WATER QUALITY MODELING: A COMPARISON OF TRANSPORT ORIENTED AND BIOCHEMISTRY ORIENTED APPROACHES

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PREFACE

The author was a rapporteur for the session on "Flow Related Transport Phenomena: Water Quality" at the International Conference on Numerical Modelling of River, Channel and Overland Flow for Water Resources and Environmental Applications, organized by IAHR, WMO, IIASA, and the Czechoslovakian Committee of IAHR, and held in Bratislava, Czechoslovakia, May 4-8, 1981.

The request to the rapporteur was to give an overview of the related subject. This formed the first part of the original report and is published here since it considers some typical features and an apparent gap in water quality modeling, and is therefore of more general interest. The papers reviewed are listed in the Appendix.

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1. INTRODUCTION

Water quality and transport are closely related ideas; nevertheless, the difference is obvious, as water quality in general results from many interconnected processes, only one of them being the transport phenomenon. A *transport model* allows one to describe the behavior of a conservative material which is an idealized substance, but only a small portion of the water quality components possess such features. Thus, the appropriateness of a transport model depends very much on how crucial the deviation caused by biological, chemical, and other physical processes is, compared to the assumed conservative behavior. If this is large, the transport equation should be extended by involving the actual reactions, which then often leads to an increase in the number of variables and equations; most of the reactions simply depend on other components of the ecosystems. Assuming that this step is fulfilled, a water quality model results, which accounts for transport phenomena (therefore often called a *coupled water quality-transport model*), consisting of a set of nonlinear partial differential equations (PDEs). At this moment however, the correctness of the development starting from the transport equation is not necessarily obvious; namely, it can easily be the case that the contribution of transport to the total changes is negligible (e.g., biological reactions dominate) and the system can be described by a simplified *water quality model* based on ordinary differential equations (ODEs). Naturally, a general decision in this respect can hardly be made, since it requires the analysis of the relative importance of different processes, which in turn depends on the characteristics of the system considered. This statement implies that it is not considered realistic to work out water quality models of general validity and this is supported by the large variety of models (order of magnitude some hundred) presented in the literature.

The classification of water quality models in general is a huge task (see for example, Cembrowicz et al., 1978). However, when analyzing the link between water quality and transport, or the role of transport in determining water quality (the objective here), the classification is much easier. Essentially two major model groups can be distinguished (note that here models in the research context are considered) in harmony with the previous explanation (a third group will be mentioned later):

(i) *transport* oriented water quality models being oversimplified with respect to biology and chemistry, and based on PDEs (Type 1);

(ii) *biochemistry* oriented models which often exclude the influence of transport and consist of a set of ODEs (Type 2).

In the first case, the word *transport* is emphasized, while in the second, *water quality*. When analyzing the modeling procedure for Types 1 and 2, essential differences can be found. These involve the basic modeling strategy, the methodologies applied, the procedure of data collection, and its interactive character with modeling. The differences can be so fundamental that frequently *a priori* assumptions are made on the relative importance of transport and biochemistry respectively, and thus there is no opportunity to perform a sensitivity analysis by the model itself. In short, there exists a certain gap between transport and biochemistry oriented water quality modeling which calls for an effort to combine the advantages of the two methods. The approaches developed in this manner can be used to create the third type of model, which is desirable but still rarely found in the literature. Models of this kind can also be called, for example, *coupled water quality-transport models*, but in this case, the emphasis is derived primarily from the relative role of the transport. One can use, for instance, the three-dimensional transport equation in some aggregated manner. Here methodological questions play an important part. Preferably, a model structure should be sought which will not *a priori* exclude the applicability of several desired techniques, such as parameter estimation or sensitivity analysis, in the course of the modeling procedures.

In recognition of the contradiction between the models of Types 1 and 2, and the rarely occurring Type 3, it was felt to be realistic to consider the given subject in the light of this discrepancy. This report is organized as follows: First, the modeling procedure is discussed in general, then the strategies applied to Types 1 and 2 are analyzed and compared. The conclusion from this will serve to provide some discussion of the features of Type 3. Examples will be presented to illustrate this.

2. MODELING PROCEDURE

2.1 Basic Steps of the Modeling Procedure

Some of the basic steps of modeling will be stressed here, rather than a general strategy for application. For this purpose, two figures in a slightly modified form are adapted from the literature (Eykhoff, 1974, and Beck, 1981) and combined in Figure 1.

At the beginning of the water quality modeling process, the "reality": the specific system (river, lake, or others) and problem (e.g., oxygen or thermal household, eutrophication) and furthermore, the objective of the study (understanding, prediction, control, planning, management, etc.) is 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 and measurement, and their dual nature is clearly expressed in Figure 1a. The first,

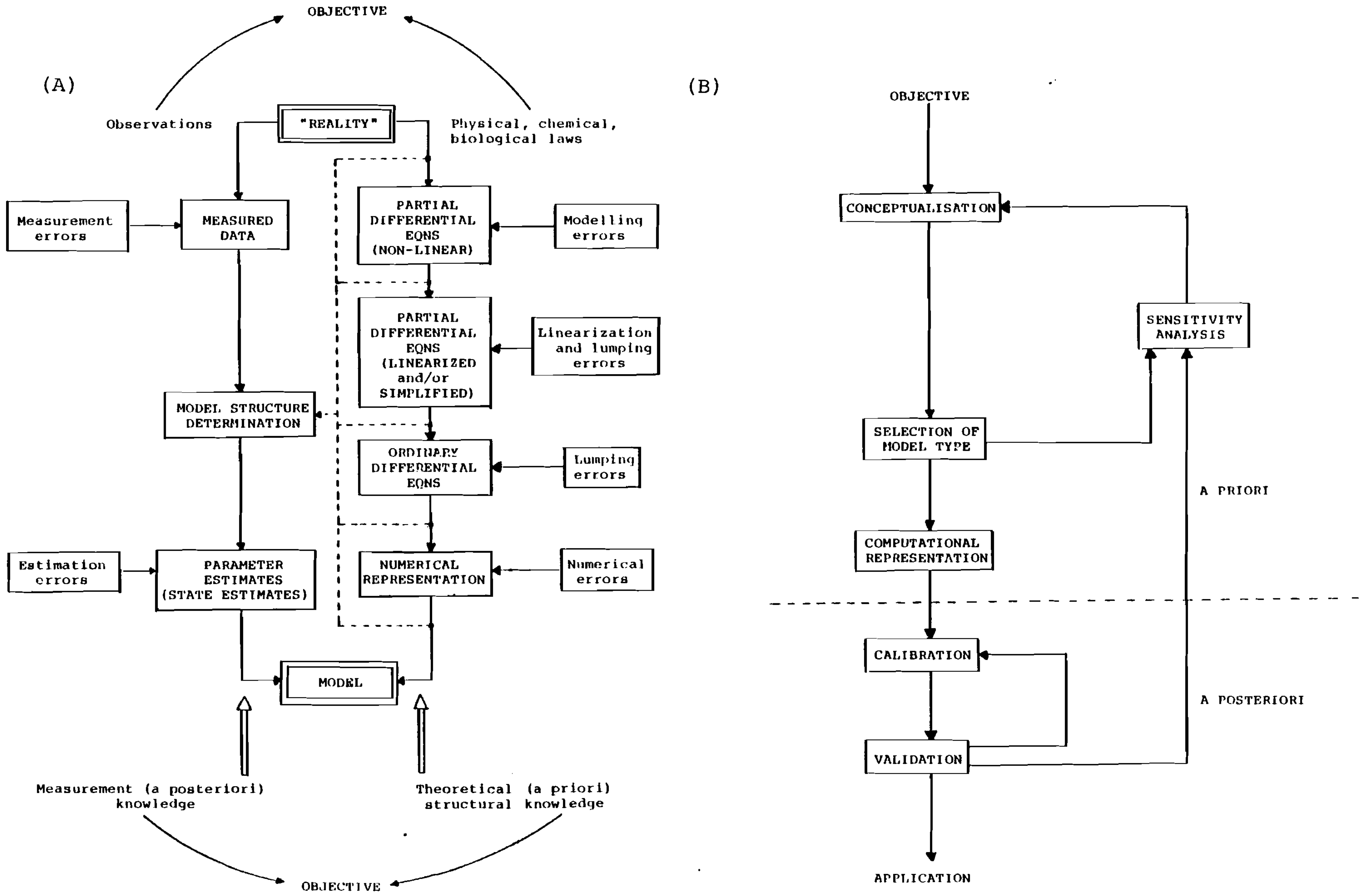

Figure 1. Illustrations of the Modeling Procedure by combining Theoretical and Measurement Knowledge (after Eykhoff, 1974 and Beck, 1981)

associated with *a priori* structural *knowledge*, is based on natural laws (such as mass and momentum conservation) and can be expressed by nonlinear partial differential equations. These latter will then often be simplified and solved for the most part, numerically.

For the development of models, some observations should be available beforehand (*a priori* measurement knowledge). This is necessary to characterize the physical system considered, select the water quality variables to be involved, establish the order of magnitude of their temporal and spatial changes, and represent the physical system in the model in accordance with them. All these steps, together with others not listed, belong to the conceptualization, *a priori* model structure determination and the selection of model type (see Figure 1b and for details, Beck, 1981). Any further progress needs systematically planned experiments and data collection of an interactive character with the model development. The sum of the information gained can be called *a posteriori* (measurement) *knowledge* (see Figure 1), which then allows for identification of the model structure (often thought to be correct on the theoretical basis), for estimation of the unknown parameters (rate constants, dispersion coefficients, etc.) and for the model validation. Note that the meaning of validation is quite broad: it may mean the successful application of the model after calibration for a new set of data, its use under changed conditions (both are extensions in time) or for example, for other reaches of the same system (spatial extension).

Thus, the model results from a procedure which incorporates the *a priori* and *a posteriori knowledge*, accounts for the plentiful errors indicated in Figure 1, and involves several loops and feedbacks. The way of combining the theoretical and measurement knowledge depends essentially on the subject considered. As two extremes, modeling in hydrology and hydrodynamics, can be mentioned. The first way is characterized by the dominant role of *a posteriori knowledge* (e.g., flood forecasting using the historical data of two gauges), while the second is characterized by structural knowledge (e.g., computation of the same flood events based on the Saint-Venant equations, if the downstream boundary condition is known).

The (*a posteriori*) model structure determination and the interaction with data (Figure 1a) can also be important for situations when the theoretical knowledge is well established. It is sufficient to mention that in nature, the conditions are not "pure", as contrasted to the assumptions used when the equations are derived. Thus, modeling errors (Figure 1a) cannot be avoided. Problems related to boundary conditions are especially important. Here as an example, the influence of dead zones near to river banks and in river beds on dispersion phenomena is referred to only in a study by Beer and Young (1980). They achieved a better agreement to measured concentrations with a dead zone time series model than with the conventional longitudinal dispersion equation. This fact suggests that the accumulation and release of dead zones exert a larger contribution (together with the time lag caused) on dispersion than the spatial non-uniformities in the water body, thus being the dominant mechanism. This calls into question the "self-evident" use of the classical dispersion equation.

Using the theoretical and accrued measurement knowledge, one can develop different models for the same problem. The obvious goal is to find the simplest but still realistic version, since accomplishing the necessary steps in the modeling framework (uncertainty and sensitivity analysis, parameter estimation, etc.) depends essentially on the model structure. The contrast among techniques available for partial and ordinary differential equations (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, the realization of the modeling procedure illustrated in Figure 1 is simply unrealistic (see also later); the data collection would 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 the spatial changes are dominant (many spatial "boxes" should be considered) and/or the number of water quality components (e.g., ecological "compartments") to be incorporated is high. Under such conditions, some compromise strategy should be looked for.

2.2 Procedure for Transport Oriented Modeling

The structure of the model is given by the transport equation, which further involves some simple biochemical reaction terms (i.e., a first order decay form). The transport equation can, in a usual case, be used to calculate the concentration in the given water body, as a function of time and three spatial coordinates. Frequently, the equation is employed simultaneously with the corresponding version of the equations of continuity and motion, thus resulting in a set of highly nonlinear partial differential equations (see Watanabe et al., 1980).

These can then be solved numerically, e.g., by the methods of finite differences or finite elements. The technique applied is generally closely related to the formulation of the boundary conditions, the assumptions made on the variation of different coefficients and the simplification related to terms involved in the equations. Further distinction depends on whether the number of independent variables can be reduced or not and the description of turbulence (Watanabe et al., 1980; Launder and Spalding, 1972). Thus, the modeling procedure is very much based on the theoretical knowledge and as seen in Figure 2, the determination or the *a posteriori* model structure is absent. Measurements are certainly important, but mainly used for finding some of the parameter values, such as roughness and mixing coefficients, or for checking the velocity field computed. The validation also has a slightly different meaning and a study on error propagation or model sensitivity is rarely done.

These features have a strong methodological background; the majority of steps indicated in Figure 1 were carried out for ordinary differential equations, but for PDEs only some very limited efforts surface in the literature (Thau, 1969; Koivo and Koivo, 1977).

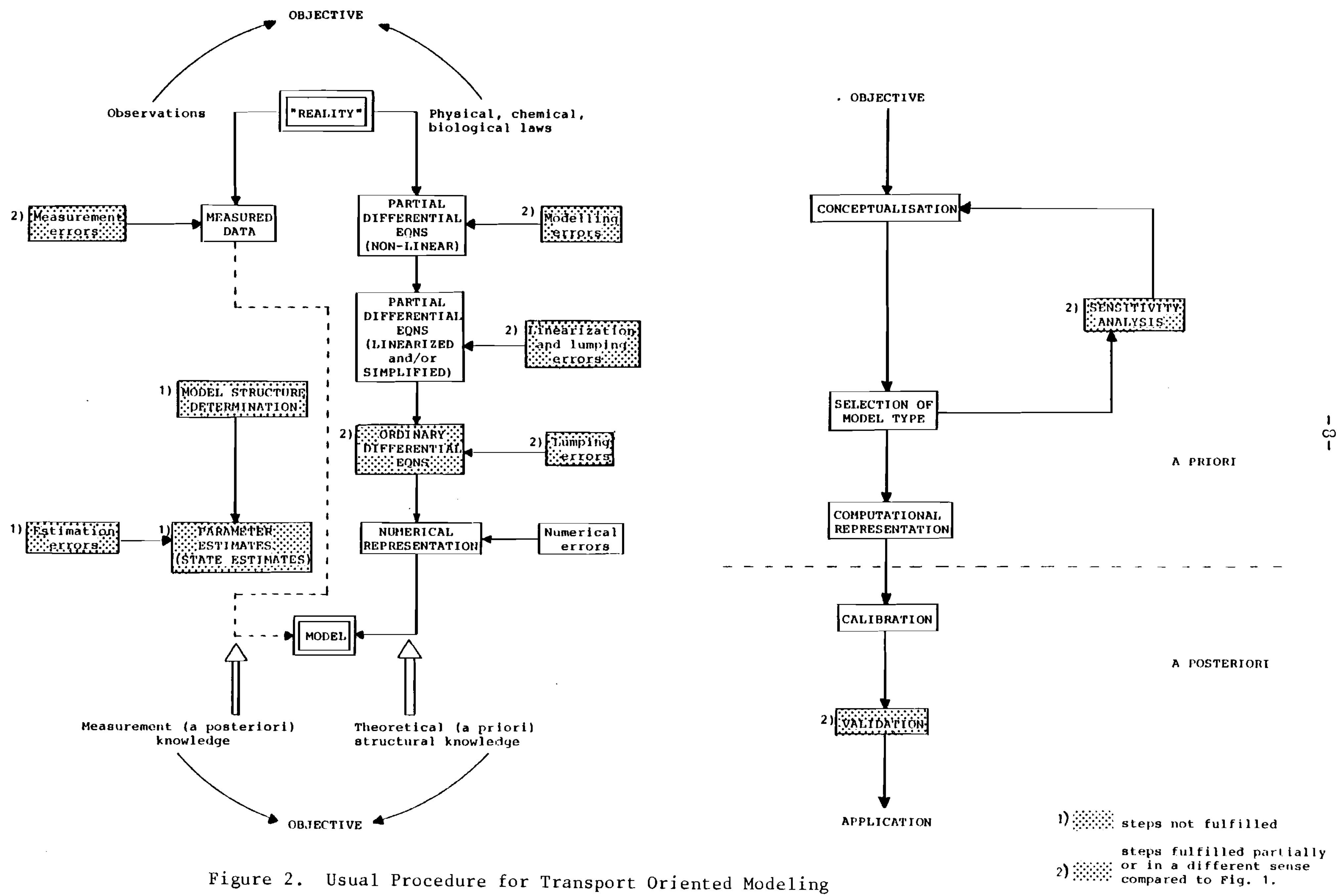

Figure 2. Usual Procedure for Transport Oriented Modeling

Generally, the numerical solution of a PDE can be replaced by the solution of N number of ODEs, but the methodological problem still remains: the number of state variables will be much larger than that of the obvervational variables, thus prohibiting the application of techniques in question.

2.3 Procedure for Biochemistry Oriented Modeling

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

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

Second, in relation to the structure and complexity of models, quite often they manifestly intend to describe subprocesses as detailed as possible, which leads to an overabundance of state variables and parameters without enough data to identify the model structure and calibrate it. These latter problems are not only due 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 Figure 1 cannot be applied. The presence of nonlinearities, empirical functions, and discontinuities increase the difficulties. Thus, in many cases the parameter estimation is downgraded to a simple trial and error fitting and there is no *a posteriori* model structure determination in a strict sense.

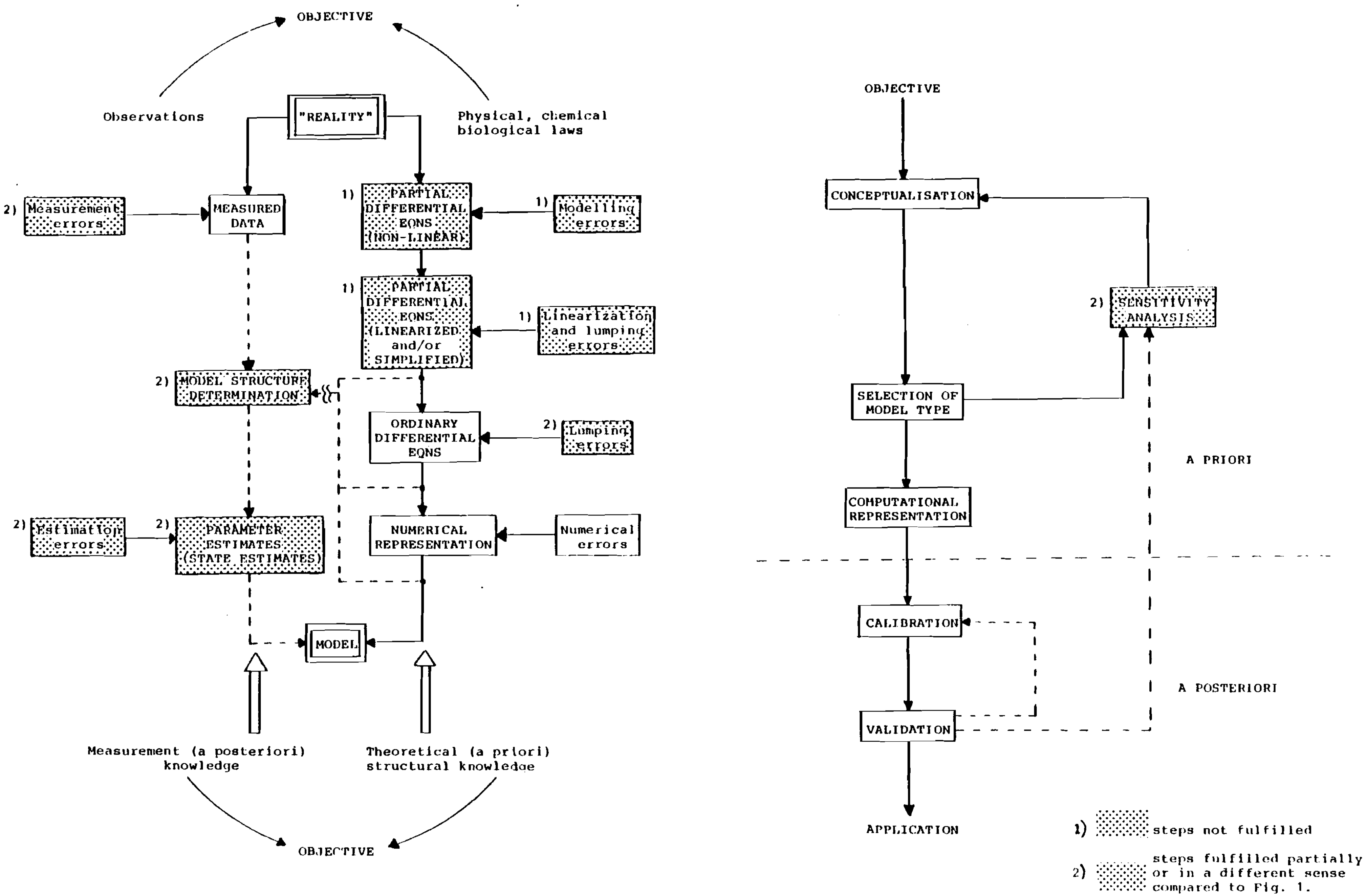

Figure 3. Procedure for Biochemistry Oriented Modeling

2.4 Conclusions and Comments on the Modeling Procedure

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

(1) none of the strategies discussed can have a general validity (Types 1 and 2);

(2) either of the two approaches excludes the possibility of model extension by *a priori* assumptions in the course of the development towards the involvement of the less emphasized phenomena; in other words, the structures are not flexible enough;

(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 ecological compartments), the scheme illustrated in Figure 1 cannot be realized in a strict sense.

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

A situation characterized by (3) is therefore considered, for which the modeling at first appears so difficult that this work may seem fruitless. The author rejects this outlook, since modeling is believed to be generally useful. It is instead suggested that Figure 1 be considered as a framework for modeling which depicts the interaction between modeling, data collection, and experiments, and moreover, many of the required steps. These need not necessarily be involved in a closed form of the model as one large unit. The way proposed is off-line in character, the idea being to separate as many subprocesses and modeling steps as possible (it is stressed here that the isolation can never be complete; therefore the aim is to apprehend the dominant features), to study them independently and then couple the distilled knowledge according to Figure 1. For example, quite often the system can be approached with a set of completely mixed reactors (Beck and Young, 1976; and Szöllösi-Nagy, 1977), to which the combined information from a transport model can be linked (van Straten and Somlyódy, 1980; and Shanahan et al., 1981). In other cases, some of the biological or chemical phenomena can be treated separately. As an example, the estimation of algal growth parameters from vertical primary production measurements can be mentioned (van Straten and Herodek, 1981; see also Example 2 for another problem).

When working out the model, some properties to seek include a *harmony* in the descriptive process, as stressed before, *flexibility*, and *simplicity*. The analysis of time and length scales, and the order of magnitudes are extremely useful in obtaining harmony (Verboom and Vreugdenhil, 1975; Harleman and Shanahan, 1980). Flexibility will allow for the testing of hypotheses simultaneously (Spear and Hornberger, 1980; Hornberger and Spear, 1980; and Fedra et al., 1981), and the extension of modification of the model at each stage in the development according to the needs. The role of simplicity is obvious if the structure of Figure 1 is kept in mind. This also extends to the numerical techniques applied, especially if PDEs are involved. Fast methods on the computer enable one to perform a numerical uncertainty and sensitivity analysis (see an example for a one-dimensional lake seiche model in Somlyódy and Virtanen, 1981), and to estimate parameter values.

In summary, all this means nothing more than a spiralling circulation focusing on the core of the problem through utilization and constant improvement of theoretical and measurement knowledge, and a combination of the most appropriate methodologies. One would hope that in this way, the study is properly completed by a reasonable model approach to the reality. From time to time, and provisionally, the conclusions could even be negative. In a field such as water quality modeling, which has a relatively short history and pronounced interdisciplinary character, this is quite self-evident.

2.5 Examples Illustrating the Modeling Procedure

The first example is related to a river problem where much emphasis was laid on determining the relative importance 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. When beginning with a PDE and aggregating it to an ODE, the majority of steps in Figure 1 could be realized.

Example 1. Study of the Cadmium Pollution of the River Sajó, Hungary.

The river is one of the tributaries of the Tisza River (Figure 4a) located in the northern part of Hungary. It is of medium size with a mean streamflow of around 30 m^3/s and a large fluctuation between 5 and 500 m^3/s. The river is characterized by a high degree of sinuosity and consequently an effective mixing. It is heavily polluted in organic materials and heavy metals, among which Cadmium is perhaps the most important of those released basically from a single point source (Figure 4a). The Cd pollution was studied intensively between 1973-78 (see Literáthy and Lászlo´, 1978); dissolved and particulate forms, spatial and temporal changes, and the bottom sediment were observed. The average load was estimated at approximately 15,000 kg/year, 60-70% of which is deposited to the sediment. On a long-term basis, the metal content of the sediment decreased exponentially downstream from the source, clearly showing the influence of accumulation. The majority of Cd was bound to the 25-50 μm fraction. Under low flow conditions, the longitudinal change of concentration had a similar character to that of the sediment pollution. At higher streamflow rates, however, the role of resuspension became apparent, also causing at times increases in the concentration in the flow direction. The influence of floods was also studied. They smoothed out the pollution pattern of the sediment through re-entrainment, convection, and repeated deposition. The character of the river suggested that anaerobic conditions in the sediment are rarely occurring. This also meant that there was 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), but the downstream river system is certainly endangered (i.e., Cd is stirred up and transported under flood conditions, then deposited and re-mobilized in reservoirs).

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 process and to perform some extrapolation on the past (no historical data were available) and future (the load was reduced in 1979 to 1/10 its size). The results are being reported in detail by Somlyódy et al., (1981).

The in situ measurements showed that the river reach studied (Figure 4a) had a rather uniform chemical environment. Two dominant mechanisms were found to relate to the changes in dissolved and particulate forms (C_D and C_P) in the water: coprecipitation and adsorption on the suspended solids (SS). The first depended 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 in the cross-section for a relatively short river length (some km). Accordingly, all three processes were assumed later in the modeling work to take place instantaneously. On the basis of frequent effluent water quality measurements, the pH and thus the C_D/C_P ratio were found to fluctuate drastically. However, due to coprecipitation and adsorption in the river, the particulate Cd was dominant, leading to accumulation in the sediment layer through settling. The deposition and re-entrainment of fine sand ($\sim$120 μm) and natural river sediment ($\sim$30 μm) were studied in a laboratory open channel and *hypotheses* were made on the probability coefficients of both processes (Sayre, 1969; Graf, 1971; and Partheniades, 1977), depending on the streamflow (they were assumed to be proportional to $(1+Q)^{-1}$ and Q, respectively).

The model developed interactively with experiments involved three state variables for Cadmium (Figure 4b): concentrations C_D, C_P, and C_S (the latter expressing the pollutant content of the sediment related to unit river length), among which SS played a controlling role (this was simply described by an SS(Q) rating curve). The adsorption was characterized by a Langmuir isotherm and the coprecipitation as a function of dilution--both based on laboratory measurements. It is noted that bioaccumulation was also studied, but not involved in the model (under the present conditions it does not exceed 1 kg). For the interaction between water and sediment, a modified, nonlinear version of Sayre's approach was used (Sayre, 1969), which distinguished 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 the equations of unsteady flow (Mahmood and Yevjevich, 1975 and Kozák, 1977) were coupled. The five PDEs were solved simultaneously by using the method of finite differences. For the transport equations, the fractional step method (Verboom and Vreugdenhil, 1975) was employed with explicit schemes, while for the flow problem an implicit scheme, followed by the economic double sweep technique for the solution of the linearized algebraic system of equations (Mahmood and Yevjevich, 1975; note that its stability should be checked carefully. For a similar matrix method where stability can be proved, see Somlyódy and Virtanen, 1981). To make the solution more economical, models for steady flow and quasi-permanent transport were also elaborated; the combination of them depended on the boundary conditions and were controlled inside the model. For the quasi-steady conditions, the transport equations were linearized: the dispersion neglected, and the solution derived by linking the analytical solution of the problem for subreaches of length Δx_i.

Figure 4c shows the appropriateness of the unsteady flow model. In this example, the upstream and downstream water levels (locations 1 and 3 on Figure 4a) were used as boundary conditions, while the Manning roughness coefficient was calibrated (k=36) independently with the help of the steady flow model and an observation of the longitudinal free surface profile.

For the transport model, the settling velocity and probability coefficient of deposition were determined from experiments and literature respectively, while the 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

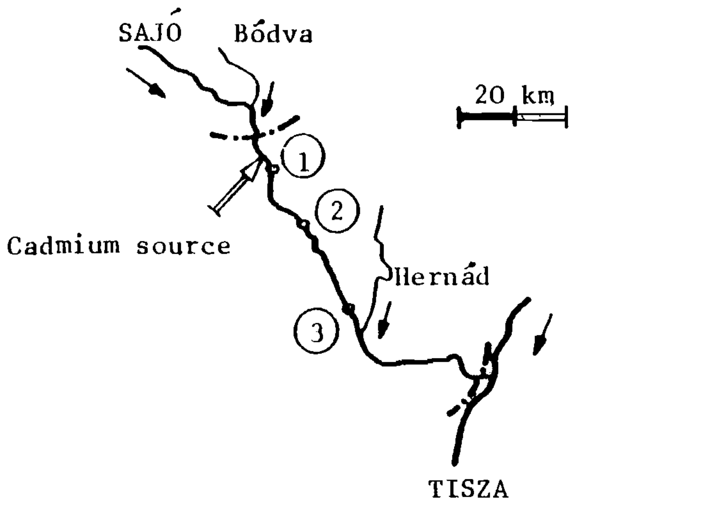

Figure 4a. The studied reach of River Sajó
—·— boundary of the reach

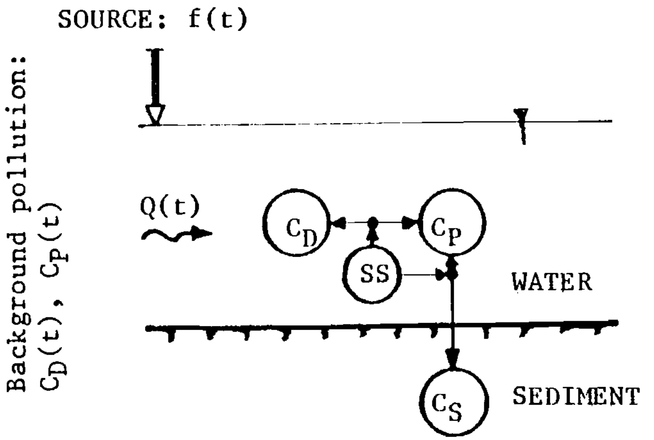

Figure 4b. State variables involved

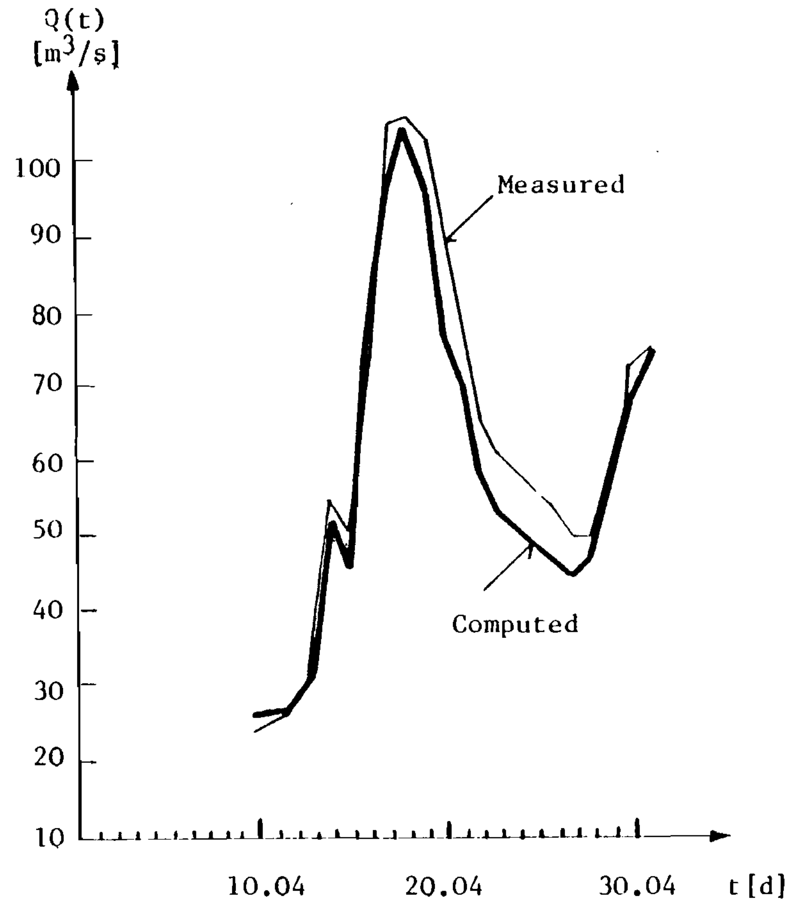

Figure 4c. Measured and computed streamflows, station 2, period 10-30.04.1975

pattern gained (Figures 5a and 1) is in reasonable agreement with observations (Somlyódy et al., 1981). Next, a specific year was considered, consisting of a six-month low flow period ($Q = 20\ m^3/s$) followed by a 30 day long flood (historical scenario, $Q_{max} = 150$) and an average regime. Figure 5a involves the particulate concentration distributions at the end of each period (2, 3, and 4 in the same sequence as before). As can be seen, during the first and third periods, deposition dominated and more than 10t Cd reached the bottom; however, it was striking to note that approximately 30% of this amount was stirred up by the flood. The corresponding $C_P(x)$ distribution is also essentially different from the two others, as it is much more uniform along the river. With regard to the dissolved Cd, it is worthwhile mentioning that on average, 60% is transformed ultimately to particulate form, which is then removed essentially by sedimentation. However, the rest of the Cd behaves like a conservative material (affected only by the dilution at the mouth of River Hernád, as the chemical environment did not change notably along the river). Accordingly, at the junction of the River Tisza, C_D is more plentiful than C_P and the background concentration upstream of the source, if Q is low, but C_P generally exceeds C_D under floods. The total Cd load reaching the Tisza River may range between 100-3000 kg/month with a variable dissolved-particulate ratio as explained before.

Figure 5b shows the effectiveness of the loading reduction already completed. If however, the load of River Tisza is considered, this management is much less efficient; in fact, 1/10 decrease at the source causes a reduction at the mouth of River Sajó between 1/2-1/5, depending on the hydrologic 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 for the future. This also means that the pollution problem is not solved unambiguously for the downstream water system.

In addressing the problem, the researchers arrived at many useful answers, but admittedly they had weak points. Recalling Figure 1, it should be stressed that an in situ data collection of a sufficiently dense sampling frequency is unrealistic in this

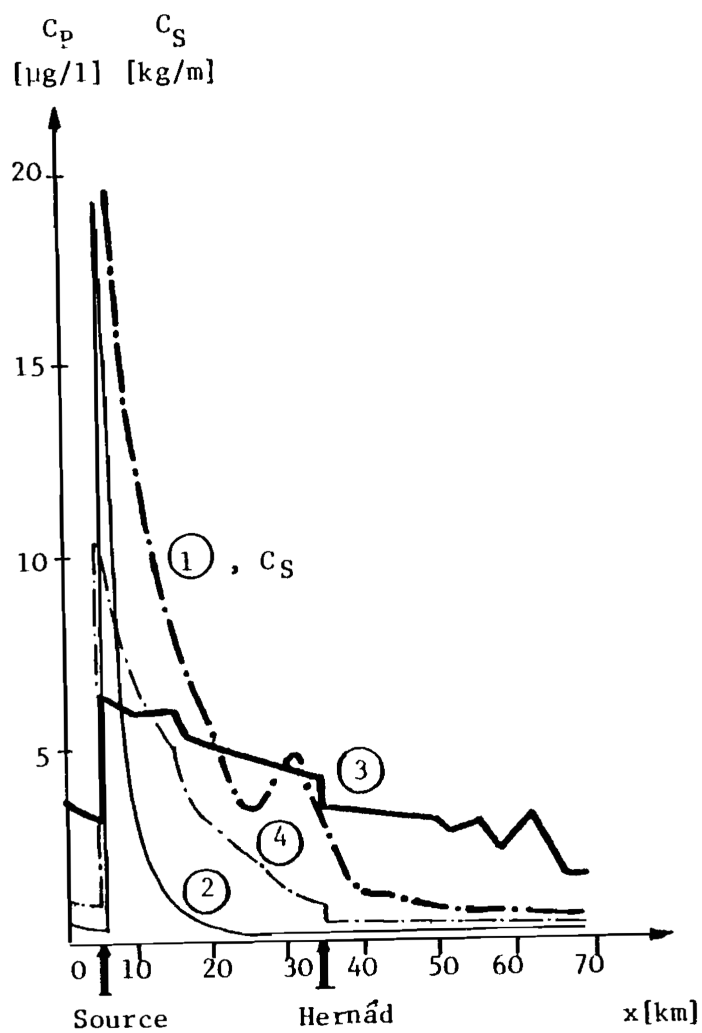

Figure 5a. Distribution of particulate and sediment Cd concentrations along the river

(1) pollutant content of the sediment after 20 years, C_S
(2) - (4) simulation of a specific year: $C_P(x)$ at different times

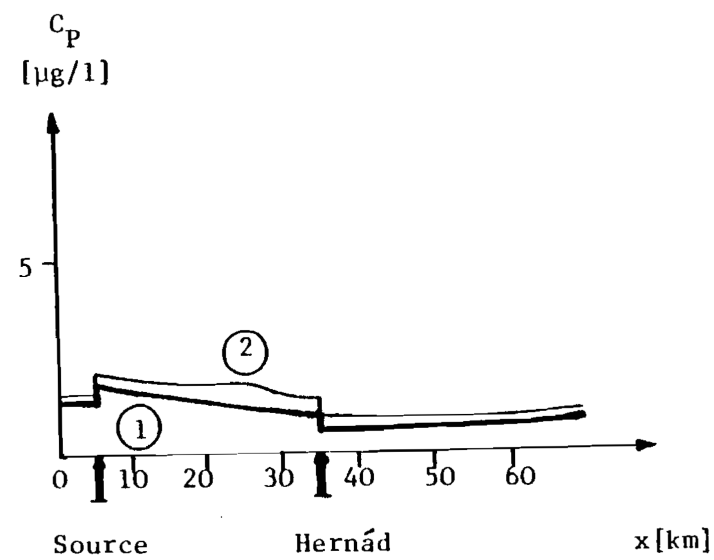

Figure 5b. Effect of load reduction

(1) Average flow conditions
(2) Higher streamflow rates

case and perhaps the strategy presented is the most reasonable. This ultimately means that an *a posteriori* model structure identification cannot be performed and the quality of the model depends essentially on the theoretical knowledge of the problem. It is felt that 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 not only is it attempted to pinpoint the behavior of the fine sediment (a rather unexplored filed), but also that of the 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 can be equally useful.

Example 2. Wind Induced Sediment-Water Interaction in Lake Balaton, Hungary

This lake is the largest shallow lake in Europe; 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 modeling work, the nutrient cycling in the lake and watershed, and furthermore, the problem of water quality management (for details, see van Straten and Somlyódy, 1980) have been researched. One of the processes of primary importance in the lake is the interaction between water and the sediment layer (and this is the common feature with the previous example) influencing both the uptake and release respectively of several dissolved and particulate, organic and inorganic, and living and non-living materials.

For studying the sediment-water interaction in lakes, several approaches are possible (see, for example, Lam and Jaquet, 1976; Sheng and Lick, 1979; and Fukuda and Lick, 1980). In this study, still a different method was chosen (Somlyódy, 1980), in the recognition that when eutrophication is considered, 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 more or less as one of the uniform areas of the lake in terms of water quality. The measurements involved Secchi depth, temperature, SS, Chl-a, and phosphorus fractions at different 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 for a characterization of the temporal changes in the light conditions, the release of phorphorus fractions, and the sedimentation. Lastly, all these processes can be incorporated into an ecological model. Only the behavior of SS is reported in this paper.

The analysis started with a simplified transport equation for describing the temporal and vertical changes of the averages 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 recognized however, that the problem had an undefined boundary condition at the bottom, $z = H$ (Somlyódy, 1980).

$$wc - E \frac{\partial c}{\partial t} = \phi_d - \phi_e \quad , \tag{1}$$

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 the boundary condition. From the observations made, it appeared that the temporal changes governed the system (see Figure 6 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 the depth, and use the ODE derived, which thus directly involves the boundary condition itself.

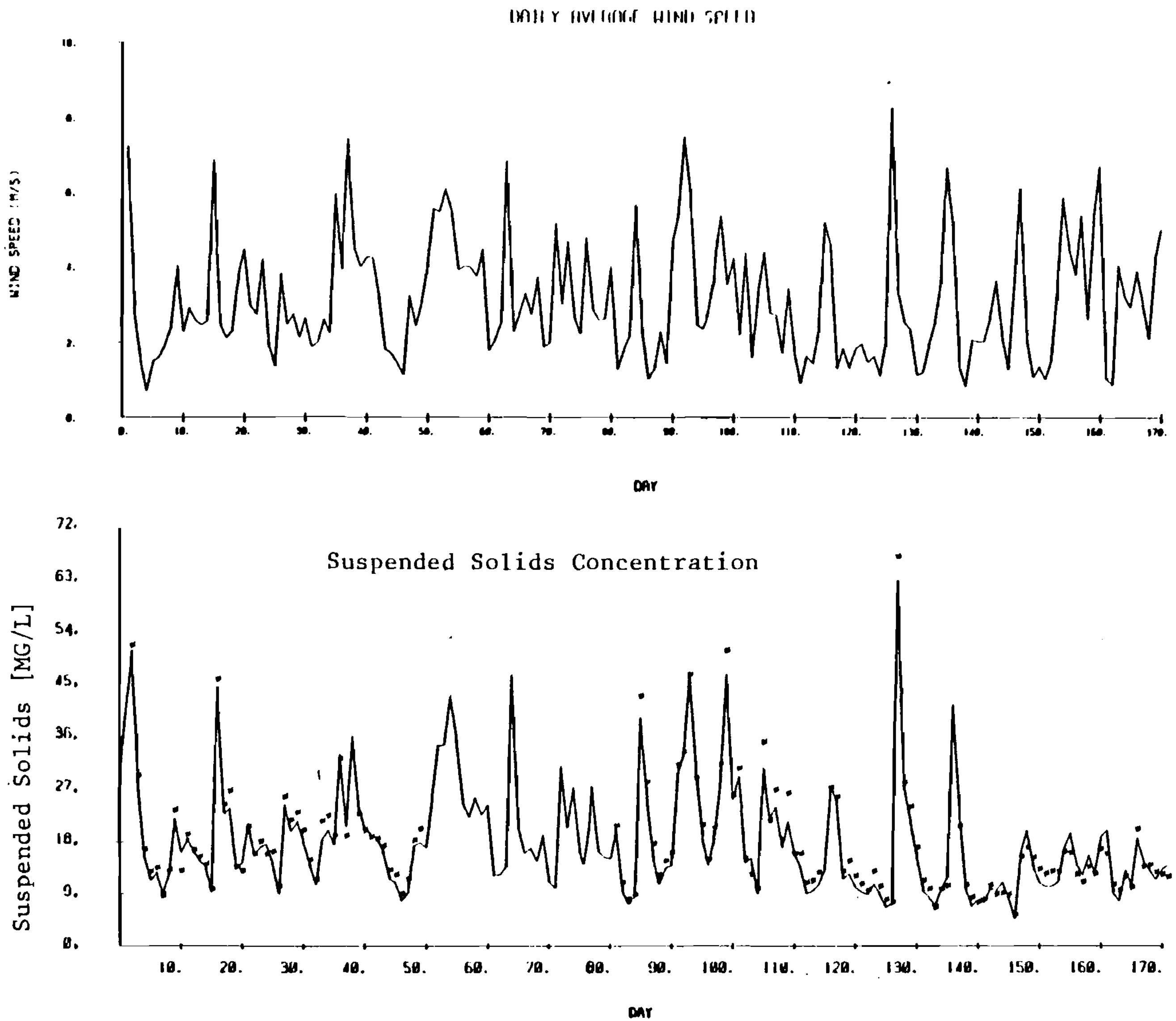

Figure 6. Identification and parameter estimation of a model for wind induced sediment-water interaction for Lake Balaton: recursive estimate of the suspended solids concentration

* Observations

In order to carry out this step, *hypotheses* were needed for the fluxes ϕ_d and ϕ_e. The deposition was characterized by its P probability as in the previous example.

$$\phi_d = Pw\tilde{c} \quad , \tag{2}$$

(here, the waved line indicates depth averaged value), while ϕ_e by an empirical relationship (Lam and Jaquet, 1976).

$$\phi_e = k\rho_w \frac{\rho_s}{\rho_s - \rho_w} w_e \quad , \tag{3}$$

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 transformulation between potential and turbulent kinetic energies often employed for stratified lakes was adopted (Stefan and Ford, 1975; Bloss and Harleman, 1979). Accordingly, under simplified conditions:

$$w_e \sim \frac{1}{H} W^n \quad , \tag{4}$$

where the power depends on the Richardson number.

Using these *hypotheses*, the depth integrated transport equation takes the following form:

$$\frac{d\tilde{c}}{dt} = -K_1\tilde{c} + K_2W^n \quad , \tag{5}$$

where K_1 and K_2 comprise on the one hand parameters listed in part before, being approximately constant for a given situation, and unknown coefficients on the other hand, derived from the hypotheses (Equations 2 to 4). Consequently, the structure of the model should be identified and the parameter values, K_1 and K_2, estimated from measurements. The feasibility of Equation (5) can be appreciated from Figure 6, which clearly shows the influence of the wind velocity on the concentration. However, a simple regression between the W and SS is not precise enough; the involvement of SS in a time series fashion improves it, thus suggesting the influence of settling and deposition.

The values of K_1 and K_2 were estimated (based on the observations of the first 50 days, see Figure 6) first by using a linear deterministic least square fitting technique by changing n systematically. Then, solutions:

$$\phi_d = 5.57\ \tilde{c}\ \mathrm{kg/m^2d} \quad \text{and} \quad \phi_e = 0.034\ W\ \mathrm{kg/m^2d}$$

were arrived at, both serving realistic order of magnitudes, for example 5.57 m/d for the sedimentation velocity and $P \cong 0.2$ if 0.3 mm/s settling velocity is assumed to belong to 20 μmm average particle size (Györke, 1978); furthermore $\tilde{c}_e = 0.6\ 10^{-2}W$ [kg/m^3] for the equilibrium concentration (W is expressed in m/s). The value $n \simeq 1$ coincides with the small Richardson number. Although the results were in harmony with the expectations, the *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; and Beck and Somlyódy, 1981, for this problem) which estimates among other things, the parameter values recursively for each time step. Thus, it can be used for the identification of model structure: it is accepted if the parameters are practically time invariant.

Figures 6 and 7 involve results gained with EKF when the value of n was also estimated. As can be seen from Figure 7, the parameters become approximately constant after the first 40-50 days (as initial parameter values, the estimates of the previous 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 was given as before, while K_2 changed in harmony with the increase in the power n. Some slight parameter changes can be observed at the end of the period; this may be caused, e.g., by the exclusion of inflow-outflow processes (or by other phenomena such as algae blooms). This suggests that the isolation of subprocesses can only be partial as was stressed before. It should be noted that as input, the absolute value of the wind speed was employed and the inclusion of a perpendicular component did not cause any refinement (the fetch is

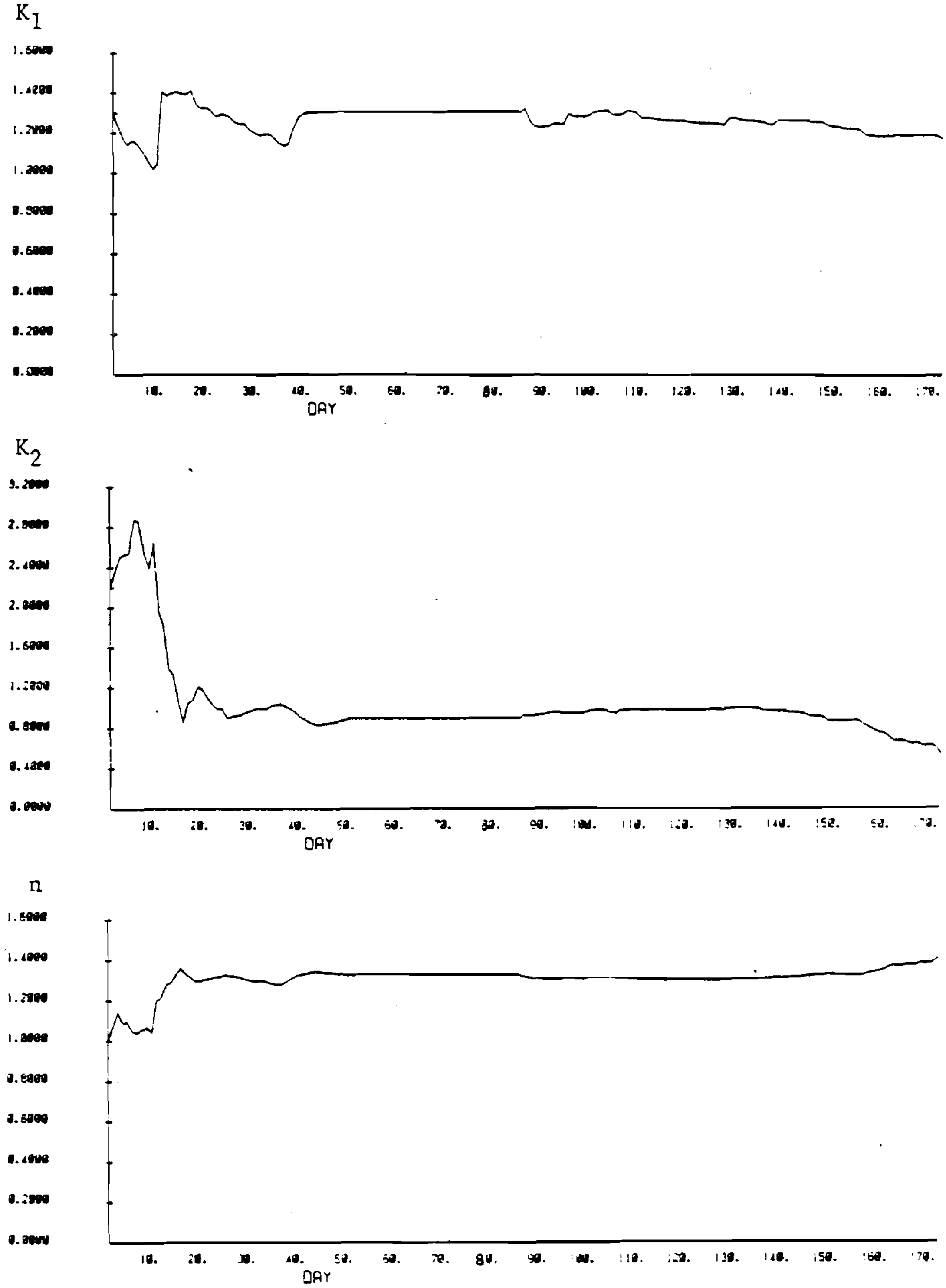

Figure 7. Recursive parameter estimates for the sediment-water interaction model

"large" independently of the wind direction). Some other phenomena (such as wave motion if $W > 50$ km/h, or pronounced longitudinal seiche) may modify the mechanism of interaction, but these rarely occur in this particular case.

Returning to Figures 6 and 7, the author stresses that for one month the middle of the total period, the model was used for prediction, since no SS measurements were available. The appropriateness of the model is also illustrated by the fact that after getting new data, the parameter values did not change. This second period served for validation, following the identification and calibration procedure (see Section 1). Figure 6 presents the reasonable agreement between observations and model calculation. Note that the plot involves the corrected value of the prediction in possession of the new measurement (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 by using an implicit finite difference method. Furthermore, having measurements for different layers, an effort has been made to estimate the vertical distribution of eddy diffusivity. This poses a slightly different problem of primary importance when the calculation of lake circulation is considered (Shanahan et al., 1981).

To summarize, the major steps of the analysis are repeated in the light of Figure 1:

(1) a problem governed by a PDE with an unknown boundary condition was considered (no *a priori* knowledge was available on the boundary condition);
(2) measurements of regular sampling frequency were performed;
(3) concluding from the observations, the PDE was simplified to ODE and hypotheses were made on the boundary condition leading to the *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.

3. CONCLUSIONS

In the report, transport and water quality related problems were discussed, involving both the connection between the two and the modeling procedures. To add one important conclusion to the others summarized in Section 2.4, it is felt that hydraulics has its 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 not a result of the sum of several processes belonging to different disciplines, but rather, their complicated interactions. The methods employed, furthermore, have to express this fundamental behavior: water quality models should be based on the description of subprocesses according to their relative importance. This can be realized in most of the cases, but it is not a simple matter of adding the particular methodologies of physics, biology and chemistry, but of development of new methodologies on a higher level which somehow comprise the tools of the individual disciplines: a language which should perhaps be established in the future for water quality modeling.

APPENDIX: LIST OF PAPERS REVIEWED

1. Baumert, H., Luckner, L., Müller, W.D., and Stoyan, G.:
   A generalized programme package for the simultaneous simulation of transient flow and matter transport problems in river networks.

2. Glos, E., Frotscher, D., Baumert, H., and Schmidt, H.:
   Analysis and simultaneous simulation of transient flow and matter transport scenarios for a lowlands river network using a generalized programme package.

3. Braun, P., and Koehler, W.:
   Ecologically oriented matter transport model for shallow rivers.

4. De Smedt, F., Ideler, W., and Van der Beken, A.:
   A water quality transport model for the channel network of Northern Belgium.

5. Michna, L.:
   Mathematical water quality modeling of a trout system for determination of an optimal advanced waste treatment level.

6. Czernuszenko, W.:
   Unsteady diffusion of solutes in natural streams.

7. Bähler, M.:
   Relations between the dispersion of a conservative substrate and the hydraulic resistance behaviour in a turbulent flow.

8. Lafleur, D.W., McBean, E.A., and Al-Nassri, S.A.:
   Design and analysis of stormwater retention ponds based on water quality objectives.

REFERENCES

Beck, M.B. 1981. A Procedure for Modelling, in Mathematical Modeling of Water Quality (G.T. Orlob, editor): Wiley Chichester (in press).

Beck, M.B., and L. Somlyódy. 1981. Identification of a Model for Wind Induced Sediment-Water Interaction in Lake Balaton. International Institute for Applied Systems Analysis, Working Paper (forthcoming), Laxenburg, Austria.

Beck, B., and P. Young. 1976. Systematic Identification of DO-BOD Model Structure, in Journal of The Environmental Engineering Division, Proceedings of the American Society of Civil Engineers, Vol. 102, No. EE5.

Beer, T., and P.C. Young. 1980. On the Characterisation of Longitudinal Dispersion in Natural Streams. Cres Report No. AS/R42, Centre for Resource and Environmental Studies, Australian National University.

Bloss, S., and D.R.F. Harleman. 1979. Effect of Wind-mixing on the Thermocline Formation in Lakes and Reservoirs. Massachusetts Institute of Technology, Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, Report No. 249.

Cembrowicz, R.G., H.H. Hahn, E.J. Plate, and G.A. Schultz. 1978. Aspects of Present Hydrological and Water Quality Modelling, in Ecological Modelling: Elsevier Scientific Publishing Company, Amsterdam, The Netherlands.

Eykhoff, P. 1974. System Identification - Parameter and State Estimation: Wiley, Chichester.

Fedra, K., G. van Straten, and M.B. Beck. 1981. Uncertainty and Arbitrariness in Ecosystems Modelling: A Lake Modelling Example, in Ecological Modelling, Elsevier Scientific Pub. Co., Amsterdam, The Netherlands.

Fukuda, M.K., and W. Lick. 1980. The Entrainment of Cohesive Sediments in Freshwater, in Journal of Geophysical Research, Vol. 85, No. C5, May 1980.

Graf, W.H. 1971. Hydraulics of Sediment Transport: Mcgraw-Hill, New York.

Györke, O. 1978. Formation of SS Concentration in Shallow Lakes and Reservoirs, VITUKI Report, 7411/2-323 Manuscript (in Hungarian).

Harleman, D.R.F., and P. Shanahan. 1980. Aspects of wind-driven circulation and mixing in eutrophication studies of Lake Balaton, in Proceedings of the Second Joint MTA/IIASA Task Force Meeting on Lake Balaton Modeling, edited by G. van Straten, S. Herodek, J. Fischer, I. Kovacs. MTA VEAB, Veszprem, Hungary.

Hornberger, G.M., and R.C. Spear. 1980. Eutrophication in Peel Inlet-I. The Problem-Defining Bahavior and a Mathematical Model for the Phosphorus Scenario, in Water Research, Vol. 14, Pergamon Press.

Koivo, H.N., and A.J. Koivo. 1978. Least-squares Estimator for Polluted Stream Variables in a Distributed Parameter Model, in Advances in Water Resources, Vol. 1, No. 4.

Kozák, M. 1977. Computation of the Unsteady Flow Motion in Open Channels, published by the Adamemiai Kiado, Budapest (in Hungarian).

Lam, D.C.L., and M. Jaquet. 1976. Computations of Physical Transport and Regeneration of Phosphorus in Lake Erie, in Journal of Fisheries Research Board of Canada, Vol. 33, No. 3.

Launder, B.E., and D.B. Spalding. 1972. Lectures in Mathematical Models of Turbulence. London: Academic Press.

Literáthy, P., and F. László. 1978. Accumulation of Bioresistant Micropollutants in a Particular Catchment in Hungary, in Prog. Water Techn., Vol. 10, Nos. 5/6.

Mahmood, K., and V. Yevjevich. 1975. Unsteady Flow in Open Channels, in Water Res., Publ., Vol. 1.

Partheniades, E. 1977. Unified View of Wash Load and Bed Material Load, in Journal of the Hydraulics Division, Vol. 96, No. EM 3, June 1977.

Sayre, W.W. 1969. Dispersion of Silt Particles in Open Channel Flow, in Journal of the Hydraulics Division, Vol. 95, No. HY 3, May 1969.

Shanahan, P., D.R.F. Harleman, and L. Somlyódy. 1981. Modeling Wind-driven Circulation in Lake Balaton. International Institute for Applied Systems Analysis: Collaborative Paper No. CP-81-7, Laxenburg, Austria.

Sheng, T.P., and W. Lick. 1979. The Transport and Resuspension of Sediments in a Shallow Lake, in Journal of Geophysical Research, Vol. 84, No. C4, April 1979.

Somlyódy, L. 1980. Preliminary Study on Wind-Induced Interaction between Water and Sediment for Lake Balaton (Szemes Basin), in Proceedings of the Second Joint MTA/IIASA Task Force Meeting on Lake Balaton Modeling, edited by G. van Straten, S. Herodek, J. Fischer, I. Kovács. MTA VEAB,Veszprem, Hungary.

Somlyódy, L., I. Licskó, J. Fehér, and B. Csányi. 1981. Study and Modeling the Transport of Cadmium Pollutant on the River Sajo, in Hidrologiai Kozlony, forthcoming (in Hungarian).

Somlyódy, L., and M. Virtanen. 1981. Application of a One-dimensional Hydrodynamic Model for Lake Balaton. International Institute for Applied Systems Analysis: Working Paper (forthcoming), Laxenburg, Austria.

Spear, R.C., and G.M. Hornberger. 1980. Eutrophication in Peel Inlet-II. Identification of Critical Uncertainties via Generalized Sensitivity Analysis, in Water Research, Vol. 14, Pergamon Press.

Stefan, H., and D.E. Ford. 1975. Temperature Dynamics in Dimictic Lakes, in Journal of the Hydraulics Division, Vol. 101, No. HY 1, January 1975.

Szöllösi-Nagy, A., 1977. On an Optimal Stochastic Water Quality Control Model, in Hidrologiai Kozlony, 10, sz (in Hungarian).

Thau, F.E. 1969. On Optimum Filtering for a Class of Linear Distributed-Parameter Systems. Presented at the Joint Automatic Control Conference, Ann Arbor, Michigan, June 26-28, 1968 by the Automatic Control Division of The American Society of Mechanical Engineers.

van Straten, G., and L. Somlyódy. 1980. Lake Balaton Eutrophication Study: Present Status and Future Program. International Institute for Applied Systems Analysis: Working Paper No. WP-80-187, Laxenburg, Austria.

van Straten, G., and S. Herodek. 1981. Estimation of Algal Growth Parameters from Vertical Primary Production Profiles. Submitted to Ecological Modeling.

Verboom, G.K., and C.B. Vreugdenhil. 1975. Basic Aspects of Mathematical Models. Chapter 9 of the Proceedings of the European Course on Heat Disposal from Power Generation in the Water Environment, Delft, 1975.

Watanabe, M., D.R.F. Harleman, and O.F. Vasiliev. 1980. Two- and Three-Dimensional Mathematical Models for Lakes and Reservoirs. Chapter 8 in Mathematical Modelling of Water Quality: Streams, Lakes and Reservoirs (G.T. Orlob, editor), in press.

Young, P.C. 1974. A Recursive Approach to Time-Series Analysis. Bulletin Institute of Mathematics and its Applications, Vol. 10.