THE USE OF MATHEMATICAL MODELS IN THE FORMULATION OF POLLUTION CONTROL POLICIES — AN OVERVIEW

A. Gerber

National Institute for Water Research, Council for Scientific and Industrial Research, P.O. Box 395, Pretoria 0001, South Africa

ABSTRACT

The principles underlying the development of mathematical models are outlined in non-mathematical terms. Some of the advantages and limitations of computer models are highlighted, especially ways in which models may be misused. The skills required for effective modelling are sketched as are major problem areas hampering the general application of models.

KEYWORDS

Computer simulation; digital model; management model; mathematical modelling; numerical modelling; prediction model; water pollution.

INTRODUCTION

The formulation and management of pollution control policies must be practised effectively and efficiently if the best possible applications to water resources are to be realized. One of the most valuable tools available to the modern water resource manager is the computer model and any professional working in this field should adapt to and use models to be truly efficient. However, model use should be tempered by an adequate awareness of the limitations, underlying assumptions and appropriateness of the model before using it as an aid in making regulatory, management, planning or policy decisions. It therefore was considered timeous that the organisers of this conference had included in the conference programme a session on the application of mathematical models to specific water quality related problem areas. The resulting discussions are expected to ultimately result in better utilization of models in formulating water pollution control strategies.

The purpose of this overview is firstly to provide a backdrop to the papers presented by highlighting several aspects of concern to model developers and users. Secondly it summarises the thoughts expressed on deficiencies inherent to current numerical models and suggestions as to how the utility of models used in studying water pollution control problems can be improved.
WHAT IS A MODEL AND HOW IS IT DEVELOPED?

A mathematical model is simply a set of equations which, subject to certain assumptions, represents one or more aspects of a physical system, for example, dissolved oxygen concentrations in an estuary. While the model itself obviously lacks the detailed reality of the system, the behaviour of a valid model duplicates the actual responses of the system. Future responses may therefore be predicted by operation of the model and manipulation of the results in a process termed 'simulation'.

The first step in developing a mathematical model is to gain an understanding of the system to be modelled. In this conceptual phase the modeller determines cause-effect relationships, the nature of the problem to be analysed and the simplified framework which best represents the system.

The second step entails translating the governing relationships identified in the first stage into mathematical equations that describe the behaviour of and inter-relationships between the various constituents being considered. This step constitutes what is termed functional representation and completes the mathematical model of the system.

Once the mathematical model is formulated the next step is to develop a computational scheme. If the set of equations can be simplified further to form a subset that is amenable to analytical solution an analytical model results. For complex applications it is usually necessary to employ special numerical techniques and a digital computer to solve the equations. The remainder of this overview is concerned mainly with such numerical models.

The last step of model development entails validation, which involves selecting appropriate values for coefficients in the model and which consequently makes a general model unique to a particular system. This phase also establishes the level of confidence in the modelling results, which is generally determined by the amount of data available. The first stage of validation is known as calibration, which involves the adjustment of model coefficients until computed results match observed data from the system. The second stage is termed verification, which entails testing the model against several other, independent, data sets from the system. If the results compare favourably with observed responses the model is considered verified.

In summary, the development and use of models involve several interrelated areas such as system conceptualization, model selection, data collection design, computer program use, history matching and prediction. Although the developer must negotiate each of the individual steps the use of models cannot be considered a step-by-step procedure. When dealing with real systems a model is never exact and complete data are never available, therefore model use is an iterative process to which one never achieves a final solution.

ADVANTAGES OF NUMERICAL MODELS

Several characteristics may be identified which combine to make the development and use of numerical models a worthwhile exercise. A selection of these are highlighted below.

Firstly, model development requires the investigator to determine and resolve data inadequacies. This needs no further explanation other than to say that inconsistent data will almost invariably result in unrealistic parameter values or the inability to match model feedback with historical system response. Models serve
to organize information of a system or processes within a system. In the hands of an experienced operator a model may thus be an excellent safeguard against the acceptance of anomalous data.

Secondly, construction of a model aids in conceptualizing system behaviour. Interaction with the model forces an accurate representation of system characteristics and checks assumptions regarding system functioning. Model results alert the investigator to the need for re-evaluating deviant field characteristics and may guide the formulation of new hypotheses regarding system behaviour. A model used in the early stages of a field study often helps in determining which and how many data should be collected. These factors may motivate investigators to frame problems in the context of models at the inception of a study irrespective of whether the models are needed for purposes of prediction or management.

Thirdly, there is no doubt that numerical models provide a means for solving extremely complex water-related problems. In-site data give only a synoptic view of the combined influence of all factors affecting the system and it may be impossible to predict future conditions accurately by analysing the statistical properties of historical data alone. A properly formulated and applied digital model provides the investigator with a means for collectively analysing large quantities of data as a coherent system. Used in this way models become powerful aids to planners in their decision-making as they may be used to demonstrate benefits or impacts which will result from manipulation and perturbation of the system. Computer-assisted simulations enable a great range of alternatives to be evaluated to furnish information which could be acquired in no other way.

Fourthly, a variety of models are available to virtually everyone in the water field. The tools are now where they belong - in the hands of those doing the local work, where the problem areas exist. This desirable state of affairs has been achieved largely due to the advent and general availability of powerful computers, even in the mini and micro frames.

Lastly, the computer code and data deck utilized in a study is a perfect record and means for transferring information as to how a problem was solved (Prickett, 1979). Armed with the information contained in the numerical code doubts as to the exact assumptions used and the step-by-step solution procedure may be resolved unambiguously. In this day of the jargon-ridden article this advantage attached to the proper use of models is not to be under-estimated.

MODEL MISUSE

There are many ways in which models may be misused. Prickett (1979) and Mercer and Faust (1981) cited overkill, inappropriate prediction and misinterpretation as common instances of model misuse in the groundwater field. These examples apply also in model applications to other water bodies.

The temptation to use an overly sophisticated computational tool for the problem at hand is sometimes difficult to resist. Overkill is evident when two- or three-dimensional models are developed when experience or application of a simple formula would do, or when complex models are used too early in a study. The degree of sophistication opted for should match the complexities of the problem, the objectives of the study and the amount of data that are available. The best approach might be to start with the simplest model and a broad description of the system followed by progressive refining of both model and data until the desired estimation is obtained. Investigators should guard against selecting a sophisticated model mainly for public relations purposes, with audience impact in mind or
to conceal the lack of input data. One needs competence in numerical modelling not only to use numerical models but also to know when not to use them.

Inappropriate prediction occurs when investigators select the wrong model or fail to recognise significant changes in conditions which have occurred between the history-match portion of a simulation and the prediction segment. One should at all times be aware that numerical models are mathematical approximations created to simplify and better understand complex, natural phenomena. As such, certain assumptions have been made in the development of the model which must be adhered to in its application. Many modellers seem to believe that numerical models can be calibrated to predict aspects such as future water quality trends regardless of the available data. This is false. The success of a calibration is directly proportional to the amount of reliable input data and the skill of the modeller. In this regard it may be well to remember the adage often seen and heard in computer installations: 'Garbage in, garbage out'. Modellers and managers alike should realise that the ability of a calibrated model to duplicate past conditions does not necessarily verify its ability to predict future behaviour.

Emphasis should be placed on the description of modelling as a tool. Numerical models are by far the most powerful tools ever available for solving problems in the water industry. Naturally the chief drawback of any powerful tool is that with only slight misuse it can bring disastrous results. The worst possible instance of misinterpretation and model misuse is to have blind faith in model results. Only by checking can we ensure that results are consistent with the data and the method of analysis. When working by hand we continually evaluate the accuracy and reasonableness of our solutions. The calculating power and speed of the computer and the finished appearance of neatly tabulated results may obscure the need for checking results. Calculations that contradict normal intuition often may be traced to some data entry mistake, an error in the computer program or misapplication of a model to a problem for which it was not designed. If interpretation of the results of modelling is not coupled with a conceptual understanding of the system being studied the exercise becomes not only a waste of time and money but a threat to the profession where it is applied. There is cause for concern when far-reaching decisions about water resources are based on poorly constructed and interpreted models and when the good water resource studies are distinguished from the bad ones on the assumption that the former are those in which numerical models are employed. These actions can only produce untenable studies and management programs, and the end result may be disillusionment and a loss of confidence in modellers and their models. Models do not eliminate the need for data gathering efforts, practical human experience, sound judgement and common sense. They are only tools which become useful when these criteria are combined with the speed and accessibility made available by the use of modern day computers.

SKILLS REQUIRED FOR EFFECTIVE MODELLING

Those who use computer models effectively are well aware that modelling can be extremely valuable during most phases of a project. Nevertheless, confusion and misunderstanding over their application still exists and the issue of how much faith should be put in computer modelling raises questions based on real concerns.

The concerns over faith in models are valid, but often misdirected. The actual issue is how much faith we can place in the human being who performs modelling. Adequate knowledge is one of the main ingredients required for successful modelling and the investigator needs a firm understanding of the following aspects in order to be effective:
(a) The hydraulics of the water body under study and the various factors influencing water movements.

(b) The strengths and deficiencies of field data collection techniques.

(c) The scientific principles governing the behaviour of the process being modelled.

(d) The theory of numerical models, particularly their capabilities and limitations.

(e) The principles of sound scientific judgement.

(f) The art of effective communication, without which the modeller risks misinterpretation by others and their dissatisfaction with models.

The modeller must have a thorough understanding of the specific system being studied, the various modelling techniques and the limitations and sources of error inherent in models to be equal to the task. To be effective these qualities must be supplemented by efficient communication throughout the project, especially with regard to clear documentation on the inherent assumptions, procedures, results, accuracies and limitations of the analysis. Models originate nothing. Results depend on the analytical skills of those who use models. Success in modelling comes to those who perceive models not as a means to analyse systems they cannot comprehend but merely as tools that permit them to perform with greater ease and speed the analyses they already know how to do.

**PROBLEM AREAS HAMPERING THE APPLICATION AND UTILITY OF MODELS**

There are several problem areas associated with all modelling applications. Inadequacies related to the use of numerical models in groundwater management as highlighted by Bachmat and co-workers (1980) are an excellent reflection of the current situation also in the other areas of model application discussed during the session. These central problems, which require continued and increased attention in an effort to accelerate the rate of improvement in the utility of numerical models applied to management situations, are outlined below.

**Data Deficiencies**

Inadequate or insufficient data are an important limiting factor in the use of models and data are often the largest single factor influencing the cost and benefits of using models. Data acquisition is an expensive, time-consuming activity and improved methods of collection would unquestionably benefit the application of models. It is fair to say that progress in data gathering techniques has not paralleled advances in the development of simulation models for water resource evaluation and management. The determination of which data affect model output most critically therefore remains a particularly important process in data collection. Testing models through sensitivity analysis to discover which additional data need to be determined or to indicate areas where added data would most significantly improve our ability to simulate system behaviour should thus be assigned high priority in any modelling study. As pointed out earlier, the application of computer models when there are few data may well turn out to be their most useful function in many studies.

**Inadequacies in Modelling**

A large number of water-quality related models have been proposed and used, ranging from very simple to very complex. Nevertheless, certain kinds of models
are yet to be developed while others have proved unsatisfactory. No attempt will be made here to identify those model types which require further refinement or the areas in which new models are needed. The reader interested in further information is referred to the papers presented during the session and published in this issue of the proceedings.

The lack of models in certain areas or the unreliability of existing ones frequently is the result of factors extraneous to modelling. An example is systems where the underlying theory has been described inadequately and the gap in scientific understanding of the controlling physical phenomena awaits further observation and the development of theories to explain them. Once the governing equations are available, their incorporation into models is a tractable problem. Similarly, poor modelling results are frequently the result not of any omission of relevant variables from the model but of failure to account for their true nature. Many pollution related variables and parameters are actually probabilistic in nature and their stochasticity should be included in the model. In this area inadequacies of modelling are often the result of data deficiencies. Further refinement awaits the development of improved data collection equipment and techniques. In the water pollution field the most pressing need in this area is probably that for continuous, on-line monitoring instrumentation.

Deficiencies in modelling occur also in more subtle ways than those referred to above. There are several areas in which barriers to the use of otherwise satisfactory models can be removed with proper effort. These include transferability and flexibility of computer codes as well as refinements with respect to computer storage, time requirements and simplicity of structure. Modellers should make every effort to ensure that they develop codes which are easy for the user both to understand and to use.

Lack of Communication

Modelling is a rapidly developing science, the increasing sophistication of which is partly responsible for the lack of confidence on the part of managers in models as decision-making tools. Many managers are not versed in the technical details of modelling and their lack of understanding of the inherent capabilities, limitations and assumptions of models may often result in distrust and rejection. This problem is compounded by professionals overselling their models, claiming that their models can perform better than is actually possible. This serious problem has led to understandable disenchantment on the part of managers and the impression that models do not produce efficient and reliable results for decision-making purposes. Modellers need to ensure that the results they produce are presented in a way that is both meaningful and compatible with decisions that must be made, and that inherent uncertainties are indicated.

While it is not reasonable to expect all managers to become well versed in modelling it is possible and necessary for managers to learn something about models through more active participation in the application of models to their problems. If this is coupled with willingness on the part of the technical expert to translate what is known in terms that others can understand instead of using camouflage jargon then not only are the accuracy and credibility of the model likely to be improved but also the use of its output. This interactive participation of managers and technical staff is particularly important in defining those factors which are critical for the application of a model to a problem and in formulating those factors in the exact terms needed for modelling.

In summary, there is a need to educate the resource managers who use models so they will know what is available to them and to train the technical expert in the art and skill of verbal articulation so that his knowledge may be transmitted with
the highest standard of lucidity. The practicality of models and their results is not purely a function of intelligence and the ability to select an appropriate level of modelling for a particular project but also of the competence on the part of all concerned to communicate with those who need the information.

Accessibility of Models

The concerns regarding accessibility of models manifest themselves in two major problem areas, namely model documentation and distribution.

Solving a problem and not giving an adequate description as to how it was done commonly occurs in the modelling business (Prickett, 1979). What is lacking is proper documentation, which should include a description of the model, a listing of the code and a user's manual. Reasons put forward for the deficiencies in present documentation vary from the disinclination of private consulting firms to distribute proprietary models at low cost, to the statement that documentation is not necessary for the immediate solution of the problem for which a model is built. Documentation of computer codes is the least exciting part of a modelling project. In fact, it usually is downright unpopular as it comes at the end of the modelling process when funds have often been exhausted and the modeller would rather move on to new assignments than endure the time-consuming effort involved in documentation. This serious state of affairs calls for action by those organisations in which it occurs. Undocumented programming, other than providing the immediate solution sought, is probably a wasted effort. Documentation needs to be done along with the code, otherwise, when the memory has faded, the code may become worthless even to the originator. Even more important, the model may contain particular features, uncertainties or assumptions which may be difficult to detect unless the code is exposed to scrutiny by others.

The existence of a computer code is not sufficient to ensure accessibility to prospective users. Documentation must be publicised and distributed otherwise potential users will not be aware of which models are available or where they may be obtained. It seems desirable to have a continuing service for the systematic collection and dissemination of information on models as they become available and as they are applied to specific situations. The development of models is an expensive process that calls for a level of expertise which is not available everywhere. If the modelling community could establish such a service then not only will unnecessary duplication of effort be avoided but they should also see more effective use of models and improved international cooperation.

GENERAL IMPRESSIONS AND RECOMMENDATIONS

The state-of-the-art session on the use of mathematical models in formulating water pollution control problems achieved its objectives of reviewing, in general terms, applications to specific problem areas. The exchanges between participants from different disciplines should aid in the definition of problems of common concern and areas of deficient knowledge. Ultimately that vitally important resource, water, stands to benefit from the dialogue initiated there.

It is a considerable disappointment that no base papers were read on the use of mathematical models in ecological monitoring and several specialized areas of concern in water pollution abatement. The latter category includes applications to the economics of sewage and industrial effluent treatment unit process simulation in wastewater treatment, real-time treatment plant operation and control as well as plant and process engineering design. It is recommended that these areas be explored for possible inclusion in the programmes of future conferences or technical seminars.
It was pointed out in earlier sections of this overview that mathematical models are, above all, practical tools. In gauging the expectations of those who participated in this session, the practical approach, dealing with problems which require solutions at local, regional or national level, dominated by far. It seems that detailed presentation of a single but relevant case study, along with the general principles involved in the application of mathematical modelling to a specific area, would greatly enhance the value of future sessions of this kind. In other words, what is needed is a convincing demonstration of what models can do. Ultimately this will lead to an awakening of interest in the application of models to water pollution problems, more open understanding and increased use of models, and fewer stones thrown at modellers.

The preceding sections of this overview outlined some general difficulties and gaps in the application of models to water resource evaluation and management. The technical nature and range of applications of models to water-related problems are so divergent, however, that it becomes impractical, if not impossible, to identify specific research priorities on the basis of the rather general nature of the state-of-the-art session. What seems necessary is the establishment of an international working group charged with assessing and issuing situation statements regarding models which, in the words of Bachmat and co-workers (1980), management needs but does not have and to examine why certain of the available models are not used. This should be done for each major issue area pertinent to water pollution control. The main tasks of the working group are considered to be as follows:

Firstly, survey and catalogue existing computer models so that an inventory may be compiled and published. Pertinent information that should be listed includes the general characteristics of the model, its conceptual and mathematical framework, the nature of the computer program, references to existing applications as well as the status of program documentation and availability. All model categories should be covered, including prediction, management and parameter estimation models.

Secondly, evaluate the research needs related to numerical models and their use in the solution of water quality problems. The findings of this phase should be ordered and formulated in terms of research priorities.

Thirdly, investigate the feasibility of establishing an internationally based information facility for the systematic collection and dissemination of information on models.

In conclusion, water quality and pollution control comprises an exceedingly complex natural system involving interrelationships between hydrology, climate and man's activities. In these times of rapid change we are concerned not only with the present but also with the future and its presently unknown chemical compounds with their equally unknown degradation products. Numerical modelling has evolved to a level at which many of its components are worthwhile tools for the investigator tackling these complex problems. Indeed, the future looks exciting as more models will be developed, more investigators will be using models effectively and low-priced computer equipment will become commonplace for general use. However, the final worth of modelling applications will continue to depend, ultimately, on the people who apply the models, their knowledge of site conditions and their understanding of modelling capabilities. Every effort should be made, therefore, to equip them with all the technical know-how, enthusiasm and facilities required for maximum exploitation of the analytical powers that have been harnessed in modern computers.
ACKNOWLEDGEMENTS

This overview is published with the approval of the Director of the National Institute for Water Research.

REFERENCES

