

WATER-QUALITY MODELLING: A COMPARISON OF TRANSPORT-ORIENTED AND ECOLOGY-ORIENTED APPROACHES

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RR-83-20

August 1983

Reprinted from *Ecological Modelling*, volume 17 (1982)

INTERNATIONAL INSTITUTE FOR APPLIED SYSTEMS ANALYSIS
Laxenburg, Austria

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FOREWORD

The water quality of rivers, lakes, and reservoirs is determined by the interaction of various biological, chemical, hydrophysical, and other processes. In the modeling of water quality, these processes should be incorporated according to their relative importance, a requirement that is, however, often neglected. Models based on *a priori* assumptions that cannot be justified later are frequently developed. The reasons for this are numerous; among them are the different levels of “theoretical” knowledge available to and “measurement” knowledge required of the analysts in various fields, as well as the methodological difficulties encountered.

Most of the water quality models developed until now have been either transport-oriented or ecology-oriented. In the first case, the description of biological and chemical processes is oversimplified, while the second type of model oversimplifies the hydrophysical and transport phenomena.

The following article discusses this apparent gap and how to overcome it.

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(Accepted for publication 11 May 1982)

ABSTRACT

Somlyódy, L., 1982. Water-quality modelling: a comparison of transport-oriented and ecology-oriented approaches. *Ecol. Modelling*, 17: 183–207.

In water-quality modelling several different directions can be distinguished according to the strategy employed and the disciplinary background used for analysis. A precise classification would be difficult to make, but the manifest difference between transport-oriented and ecology-oriented water-quality models creates at least two obvious groups. In the first case, the description of biological and chemical processes is oversimplified, while in the second, the same applies to transport phenomena. Both approaches determine the level of involvement of the respectively less emphasised phenomena by a priori assumptions. This paper discusses this apparent gap and how to overcome it. No overall procedure is given; instead, a framework is suggested which is based on establishing the relative importances of the various subprocesses determining water quality and proceeding to the corresponding model structure. This should allow the proper combination of knowledge gained from theory and observations, and, furthermore, the elaboration of essential modelling steps such as parameter estimation and model identification. To illustrate, two examples are presented—one concerns heavy-metal pollution of a river, the second involves a lake for which the wind-induced interaction between water and sediment was analysed. In the first situation, a one-dimensional, coupled hydrodynamic-transport-water-quality model for three cadmium compartments was adopted. For the second problem, it was necessary to determine the unknown boundary condition at the lake bottom. This latter was achieved by simplifying the governing transport equation into an ordinary differential equation and introducing some simplifying hypotheses. Given data from regular, intensive observations, the calibration, identification and validation of this model were carried out using the extended Kalman filtering technique.

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INTRODUCTION

Water-quality models can be imagined as structures having three axes specified respectively by time, space and the degree of detail of the ecological component. The first axis defines whether the model is dynamic or steady, the spatial resolution concerns the number of “boxes” or segments, while the third axis defines the number of state variables or compartments. In principle, the location of a model in this three-dimensional space should follow from the dynamics and relative importances of the various subprocesses in the entire system under study. Depending on the character of the problem many combinations exist, and this fact is well reflected by the large number of water-quality models published in the literature.

Considering only space and ecology as the axes, two extreme types of model can be distinguished: a *transport model* for a conservative material (with considerable detail in space for a single compartment), and an *ecological model* of a system under the assumption of complete mixing (with considerable ecological detail for a single box) *. At first glance there is no difficulty in developing, between these two extremes, models appropriate for the features of a particular water-quality problem that is being studied. For instance, it is possible to start with a transport equation and apply it to all of the ecological compartments by adding the various reaction and interaction terms. Bearing in mind that the transport equation needs input from hydrodynamic equations (unless a purely empirical approach is adopted), a *coupled transport–water-quality model* consisting of a set of nonlinear partial differential equations (PDE’s) results. It is arguable, however, whether or not this procedure is feasible.

We are concerned here with differences in the levels of theoretical knowledge available from the various disciplines which should be integrated in a model. For example, hydrodynamics and transport phenomena have a quite solid theoretical background compared to the biology and chemistry of lakes or rivers. Consequently, for the latter, data (that is, in situ and laboratory observations —so-called measurement knowledge) are extremely important in establishing a model, in estimating its parameters and in identifying the model structure. On the other hand, all these steps should be done within the framework of the coupled transport–water-quality model, the robust structure of which—associated with the PDE formulation—does not favour the incorporation of measurement knowledge. Moreover, this structure excludes in practice the application of present-day estimation and identifica-

* It is noted that in this paper hydrodynamic and transport phenomena are considered not to be subsumed within ecology.

tion techniques, and testing of hypotheses concerning the reaction and interaction terms, and thus indirectly the understanding of the biological and chemical processes which is the precondition of any practical use of the model. Thus our conclusion is that it is not realistic to generate water-quality models of general validity: even a strict modelling procedure must be relinquished, and only a framework retained. These statements are supported by the large number of existing models.

The classification of water-quality models in general is a huge task (see for example, Cembrowicz et al., 1978). However, by analyzing simply the degrees of detail along the spatial and ecological axes, the classification is made much easier (although it can be argued that it is still artificial). Most known models are near to one of the two extreme groups mentioned previously (one reason for this is the generally specific and differing training of various analysts). Accordingly, it is possible to distinguish (i) *transport-oriented* water-quality models, which are oversimplified with respect to biology and chemistry, and based on PDE's (Type 1); and (ii) *ecology-oriented* models, which often exclude the influence of transport and consist of a set of ordinary differential equations (ODE's) (Type 2).

Essential differences can be found in the modelling procedures for Types 1 and 2. These involve the basic modelling strategy, the methodologies applied, and the procedure for data collection and its interaction with the modelling process. The differences can be so fundamental that a priori assumptions are frequently made concerning the relative importance of transport and ecology respectively, and thus there is no opportunity to perform sensitivity analysis on the model subsequently developed. In short, there exists a certain gap between transport- and ecology-oriented water-quality modelling which calls for an effort to combine the advantages of the two methods. Approaches developed in this manner constitute a third type of model (Type 3) which is desirable but still rarely found in literature. Models of this kind may also be termed coupled transport-water-quality models, but in this case the emphasis lies in a consistent and balanced combination of the descriptions of transport and ecology rather than on the mechanism of coupling. For instance, a three-dimensional transport equation may be used in some aggregated manner. Here methodological questions play an important part. Preferably, a model structure should be sought which will not exclude a priori the application of several desired techniques, such as parameter estimation or sensitivity analysis, in the course of the modelling procedure.

Considering the contradiction between models of Types 1 and 2, and the infrequent occurrence of Type 3, it was felt realistic to consider the given subject in the light of this discrepancy. This paper is organised as follows. First, the modelling procedure (in the research context) is discussed in

general, and then the strategies applied to Types 1 and 2 are analysed and compared. The conclusion from this serves to provide some discussion of the features of Type 3: examples are presented to illustrate this.

MODELLING PROCEDURE

Basic steps of modelling procedure

Some of the basic steps of modelling are stressed here, rather than a general strategy for application. For this purpose, two figures have been adapted in slightly modified form from the literature (Eykhoff, 1974; Beck, 1982) and combined in Fig. 1.

At the beginning of the water-quality modelling process, the specific system (river, lake, etc.) and problem (e.g., oxygen or thermal region, eutrophication) and, furthermore, the objective of the study (understanding, prediction, control, planning, management, etc.) are considered. Starting with this information, the intention is to devise a model conforming as accurately as possible to the stated objective. In developing the model, two different fields of knowledge can be drawn upon (Eykhoff, 1974): theoretical knowledge and measurements. Their dual nature is clearly expressed in Fig. 1(a). The first associated with a priori *structural knowledge*, is based on natural laws (such as mass and momentum conservation) and can be expressed in terms of nonlinear PDE's. These latter are then often simplified, and solved for the most part numerically.

In developing a model, some observations should be available beforehand (a priori measurement knowledge). This is necessary in order to characterise the physical system considered, to select the water-quality variables to be involved, and to establish the orders of magnitude of their temporal and spatial changes, so that the physical system may be reflected in the model. All these steps, together with others not listed, belong to the stage of conceptualisation, a priori model structure determination, and selection of model type (see Fig. 1(b) and for details, Beck, 1982). Any further progress requires systematically planned experiments and data collection in interaction with model development. The sum of the information gained may be termed *a posteriori (measurement) knowledge* (see Fig. 1), which then allows identification of the model structure (often considered to be correct on some theoretical basis), estimation of unknown parameters (rate constants, dispersion coefficients, etc.), and validation. Note that the meaning of validation is quite broad: it may mean the successful application of the model after calibration to a new set of data, its use under changed conditions (both are extensions in time) or, for example, for other reaches of the system for which it was established (spatial extension).

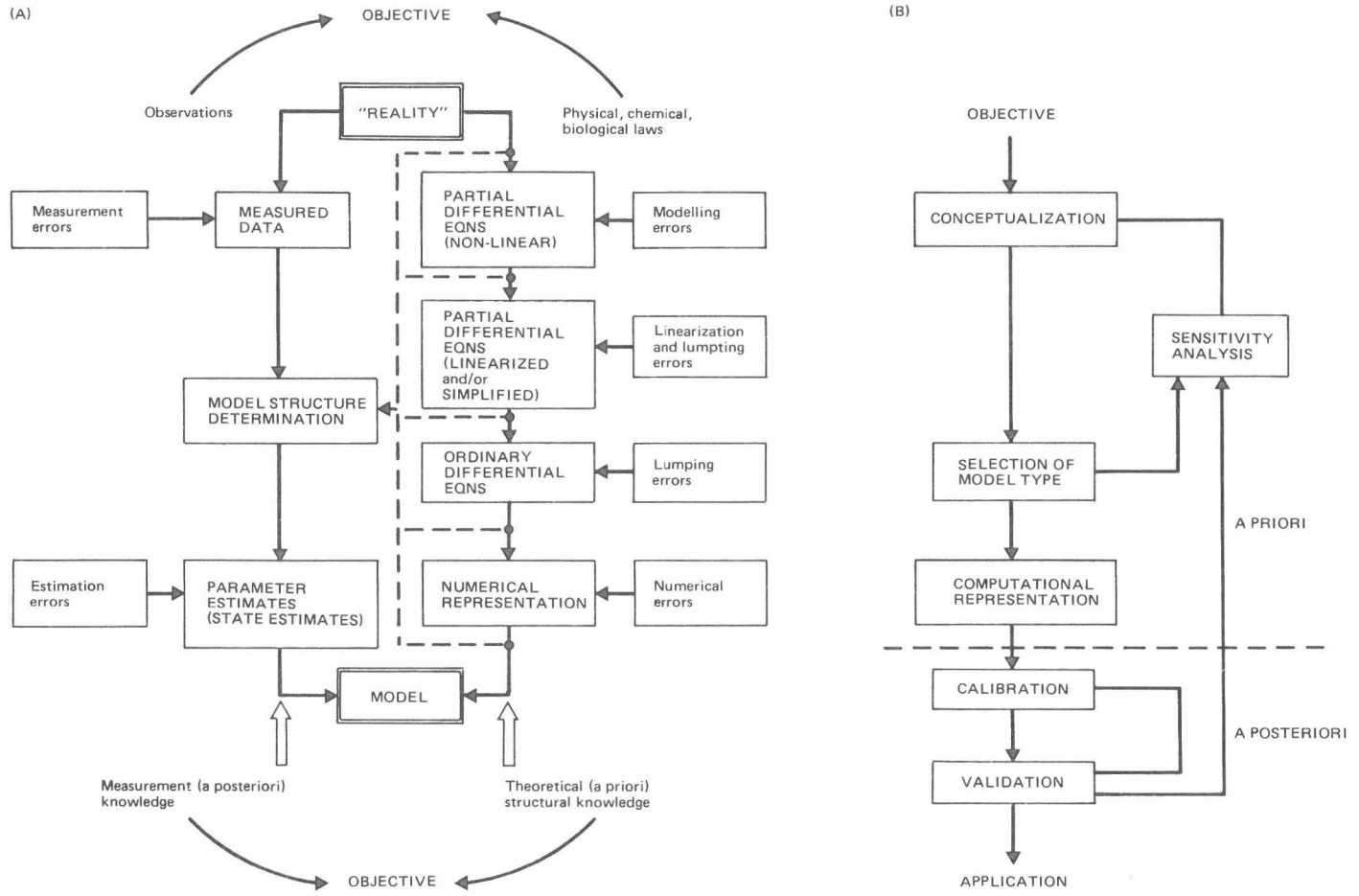


Fig. 1. Illustrations of modelling procedure combining theoretical and measurement knowledge (after Eykhoff, 1974; Beck, 1982).

Thus, a model will result from a procedure which incorporates both a priori and a posteriori knowledge, will account for the plentiful errors indicated in Fig. 1, and involve several loops and feedbacks. The way in which the theoretical and measurement knowledge are combined will depend essentially on the subject considered. For instance, as two extremes, modelling in hydrology and in hydrodynamics may be mentioned. The first is characterised by the dominant role of a posteriori knowledge (e.g., flood forecasting using historical data from two gauges), while the second is characterised by structural knowledge (e.g., computation of the same flood events based on Saint Venant equations).

The (a posteriori) model structure determination and interaction with the data (Fig. 1(a)) can be important also in situations when theoretical knowledge is well established. For example, in Nature, conditions are not "pure", in contrast to the assumptions often used when modelling equations are derived: thus, modelling errors (Fig. 1(a)) cannot be avoided. Problems related to boundary conditions are especially important. As an example, the influence of dead zones near to river banks and in river beds on dispersion phenomena (Beer and Young, 1980) may be cited. Better agreement with measured concentrations was obtained using a dead-zone time-series model than using the conventional longitudinal dispersion equation. This fact suggests that the accumulation and release of dead zones exert a larger contribution (together with the resulting time lag) on dispersion than do spatial nonuniformities in the water body, and are thus the dominant mechanism. This calls into question the "self-evident" use of the classical dispersion equation.

Using the theoretical and measurement knowledge accrued, different models can be developed for the same problem. The obvious goal is to find the simplest but still realistic version, since accomplishing the necessary steps in the modelling framework (uncertainty and sensitivity analysis, parameter estimation, etc.) depends essentially on the model structure. Here a distinction between techniques available for PDE's and ODE's (or for distributed- and lumped-parameter models) is especially apparent.

It should also be noted that if the number of state variables is too large, realisation of the modelling procedure illustrated in Fig. 1 will be simply unrealistic (see also later); data collection will be too expensive (this can also be the case when only a few state variables are involved, but specific measurement techniques are required). This situation may occur if spatial changes are dominant (many spatial "boxes" must be considered) and/or the number of water-quality components to be incorporated is high. Under such conditions, some compromise strategy should be looked for.

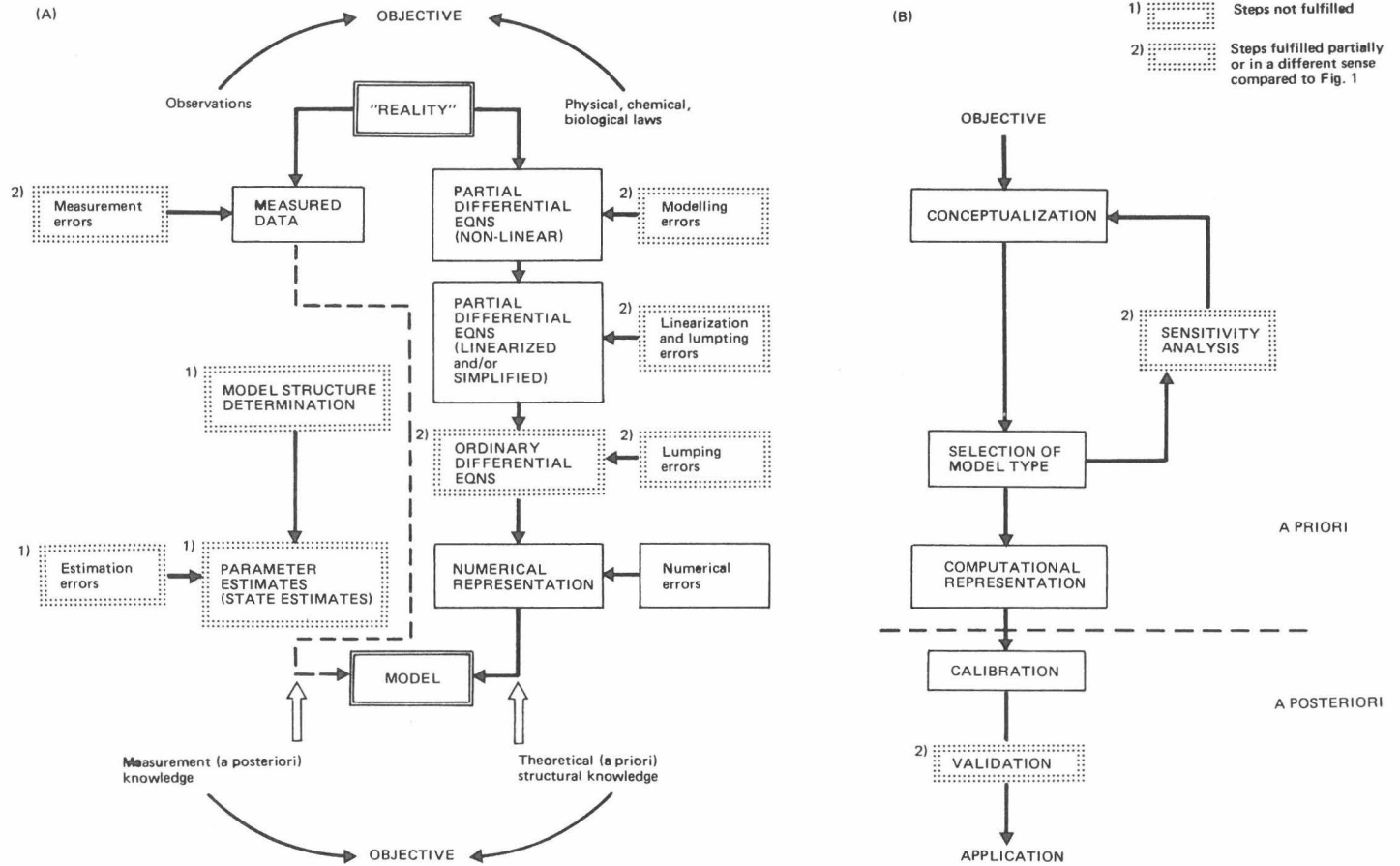


Fig. 2. Usual procedure for transport-oriented modelling.

Procedure for transport-oriented modelling

The structure of this type of model is given by the transport equation, which further involves some simple biochemical reaction terms (i.e., a first-order decay). The transport equation can usually be used to calculate concentrations in a given water body as a function of time and three spatial coordinates. Frequently, the equation is employed simultaneously with the corresponding versions of the equations of continuity and motion, thus resulting in a set of highly nonlinear PDE's (see Watanabe et al., 1982).

These can then be solved numerically, for example by the methods of finite differences or finite elements. The technique applied is generally related closely to the formulation of the boundary conditions, the assumptions made concerning variations the various coefficients, and simplifications related to terms involved in the equations. The choice further depends on whether or not the number of independent variables can be reduced, and on the description of turbulence (Watanabe et al., 1982; Launder and Spalding, 1972). Thus, the modelling procedure is based very much on theoretical knowledge, and as seen in Fig. 2, a posteriori determination of model structure is absent. Measurements are certainly important, but are used mainly to determine values for some of the parameters, such as roughness and mixing coefficients, or to check the computed velocity field. Validation also has a slightly different meaning, and a study of error propagation or model sensitivity is rarely done.

These features of the modelling procedure imply strong constraints on methodology: the majority of steps indicated in Fig. 1 may be carried out for ODE's, but for PDE's only very limited applications appear in the literature (Thua, 1969; Koivo and Koivo, 1977).

Generally, the numerical solution of a PDE can be replaced by the solution of N ODE's, but the methodological problem still remains: the number of state variables (here the product of the numbers of compartments and boxes) will be much larger than the number of observed variables, thus prohibiting the application of the techniques in question.

Procedure for ecology-oriented modelling

At first glance, the strategy here (Fig. 3) is much more similar to the desired procedure than in the previous case, and there is a more balanced utilisation of both theoretical and measurement knowledge. This is, however, quite obvious, since, as noted previously, the theoretical basis for describing the biological and chemical processes that occur in rivers and lakes is much less explored than is that of transport phenomena. Consequently, the data are more important.

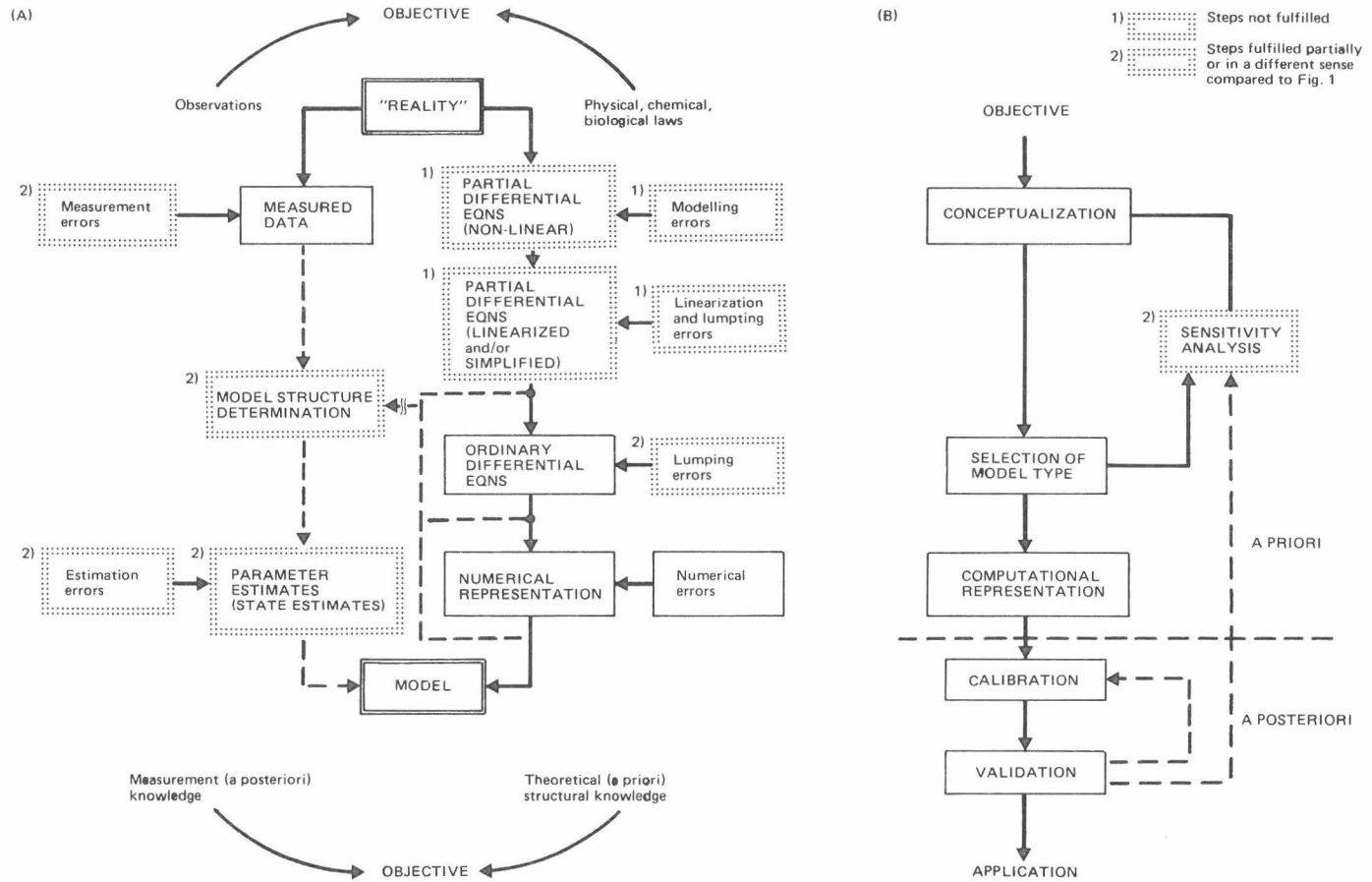


Fig. 3. Usual procedure for ecology-oriented modelling.

If the specific steps of the modelling process are studied more carefully, the impression is not so satisfactory. The first feature apparent is the nearly complete exclusion of transport which—it should be stressed—may influence not only spatial changes, but also the dynamics of the system.

Second, concerning their structure and complexity, models of this type quite often set out explicitly to describe subprocesses in as detailed a manner as possible, which leads to an overabundance of state variables and parameters with insufficient data to identify the model structure and calibrate it. These latter problems are due not only to data scarcity, but also to the structure of the model. If the number of state variables exceeds some limit (between 5 and 10), most of the analytical techniques indicated in Fig. 1 cannot be applied. The presence of nonlinearities, empirical functions and discontinuities increases the difficulties. Thus, in many cases parameter estimation is downgraded to a simple trial-and-error fitting, and there is no a posteriori model structure determination in a strict sense.

Conclusions and comments on modelling procedure

From the previous arguments, at least three conclusions can be drawn:

(1) neither of the strategies discussed (Types 1 and 2) can have general validity;

(2) both approaches by their a priori assumptions exclude the possibility of model extension in the course of development towards the involvement of the respectively less emphasised phenomena; in other words, the structures are not sufficiently flexible;

(3) if the number of essential state variables is high (regardless of whether the cause is an increase in the number of spatial boxes or of ecological compartments), the scheme illustrated in Fig. 1 cannot be realised in a strict sense.

Thus, it does not seem to be realistic to elaborate a general water-quality model or a widely applicable modelling procedure. Subsequently, no overall rules are presented here. Rather, some principles believed to be essential are discussed.

A situation characterised by conclusion (3) is therefore considered, for which modelling might at first appear so difficult as to be fruitless (the author rejects this outlook, since modelling is believed to be generally useful). It is instead suggested that Fig. 1 be considered as a suitable framework for modelling, depicting the interaction between modelling, data collection and experiments, and, moreover, many of the steps required. These need not necessarily be applied to a closed form of the model as one large unit. The method proposed is of an indirect nature, the idea being to separate as many subprocesses and modelling steps as possible (it is stressed

here that the isolation can never be complete, therefore the aim is to apprehend the dominant features; see for example, Van Straten and Herodek, 1981, Section 2.5), to study them independently, and then couple according to Fig. 1 the resulting knowledge.

The example is Shanahan's work (1981) for the Lake Balaton eutrophication study (van Straten and Somlyódy, 1980). In order to find the proper balance between transport and ecology, Shanahan first worked out a two-dimensional lake circulation model. Next, he aggregated from the convection and dispersion terms a one-dimensional dispersion equation, which is acceptable for this particular long, narrow lake. Subsequently, he coupled the dispersion equation with van Straten's (1980) phosphorus-cycle model, which has four state variables, and assumed originally that the lake could be subdivided into four interconnected boxes (where the interconnection was specified by hydrological throughflow and a bulk return-flow velocity subject to calibration). In the course of the analysis the parameter values of the original model were maintained. Finally, the simulation results of the "continuous" and four-box model were compared.

From the comparison, Shanahan concluded that:

(i) the coupled transport-water-quality model obviously reflected better the spatial details and local influences;

(ii) the four-box model underestimated the various phosphorus concentrations for one of the basins, while the basin-wide averages were satisfactory for the rest of the lake;

(iii) the return-flow velocity could not be used, since the four-box formulation introduced a priori artificial dispersion which was higher than the wind-induced dispersion.

An additional conclusion which can be drawn from Shanahan's results is that:

(iv) the four-box model with its ODE structure and all the advantages associated with this can be reasonably maintained for practical purposes and subsequent analysis.

There are further important guidelines for developing such a model. For instance, some desirable attributes include a *balance* in the descriptive process and, as stressed before, *flexibility* in the approach, and *simplicity*. The analysis of time and length scales and of orders of magnitude are extremely useful in obtaining an appropriate balance (Verboom and Vreugdenhil, 1975; Harleman and Shanahan, 1980; Shanahan et al., 1981; Shanahan, 1981). Flexibility allows simultaneous testing of hypotheses (Spear and Hornberger, 1980; Hornberger and Spear, 1980; Fedra et al., 1981) and subsequent modification of the model at each stage in its development, according to necessity. The role of simplicity is obvious if the structure of Fig. 1 is kept in mind. This also extends to the numerical techniques applied,

especially if PDE's are involved. Fast computer methods enable numerical uncertainty and sensitivity analyses to be performed (as for the one-dimensional lake hydrodynamic model discussed in Somlyódy and Virtanen, 1982) and parameter values to be estimated.

In summary, this process represents no more than a spiralling path focussing on the core of the problem studied, through the utilisation and constant improvement of theoretical and measurement knowledge, and a combination of the most appropriate methodologies. It is hoped that by adopting this approach, a study will be properly completed with a reasonable model eventually approximating reality. Of course, from time to time, although only provisionally, conclusions may even be negative. For a field such as water-quality modelling, which has a relatively short history and pronounced interdisciplinary character, this is self-evident.

Examples illustrating the modelling procedure

The first example here is related to a river problem where much emphasis was laid on determining the relative importances of various processes. The results were quite satisfactory on an experimental basis, although the model remained transport-oriented. The second study, concerning a lake problem, illustrates a nearly ideal case, where, beginning with a PDE and aggregating it to an ODE, the majority of the steps in Fig. 1 could be realised.

Example 1. Study of cadmium pollution of River Sajó, Hungary

The River Sajó is one of the tributaries of the River Tisza (Fig. 4) located in the northern part of Hungary. It is of medium size, with a mean streamflow of $\sim 30 \text{ m}^3 \text{ s}^{-1}$, showing large fluctuations (between 5 and $600 \text{ m}^3 \text{ s}^{-1}$). The river is characterised by a high degree of meandering, and consequently by effective mixing. It is polluted heavily with organic materials and heavy metals, among which cadmium is perhaps the most important

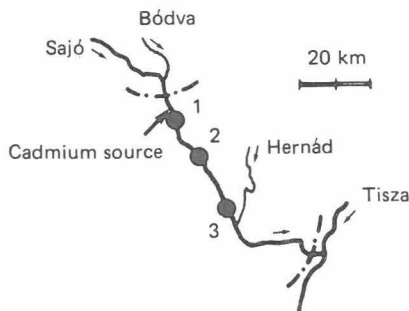


Fig. 4. The reach of the River Sajó studied: - · -, boundary of reach.

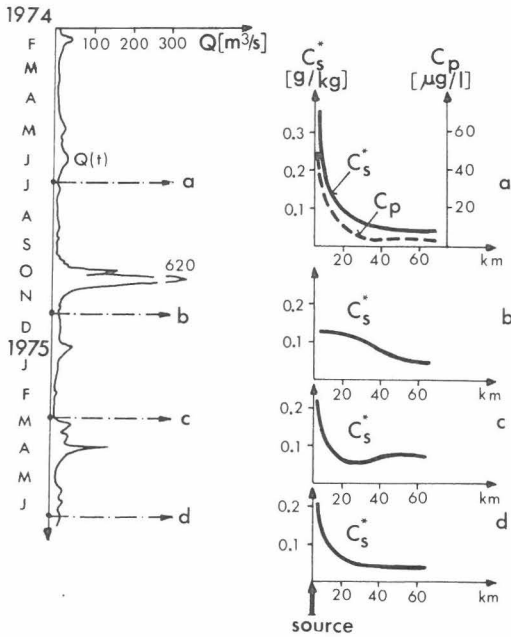


Fig. 5. Pollution pattern of the River Sajó under various streamflow conditions (taken from Litheráthy and László, 1977): note that C_s^* is the cadmium amount of the sum of ignition loss and the acid-soluble part of the sediment.

of those released basically from a single point source (Fig. 4). Cadmium pollution was studied intensively in the period 1973–1978 (see Litheráthy and László, 1978); dissolved and particulate forms, spatial and temporal changes, and bottom sediment were observed. The average load was estimated, on the basis of discharge and water concentration data, as $\sim 15\,000$ kg per year, 60–70% of which is deposited as sediment. On a long-term basis, the metal content of the sediment decreases exponentially downstream from the source, showing clearly the influence of accumulation (see Fig. 5(a), which illustrates the changes of the particulate and sediment cadmium concentrations, C_p and C_s^* , respectively). The majority of the cadmium is bound to the 25–50 μm fraction. Under low flow, the longitudinal change of concentration is similar to that of the sediment pollution (Fig. 5(a)). At higher streamflow rates, however, the role of resuspension becomes apparent, sometimes causing increases in concentration in the flow direction. The influence of floods was also studied. They smooth out the pollution pattern in the sediment through re-entrainment, convection and repeated deposition (Fig. 5(b)). After a flood, the sediment pollution is re-established (Fig. 5(c) and (d)). The character of the river suggests that anaerobic conditions rarely occur in the

sediment. This means that there is no direct toxic danger to the river itself (it now has a very poor ecosystem as a result of many different types of pollution during the last 30–50 years), since most of the cadmium is present in particulate form and essentially no dissolution mechanism acts. The downstream river system is, however, certainly endangered when cadmium is stirred up and transported under flood conditions and then deposited and remobilised in reservoirs having large retention times.

With this preliminary knowledge about the system, it was decided to continue the study with the aim of building a model simultaneously with appropriate in situ and laboratory measurements. The objectives of the analysis were to gain an understanding of the processes and to perform some extrapolations to the past (no historical data were available) and future (the load was reduced in 1979 to 1/10 its previous size). The results will be reported in detail elsewhere (Somlyódy et al., 1982).

The in situ measurements showed that the river reach studied (Fig. 4) has a rather uniform chemical environment. Two dominant mechanisms were found concerning the changes in dissolved and particulate forms (C_D and C_P) in the water: co-precipitation, and adsorption onto suspended solids (SS). The first depends on the dilution in the plume, the second on SS concentration—both processes having the same time scale (some hours) as the mixing of pollutants over the cross-section along a relatively short river length (some km). Accordingly, all three processes were assumed in later modelling work to take place instantaneously. On the basis of frequent effluent water-quality measurements, the pH and thus the ratio C_D/C_P were found to fluctuate drastically. However, owing to co-precipitation and adsorption in the river, particulate cadmium is dominant, leading to accumulation in the sediment layer through settling. The deposition and re-entrainment of fine sand ($\sim 120 \mu\text{m}$) and natural river sediment ($\sim 30 \mu\text{m}$) were studied in a laboratory open channel and hypotheses made concerning the probability coefficients for the two processes (Sayre, 1969; Graf, 1971;

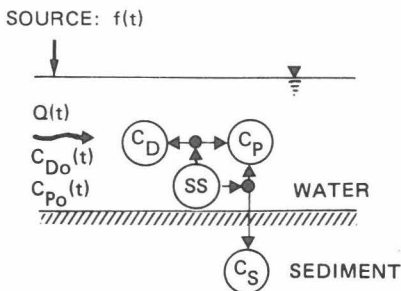


Fig. 6. State variables involved in cadmium model.

Partheniades, 1977), depending on the streamflow Q (they were assumed to be proportional to $(1 + Q)^{-1}$ and Q , respectively).

The model developed interactively with the experiments involved three state variables for cadmium (Fig. 6): the concentrations C_D , C_P and C_S (the latter expressing the pollutant content of the sediment per unit river length), for which SS played a controlling role (this was described simply by an $SS(Q)$ rating curve). Adsorption was characterised by a Langmuir isotherm, and co-precipitation as a function of dilution—both on the basis of laboratory measurements. Bioaccumulation was also studied but was not included in the model (under the present conditions it does not exceed 1 kg/yr.). For the interaction between the water and the sediment, a modified, nonlinear version of Sayre's approach (1969) was used which distinguishes between the total polluted sediment and the upper, available layer. For all the state variables a transient, one-dimensional transport equation was established (accounting for convection and dispersion in addition to the processes listed above), to which equations of unsteady flow (Mahmood and Yevjevich, 1975; Kozák, 1977) were coupled. The five PDE's were solved simultaneously using the method of finite differences. For the transport equations, the fractional step method (Verboom and Vreugdenhil, 1975) was employed with explicit schemes; for the flow problem, an implicit scheme was used followed by application of the economical double-sweep technique to solve the linearised algebraic system of equations (Mahmood and Yevjevich,

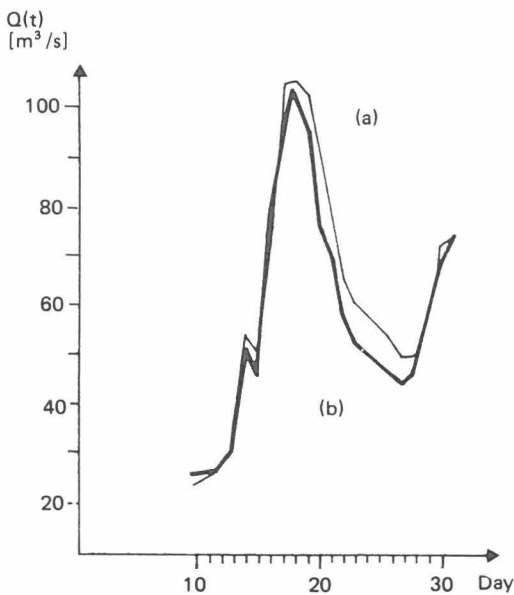


Fig. 7. Measured and computed streamflows: station (2), period 10–30.04.1975.

1976). To make the solution more economical, models for steady flow and quasipermanent transport were also elaborated; their combination depended on the boundary conditions and was controlled inside the model. For the quasisteady conditions, the transport equations were linearised, dispersion neglected, and the solution derived by linking the analytical solutions of the problem for subreaches of length Δx_i .

Figure 7 shows the appropriateness of the unsteady-flow model. In this example, the upstream and downstream water levels (locations 1 and 3 in Fig. 4) were used as boundary conditions, whereas the Manning roughness coefficient was calibrated ($k = 36$) independently with the help of the steady-flow model and observations of the longitudinal free-surface profile.

For the transport model, the settling velocity and probability coefficient of deposition were determined from experiments and the literature, respectively; re-entrainment was determined through model calibration. As a subsequent step, the pollutant content of the sediment was calculated assuming 20 years' permanent discharge and average streamflow rates for each month. The pattern obtained (Fig. 8, curve 1) is in qualitatively good agreement with observations (Somlyódy et al., 1982, Fig. 5). next, a specific

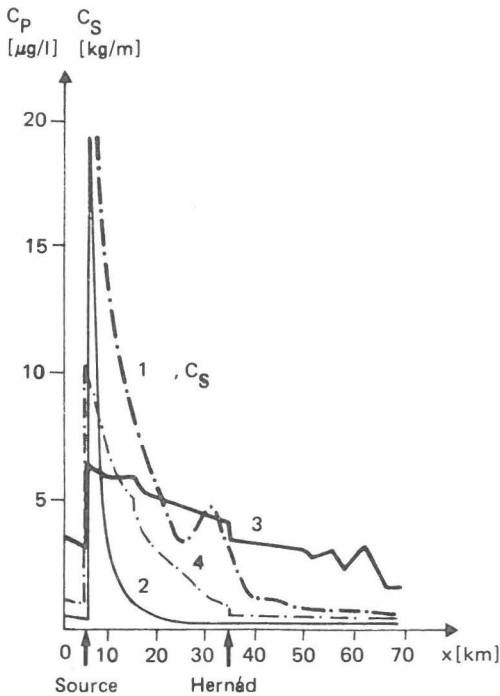


Fig. 8. Distribution of particulate and sediment cadmium concentrations along river: ①, pollutant content of sediment after 20 years (C_s); ②–④, simulations of specific years (C_p).

year was considered, consisting of a six-month low-flow period ($Q = 20 \text{ m}^3 \text{ s}^{-1}$) followed by a 30-day flood (historical scenario, $Q_{\text{max}} = 150 \text{ m}^3 \text{ s}^{-1}$) and an average regime. Figure 8 indicates the concentration distributions of particulate matter at the end of each of these periods (curves 2, 3 and 4, respectively). As can be seen, during the first and third periods, deposition dominates and more than 10 tonnes of cadmium reaches the bottom; however, it is striking that $\sim 30\%$ of this amount is stirred up by the flood. The corresponding $C_p(x)$ distribution is also essentially different from the two others, being much more uniform along the river. $C_s(x)$ is modified similarly, showing a more homogeneous pattern (Fig. 5). With regard to dissolved cadmium, it is worth mentioning that on average 60% is transformed ultimately into particulate form, which is then essentially removed by sedimentation. However, the remainder of the cadmium behaves conservatively, being affected only by the dilution at the mouth of the Hernád river, as the chemical environment does not change notably along the Sajó. Correspondingly, at the junction with the River Tisza, if Q is low then C_D is greater than both C_p and the background concentration upstream of the source; however, C_p generally exceeds C_D under floods. The total cadmium load reaching the River Tisza ranges between 100 and 3000 kg per month, with a variable ratio of dissolved and particulate matter, as explained before.

Figure 9 shows the effectiveness of the reduction in loading already completed. However, if the load reaching the River Tisza is considered, this management appears much less efficient; in fact, the decrease at the source to $1/10$ of the previous load causes a reduction at the mouth of the River Sajó to between $1/2$ and $1/5$, depending on the hydrological regime. The reason is quite obvious: the rather thick polluted sediment layer is not affected by the change in the system and may act as a secondary source in the future. This also means that the pollution problem has not been solved definitively for the downstream water system.

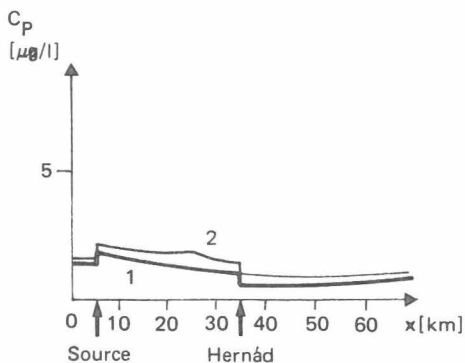


Fig. 9. Effects of load reduction: ①, average flow conditions; ②, higher streamflow rates.

In the course of this research, no quantitative comparisons were given with the observations. The reasons are twofold:

(i) the amount and quality of available data permit only conclusions concerning general trends in the behaviour of the system (Fig. 5);

(ii) in the course of the sediment analysis, C_s was expressed as a fraction of the sediment (the sum of the ignition loss and the acid-soluble part of the dry substance; see Fig. 5). However, the ratio of this fraction to the total amount of sediment is known only with great uncertainty, and consequently the amount of cadmium accumulated, per unit length of the river bed cannot be derived appropriately for the purposes of model comparison. Recalling Fig. 1, it is also stressed that a sufficiently dense sampling of the sediment and the associated chemical analysis would be too costly and cannot be realised in practice.

From the previous reasoning it follows that, although the researchers arrived at many useful answers, the analysis admittedly has weak points. Returning to Fig. 1, the calibration was done on the basis of an annual mass balance, and no validation was performed. Owing to the lack of data, an a posteriori model structure identification could not be done, and the model therefore depends essentially on theoretical knowledge. The transitions between dissolved and particulate fractions were explored satisfactorily, and thus the a priori knowledge improved; however, the same cannot be said for the interaction phenomenon. This is a problem where it was attempted to determine not only the behaviour of fine sediment (a rather unexplored field), but also that of metal pollution associated with the sediment layer. Thus, the description of one of the subprocesses leaves much to be desired, which in turn leaves open the question of whether the involvement of a coupled unsteady-flow-transport model is really required or a simpler, lumped model could be equally useful.

Example 2. Wind-induced sediment-water interaction in Lake Balaton, Hungary

Lake Balaton is the largest shallow lake in Europe; it is a typical wind-affected water body. During the past few years, the eutrophication of the lake has been studied in detail. Through both experimental and modelling work, nutrient cycling in the lake and watershed have been researched and, furthermore, problems of water-quality management considered (for details, see van Straten and Somlyódy, 1980; Somlyódy, 1981). One of the processes of primary importance in the lake is the interaction between water and the sediment layer (which is the feature in common with the previous example), which influences both the uptake and release of various dissolved and particulate, organic and inorganic, living and non-living materials.

Several approaches are possible for studying sediment-water interaction

in lakes (see for example, Lam and Jaquet, 1976; Sheng and Lick, 1979; Fukuda and Lick, 1980). In the study considered here a still different method was chosen (Somlyódy, 1980), on the basis that when considering eutrophication not only physical processes should be examined. Daily measurements were performed for 6 months at the midpoint (depth $H = 4.3$ m) of the Szemes basin (width 7 km, surface area 186 km^2), which can be considered an area of the lake that is approximately uniform in terms of water quality. The measurements involved Secchi depth, temperature, SS, chlorophyll-*a*, and phosphorus fractions at various vertical locations. Wind velocity and direction were recorded continuously, from which hourly averages were calculated. The objective of the first part of the analysis was to describe the dynamics of the suspended solids as a function of wind. This then allows characterisation of temporal changes in light conditions, of the release of phosphorus fractions, and of sedimentation. Finally, all of these processes could be incorporated into an ecological model. Only the behaviour of SS is reported here.

The analysis started with a simplified transport equation describing the temporal and vertical changes of average SS concentration in the basin, neglecting inflow and outflow (the prevailing wind direction is approximately perpendicular to the axis of the lake and the basin). It was recognised, however, that the problem had an undefined boundary condition at the bottom, $z = H$ (Somlyódy, 1980), i.e.,

$$wc - E \frac{\partial c}{\partial z} = \phi_d - \phi_e \quad (1)$$

where c is concentration, w is settling velocity, E is vertical eddy viscosity, and ϕ_d and ϕ_e are the fluxes of deposition and resuspension, respectively. In fact, one of the objectives of the measurements was to formulate this boundary condition. From the observations made, it appeared that the temporal changes governed the system (see Fig. 10 for the depth-integrated values and daily average wind speed). The $c(z)$ profiles were quite uniform, except for the vicinity close to the bottom, where the expected sudden increase could be observed. Accordingly, it was decided not to determine the unknown boundary condition from the PDE formulation (a rather tedious procedure), but to integrate the turbulent diffusion equation along depth and use the ODE derived, which thus directly involves the boundary condition itself.

In order to carry out this step, hypotheses were needed concerning the fluxes ϕ_d and ϕ_e . Deposition was characterised by its probability, as in the previous example:

$$\phi_d = Pw\bar{c} \quad (2)$$

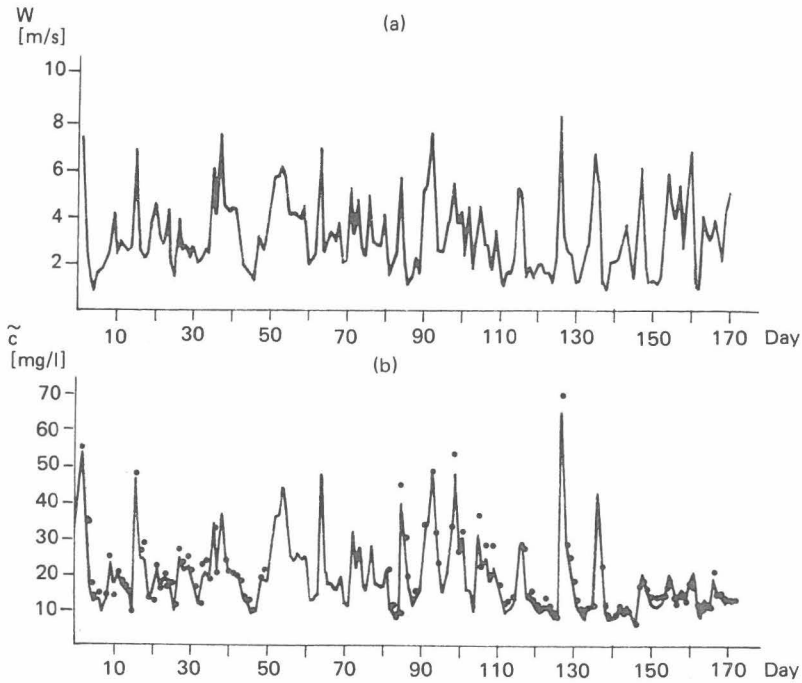


Fig. 10. Identification and parameter estimation of a model for wind-induced sediment–water interaction for Lake Balaton: recursive estimate of concentration of suspended solids (*, observations).

(here, the tilde indicates a depth-averaged value), while ϕ_e was characterised by an empirical relationship (Lam and Jaquet, 1976):

$$\phi_e = k\rho_w \left[\rho_s / (\rho_s - \rho_w) \right] w_e \quad (3)$$

where ρ_s and ρ_w are sediment and water densities, and w_e is entrainment velocity. To find w_e , the concept of energy transformation between potential and turbulent kinetic energies as often employed for stratified lakes was adopted (Stefan and Ford, 1975; Bloss and Harleman, 1979). Accordingly, under simplified conditions,

$$w_e \approx (1/H)W^n \quad (4)$$

where the power n depends on the Richardson number.

Using these hypotheses, the depth-integrated transport equation takes the form

$$d\tilde{c}/dt = -K_1\tilde{c} + K_2W^n \quad (5)$$

where K_1 and K_2 constitute on the one hand parameters listed in part before, being approximately constant for a given situation, and on the other hand

are unknown coefficients derived from the hypotheses (eqs. 2–4). Consequently, the structure of the model should be identified and the values of K_1 and K_2 estimated from measurements. The feasibility of eq. 5 can be appreciated from Fig. 10, which clearly shows the influence of wind velocity on concentration. However, simple regression between W and SS is not sufficiently precise; involvement of SS in a time-series fashion improves the result, thus suggesting an influence of settling and deposition.

Values of K_1 and K_2 were estimated (based on observations made during the first 50 days; see Fig. 10) first using a linear, deterministic least-square fitting technique, by changing n systematically (Somlyódy, 1980). Then, the solutions $\phi_d = 5.57\bar{c} \text{ kg m}^{-2} \text{ d}^{-1}$ and $\phi_e = 0.034W \text{ kg m}^{-2} \text{ d}^{-1}$ were obtained, both of which are of a realistic order of magnitude; for example, a sedimentation velocity of 5.57 m d^{-1} and $P \approx 0.2$ are obtained if a settling velocity of 3 mm s^{-1} is assumed for the $20 \mu\text{m}$ average particle size (Györke, 1978); furthermore, $\bar{c}_e = 0.6 \times 10^{-2} W \text{ kg m}^{-3}$ for the equilibrium concentration (W is expressed in m s^{-1}). The value $n \approx 1$ corresponds to the small Richardson number. Although the results are in agreement with expectations, a posteriori model structure determination was obviously not done.

For this purpose, as a second step, the extended Kalman filter (EKF) method was applied (see for example, Young, 1974; Beck and Young, 1976; Beck and Somlyódy, 1982) to estimate parameter values recursively for each time-step. The model structure can be considered adequate if the parameters as estimated are (approximately) time invariant.

Figures 10 and 11 show the results of the EKF analysis with the value of n being estimated simultaneously. As can be seen from Fig. 11, the parameters become approximately constant after the first 40–50 days (as initial parameter values, estimates from the preceding analysis were applied), resulting in essential information beyond that gained in the preliminary study: the structure of the model is satisfactorily correct. For K_1 , the same value is obtained as before, while K_2 changes according to the increase in the power n . Some slight parameter changes are observed at the end of the period; these may be caused, for example, by the exclusion of inflow–outflow processes (or of other phenomena, such as algal blooms). This suggests that the isolation of subprocesses can only be partial, as stressed before. It should be noted that the absolute value of the wind speed was employed as input, and the inclusion of a perpendicular component did not yield any refinement (the fetch is “large” independent of the wind direction). Certain other phenomena (such as wave motion if $W > 50 \text{ km h}^{-1}$, or pronounced longitudinal seiche) might modify the mechanism of interaction, but these occur rarely in this particular case.

Returning to Figs. 10 and 11, it is stressed that for one month in the middle of the total period the model was used for prediction, since no SS

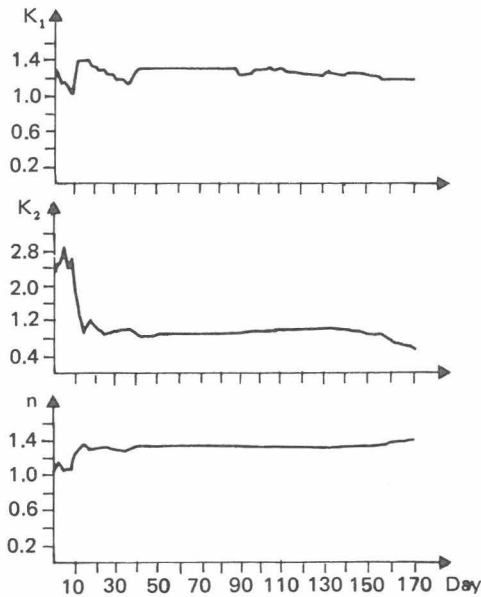


Fig. 11. Recursive parameter estimates for sediment-water interaction model.

measurements were available. The appropriateness of the model is also illustrated by the fact that after including new data, the parameter values did not change. This second period served for validation, following the identification and calibration procedure. Figure 10 shows reasonable agreement between the observations and model calculations. Note that the plot involves the corrected value of the prediction including the new measurements (except between days 50–80); a deterministic prediction has slightly higher deviations from the observed values.

After determining the boundary condition as described above, the original PDE can be solved easily. In fact, this was done using an implicit finite-difference method. Furthermore, since measurements were made for various layers, an effort was made to estimate the vertical distribution of eddy diffusivity: a critical problem to be solved when establishing a three-dimensional lake circulation model (Shanahan et al., 1981).

To summarise, the major steps of the analysis may be repeated with reference to Fig. 1:

- (1) a problem governed by a PDE with an unknown boundary condition was considered (no a priori knowledge was available concerning the boundary condition);
- (2) measurements of regular sampling frequency were performed;
- (3) on the basis of the observations, the PDE was simplified to an ODE

and hypotheses were made concerning the boundary condition, leading to an a priori model structure;

(4) by combining the theoretical and measurement knowledge, the model structure was identified and the parameters estimated with the help of the EKF method; finally, the model was validated.

CONCLUSIONS

In this paper, transport- and water-quality-related problems have been discussed, involving both the relation between the two types and the appropriate modelling procedures. To add one important conclusion to those summarised above, it is felt that hydraulics has well-established tools for solving many flow-related tasks (the same is true for biology or chemistry). The situation is, however, slightly different when considering water quality, which is a result not of the sum of several processes belonging to different disciplines, but rather, of their complicated interactions. The methods employed should express this fundamental behaviour: water-quality models should be based on the description of subprocesses according to their relative importance. This can be realised in most cases, but it is not a simple matter of adding the particular methodologies of physics, biology and chemistry, but of the development of new methodologies on a higher level which somehow comprise the tools of the component individual disciplines: a language which should perhaps be established in the future for water-quality modelling.

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