest: it has yielded a combination of insight and an understanding of how to organize solution approaches at the strategic level, for example, by exploiting in an albeit naive Popperian spirit the notions of falsifying confident hypotheses and of speculating about relatively uncertain hypotheses (Popper, 1959). There has been some success, notably in Young's challenge to the strongly entrenched conventional view of advection– dispersion models for stream water quality (Beer and Young, 1983; Young, 1983) – a case of sharply focusing analysis on a relatively simple model structure. And there have been failures too, not so much of method, but in the strategy of solution (Beck, 1982b) – a case of attempting to tackle the "diffuse" character of more complex, but still modest, model structures with a significant biological content (seemingly just as intractable problem situations now as always).

Scant reward for the investment of much effort has also been a characteristic of case studies of the supposedly more straightforward problem of estimation, though here rather larger-scale models have been tackled, with up to 12 state variables and 20 parameters, for example, in Di Toro and van Straten's analysis of a phytoplankton model for Lake Ontario (Di Toro and van Straten, 1979; van Straten, 1983). The essential, and almost universal, difficulty has been that of identifiability (Beck, 1984). There are several reasons for this, although they can be summarized as being a function of too many parameters to be estimated with too few field data derived from "experiments" that are very poor approximations of the ideal experiments of laboratory science. Or, in terms of our previous discussion of scale, the size of the state-parameter vector to be estimated (in effect, the degrees of resolution in the spatial, temporal, and ecological dimensions) is in principle much greater than the degree of resolution in the available field data (in effect, the frequencies of sampling in these same dimensions). For distributed-parameter models the problem of identifiability is thus likely to be endemic, although there has been some progress in estimating the parameters of such models for stream water quality (Thé, 1978) and groundwater systems (McLaughlin, 1978, 1979a, b, c). The classic manifestation of identifiability is the occurrence of a fitting-function hypersurface that, in contrast to the elliptical contours of Figure 9(b), is degraded into a valley-like or, worse still, flat surface. In this event many combinations of parameter values turn out to be more or less the "best" estimates, and these estimates will have large errors of estimation, that is, the estimates are quite uncertain.

There are not many avenues of escape from this impasse, except for the obvious: the prudent transformation of ill-posed problems to better-posed problems of estimation, which is a possibility (Beck, 1984); a retreat to speculative simulation modeling and the ubiquitous Monte Carlo simulation (as advocated by Fedra, 1983b); or, putting one's faith (probably correctly) in technological innovation, to adopt the view that the current constraints on the availability of field data are not destined to persist in the future. On this last point, there is a further pragmatic consideration to be added to the three quoted in Section 2.3.2. Consider, for example, the ever growing potential for generating data from environmental monitoring networks (as discussed by Marsili-Libelli, 1980; Caddy and Whitehead, 1981; Whitehead and Caddy, 1982). There is thus the possibility:

(C4) that future constraints on model development may well be dominated by the inability to absorb and interpret the diagnostic evidence of data analysis.

To summarize, therefore, there is a paradox. On the one hand, there are too few data to assess rigorously many of the contemporary models and, on the other hand, there is a potential for confusion were adequate amounts of data to become available (Beck, 1983b).

2.4.4 Relevance to Management

Having burrowed down to a philosophical level in this discussion of field data analysis, the pragmatist will surely ask the question: what is the practical significance of model structure identification and estimation? He sees the difficulties and expense of collecting field data, the apparently meager results of arduous analysis, and perhaps the (misleading) appeal of the comprehensive (general-purpose) simulation model to dispense with such difficulties.

A quotation from Biswas's (1981a) book on models for water quality management provides a provocative starting point for a response:

> Recognizing that a model is only an approximation of the real system, it appears logical to visualize that water quality modeling is merely curve fitting in a river system .... [The] statistical theory of estimation and hypothesis testing are all useful in model building.... On the other hand, failure to recognize the quality modeling as curve fitting has, in part contributed to the making of water quality modeling a field of ambiguity and mystery. Too often the calibration/verification procedure is described as a distinct and creative step in water quality modeling. However, it is merely, in fact, an ad hoc procedure to fill partially the role of estimation and hypothesis testing (deLucia and McBain, 1981).

In spite of the confusing ambiguity of this statement, it is apparent from other statements by these authors that following the *a posteriori* steps of model development *is* thought to be a good thing (in this instance for the purposes of management in the St. John River, USA). There is strong disagreement, however, between the position of this review and the above-implied assertion that the *a posteriori* phase of model development is not a "distinct and creative" step in water quality modeling. It is not, as these authors say, "merely curve fitting", if this is meant to imply that fitting the curve to the data is an end in itself; rather, it is a means to an end, and what is revealed about the model structure in the process of making the model fit the data is much more important (Beck, 1982b). The essence of the argument for a change of perspective (in Section 2.4.1) is intended precisely to dispel the illusion that "calibration" does not involve a critical questioning of, and creative speculation about, prior hypotheses. But if deLucia and McBain's comments represent a consensus on the role of field data analysis, and one expressed by authors favorably disposed toward the topic, then it is indeed important to answer the pragmatist's question.

First, a personal view expressed in the introduction to this review was one of two streams of development: the resolution of issues of management; and the retrospective distillation and prospective catalysis of this process through the development and application of mathematical models. This section, above all, has been concerned with the scientific basis for the latter. And because there are two such streams of development, where the latter may well only indirectly influence the former, and after some delay, it is far easier to say that a particular decision was *not* influenced by any model than to demonstrate otherwise. This much is conceded. The workings of a catalyst, by definition, are not visible in the composition of the end-product.

Second, however, if water quality modeling and management are supposed to be scientific, it is difficult to argue that the *a posteriori* phases of modeling, as defined here, can be entirely dispensed with. The alternative is to argue that all matters of practical significance to decision making can be deduced from existing *a priori* theory, which at the present seems to be a hardly (if ever) tenable position.

Third, precisely because there have been too few exercises in conducting the *a posteriori* steps of model development (because these steps of the procedure are felt to be unsystematic or *ad hoc*), there should, in the short-term future, be an increasingly suspicious and critical attitude toward models applied purely (or predominantly) on the basis of *a priori* theoretical considerations. The scientific respectability of a subject, irrespective of pragmatic management considerations, should not continue to survive without the accruing of corroborative evidence for these prior theories.

Here, then, let us leave the arguments about the usefulness or otherwise of field data analysis. What has been said is really a response to something of an open question: a result of critical introspection, with no illusions about the universal need for mathematical models, or about the inviolate accuracy of models. But if management calls for a model, it is better that the way in which the model is to be developed is felt generally to be on a sound scientific footing.

Less contentious is the practical potential of speculative simulation modeling, since it clearly addresses common problem situations and would satisfy the pragmatist's concern to avoid expensive data collection exercises. He takes the risk, however, that the outcome of such an analysis, being rigorously consistent with the few data that *are* available, may be vague and not clear-cut (e.g. Fedra *et al.*, 1981). Equally practical is Thomann's verification analysis (Thomann, 1982; see also Ambrose and Roesch, 1982), which covers some of the simpler statistical techniques that can be employed as *a posteriori* checks and balances on the adequacy of a model (the last step in the procedure of Figure 7).

In practical terms there are other, less obvious ways in which model structure identification and estimation affect the application of models for management purposes. They have to do with uncertainty, making predictions, and prediction error propagation.

2.5 VALIDATION, PREDICTION, AND PREDICTION ERROR PROPAGATION

The topics of validation and prediction stand at the point of transition between model development and the application of the model to problem solving. Whatever the benefits of model development in terms of acquiring understanding or as a framework for organizing and interpreting experimental data, the ultimate test of a model is whether it can be believed as a mechanism for prediction. And the most searching question almost invariably posed is whether predictions can be made of conditions expected in the future that will be substantially different from those observed in the past (this is sometimes also given as an operational definition of validation).

These critical questions of prediction and validation indeed sharpen the focus of discussion about current limitations in the approaches to water quality modeling. For instance, one can pose the following dilemma (Beck, 1981a, 1983b). With a "large", complex simulation model – the kind of general-purpose model developed principally on the basis of the *a priori* steps of the modeling procedure – it may well be possible to predict the "correct" future, but one would have little or no confidence in that prediction. With a "small" model – the kind of model that might result from a rigorous application of the *a posteriori* steps of model development – it may be that an "incorrect" future is predicted, and, worse still, one might place considerable confidence in that prediction. The purpose in stating such a dilemma is not to suggest that it should be resolved, even if that were possible, but rather to emphasize both the role of uncertainty and the importance of the connection between historical data analysis (the *a posteriori* phases of model development) and prediction. This relationship between the identification of past behavior and the prediction of future behavior, in terms of accounting for uncertainty, can loosely be summarized as in Figure 10; the *a posteriori* parameter estimation errors can be thought of as a synopsis of the process of fitting the model to the data. Recall, therefore, the problem of identifiability and the literal interpretation of curve fitting. Let us suppose that the model can be made to fit the data arbitrarily well, but that the unavoidable results of this are that some of the parameters and unobserved state variables must be varied arbitrarily, or that many combinations of parameter values yield equally "best" estimates and these estimates are accordingly poorly defined (i.e. highly uncertain). Both results may be of no consequence whatsoever in terms of replicating past behavior, but they would certainly have significant implications should the model be used for prediction. They would, in general, lead to ambiguous statements about future behavior, and even this ambiguity might not be discernible against a background of high uncertainty (Beck, 1983b).

In this section we are therefore broadly concerned with the following problem: a model having been derived, it is to be used to make statements about conditions other than precisely those under which it was derived, and it is important to know what confidence can be attached to these statements. There are several familiar problems covered by this definition, and some examples are given here:

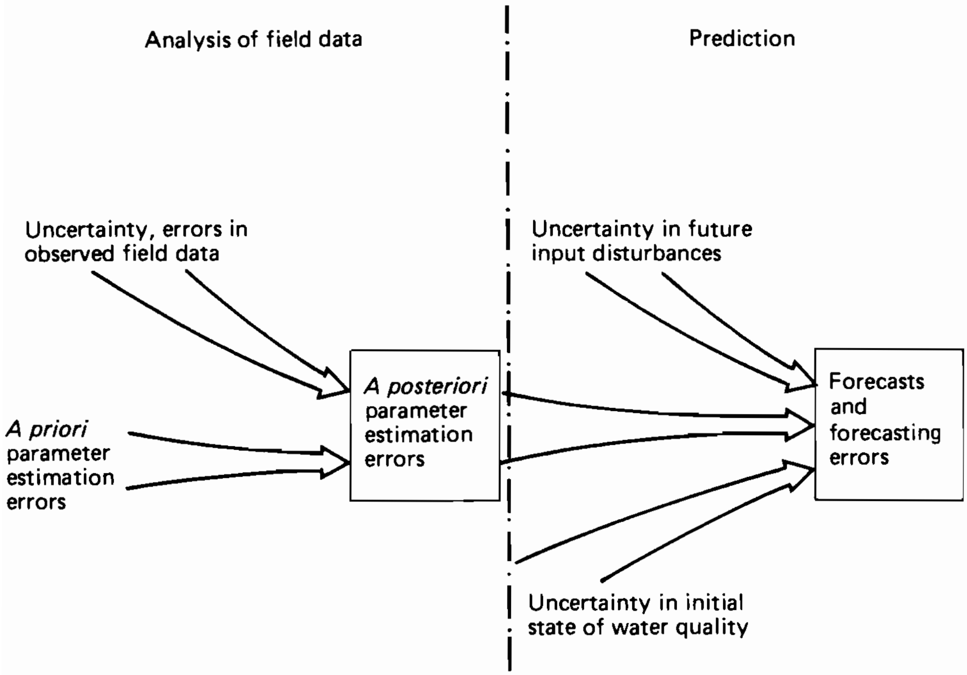

FIGURE 10 Sources of error and uncertainty and the connection between prediction and the *a posteriori* steps of model development.

(1) *Validation*: Given the model structure and parameter estimates, determine behavior under different (observed) input conditions for comparison of the output response with observed behavior.

(2) *(Conventional) sensitivity analysis*: Given the model structure and parameter estimates, determine changes in the output model responses due to changes in the estimated values of the parameters.

(3) *Prediction error propagation*: Given the model structure and parameter estimates (subject to uncertainty), determine future behavior under different (assumed) input conditions.

(4) *Reducing uncertainty*: Determine which sources of error (uncertainty) contribute most to the uncertainty of the predicted responses, and design experiments in order to reduce this uncertainty.

Of these, *sensitivity analysis* has already been discussed, albeit very briefly, and will not be considered further.

Taken in the narrow operational sense defined above, there have been few documented case studies in *validation*, although the work of Thomann *et al*. (1974a) on the Potomac Estuary, USA, and of Jørgensen *et al*. (1978) on the effects of sewage diversion from Lyngby Lake in Denmark are notable exceptions. Validation can, of course, be seen as a more philosophical matter, particularly in the (obverse) Popperian sense of seeking invalidation of a model (e.g. Holling, 1978; Young, 1978, 1983), and particularly within the domain of systems ecology (Caswell, 1976; Mankin *et al*., 1977; Cale *et al*., 1983). But such discussions of validation, like the earlier discussion of model structure identification, are directed toward the scientific basis for modeling and we shall mention them here only in passing.

2.5.1 Prediction Error Propagation

The interest in prediction error propagation (or "error analysis") has similarly been stimulated by a mood of critical self-appraisal. In concert with the emergence of Thomann's verification analysis and with the changing perspective reflected in the discussion of model structure identification, error analysis is also a reaction (perhaps unspoken) to the trend toward the development of ever larger-scale simulation models; undoubtedly it is a movement away from determinism. In 1979, when summarizing the state of this new area of analysis, O'Neill and Gardner (1979) observed that "the real challenge lies with [the] complex ecosystem models that have been developed over the past decade."

The crux of the problem of prediction error propagation is defined succinctly in O'Neill's (1973) original contribution to the subject. He noted that the error in the prediction from a model should decrease with a decreasing degree of model aggregation (in an ecological, as opposed to spatial or temporal, sense in this case). However, he noted also that precisely this increasing refinement of detail – more complex kinetic expressions, more state variables – would tend to increase the prediction errors resulting from the necessarily increasing number of model parameters with uncertain values. For instance, errors of 10% (expressed as a coefficient of variation) in the parameter values were found to yield errors of prediction greater than 100%.

In the decade or so of subsequent research a principal focus of debate has been about which method of analysis should be used, although individual studies were often not conceived as intentional forays into this debate. On the one hand, there is Monte Carlo simulation (represented by the studies of Tiwari *et al.*, 1978; O'Neill and Gardner, 1979; Gardner *et al.*, 1980, 1981, Hornberger, 1980; Fedra *et al.*, 1981), and on the other hand, first-order, and possibly higher-order, error analysis (as illustrated by, for example, Argentesi and Olivi, 1976; Reckhow, 1979a, b; Scavia, 1980a; Dettinger and Wilson, 1981; Beck, 1983b; McLaughlin, 1983). There have followed inevitably a number of comparative studies, some of which argue that the two approaches give essentially similar results (Walker, 1982; Malone *et al.*, 1983), while others have quite clearly revealed significant differences (Scavia *et al.*, 1981a), particularly with respect to drawing inferences about solutions to the problem of reducing prediction uncertainty (Gardner and O'Neill, 1983).

In effect, the issue of which method is superior is no longer an issue; when the computing power is available, there can in general be no strong argument against the use of Monte Carlo simulation. This does not mean that there can be no argument in favor of a first-order error analysis (indeed, such an argument will be given below). However, the assumptions necessary for the derivation of the algorithms of a first-order analysis are always likely to be restrictive, and they are, strictly speaking, frequently violated by the large errors now known to be characteristic of the models under study (Scavia *et al.*, 1981b; van Straten, 1983). Unlike the areas of model structure identification and estimation, which are in need of significant methodological progress, the methods of prediction error analysis have, by and large, delivered the answers sought to the questions posed. As a general conclusion it is perhaps not so much new methods but new questions in the analysis of prediction that are now needed (Beck, 1984); one such question will be discussed in Section 4. O'Neill and Gardner's "challenge" of the larger, more complex models has not yet been met, except for one outstanding case study of a phytoplankton model for Saginaw Bay, Lake Huron (Scavia *et al.*, 1981a, b). But already these and other results provide plenty of ammunition for those who would argue that models, and especially the larger ones, give predictions that are highly uncertain (with coefficients of variation of upward of 700%, if such a statistic then has any real meaning). And to be able to predict only that all things are more or less equally probable is no basis for decision making. Of course, this does not prevent one from *believing* that reality is more orderly and predictable than these results would suggest. A recent study by Kremer (1983) lends considerable support to this belief by pointing out a possible source of overestimation of prediction error magnitudes that is inherent in the assumptions underlying most of the earlier applications of Monte Carlo simulation.

2.5.2 Reducing Uncertainty: An Iterative Cycle

This same belief would also be persuasive for assuming that further experimental work could be planned in order to reduce some of the critical uncertainties of model predictions. Thus it is that the discussion of the procedure for modeling (Figure 7) has turned a full circle back to the topic of experimental design. One iteration through the cycle of experiment → identification (field data analysis) → prediction has been completed; in a Bayesian spirit, the "posteriors" of the first iteration have become the "priors" for the second iteration. The analogy is apt. The problems of each of the three stages of the cycle can be addressed in the Bayesian framework of filtering theory and recursive estimation: for experimental design (Canale *et al.*, 1980); for identification (Beck, 1979); and for prediction error propagation

(Beck, 1983b). We may note in passing that although this topic is not a large one it is sufficiently independent to have justified a specialized conference on the application of filtering theory to hydraulics, hydrology, and water resource systems more generally (Chiu, 1978). For most of the related algorithms of practical interest the equations for the propagation of error are those of a first-order error analysis, and it is this conceptual link with the iterative cycle of experiment → identification → prediction that may prove to be the strongest argument in favor of the continued use of first-order error analysis (Beck, 1984).

It would be premature to expect there to have been many case studies in the design of experiments to reduce model prediction uncertainty. The subject of error analysis in water quality modeling is barely old enough for even one iteration through the cycle of analysis to have been completed. Again, the work related to a phytoplankton model for Saginaw Bay, Lake Huron is especially notable (Scavia *et al.*, 1981a; Canale *et al.*, 1980). The specification of the experimental design problem in the present context, however, has somewhat different objectives from those to be discussed in the next section; certain distinctions should be made. Here, the specific purpose is to design an experiment to improve a model for the relationships between "causes" and "effects", not to characterize, or to monitor in accordance with, a probability distribution (equally so a model) for the variability of either the "causes" or the "effects". These latter are objectives of management, not of model development for its own sake. In terms of the model of Table 1, the problem here is: given a (prior) model and (prior) knowledge of the internal description of the system's behavior ($\boldsymbol{x}$,$\boldsymbol{\alpha}$) *and* their associated uncertainty, determine a measurement strategy for $\boldsymbol{u}$ and $\boldsymbol{y}$ (the observable "causes" and "effects") in order to improve the (posterior) knowledge of $\boldsymbol{x}$ and $\boldsymbol{\alpha}$. But even the best of such planned experiments are passive, in the sense of being unable to manipulate $\boldsymbol{u}$ to perturb $\boldsymbol{y}$ in a deliberate fashion and thereby to learn something of the system's behavior in the classical manner of laboratory science. And it is this fundamental barrier to progress that cuts across the path of what might otherwise be the more straightforward development of water quality modeling (Beck, 1982b).

3 POLLUTION PROBLEMS AND THE APPLICATION OF MODELS FOR MANAGEMENT

It is all very well for the purist to talk in rigorous scientific terms about uncertainty and the limits to the predictive capabilities of current water quality models. But he who has little confidence in the predictions of his model may jeopardize his case in providing advice for the resolution of issues of management. Does it not merely confuse the issues to give advice couched in the hesitancy of uncertainty? Perhaps in this instance the distinction of the two trains of development in modeling and management and the smoothing effects of their delayed interactions work to the advantage of modeling. In spite of uncertainty, broad strategies for action do emerge; indeed, there are those who would argue that these strategies are all the more robust and adaptable for having considered uncertainty (Holling, 1978).

In at least two directions, an "institutionalizing" of modeling in the standard-setting procedure (Water Pollution Control Federation (USA), 1981) and the emergence of probabilistic water quality standards (National Water Council (UK), 1978), we shall see again a slow changing of perspective at the beginning of this part of the review, Section 3.1. Section 3.2 then surveys briefly some selected issues in management and the role of optimization, and Sections 3.3 to 3.6 follow through the sequence of four pollution problem categories introduced in Section 2 and Figure 1: easily degradable organic wastes; eutrophication; the nitrate problem; and toxics.

3.1 STANDARD SETTING AND MONITORING

In 1981, the US Water Pollution Control Federation published the first three of eight position papers on water pollution issues that it had "identified ... as being top priorities for professional attention during the next decade" (Water Pollution Control Federation, 1981). One of these issues was that of "improving water quality criteria and standards". The position paper on this issue noted the "general switch from stream quality to effluent quality control ideas in 1972", and went on to argue that the "neglect [of] water quality standards ... has meant that the arts of stream sampling and modeling have not improved significantly." In proposing as an objective the elucidation of ways to enforce standard-setting programs, the position paper recommended *inter alia* (Water Pollution Control Federation, 1981):

> Analyzing the wasteloads for water quality-limited streams using verified mathematical models that are calibrated with local information.
>
> Consider setting aside some of the stream's capacity as a reserve for future discharges and as a hedge against errors or inaccuracies in the predictions made with the model.

Here, then, at the forefront of a strategy for management, is official recognition of uncertainty and the role of the mathematical model.*

Earlier, in 1978, the UK National Water Council published a policy statement in which it recommended that, in effect, the Regional Water Authorities of England and Wales should manage water quality by assessing the existing or future uses of a water body, thus to specify water quality objectives related to these uses, and hence declare the conditions to be met by polluting discharges as management took action to move toward those objectives (National Water Council, 1978). This statement of UK policy has at times been seen as quite at odds with the (assumed) preferred policies of the European Economic Community (EEC), the main issue of the debate falling precisely (as in the USA) on the different implications of adopting "stream standards" or

*Though it should not escape notice that R.V. Thomann, whom we assume to be an advocate of modeling, is acknowledged as a member of the task group for this position paper.

"effluent standards" as the primary instruments of policy (Haigh, 1984). Nevertheless, following the lead of the National Water Council's policy statement, various authorities in England and Wales prepared declarations of what they considered to be suitable standards for in-stream water quality (e.g. Bedford Ouse Study, 1979; Price and Pearson, 1979). These standards, other standards developed in conjunction with the program for water quality protection within the EEC (Mance and O'Donnell, 1984), and standards specified for effluent discharge quality characteristics are notably declared with the inherent assumption of the probabilistic nature of water quality. The argument is no longer about whether the uncertainty or variability of conditions can be formally acknowledged, but about how to monitor compliance of actual performance with a desired performance defined in such terms (Warn and Matthews, 1984). To these developments in the UK can be added the authority of the US WPCF position paper in its recommendation to develop and implement the concept of allowing an acceptable frequency of noncompliance with standards (Water Pollution Control Federation, 1981).

These changes at a strategic policy level are shifts of attitude away from a rigid uniformity toward a more flexible acceptance of the complexities of the variability of water quality. Translated down to the level of future monitoring practice, their implications are almost certainly that sampling and network design will likewise become more complex, especially when viewed against a background of technological development, as we shall see in Section 4. The important questions at this point in the review, however, are those concerning the use of systematic methods for solution of current network design problems. It is appropriate first to define the sort of relationships on which data are required.

Within any strategy of management there is an implied logic of known cause-and-effect relationships:

(i) between the stipulation of the allowable levels of constituents in a polluting discharge and the effects of these constituents on the attainment of an environmental quality objective; and

(ii) between the stipulation of the composition of an environmental quality objective and its "effects" on the intended use of a water body and its flora and fauna.

It is helpful for the subsequent discussion to distinguish these as two "input—output" couples (as u–y couples in terms of the model of Table 1), where the output of the first is the input to the second couple. We shall, however, consider only the first couple as the domain of interest to monitoring network design. Monitoring public health in response to the consumption of water, such as the identification of relationships between water softness and cardiovascular mortality, nitrates and stomach cancer, and the effects of bathing in polluted waters, will not be of concern here (see, e.g., Cabelli *et al.*, 1979; Shaper *et al.*, 1980; Fraser and Chilvers, 1981).

The objectives for monitoring water quality are more or less self-evident. Omitting the case where experiments are conducted for the express purpose of model development (already discussed in Section 2), they are generally agreed to cover four broad, but not necessarily distinct, items:

(i) for enforcement purposes, the detection of violations of desirable or legal standards for acceptable water quality;

(ii) the detection of long-term trends or changes in the degree and type of variability in the overall state of water quality;

(iii) the provision of background data for the purposes of management in the broadest sense;

(iv) the protection of water supply abstractions.

The objective, as Lettenmaier (1979) has emphasized in a review article, suggests the solution approach to the design problem.

The degree of sophistication of the solution is dependent upon the amount of prior knowledge brought to bear on the problem. At the first iteration, in a state of some ignorance, it may suffice to make some simple assumptions about the distribution of a variable and to determine the number of samples required to estimate various statistics of this distribution with a chosen level of confidence (Reckhow (1978) and Ellis and Lacey (1980) are illustrative of this class of problems). For example, the objective might be to estimate the variability in nutrient loading delivered by a tributary to a lake, without searching for the causes of this variability. The assumption about the underlying probability distribution is indeed a model, but not of the kind defined in Table 1, except in the most trivial of its reduced forms. The purpose of the design solution is tantamount to seeking essentially *univariate* characterizations of a collection of causes ($\boldsymbol{u}$) and a collection of effects ($\boldsymbol{y}$). This would not, however, debar the possibility of establishing (multivariate) cause-and-effect relationships once the data have been collected. At a second iteration, with presumably much more prior information, more sophisticated methods of network design can be employed. Almost certainly the problem will be predicated on the assumption that *multivariate* relationships prevail, including the input—output couples discussed above, and it will accordingly be necessary to posit a model of these relationships. As with the earlier discussion of designing experiments for model identification, approaching these "second-generation" problems within the framework of filtering theory has been most popular (Moore, 1973; Lettenmaier and Burges, 1977; Kitanidis *et al.*, 1978; McLaughlin, 1978; Pimental, 1978). But here the model is not the objective of the analysis; it reflects a summary of the prior knowledge germane to the economy and effectiveness of the design.

Like the experiment → identification → prediction cycle, systematic solution of the monitoring-network design problem is barely mature enough to have completed its first iteration. It is not surprising, therefore, that *in situ* field data for the purpose of (multivariate) model development have not been readily available from the essentially univariate designs of existing monitoring networks. Nor is it surprising that the WPCF position paper laments the lack of progress in sampling-program design and modeling when the burden of standard setting has rested predominantly with the need to think in the essentially univariate terms of polluting discharge "causes" alone. There is certainly ferment in the present state of thinking about water quality monitoring (Rickett and Hines, 1978; Lee and Jones, 1983; van Belle and Hughes, 1983), which seems likely to evolve toward a two-tiered system of routine (background) monitoring coupled with intensive, synoptic surveys. The plea of Ward and Loftis (1983) that the probabilistic nature of water quality be incorporated into management strategies is unlikely to go unheard. And the subject of water quality modeling can only be a beneficiary of these developments.

3.2 MANAGEMENT AND THE ROLE OF OPTIMIZATION

Having assimilated the information derived from monitoring, which may indicate that actual performance does not match desired performance, or that understanding of the relationships between causes and effects has changed significantly, management may contemplate action to manipulate the causes ($\boldsymbol{u}$) to bring about certain desired effects ($\boldsymbol{y}$). It may take this action in three phases, to each of which modeling may be relevant (these definitions are based on Jamieson, 1978, 1979):

(1) *Planning* – for which, to meet the longer-term strategic objectives, models may be required to screen a large number and variety of possible regulatory options with a view to isolating a few that are attractive because they represent "optimal" or "near-optimal" solutions (see also Loucks, 1978).

(2) *Design* – where, a restricted number of attractive options having been identified, a more detailed analysis of the design of the required engineering facilities (for treatment, storage, and so forth) is conducted, together with the development of tentative operating rules and an assessment of the expected performance of these facilities.

(3) *Operation* – for which models may be used both in the detailed design of process operational control schemes and as a support service in the implementation of shorter-term, day-to-day management, where satisfaction of the planned objectives (possibly in a least-cost fashion) is desired (see also Beck, 1981b).

The hierarchical character of these aspects (as emphasized by Jamieson) and the underlying questions of scale and of aggregation–disaggregation run parallel to what has been said in Section 2 about problem decomposition and model development. As an illustrative introductory example, the study by Stehfest (1978) (see also Rinaldi *et al.*, 1979) typifies the use of modeling for planning purposes, specifically for the allocation of wastewater treatment capacity for the Rhine River (FRG). At the opposite end of the spectrum, the (theoretical) studies of real-time process control schemes for maintaining satisfactory river DO levels are illustrative of the application of models to problems of operational management (e.g. Young and Beck, 1974; Whitehead, 1978; Gourishankar and Lawal, 1978).

Cutting across the management problem in a different direction, one can identify several important questions that might be asked of any proposed solution (i.e. course of action):

(1) Is the solution stable, or is it likely to induce radical changes of behavior?

(2) Is it sensitive to current uncertainties?

(3) Does it increase or decrease the probability of managing contingencies successfully?

(4) Is it "acceptable" within certain broad bounds?

(5) Is it, more precisely, "optimal", or economically efficient?

The analysis of stability has long been of considerable interest in systems ecology. There have been a few applications of this analysis to models of the phytoplankton systems of concern to water quality management (e.g. Ikeda and Adachi, 1978; Adachi and Ikeda, 1978; Duckstein *et al.*, 1979; and van Nguyen and Wood, 1979; the last two are applications of catastrophe theory); the effects of a toxic substance on the stability of populations in ecological systems have also been analyzed (Hallam *et al.*, 1983). But these have been largely theoretical analyses, and the question of instability as a consequence of a contemplated action does not appear to have been articulated in the context of management. Demands at the policy level for the recognition of uncertainty have, as we have seen, already been made; and in one way or another such uncertainty can be incorporated into the application of models for management purposes (Lohani and Thanh, 1979; Lohani and Saleemi, 1982; Somlyody, 1982a, b, 1983b; Reckhow, 1983; Fedra, 1983a).

The overwhelming majority of published studies, however, have focused on the fifth question of determining "optimal" solutions* and, in particular, solutions to the management of easily degradable wastes in a river system. Indeed, these "paradigm" problems and solutions have become so well established that they have achieved textbook status (e.g. Stark and Nicholls, 1972; Rinaldi *et al.*, 1979; Loucks *et al.*, 1981; Smith *et al.*, 1983). Reports on a number of the by then already "classic" case studies were assembled by Deininger (1975); they were predominantly analyses of the planning aspect of management.

To introduce the following four sections of the review, let us take stock of the achievements. First, there is a notable gap between the macroscopic nature of economic analyses required for the purposes of planning and the relatively microscopic (and, thus far, often impractical) details of studies on operational control system synthesis. There do not appear to have been any studies in the middle ground that address detailed questions of design–operation interactions in water quality management. Second, there has been little or no systematic study of formal approaches to the pertinent questions of management other than that of seeking economically efficient

*Meaning here that the model of behavior is embedded usually as a constraint set in a general constrained optimization problem.

solutions among the various alternatives. Admittedly, all other questions might be of secondary importance but that does not necessarily justify what seems to have been their almost complete neglect. Third, subsequent to the early 1970s few, if any, major case studies have been initiated in which the focus on optimal solutions was as clear as it had been in the earlier (prototype) projects (and one is tempted to ask why). The application of mathematical programming now seems, however, to be enjoying something of a renaissance, although this time more evenly distributed among the problems of easily degradable wastes (Marsili-Libelli, 1982), eutrophication (Bogardi *et al.*, 1983; Chapra *et al.*, 1983; Somlyody, 1983b), and nitrates (Moosburner and Wood, 1980), and for groundwater management more generally (Willis, 1979).

3.3 EASILY DEGRADABLE ORGANIC WASTES

It was argued earlier (in introducing Section 2) that the classical studies of Streeter and Phelps (1925) on the equally classical problem of gross pollution, as defined by the degradation of waste organic matter (BOD) and its interaction with dissolved oxygen (DO), can be viewed as the origin of water quality modeling. Figure 11 is an interpretation of the major historical developments of the subject in support of such an argument. Given, however, the prodigious number of papers dealing both with DO–BOD interaction and with modifications or applications of the Streeter–Phelps model, this part of the review will be restricted to the salient features of the subject's historical development, its range (particularly in the light of the methodological features discussed in Section 2), and its demonstrable successes in practice.

According to Figure 11, developments between the original work of Streeter and Phelps and the current agenda of problem areas can be separated into two phases. The first, beginning in the mid-1960s, produced a rich critique of the limitations of the Streeter–Phelps assumptions; each of the current problem areas can be said to have been foreshadowed in this critique. All of the modifications proposed at that time involved additions and/or subdivisions of source and sink terms for the two state variables of DO and

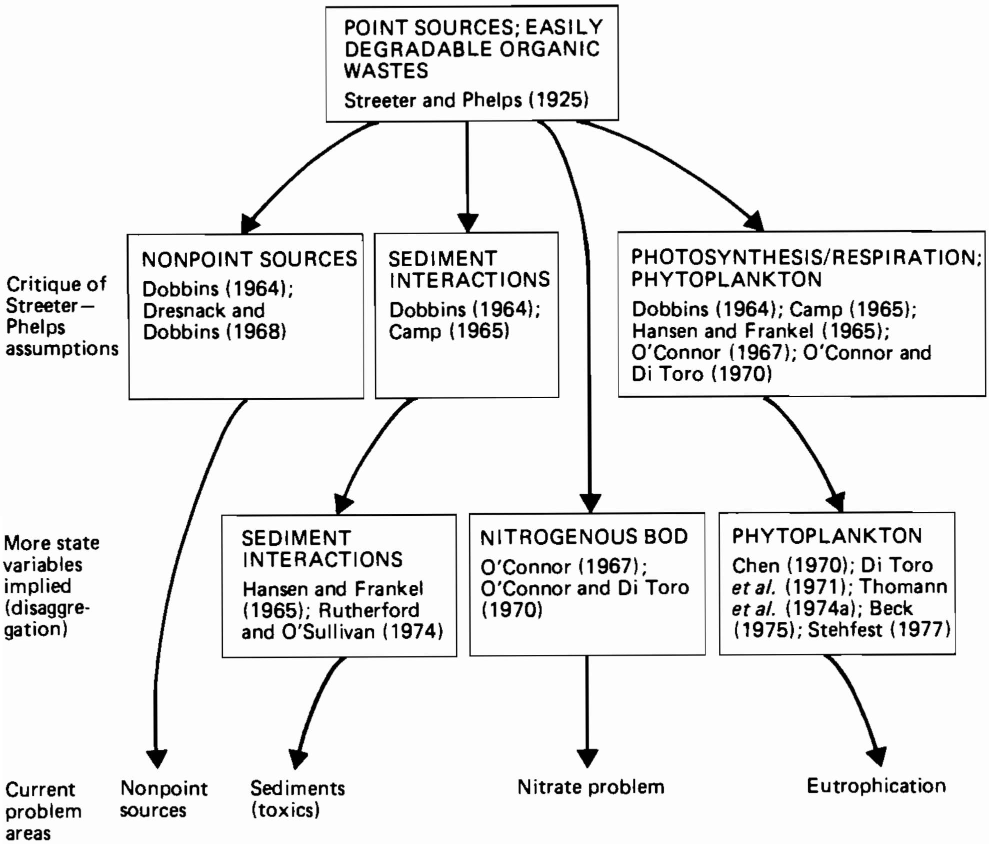

FIGURE 11 Developments, in two phases, from the original work of Streeter and Phelps (1925); the connection with today's toxics problem is admittedly tenuous.

BOD. It was the implicit or explicit addition of more state variables – for example, the separation of BOD into carbonaceous and nitrogenous components or a separate mass balance for phytoplankton – that marked the beginning of the second phase of developments toward the end of the 1960s. In other words, there was a progressive conceptual disaggregation of the macroscopic variables characterizing gross pollution, which, in its most obvious trend, has tended subsequently to pass through a concern with estuarine water quality problems (Di Toro *et al.*, 1971; Thomann *et al.*, 1974a; Orlob, 1976) toward the problem of lake eutrophication (Thomann *et al.*, 1979; Di Toro and Matystik, 1980). Many of the developments indicated in Figure 11 are evident in the evolution of a uniquely comprehensive study of the Neckar River, FRG (Hahn and Cembrowicz, 1981).

The range of studies on the problems of modeling and managing easily degradable organic matter is enormous; we can only attempt to sketch here the frontiers of this range in certain directions. First, in terms of spatial scale the models developed for the St. John River, Canada (Biswas, 1981b), the Upper Cauca River, Columbia (Bartone, 1975), and a 450 km stretch of the Rhine River, FRG (Stehfest, 1977, 1978) are typical of the larger, regional analyses. Second, the two case studies of the Cam and Bedford Ouse Rivers in the UK (Beck, 1975; Bedford Ouse Study, 1979; Whitehead *et al.*, 1981a) are representative of the most detailed analyses of short-term temporal variations in DO–BOD interaction. Third, these same studies of the Cam and Bedford Ouse Rivers are illustrative of some of the most recalcitrant problems of model structure identification and estimation that have been mentioned in Section 2.4 (see also Beck, 1983b). Fourth, the studies of the Bedford Ouse (Bedford Ouse Study, 1979; Whitehead and Young, 1979), the Canadian section of the St. John River (Biswas, 1981b), and the Hsientien basin, Taiwan (Lohani and Thanh, 1979) are notable for giving more detailed considerations of the uncertainty and variability of expected future behavior (in part due to precipitation-discharge variability) than most of the other studies reported in the literature. Lastly, the discussion by Rinaldi *et al.* (1979) of planning an optimal allocation of wastewater treatment and artificial in-stream aeration capacities for the Rhine River, together with the ambitious study by Spofford *et al.* (1976) of regional residuals management in the Lower Delaware Valley, USA, indicates the impressive extent to which techniques of mathematical programming have been applied to the management of easily degradable organic wastes.

If, however, as the survey by Cembrowicz *et al.* (1978) says, the Streeter–Phelps model continues to be widely applied in water quality planning studies, this begs the question, among others, of how far the considerable research effort of the past two decades has brought us. It is significant to note how fertile was the period of the mid-to-late 1960s, when many original contributions were made: in applying stability analysis (Thomann, 1963); the application of dynamic programming (Liebman and Lynn, 1966); the application of linear programming (Revelle *et al.*, 1968); consideration of the time-variable and operational aspects of management (Thomann *et al.*, 1968); in the application of distributed-parameter control theory (Tarrasov *et al.*, 1969); and in the publication of a text on systems analysis and water quality management (Thomann, 1972). Even if one were to argue that some of these were contributions of a more theoretical character, the progress since that time has been modest in comparison. It is as though these early innovations were premature and have since lain dormant; perhaps, as this review will show, their time has now come.

There is, of course, a distinction between success in theory and success in practice; as too there is a distinction between factors influencing the making of a decision and the factors proving the conclusion that management has been successful. What practical successes, therefore, have been claimed for the management of easily degradable organic matter, and have these successes been achieved in river basins that have been the subjects of modeling? In 1979, a report of the Organization for Economic Cooperation and Development (OECD, 1979) observed that:

> The quality of fresh water has improved in that pollution by suspended solids and oxidizable matter (BOD) has stabilized or decreased in countries where action has been taken ....

But at what cost, one wonders, when in the same year the US Water Pollution Control Federation opened one of its White Papers as follows (Hill *et al.*, 1979):

> Of all areas of consideration involved in the planning, design, and construction of wastewater treatment facilities, operation and maintenance (O and M) is the fundamental measurement of a facility's performance; this is also many times the area most overlooked during the planning phase. That only half of all treatment facilities in the U.S. are meeting their design standards for biochemical oxygen demand and suspended solids clearly exemplifies the result of poor O and M.

More specifically with respect to the benefits of modeling, the following comments from four case studies are especially revealing:

(1) DeLucia and McBain (1981) conclude from the St. John River, USA, study that: "the model for prescriptive purposes [i.e. a model for determining least-cost optimal solutions] was of more limited use than the model for descriptive purposes [i.e. a model used simply for simulating scenarios]. ... it was the potential for wide application and for EPA sponsorship that led to the prescriptive model development."

(2) For the Neckar River, FRG, study, Hahn and Cembrowicz (1981) state in retrospect that: "Early and realistic impacts on planning and decision making stemmed from results obtained with relatively simple simulation models. Only recently results from optimization models have found acceptance by the practising and administrating engineers."

(3) Woodward (1980) records "20 years of improvement" for the quality of the Trent River, UK, yet he notes that "the Trent Economic Model is ... now of minimal use to the Severn–Trent Water Authority as a management tool" (admittedly, however, because of extenuating circumstances associated with a major change in institutional arrangements for water quality management).

(4) For the estuarine part of the Thames River, UK (a much publicized case of improvement), Casapieri and Owers (1980) present predictions from a model that "contributed to the decision" not to incur the additional expenditure of upgrading treatment facilities that would yield benefits of only marginally better water quality.

Two points can be concluded from this small sample of comments. First, there is the suggestion from the first two cases – supported also explicitly in other observations by Woodward and implicitly by Casapieri and Owers – that it is modeling in the context of simulating scenarios, rather than in determining directly optimal investment patterns, that has been the more demonstrably useful application. Second, these comments are, at most, weak affirmatives. The statement that the results of modeling "contributed" to the making of a decision is more direct than most but nevertheless circumspect.

3.4 EUTROPHICATION

Unlike the problem of easily degradable organic wastes, where most contemporary analyses can be seen to share a common historical origin, the study of modeling eutrophication is characterized by at least four slowly converging lines of development. The first, as noted in the preceding section, emerged from the adaptation of stream DO–BOD models with the introduction of mass balances for phytoplankton, in particular for estuarine systems (although for these systems it could alternatively be argued that such modifications were stimulated primarily to account for the relationship between DO and the nitrogen cycle; see, for example, Orlob, 1976; O'Connor *et al.*, 1976). The second was an outgrowth from studies in the early 1960s on simple thermal energy budget modeling for lakes, and passed likewise through a phase of concern with DO–BOD interaction (e.g. Markovsky and Harleman (1973); also Orlob (1981, 1983b) summarizes the chronology of this line of development). The third line, apparently somewhat independent of the other developments, was an approach of distinctively limnological origins concentrating essentially on simple nutrient budget models and regression relationships (e.g. Vollenweider (1969); also Reckhow (1979a) chronicles the development of this line). The fourth strand in the development of models relevant to eutrophication problems, and one that represents quite the opposite end of the spectrum to the simplicity of the Vollenweider models, is the contribution of complex ecological models from what might be called the context of systems ecology (e.g. Park *et al.*, 1974, 1975; Park, 1978; Chen and Orlob, 1975; Chen and Smith, 1979; Jørgensen, 1976; Walters *et al.*, 1980). Various aspects of these differing approaches have been brought together in the much studied case of Lake Ontario, USA/Canada (Scavia and Chapra, 1977; Canada Centre for Inland Waters, 1979; see also Thomann *et al.*, 1979; Scavia, 1980b).

To say that these developments were all problem-driven, in the sense that the models were constructed for solution specifically of the eutrophication problem, would not be altogether accurate. It is perhaps better to say that the eutrophication problem has been a meeting place of disciplines. It is both difficult and unnecessary to disentangle developments that were probably of a more theoretical nature. Nor were all the models developed for lake water quality necessarily intended to be "eutrophication" models. It is indeed easy to make an exclusive association of eutrophication with lakes and reservoirs; yet clearly the same effects of a eutrophic situation – excessive growths of algal populations – are evident in slowly flowing lowland river systems (Beck, 1975, 1982b; van Straten and de Boer, 1979; Whitehead *et al.*, 1981b) and shallow estuarine systems (Hornberger and Spear, 1980).

For the North American Great Lakes alone, Sonzogni and Heidtke (1980) note that well over a hundred models have been developed during the past fifteen years, although not all were intended to address the problem of eutrophication. Not surprisingly, however, the number of publications on eutrophication modeling is enormous, and again for the purposes of this review it is possible only to sketch the frontiers of progress in certain directions. In terms of spatial scale, clearly the largest of all lake systems, Lake Baikal, USSR (Menshutkin *et al.*, 1980; Paul *et al.*, 1980) and the North American Great Lakes (e.g. Thomann *et al.*, 1979; Di Toro and Matystik, 1980; Bierman *et al.*, 1980), present no barriers, in principle, to the application of detailed models. Along the ecological dimension, it is customary to consider in detail the phosphorous and nitrogenous nutrient cycles (e.g. Leonov, 1980a, b), these generally being regarded as critical factors for phytoplankton growth. However, the carbon (Canada Centre for Inland Waters, 1979) and silicon cycles (Bierman *et al.*, 1980) have also been simulated, but much less frequently. In terms of the greatest degree of ecological complexity, the model of Chen and Smith (1979) must surely be able to claim pre-eminence. Their model differentiates ecological detail into 15 classes of substances with subdivision of the phytoplankton, zooplankton, and fish classes into multiple groups, where the fish are considered to have three life-stages. Moreover, it resolves the spatial variability of the lake's behavior into 715 surface areal elements and seven vertical layers, and simulates temporal variations on a day-to-day basis. On a plot of the degrees of resolution in the three dimensions of spatial, temporal, and ecological detail such a model would stand far from the origin.

From the point of view of model structure identification and estimation, the studies of the Canada Centre for Inland Waters (1979) on Lake Ontario and of Scavia (1980a), Di Toro and van Straten (1979), and Jørgensen *et al.* (1981) are among some of the more sophisticated analyses. The work of Scavia and colleagues (Scavia, 1980a; Scavia *et al.*, 1981a, b), and similarly of Fedra *et al.* (1981), is indicative of recent advances in the analysis of uncertainty and prediction error propagation.

Against such a massive effort applied to model development, the application of these models to the resolution of management issues appears somewhat humble. Most such studies have generally assumed a forecasting horizon of about a decade under various scenarios for reduction in external phosphorus loadings (e.g. Canada Centre for Inland Waters, 1979; Thomann and Segna, 1980; Jørgensen, 1981) and have occasionally assessed potential deterioration (or recovery) of water quality over somewhat longer, 15–20-year (Di Toro and Matystik, 1980; Chapra, 1980) and 40–50-year planning horizons (Di Toro *et al.*, 1975). There are few examples, in comparison with the case of easily degradable organic wastes, of studies where a model characterizing the status of eutrophication has been embedded in a formal optimization framework for determining control policies; the work of Hughes (1982) and Somlyody (1983b) on Lake Balaton, Hungary, and the study by Chapra *et al.* (1983) of all five of the North American Great Lakes are notable exceptions. The analyses of Somlyody and Chapra *et al.* are remarkably similar: the former adopts a yearly peak chlorophyll *a* concentration as a measure of water quality and seeks to maximize improvement in water quality subject to budgetary constraints; the latter takes total phosphorus concentration as its measure and looks for a minimum-cost solution to the achievement of specified water quality standards.

The task of assimilating the significance of this vast research effort is formidable and we shall, accordingly, offer but some tentative summarizing observations, first on developments of a more theoretical nature. The question of a compatible combination of hydrodynamics with ecology has been a dominant concern (as discussed in Section 2.3.2 with regard to questions of scale). O'Connor *et al.* (1976) voiced a commonly held opinion, and one already encountered in this review, when they stated that:

> The substantial difficulty in constructing models of the ecologic system is primarily related to the lack of a basic scientific set of laws on biological behavior. This is in contrast to the state-of-the-art of modeling hydrodynamic phenomena where the basic equations governing fluid are known.

Harleman reiterates the same point (Jørgensen and Harleman, 1978):

> Hydrophysical models for lakes and reservoirs are at a fairly advanced level of development in contrast to the state of ecological modeling.... One area that has received relatively little attention is the coupling between hydrophysical and ecological models.

It is revealing, therefore, to find subsequently a cautiously contradictory statement by Orlob (1981) that:

> Recently, the state-of-the-art of modeling eutrophic systems has advanced rapidly in characterizing the biodynamic behavior of lakes, perhaps even outdistancing our present capability to describe rigorously the internal circulation of natural water bodies.

Clearly, there will always be problems to be solved. Any number of topics requiring further attention can be listed – many are, for example, in Scavia (1979). However, the central question of representing the structure of algal population dynamics still remains, not unanswered, not yet entirely satisfactorily answered, but certainly partially answered in a multitude of different ways. There is an impression that here an essential element of understanding is missing: it is articulated in Straskraba's work on self-organizing phytoplankton systems (Straskraba, 1979, 1983; Radtke and Straskraba, 1980), and equally so in Fedra's (1981) paper on hypothesis testing (model structure identification) and in the resort to catastrophe theory (e.g. Kempf and van Straten, 1980). Harris (1980) has gone so far as to suggest a change of paradigm, in the sense of Kuhn (1970), for the way in which phytoplankton ecology is viewed (he also makes some fairly raw comments on models and management). There is no shortage of prior hypotheses about algal growth kinetics, although gone is the time when it was believed that increasing model complexity could be equated with closing in on the "truth". But this is certainly not to disdain the achievements of the past. In short, water quality modeling in relation to the eutrophication problem has passed through a period of rich synthesis – this becomes particularly striking, for example, on reading Scavia's (1980b) paper. There has been a phase of bringing together the many and diverse results of laboratory analyses and field studies – model development, as Bierman *et al.* (1980) state, as "a quantitative framework for organizing and interpreting experimental data". It is evident in the questions of uncertainty and verification that now is a time for critical, reflective analysis of the hypotheses assembled during the phase of synthesis.

Compared with the subject of easily degradable organic wastes, eutrophication appears as a substantially more complex and difficult problem. There are more open questions regarding understanding; a less obviously regular and robust relationship between discharged wastes and observed environmental response; a much stronger influence on this response from input disturbing factors (solar radiation, temperature) that cannot be manipulated; the technically feasible regulatory actions are likely to involve a wider sector of the institutional structure of society (e.g. those that affect land-use practices); and, if all else is considered inadequate (and if one is particularly pessimistic), there is no such broadly accepted position of retreat equivalent to the Streeter–Phelps model. Judged in the same terms as earlier, the sophistication of many of the models of the eutrophication process (e.g. Chen and Smith, 1979) must be seen as quite incompatible with management's relatively crude capacities for monitoring and regulatory action. It cannot be assumed that reducing point and (much less easily) nonpoint discharges of phosphorus loads will bring about persistently reduced magnitudes of algal blooms, as it could that a reduction in BOD loads would lead to consistently better regimes of stream DO concentrations.

Thus, how relevant has modeling been to the management of eutrophication, and what success has management achieved? The report on the Canada Centre for Inland Waters (1979) study of Lake Ontario presents one of the more thorough and lucid responses to the first of these questions (see also Simons and Lam, 1980). It concludes as follows:

> The major gaps in our knowledge, be it primary production or hydrodynamic circulation, are still to be addressed by highly specialized disciplinary research. In recent years, computer modeling has developed into a powerful and exciting addition to the more conventional sciences, but the immediate practical benefits with regard to environmental management may have been somewhat oversold.

It admits a negative response, although this does not have to be interpreted as a more general conclusion. Such pessimism would not be shared by Sonzogni and Heidtke (1980), nor does it have to be shared on behalf of management *irrespective* of modeling. The same report from the Canada Centre for Inland Waters notes, significantly, that for Lake Ontario:

> Both the phosphorus and the phytoplankton levels appear to have peaked around 1970 to 1971 and display statistically significant decreasing trends since that time .... It appears, therefore, that the combination of improved sewage treatment and the ban on phosphorus in detergents has resulted in a significant decrease of concentrations in the lake.

The "success" of these measures is reiterated by Chapra (1980), although he points out the potential difficulties of distinguishing between the effects due to natural variability and those resulting from management activities. The possibility for similar ambiguities is also evident in cases reported by Fedra (1980b) and Jørgensen *et al.* (1978).

If, however, there has been success in the management of eutrophication, can it be seen to have been associated with modeling? Chapra's (1980) analysis for Lake Ontario suggests that "success" can be attributed to legislation passed early in the 1970s, a time at which the associated developments in modeling had just begun. And in 1975, the Committee on Public Works and Transportation of the US House of Representatives, in reviewing the effects of the 1972 amendments to the Federal Water Pollution Control Act (as embodied in Public Law 92-500), reported that:

> where [improved water quality] is being achieved, along Lake Erie beaches, in the Hudson River, the Willamette River, and other lakes and streams, it is the result of earlier state and federal legislation, and particularly the 1965 Federal Act. [Committee on Public Works and Transportation of the US House of Representatives, 1975]

It is time to assess not only the dynamics of the response of water quality to the manipulation of waste inputs, but also the dynamics of the institutional processes whereby action is implemented in response to a perceived problem.

Let us suppose the tentative conclusion can be made from the quote above that it takes roughly 10 years from the drawing up of legislation to an observable response in the (natural) system. This time constant would cover partly the responses of both the institutional and natural processes. It has been observed elsewhere that it takes between seven and 11 years from conception through approval to the completed construction of a treatment plant (Water Pollution Control Federation, 1981). There are other cycles, and parts of cycles, for monitoring and for analysis (the experiment → identification → prediction cycle), all of which are unlikely to have characteristic dynamics that are much faster in their responses. Now let us make a rather strong assertion and gross simplification that the institutional and natural dynamics of water quality management have the following logical sequence:

(i) perception of problem (monitoring, and some analysis);

(ii) drawing up of legislation, setting of objectives, and reorganization of appropriate institutional structure, where necessary (some further analysis);

(iii) elaboration of course of action, construction of facilities for monitoring and control (yet more analysis);

(iv) natural response of water body to actions taken.

In this light, the question of the usefulness of models to eutrophication management must appear to be premature. Or, at least in comparison with the problem of easily degradable organic wastes, the relative "youth" of the (perceived) eutrophication problem and the relatively large aggregate period of time required to follow through the causal chain of the above assertion combine to reduce the possibility of making an informed judgment at this time. Again, however, it is important to note the distinction between the time at which the use of a model influences the making of a policy and the subsequent association of success with that policy. The long time lag between almost any modeling exercise and a discernible response in practice must surely lower the probability, especially in the absence of careful retrospective analysis, of being able to relate the success of management unambiguously to the influence of modeling.

3.5 THE NITRATE PROBLEM

While the OECD article quoted earlier (OECD, 1979) saw an improving status in the management of easily degradable organic wastes, it observed that pollution by nitrogen (and phosphorus) compounds was a cause for increasing concern and drew particular attention to the rising concentrations of nitrates in several West European rivers. Whether the nitrate problem is really a "problem" – and whether it might more appropriately be labeled a nitrogen cycle problem – is a question that has attracted much discussion (e.g. Shuval, 1980; Zwirnmann, 1982; Royal Society, 1983). It is undoubtedly, however, an interesting problem, especially from the points of view of problem succession, problem perception, and problem interaction:

(1) It has emerged from and succeeded the problem of easily degradable organic wastes (e.g. in the Thames and Bedford Ouse Rivers in the UK: Whitehead *et al.*, 1981b; Whitehead and Williams, 1982; Blake, 1982).

(2) There is a growing awareness that not only is nitrate associated with methaemoglobinaemia but also "new scientific evidence is becoming available concerning the formation of carcinogenic nitrosamines" (Shuval, 1980), which assures it a future as a toxic or micropollutant problem, if not as a nitrate problem.

(3) It cannot necessarily be isolated either from the problem of easily degradable organic wastes – in fact, producing nitrate in waste-water treatment can be seen to be beneficial for the management of that (earlier) problem – or from the problem of eutrophication, or from the toxicity problems of ammonium-N discharges (Boner and Furland, 1982) (some of the reasons for this will be discussed later and have also been discussed elsewhere (Beck, 1981b)).

This last point, in particular, emphasizes the limitations in classifying pollution problems as distinct, although the strong association of the nitrate problem with groundwater systems makes it a problem worthy of independence.

The nitrate problem seems to have been identified as such, or as a problem requiring urgent action, during the 1970s. It is a relatively recent problem, a contemporary even of modeling, although the origins of its causes can be traced much further back (e.g. Onstad and Blake, 1980; Sexton and Onstad, 1980); it is, moreover, a problem restricted to specific regions with certain climatic characteristics (Golubev, 1980). Not surprisingly, therefore, the research effort allocated to it, as a problem of water quality modeling, is not nearly as great as that given to the study of easily degradable organic wastes and eutrophication. This review will accordingly be restricted to a brief discussion of a small sample of case studies.

There are two separate historical lines of development for modeling associated with the nitrate problem. One, as already suggested, was foreshadowed in O'Connor's (1967) concern with nitrogenous BOD in river systems (see also Garland, 1978), and has subsequently developed through more detailed considerations of nitrification and the nitrogen cycle as a whole (Thomann *et al.*, 1974a, b; Najarian and Harleman, 1977), although latterly such interest has been quite specifically focused on eutrophication problems in estuaries. These developments represent the scientific basis for the current work rather than reflecting its problem orientation. The second line of development has been exclusively concerned with nitrate pollution of groundwater systems. In this case, developments have been clearly stimulated by the problem, with attention focusing on the purely physical movement of dissolved nitrate through the unsaturated and saturated zones of the system (e.g. Mercado, 1976, 1980; Oakes *et al.*, 1981; Oakes, 1982). It is perhaps counterintuitive to imagine that these two conceptually distinct themes – at least in their polar extremes of resolution along the ecological dimension – should find a natural point of convergence. However, the surface- and groundwater characteristics and problems of the Thames River basin provide just such a natural focus and are the subject of a major case study (Thomson, 1979; Sexton and Onstad, 1980; Whitehead *et al.*, 1981b; Blake, 1982).

Altogether, the impression is one of a balanced development of models for application to the nitrate problem. The models range, as we have seen, from the partial differential equations of solute transport through to the simple linear algebraic constraint equations in the formulation of optimization problems for land-use planning (Moosburner and Wood, 1980) and for blending operations with nitrate-rich waters intended for potable supply (Jowitt, 1984). The problem is extensive in character, and the models have had to follow the contours of the problem, rather than being a problem of intensive character (such as the kinetics of phytoplankton growth) where model developments might have followed disciplinary contours.

It has already been argued in the preceding section that the question of the usefulness of modeling to management is premature. If this argument is valid for the eutrophication problem, it is even more so, except in two important respects, for the nitrate problem. The natural response time of aquifer systems is long, comparable to, and often longer than that of large lakes. Mercado (1980), for example, in his study of the coastal aquifer of Israel, is concerned with a forecasting horizon of 50 years from 1970 to 2020. Oakes (1982), reporting on studies of Triassic sandstone and chalk catchments in the United Kingdom, has computed changes in water quality over three centuries from 1800 to 2100.

Our two reservations about the prematurity of determining the usefulness of models to management are as follows. First, for the Thames study it is pertinent to note that:

(i) the authority responsible for management took and retains the initiative for model development; and

(ii) unlike the earlier study of easily degradable organic wastes in the Trent River (see Section 3.3 and Woodward, 1980), no major reorganization of the institutional framework for implementing control is expected in the near future.

Both points augur well for the use of models in influencing the making of a decision. Second, as clearly apparent in the Thames study (Sexton and Onstad, 1980; Blake, 1982) and as evident in the introduction and operation of a telemetered monitoring network for the Bedford Ouse River, UK (Whitehead *et al.*, 1981a, b; Caddy and Whitehead, 1981; Whitehead and Caddy, 1982), the nitrate problem is also a problem of high-frequency, short-term variations that influence markedly the reliability of potable water supplies. The accompanying use of models in decision support systems for day-to-day operational water quality management may well place the nitrate problem at the leading edge of a response to the critical question we have posed for this review.

With regard to the problems that have preceded, management of the nitrate problem, with point and nonpoint sources to be controlled and potable water supplies to be protected, can be viewed as essentially similar to management of the eutrophication problem. But the separation of the time scales relevant to management, with their respective associations with long-term planning and short-term operation (and equally, planning for contingencies), makes the nitrate problem, for reasons that will become clear, a better topic for discussion in an agenda of problems for the future (Section 4).

3.6 TOXICS

In complete contrast to the nitrate problem, where attention is focused more or less on one substance alone, the toxics problem covers an enormous range of substances. Because, therefore, of the heterogeneity of substances and problems that may be called "toxic" (especially under our loose heading), and because of the relative newness of the research effort applied to this topic, it hardly seems reasonable to look for strong and distinct lines of historical development. There are, nevertheless, certain themes that characterize the admixture of current studies and thus afford a basis for a review:

(i) a distinct separation of the time scales of interest;

(ii) determination of the *aggregate* relative importance of mechanisms governing ambient concentrations of substances and of routes to the bioaccumulation of substances in organisms;

(iii) the partitioning of the substance between water and sediments.

First, however, it is important to clarify the issues for management. Let us recall, therefore, the two input–output couples that stand at the apex of any strategy for water quality management (Section 3.1). For the toxics problem the first such couple expresses the relationship between a waste input and the resulting ambient concentration of the contaminant in the receiving water body. In theory, if for the moment we are not considering the exposure of a human population, its output describes everything about the "environment" of an organism in this water body; the model of Lassiter *et al.* (1978), for example, is addressed to this first couple. The second input–output couple relates the response of the organism, as measured by mortality or the concentration of the contaminant in certain tissues, to the conditions of its "environment". Typical of a model that concerns itself with the simulation of this second couple alone is the work of Norstrom *et al.* (1976). There are other models, of course, that cut across these distinctions, included among which is one of the prototype studies in the field (Harrison *et al.*, 1970). The clarity with which the preceding pollution problems have been dealt with stems in part from the assumption that knowledge of the second input–output couple (including, for example, that public health effects are irrelevant) has allowed *relatively* clear targets to be set for the regulation of waste inputs. This assumption cannot (as yet) be made for the toxics problem. The consequences are targets of complete elimination of the discharge of certain substances (in which case modeling is not a relevant matter); conservative but "unattainably" stringent targets; or simply uncertain targets. Quite apart from the uncertainty in understanding the first input–output couple, it is therefore *changes* in the knowledge of the second couple that will influence significantly the ways in which management of the first couple can be approached. A second distinctive feature of the toxics problem is the shift of emphasis toward pollutants of industrial origin, and the need to consider not only present-day pollutants but also categories of pollutants not yet released into the environment (Lassiter *et al.*, 1978). The problem of prediction assumes, therefore, a new dimension. The issue of testing and registering the properties of the myriad pertinent chemicals is itself a severe problem of management (Sharefkin, 1982). And given this explosive growth in the variety of chemicals that might have to be monitored, in particular for the operational protection of water supply intakes, it is not surprising to see a growing literature on the need to deploy biological monitors providing an *integrative* response to a multitude of possible disturbances of ambient water quality (Wallwork, 1980; Montgomery, 1980; Lee and Jones, 1983; van Belle and Hughes, 1983).

The steady discharge of a small amount of a toxic substance and its related equilibrium distribution in an aquatic ecosystem are quite a different problem of management from that of the sudden, accidental discharge of a large amount of the same substance in a matter of minutes. The time scales of interest are fundamentally different. For example, the studies of Lam *et al.* (1976), Orlob *et al.* (1980), Voss *et al.* (1981), and Chapman (1982) are all concerned with accidental spillages of substances and subsequent pollutant plume transport and dispersion; the *transient* evolution of the plume is of critical importance. The models are straightforward adaptations of the classical advection–dispersion equations for conservative substances, with some accounting for metal-ion complexation with dissolved organic matter or suspended solids (Orlob *et al.*, 1980) and for precipitation, sedimentation, and redissolution (Chapman, 1982). Essentially the resolution of ecological detail is nil, although the effects of a given pollutant concentration may be translated through simple empirical relationships to the quantification of levels of fish mortality and reduction in primary production (Lam *et al.*, 1976). The resolution of temporal detail is very high: at the extreme, of the order of minutes (Chapman, 1982).

At the other extreme, the behavior of the system can be considered to be invariant with time; rather, the steady-state solution for "advection and dispersion" of the pollutant along an ecological continuum is the behavior of interest, as discussed earlier and as so aptly described by Thomann (1978, 1979). In this case, the overall thrust in the development of models has been to gain insight into the aggregate functioning of the system (to be able to connect the levers of policy to the response of the system), and to determine for specific examples (PCB, lead, and cesium) the relative balance between direct ingestion of contaminated water and food-chain transfer as the routes to bioaccumulation of toxicants in top predators (Thomann, 1979, 1981). These are components of the second theme of this review of the toxics problem. The basis for these models clearly has its origin in the compartmental ecosystem models that were being developed during the early 1970s; the point of transition is marked in the analysis by Thomann *et al.* (1974b) of the distribution of cadmium in western Lake Erie (the model by Park *et al.* (1980) has similar conceptual origins). In much the same spirit of seeking insight through the simplifying assumption of steady-state behavior, Schwarzenbach and Imboden (1984) have studied the relative importance of mixing characteristics and of transfer/reaction kinetics (for gas exchange, sorption/desorption, hydrolysis, and photolysis) in determining spatial concentration patterns of hydrophobic organic pollutants in lakes (in this case, however, with no reference to the consequences of biological uptake).

The third theme of the review, to which we have alluded in the review of easily degradable organic wastes (Figure 11), concerns partitioning of the toxic substance between water and sediments. Illustrative of this less distinct theme are Somlyody's (1978) analysis of cadmium distribution in the Sajo River, Hungary (see also Somlyody, 1982b), and two papers by O'Connor *et al.* (1983) and Halfon (1984), both of which are studies of the clearance of persistent chemicals (respectively, Kepone and mirex) from an aquatic environment following cessation of their manufacture and discharge. (Schnoor and McAvoy's (1981) study of dieldrin clearance from a reservoir following a ban on pesticide application is of a similar character.) The model for the estuarine problem studied by O'Connor *et al.* employs a detailed description of bed-sediment transport – the bed being separated conceptually into a transport layer and a stationary component – and of contaminant diffusion between the overlying water column and the interstitial waters of the sediment layers. Halfon's model, while being less detailed in its account of transport factors, postulates three states in which the pollutant can be found in the sediment bed: in the interstitial water, adsorbed on the sediment particles, and in benthic organisms. This model can claim the unchallenged distinction of a prediction horizon of four millennia, which, juxtaposed with the transients of the order of minutes in Chapman's (1982) study, demonstrates dramatically the differences in the types of problem addressed under the heading, "toxics".

To impose any further order on such an immature and heterogeneous problem area would be artificial. Only a few isolated references to the use of models for management and for prediction of the consequences of regulatory action can be quoted (Mercado, 1980; Schnoor and McAvoy, 1981; Somlyody, 1982b). Of these, Mercado's analysis of the accumulation of heavy metals in the coastal aquifer of Israel is probably the most comprehensive. The problem he addresses is due to the land application of sewage reclaimed for the purposes of spray irrigation and the use of the aquifer for potable supply. Mercado's form of solution is to map out the degrees of treatment required for the sewage as a function of the spatial location at which the sewage is applied above the aquifer. Beyond this, however, Schnoor and McAvoy (1981) note that the results of their study regarding declining dieldrin residue levels "aided" the local conservation commission in its decision to lift a ban on commercial fishing – a rare statement indeed for the whole of this review. In short, the development (and application) of models for the toxics problem awaits its period of synthesis. Its immaturity, debilitating lack of quantitative data, and the concern for distinguishing among the relative significances of multiple hypotheses on the key mechanisms of behavior, would all seem to make it well matched to the character of speculative simulation modeling (Section 2.4.2). As new evidence is assembled it can be expected that the collective toxics problem will be subdivided and reorganized as the issues themselves, such as the effects of acid precipitation (Haines, 1981; Christophersen *et al.*, 1982), are perceived, or demand to be recognized, as new pollution problem categories in their own right.

4 AN AGENDA OF PROBLEMS FOR THE FUTURE

Past trends having been examined, there are two traditional aspects of prediction that will help define an agenda, albeit speculative, of problems for the future. For example, interpolation is a conventional way of specifying what is needed to cover any outstanding gaps in past achievements, and extrapolation suggests what would follow from the trends already established. These represent essentially "smooth" developments in a subject. For instance, the growth of interest in the problems of impounded river sections, which represent a convergence of river-like and lake-like problems, is a fairly predictable development. It is obvious that new pollution problems will emerge, but this does not mean that modeling for the purposes of solving these problems will be conducted in any radically different fashion. That is to say, the pollution problems may have different physical, chemical, and biological attributes, but it is hard to imagine that the procedure of model development would be radically different from that of Figures 6 and 7 or that the models developed would be essentially different from that of Table 1. Indeed, as with all matters of prediction, it is just as difficult (if not impossible) to speculate about significantly abrupt changes in the development of a subject as it is to predict abrupt changes in the behavior of a system.

Let us summarize some of the trends identified in this review. (Other trends have been commented upon by O'Connor (1982) and Orlob (1983a).) At the core of the strategies for managing water quality there has been a shift away from determinism toward the statement of water quality standards in probabilistic terms (Ward and Loftis, 1983); and even beyond this, there is now a movement toward the use of fuzzy logic for such purposes (Jowitt and Lumbers, 1982). A similar trend is clearly apparent in the prevailing views on model development, as already emphasized in Section 2. The technology of water quality management has also changed dramatically in the past 10–15 years, these changes being especially notable in the areas of instrumentation, computing, and automation (e.g. *Water Science and Technology*, 1981; Institution of Water Engineers and Scientists, 1981). The trend is, most significantly, toward a much higher frequency of sampling of water quality measurements (as well as the detection of pollutants at ever lower concentrations). Again, we have already alluded to the effects of this trend on the *a posteriori* steps in model development (Section 2.4.3). A third trend, which is inextricably interwoven with these changes in policy and technology, is discernible as a steady expansion in the time scales of interest as the problems progress from the concern with easily degradable organic wastes, through eutrophication and the nitrate problem, to the discharge of toxic substances. Streeter and Phelps's (1925) analysis was not *explicitly* concerned with changes with time; the study of eutrophication, as Simons and Lam (1980) note, focused on seasonal and longer-term (decade) dynamics; the nitrate problem has generated interest in behavior over periods of hours (Whitehead, 1980) and centuries (Oakes, 1982); and the culmination of this trend are the analyses of Chapman (1982) and Halfon (1983) referring, respectively, to time scales of minutes and millennia for problems associated with the fate of toxic materials in aquatic environments.

A fourth observation, which refers not to a trend but to the gaps in past studies, is that of all the questions that could have been asked of proposed strategies for management, one alone (is the solution economically optimal?) has claimed an arguably disproportionate amount of attention. Systematic studies of management have rested largely on a strategy of longer-term planning, leaving shorter-term operational aspects to the *ad hoc* accumulation of scattered empirical experience (Beck, 1981b). And finally, another observation: the urban, industrial, and agricultural developments in river basins continue (almost) unabated. Water is of necessity used more *intensively* and the activities affecting and affected by water quality increase in number; the intensively used water resource systems of Israel (Shuval, 1980) and the Thames River basin in England (Blake, 1982) mark points well along the scale of development. It is a truism that life becomes more complex.

It is the purpose of this section to pick out from this macroscopic mesh of trends and observations a few salient themes that may be indicative of the directions of research in the near future. In this our primary concern will be with changes in the issues of management, although we shall begin with a question of method.*

4.1 ANALYZING ACCEPTABLE FUTURE BEHAVIOR

Two contemporary questions to which the application of models for water quality management has been addressed can be paraphrased as:

> *Contemporary question (1):* Given a model of the response of the system (lake, stream, etc.) to changes in a set of decision variables, *and* a model of the costs/benefits associated with these decision variables, determine (according to some criterion) an optimal course of action (set of decisions).
>
> *Contemporary question (2):* Given a contemplated course of action (a set of changed inputs or model parameter values, for example) and a knowledge of the present state of the system, determine the response of the system in the future.

The motivation and direction of these questions assume that, in a sense, a uniquely optimal course of action exists and the attributes of nonoptimal solutions are intrinsically not of interest, and that one starts from knowledge of the present in order to state something about the future.

Such questions will always be of interest, but they are not the only way of examining what might happen in the future. Consider, for example, the following opportunities facilitated by the conceptual framework of speculative simulation modeling:

*A more detailed statement of possible future developments with respect to problems of system identification and the analysis of uncertainty is given elsewhere (Beck, 1984).

Revised question (1): Given a definition of future acceptable (B) and unacceptable ($\bar{B}$) behavior and a model (subject to uncertainty), determine which changes of inputs and model parameter values (broad courses of action) lead to either class of behavior.

Revised question (2): Given a definition of future essentially similar (B) and radically different ($\bar{B}$) behavior and a model (subject to uncertainty), determine a response equivalent to that of revised question (1).

In contrast, these revised questions do not assume a unique course of action. Rather, they are based on the idea of a broad range of actions, or at least, for example, a broad range of performance once the control facilities have been put into practice – actual performance is rarely identical with planned performance. Just as with the analysis of past behavior, there is no assumption of the notion of a degree of closeness to a "best" solution. The objective of the associated analysis is two-sided, in the sense that the causes of both acceptable (essentially similar) and unacceptable (radically different) future behavior are intrinsically of interest. Lastly, we note that these revised questions start by stating something about the future and move backwards, as it were, to an examination of whether such a future is "reachable" from the present, given the uncertainties of present knowledge.

There is perhaps nothing new about these questions, and Spear and Hornberger (1983) have themselves already recognized this same potential of their approach in process control system design. Nevertheless, they open up ways of looking at the "acceptability" and "stability" of proposed management strategies and even of approaching the problem of speculating about whether abrupt changes of behavior are likely to be induced. In this review the use of models for assessing the consequences of major civil engineering projects has not been discussed, but the potential of the revised questions as vehicles for addressing such problems is considerable. The approach is simple and flexible, as pointed out earlier, and there is undoubtedly uncertainty about the way in which a proposed reservoir project, for instance, will affect the aquatic ecology and water quality of a river basin. The complexity of the future behavior definition, which reflects the complexity of the problem at hand, does not deny the simplicity of the mechanics of deriving a solution. The difficulty lies precisely in defining a suitable model structure, into which it would be necessary to parameterize the design features of the project, and in defining the expected behavior of interest, which would be required to map out all the desirable and undesirable consequences of the project.

4.2 INTERACTIONS

The "linear" classification of independent pollution problems, as in Figure 1 and Section 3, is clearly a distorting simplification. It is easy to argue that interactions among the problems and the facilities for their management are significant, have been underestimated in the past, and are likely to be much more important in the future. Let us take as a good example the nitrate or, more appropriately here, nitrogen-cycle problem.

Ammonium-N can be removed, and nitrate-N produced, at a cost, during wastewater treatment; both can be dissipated, and nitrate produced, within the receiving water body; and both ammonium and nitrate can be removed, or diluted in the case of nitrate, and at a cost, during the purification of water abstracted for potable supply. The decision to nitrify, and possibly to nitrify/denitrify, a waste discharge affects the removal of easily degradable oxygen-demanding organic materials. The regulation of eutrophication through phosphorus removal can be nullified, as indeed it has been, by the release of phosphorus from in-lake sediments under anaerobic conditions arising from the settling and oxidation of particulate matter from a non-nitrified effluent discharge. The variability of in-stream nitrate concentrations in some river basins, such as the Thames, is a function of a longer-term trend due to the base flow deriving from groundwater and of shorter-term fluctuations deriving from precipitation/surface runoff events and treatment plant activities (as in Figure 12). To summarize, there are in fact a number of interactions to be considered:

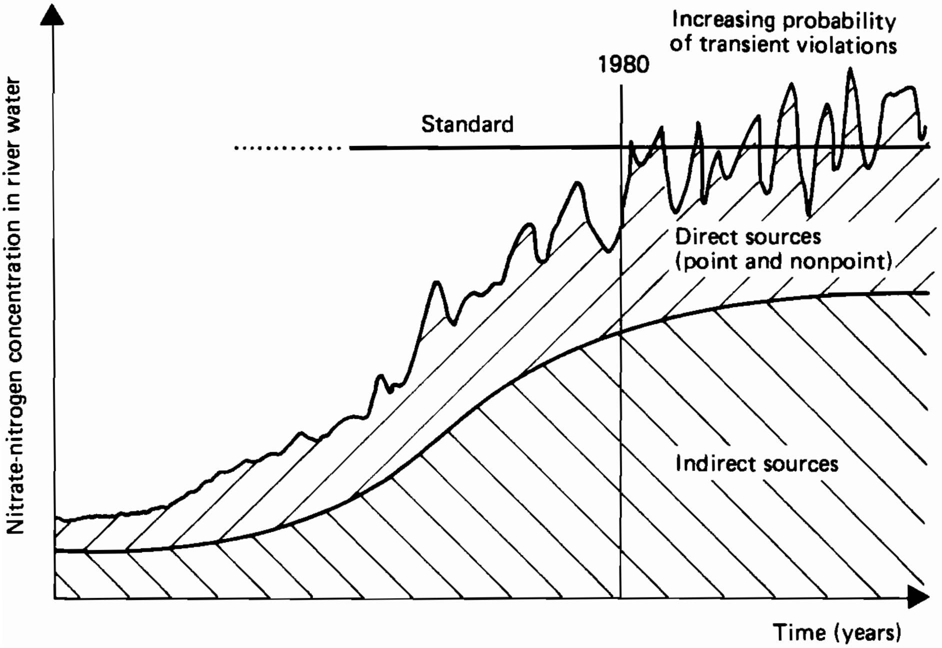

FIGURE 12 Long- and short-term changes in river nitrate-nitrogen concentration, showing the increasing probability of transient violations of standards (e.g. World Health Organization, 1970). The long-term trend is due to "indirect" sources of nitrate transported via aquifer systems; the short-term variability is due to local surface runoff and treatment plant activities.

(1) The costs and benefits of managing one pollution problem cannot be separated from the costs and benefits of managing the other pollution problems.

(2) The costs of solving a single problem depend upon an interplay between manipulations of the first and second input–output couples of the management strategy (or, more straightforwardly, costs can be balanced over removal of the waste before discharge, its assimilation in the environment, or its removal prior to consumption).

(3) The "technologies" of pollutant removal are interactive.

(4) There are interactions between the components of management intended for regulation of the long- and short-term variability of pollutant concentrations – in other words, design–operation interactions are important.

Again, there is nothing particularly novel about these observations, although certainly points (2) and (4) are quite different in perspective from the classical problems associated with the management of easily degradable organic wastes. There have been few studies, if any, of *joint* cost minimization of wastewater treatment and water purification facilities, because the treatment of easily degradable organic wastes and their effects on in-stream DO concentrations are not critical determinants of the suitability of a water source for potable consumption. And there have been few studies of the trade-offs between changing treatment plant design and construction and/or adapting plant operating schemes, because until recently the latter was thought to be neither necessary nor feasible (Beck, 1981b). In these respects, the work of Herbay *et al.* (1983) is an important first step in translating the framework for economic analysis in water quality management from a preoccupation with planning to a more balanced assessment of the costs of both construction and operation. The key questions for water quality management in the future will perhaps center less on determining how much more waste to treat and more on how to treat it differently. When more than one type of pollutant is to be removed from a waste discharge, it is unlikely that all classes of pollutants can be removed at maximum efficiency, and trade-offs among operations at less than maximum efficiencies will need to be evaluated.

4.3 TIME, CONTINGENCIES, AND THE CHANGING CHARACTER OF POLLUTION PROBLEMS

In the introduction to Section 4 a special point was made of the shifting focus in the time scales of concern in the management of the different pollution problems. The problems of water pollution control do not simply alter the focus of attention from one category of pollutants to another; the changes are more subtle and perhaps more fundamental.

In 1979, a report of the Organization for Economic Cooperation and Development (OECD, 1979) concluded that water quality in the rivers and lakes of several industrialized nations was observed to be improving. Of course, such a statement must be qualified by adding that it was water quality as gauged by *average* (equilibrium) levels of (in this instance) suspended solids and easily degradable organic matter that was improving. Thus, precisely because of past success in management there is now a greater responsibility to prevent failures in the system of pollution control. A greater number of (more sophisticated) treatment facilities need to be operated in order to maintain the control effort and therefore, in absolute terms, there is a greater probability of failure. Any failure, or transient pollution event, will moreover be readily noticed in a river restored to a good average quality; and in an intensively used system a failure in one component is more likely to affect adversely the performance of other parts of the system. The transient and damaging effects of accidental spillages or extreme meteorological events would hardly have been noticeable, and therefore not an issue of management, under conditions in the past where receiving water bodies were, on average, heavily polluted (as depicted by Figure 13). It is as though water quality management has created for itself (quantitative) hydrology's classic problem of the flood: what is of concern is not merely the average, equilibrium water quality to be achieved in the future but also the probabilities and magnitudes of fluctuations about this equilibrium level. Whereas studies were once conducted with the assumption of, say, an average low-flow condition, which *a priori* removes transient meteorological conditions from consideration, the need to distinguish between the controllable and uncontrollable (e.g. meteorological) input contributions to the variability of water quality is likely to become more apparent (as indeed pointed out by Ward and Loftis, 1983). For example, in a 1980 survey of the state of river quality in England and Wales, the National Water Council (1981a) observed that, on the positive side, "The principal reason for improvements [since 1975] ... is investment in new

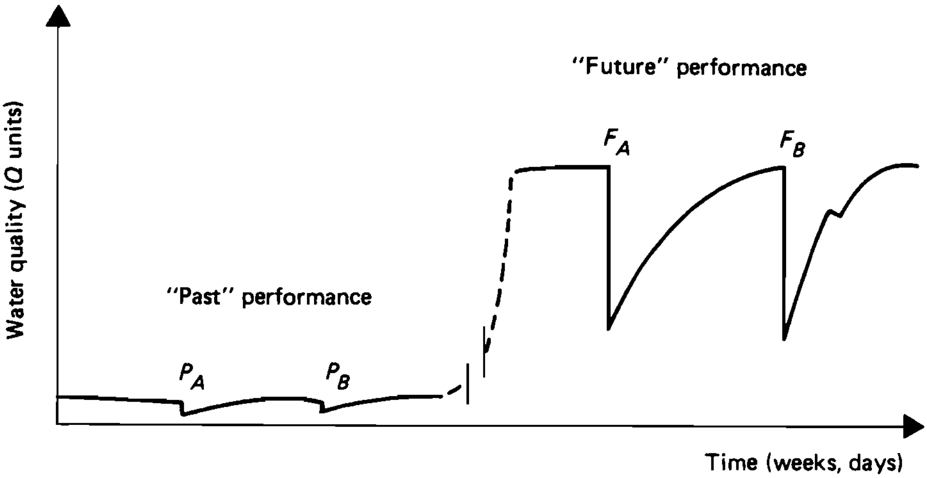

FIGURE 13 Past (P) and future (F) performance in water quality management, where P_A, P_B, F_A, and F_B represent transient pollution events against relative background, average, or "equilibrium" conditions.

and extended sewage treatment works and trunk sewers." On the negative side, however, it was observed that "Weather is significant for water quality in that rain can provide greater dilution of effluents but it can also increase the diffused pollution from urban runoff and land drainage."

In short, the point is that management sees it necessary to address itself explicitly to managing variations of water quality in time and not implicitly, as it was doing, to regulation "once and for all time". This has ramifications at several levels. It involves planning for the implementation of seasonal waste treatment policies and planning for protection against contingencies; and it involves subsequent operation on a seasonal basis in a context where contingencies can, and will, occur. Yet again there is nothing surprisingly new about this. Seasonal management policies have long been advocated, as already mentioned in Section 3.3 (Thomann *et al.*, 1968; Lettenmaier and Burges, 1975); perhaps it is rather that the time is now ripe for such policies and the analysis they require (Water Pollution Control Federation, 1981; National Water Council, 1981b; Cockburn and Furley, 1981; Boner and Furland, 1982; Kuchenrither *et al.*, 1983). The problems of protecting water supply abstractions from the effects of transient pollutions are widely appreciated (Wallwork, 1980; Caddy and Whitehead, 1981; Whitehead and Caddy, 1982) and there is a growing interest in the degradation of water quality by stormwater overflows (Cockburn and Furley, 1981; Ferrara and Hildick-Smith, 1982). Such changes of outlook are quite consistent with the general movement toward the notion of variability of performance that is captured in probabilistic standards for water quality.

The implications for the development and application of models are less self-evident. They suggest that, for example:

(1) Compact, simple dynamic models (especially in a discrete-time, difference-equation format) may be used in decision support systems for *operational* management (e.g. Whitehead and Caddy, 1982).

(2) Wastewater treatment plants may need to be operated in a manner that seeks to attenuate both within-plant disturbances (a traditional objective) and within-river disturbances; changing priorities for the control of in-stream quality may necessitate the switching of treatment plant operations among substantially different modes. In other words, the analysis of such problems may require the *combination* of dynamic models for treatment processes and in-stream processes (Jowitt *et al.*, 1984); and the assumption of waste discharge characteristics as essentially exogenous input variables may no longer suffice to resolve some of these issues.

(3) A new aspect of analysis will be the design of management strategies that attempt to alter in some way the (probability) distributions of pollution event *durations*, i.e. the periods for which certain critical concentrations of pollutants are exceeded. For instance, in the scenario of Figure 12 one would be concerned to know not only how high a peak nitrate concentration might be, but also for how long it would exceed the World Health Organization limit.

4.4 HISTORICAL ANALYSIS

It is perhaps paradoxical in an agenda of problems for the future to propose a careful analysis of the past. But *if* one is really concerned with the question of the usefulness of modeling to management, the slow dynamics of management (of which we have earlier made mention) demand the observation of research and development activities over a long period of time. Thomann (1982) has similarly remarked on the need for "post-auditing of models after environmental control procedures [have been] implemented". However, certain aspects of the nature of research funding and technological development are not favorable to the historian of water quality modeling and management. The innovation of new technology – in particular, the influence of new electronic engineering devices in the water industry on the capacity to observe and to collect data – would seem to stimulate a much greater potential to perceive even more problems. This potential, coupled with a highly adaptive research-funding mechanism (that the scientist should work on relevant, contemporary problems), increases the possibility of attention being shifted away from the "old" problems before it can be established whether they have been solved. But unfavorable though these developments may be to the carrying out of historical analysis, they in fact make it all the more urgent because of the widening gap between the rates of problem "discovery" and "resolution".

5 CONCLUSIONS

This review has cut across the field of water quality modeling and management in two directions: from the perspective of methodological developments (Section 2); and from the perspective of the issues of management and the evolving succession and interaction of these issues (Sections 3 and 4).

In the very broadest of terms, brute computing power is now rarely an overriding constraint. The analyst can enjoy considerable freedom and flexibility in the formulation and solution of his problems. Contemporary changes in the style of computing will also have a profound effect on the way models can be used in practical decision support systems. Flexible, modular sets of linked simulation models may well become commonplace, although so far they have not been widely developed; another growth area may be the incorporation of models in operational forecasting and control activities.

Such a positive view of the future, however, does not mean that the development and application of water quality models are without constraints. The mood of uncertainty, which has come to dominate the outlook of the subject, has brought about a rethinking at several levels: in the philosophical basis for model building; in the basis for standard setting and monitoring; and in the interpretation of results from the application of models. From this last point, in particular, have emerged a number of pragmatic considerations on the use of models for management purposes. For example:

(i) the results from a comprehensive, highly refined model might be so copious as to be incomprehensible to the analyst without some form of aggregation;

(ii) the detail of the model is not compatible with current monitoring and data retrieval capabilities; or

(iii) again, the detail of the model is inconsistent with the relatively crudely effective policy options available to management.

Particularly the second of these considerations has been sharply illuminated by the modest progress in evaluating water quality models by reference to *in situ* field data. There will always be a gap in any area of study between the leading edge of the theories (models) postulated and the experiments subsequently designed to test these theories. A principal reason for the present concern with the analysis of uncertainty is that the trend of the early 1970s toward ever more complex models created an unacceptably large gap between "theory" and "experiment".

The general state of the subject is therefore one in which acceptable courses of action, variability of behavior, and probabilities of events are increasingly being seen to be as important as optimality, average behavior, and determinism. More specifically, the following conclusions can be drawn:

(1) *Methodological questions*. The most significant innovation of recent years has been the development of speculative simulation modeling for the preliminary analysis of possible behavior patterns when field observations are sparse. The majority of approaches to the more conventional problem of model parameter estimation (model calibration) have suffered generally from a lack of model identifiability and inadequate prior identification of model structure. While the analysis of prediction error propagation has revolved around the issue of which is the best analytical method to use, the more important questions of the connection between identification and prediction, of ambiguities in predictions, and of the fundamental nature of making predictions have been largely overlooked.

(2) *Optimal management strategies*. The application of optimization techniques, particularly for planning purposes, and for the management of easily degradable organic wastes, seems to have had a "golden age" during the decade from about 1965 onwards. What little evidence there is suggests that management has preferred to act upon the results of models used in the context of simulating the possible consequences of predefined, and therefore not necessarily optimal, courses of regulatory action. Optimization is, however, enjoying something of a revival at present.

(3) *The management of easily degradable organic wastes*. This has been dominated by the continuing success of the assumptions of Streeter and Phelps (1925), and perhaps so much so that they have risen deceptively above dispute (see, however, Beck, 1982b). One possibly significant change of emphasis in the future may be an increasing concern with intermittent pollution by stormwater overflows.

(4) *Eutrophication*. In almost all respects, eutrophication is a more difficult problem to solve than that of easily degradable organic wastes. The associated developments in modeling have been a focal point for the convergence of (scientific) disciplinary interests. It was this problem, perhaps simply because of timing, that set in motion the movement toward extremely complex hydrodynamic–ecological models for water quality. The topic is outstanding for the act of synthesis – of assembling in mathematical format a multitude of hypotheses from diverse laboratory and partial field studies – that accompanied the development of the models. But despite this, a fairly strong case can be made in favor of arguing that the central issue of characterizing the dynamics of algal populations is still not resolved.

(5) *The nitrate problem*. In contrast to eutrophication, which stimulated interaction among scientific disciplines, the nitrate problem has brought together and emphasized interactions among the various components of water resources management: aquifer systems; surface waters; wastewater treatment; water purification; long- and short-term dynamics. In this respect it is a problem that may force new directions upon the development of the subject of water quality modeling.

(6) *Toxics*. If the problem of easily degradable organic wastes can be regarded as being part of a "classical theory" of pollution control, the toxics problem will undoubtedly be a part of what may become a "modern theory". Unlike the other problems, where the effects of the discharged pollutants on the "consumption" of water resources (literally, or as public goods) were relatively clear-cut, management of the toxics problem is beset with formidable difficulties in the basic matter of quantifying the relationships among causes and effects. It appears to have benefited from the lessons learned in tackling the eutrophication problem. The early development and application of models have been marked, at least in part, by an exploitation of as many simplifying assumptions as possible in order to gain initial insight at a macroscopic level.

Finally, it is in the nature of a review that it demands distillation of the issues of the past and thoughtful speculation about the likely issues of the future. There is inevitably bias in this process, which seems to be so succinctly put in a graffito once seen in Cambridge, England:

The real issue is who is deciding what the issues are to be.

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