

Working Paper

DESERT DEcision Support System for Evaluating River Basin sTrategies

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WP-95-23

February 1995



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ABSTRACT

An integrated PC-based software package for decision support in water quality management on a river basin scale has been developed. The software incorporates a number of useful tools, including an easy-to-use data handling module with a dBase style database engine, simulation and calibration of hydraulics and water quality, display of computed data with the help of external spreadsheet software, and optimization based on dynamic programming algorithm. The main utility of the package is to provide useful and powerful instrument for water quality assessment and decision making in emission control, including selection of wastewater treatment alternatives, standard setting and enforcement at the river basin level. Two versions of the decision support software are presented, the current version and development of a follow-up program with extended features.

1. INTRODUCTION	1
2. OVERVIEW OF THE CURRENT VERSION OF DESERT	3
2.1 Background and design guidelines	3
2.2 Data management unit	3
2.3 Display unit	4
2.4 Hydraulic unit	4
2.5 Water quality simulation unit	5
2.6 Data transfer unit	6
2.7 Calibration unit	7
2.8 Optimization unit	7
2.9 Post-analysis checking unit	8
3. DESERT V. 1.0	8
3.1 Extensions to the DESERT 0.5	8
3.2 Target software and hardware	9
3.3 Data management	9
3.4 Hydraulics	10
3.5 Water quality modeling	10
3.5 Data transfer unit	13
3.6 Example	13
4. CONCLUSIONS	15
REFERENCES	16
APPENDIX 1. KEY WORDS OF “MODUS” MODEL DEFINITION LANGUAGE	17

DESERT
Decision Support System for Evaluating River Basin Strategies

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1. INTRODUCTION

Water quality assessment on a river basin scale is very tedious and difficult task. Most often the goal is a suitable pollution control scheme which would present a compromise between the available budget for prevention measures and would ensure acceptable water quality. In the course of this work, priority water quality problems for the basin are identified first together with the water quality goals or guidelines. After data is collected and a problem identified, it is necessary to evaluate environmental consequences of the possible control decisions. In this, water quality simulation models proved to be an indispensable assessment tool (Thomann and Mueller, 1987). The procedure involves selecting appropriate models, calibration and validation of the models and, finally, decision analysis stage (Somlyódy et al, 1994). The flow chart of models application in a river basin scale assessment is shown on Figure 1.

Most often, during the course of assessment different tools are used, e.g. spreadsheet for data analysis, modelling software for simulation, optimization packages for decision analysis, and plotting programs for presenting the results. The tools usually are disparaged or only loosely connected, therefore data conversion is difficult and requires special efforts. The whole process of analysis is off-line, slow and prone to frequent converting errors. Policy selection on the river basin scale would greatly benefit from integration of the operations of data analysis, modelling, optimization etc. Therefore, one of the main requirements to decision support software is its ability to integrate analysis, modelling, optimization and presentation tools. These are the major design guidelines for the DESERT software tool described below (see also Somlyódy et al, 1994).

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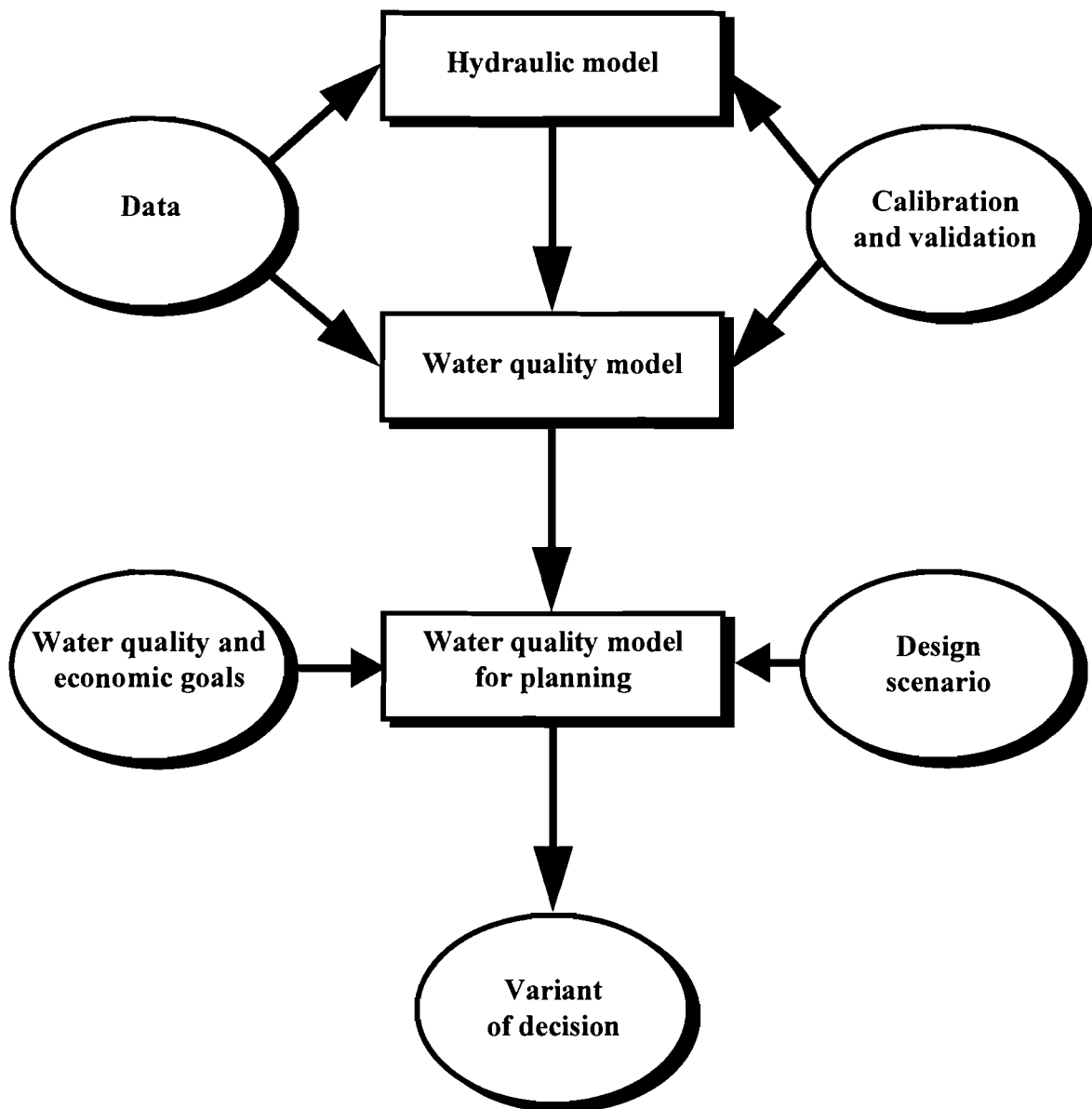


Figure 1. Decision support for water quality management in a river basin scale.

2. OVERVIEW OF THE CURRENT VERSION OF DESERT

2.1 Background and design guidelines

A software package for integrated analysis of water quality management problems on a river basin scale was designed and implemented in the Water Project of International Institute for Applied Systems Analysis (IIASA) in co-operation with the Institute for Water and Environmental Problems, (Barnaul, Russia). The first version of the software was used for assessing the water quality management problem of the Nitra River basin in Slovakia (Somlyódy et al, 1994). The Nitra River was one of the case studies in a larger policy oriented research project conducted in IIASA, which is aimed at development of viable emission control strategies for countries in Central and Eastern Europe (Somlyódy et al, 1994). The objective of the Nitra study was to develop a regional wastewater treatment policy, including the identification of an optimal, least-cost management strategy out of many feasible treatment and upgrading alternatives. Integration, ease-of-use and of results presentation were taken as objectives of software development. The “generic” nature of the tools was another concern, so that the software could be easily applied to other river basins with only minimal changes. Therefore flexible data structure and management were important issues. Figure 2 illustrates the interaction between the software elements.

2.2 Data management unit

A river basin scale assessment requires manipulation and storage of various data on the river network, effluents, treatment plants, monitoring data etc. This data usually is in non-coordinated format and poorly integrated. Data preparation, manipulation and storage can be done successfully using database management systems. However, as usual in practice of water quality management input data is stored in columnar ASCII text files, as this is the format readable by traditional water quality simulation FORTRAN programs. Therefore, most of the ordinary database engine functions like indexing, browsing, inserting and deleting records are not available for the simulation software. In this study, a dBase style relational database engine was used for data manipulation and input (Figure 2). The main advantage is the ability to use powerful dBase compatible database management software for data preparation, selection, editing, etc. The data structure is flexible and oriented to generic river basin scheme.

2.3 Display unit

River basins consist of spatially distributed objects, such as river stretches, gauging and effluent points, sampling locations, weirs etc. So the best way to represent a river basin is to display a scheme of spatial the locations of all available objects. Such rendering is handled by the display unit. The display unit draws the river basin in a symbolic way and is capable of scaling, scrolling and selecting particular river objects (Figure 3). The input data for the display unit are vector files in the format of the commercial MapViewer (TM) mapping software from Golden Software, Inc., although they can be easily produced manually or from other formats if need be.

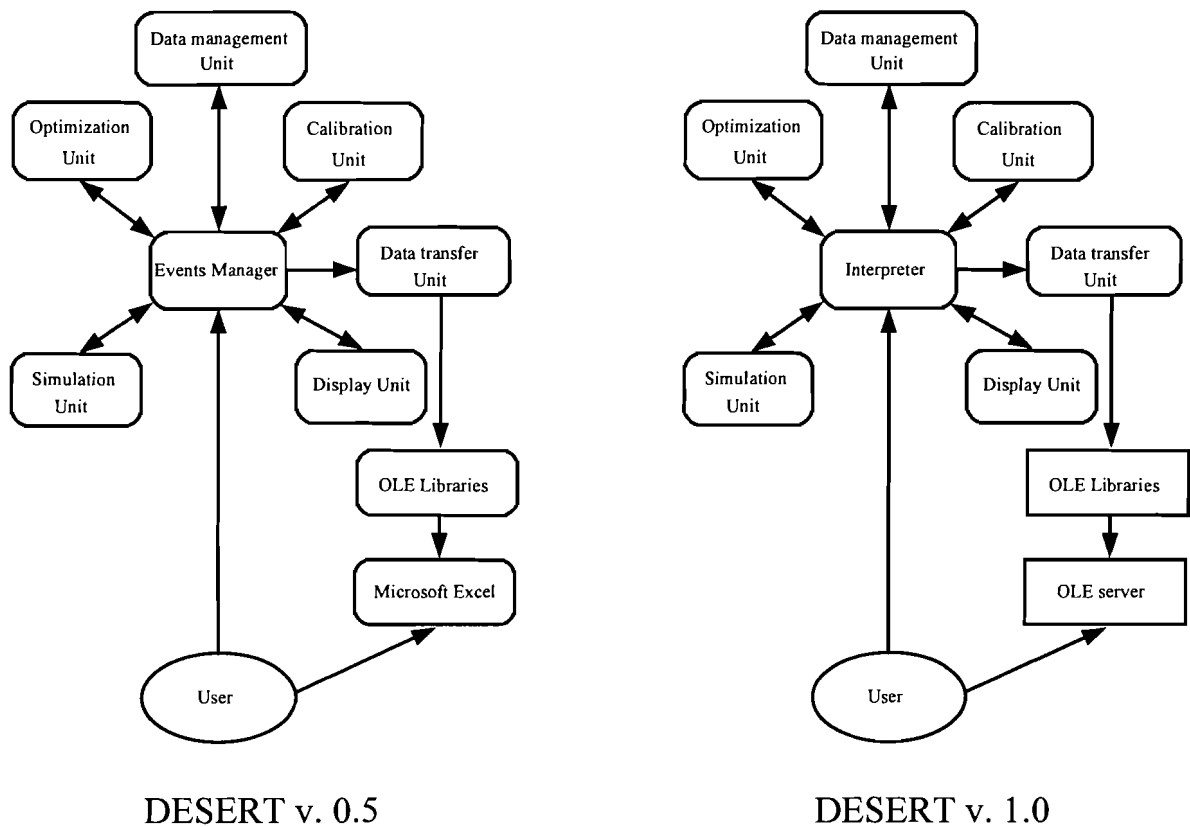


Figure 2. Outline of the two versions of DESERT

2.4 Hydraulic unit

Prior to any water quality modelling, it is necessary to compute hydraulic characteristics of the waterbody such as flow, travel time, water elevation etc. Hydraulic models for rivers and open channels are based on mass continuity and moment equations from fluid mechanics (Antontsev e.a., 1986). For a steady-state situation which is typical for low-flow periods they can be

simplified by omitting terms which are responsible for dynamic behavior of the flow. The friction term in the momentum equation is usually represented by quadratic law of resistance. In current version of DESERT, this simplified version of steady state hydraulic model is used:

$$\frac{\partial h}{\partial x} = - \frac{Q|Q|}{K^2} \quad (1)$$

where x is the coordinate along the river or channel,

Q is the stream flow rate,

h is the local depth of the river or channel,

K is the resistance parameter, calculated from Manning's equation.

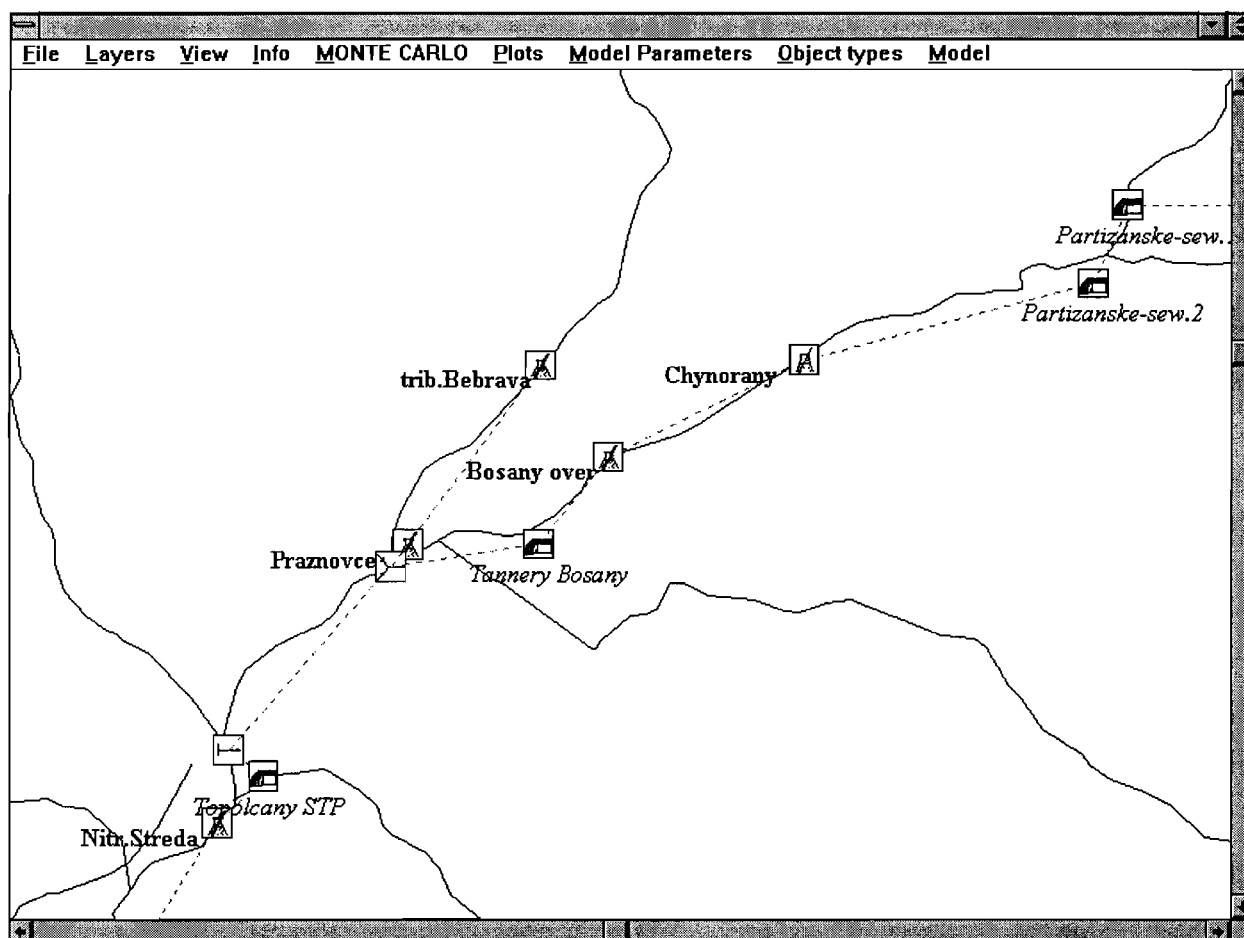


Figure 3. The main window of the DESERT 0.5

2.5 Water quality simulation unit

The following set of mathematical models is available in current version of DESERT (for a more complete reference see Somlyódy and Varis, 1992):

- The original DO-BOD Streeter-Phelps model (two parameters);
- The same model with the incorporation of sedimentation of particulate organic material (three parameters);
- As above, but with sediment oxygen demand (four parameters);
- A three state variable model with nitrogenous BOD (five parameters).

For the last model, the governing partial differential equations can be written as follows:

$$\frac{\partial(A \cdot L)}{\partial t} + \frac{\partial(Q \cdot L)}{\partial x} = -K_r A \cdot L \quad (2)$$

$$\frac{\partial(A \cdot N)}{\partial t} + \frac{\partial(Q \cdot N)}{\partial x} = -K_n A \cdot N \quad (3)$$

$$\frac{\partial(A \cdot C)}{\partial t} + \frac{\partial(Q \cdot C)}{\partial x} = k_a B \cdot (C_s - C) - K_d A \cdot L - K_n A \cdot N - B \cdot K_{SOD} \quad (4)$$

where:

L - carbonaceous biological oxygen demand (CBOD) in mg/L,

N - nitrogenous biological oxygen demand (NBOD) in mg/L,

C - dissolved oxygen concentration in mg/L,

x - coordinate along the river, m,

t - travel time in days,

Q - streamflow in m³/d,

A - cross-section area in m²,

B - stream width in m,

K_r - carbonaceous BOD removal rate in 1/d,

k_a - oxygen exchange coefficient in m/d (see O'Connor and Dobbins, 1956)

K_d - CBOD oxygenation rate in 1/d,

K_n - NBOD oxygenation rate in 1/d,

K_{SOD} - sediment oxygen demand in g/m²/d,

C_s - saturation concentration of dissolved oxygen in mg/L.

Furthermore, algae and phosphorus could also be incorporated into the model in a fashion similar to QUAL2E (Brown and Barnwell, 1987).

2.6 Data transfer unit

Simulation results must be presented in some suitable way: as a table, chart or plot. It is not a simple task, since simulation data is usually multidimensional. Moreover, it should not be limited to just simple plotting, but also allow for postcomputational processing, statistical

analysis and curve fitting. Commercial spreadsheet packages such as Microsoft Excel, Lotus 1-2-3, Corel Chart etc. can easily handle this task. In Microsoft Windows 3.1, the data transfer mechanism permitting linkage of applications is based on OLE (Object Linking and Embedding) protocol. With this facility DESERT software makes use of OLE server applications, including spreadsheets. In this particular case Microsoft Excel spreadsheet software was used as the plotting and analysis server. The data transfer unit facilitates transfer of simulation data through OLE libraries to Microsoft Excel, where data can be independently processed, stored, plotted and so on.

2.7 Calibration unit

Calibration procedure is especially important in water quality management, since in the state-of-the-art approach all the uncertainty associated with the modelling process is treated as parameter uncertainty. The following stochastic methodologies for parameter estimation are implemented in the software:

1. Hornberger-Spear-Young behaviour definition method (Hornberger e.a., 1980);
2. Bayesian estimation based on mean-variance approach (linear model only; Masliev and Somlyódy, 1995);
3. Dempster-Shaffer method based on mean-variance approach and contiguous parameter frame (linear model only; Masliev and Somlyódy, 1995).

All the above techniques provide *a posteriori* distribution in parameter space instead of a single parameter value as an outcome of the calibration procedure. Based on this distribution, an estimation is made of the uncertainty associated with the modelling process in the post-analysis checking unit (see below). Other inherent uncertainties (such as uncertainty in temperature, river streamflow etc) could be taken into account in a sensitivity fashion.

2.8 Optimization unit

Usually water quality management problems can be formulated as a search for suitable regional wastewater treatment policy. This is done with the help of water quality model in conjunction with optimization routine allowing to identify suitable decisions with respect to the given objective and water quality goals (Figure 1). One of the most common objective functions is the summary investment cost of the control alternatives. However, depending on the study, other objective functions can be used, including a multi-objective assessment in the case there are several conflicting objectives. There are many techniques that can be applied to identify optimal water quality control strategies. Our preference falls to dynamic programming (DP) (Bellman, 1957). The efficiencies of DP method can be summarised as follows:

- The method is generic - the solution algorithm does not depend on the complexity of model, linearity or non-linearity, number of state variables, etc.
- It decomposes a problem into a sequence of smaller scale subproblems. In the case of water quality assessment in a river stretch a subproblem is emerging at each water quality control point along the river reach. Therefore, this method is applicable to the problem of water quality management on a river.

The main drawback of the DP technique is the rapid increase in memory requirements as the number of state variables increases (“the curse of dimensionality”). Virtual memory in Windows 3.1 is a partial solution to this problem, but at the expense of computational speed.

2.9 Post-analysis checking unit

Since there are many uncertainties inherent in the modelling procedure, it is necessary to investigate their impact on the effectiveness of the final decision (Figure 1). The task of the final unit is to analyse *a posteriori* the effect of parameters uncertainty on the optimal solution. This estimation can be provided in two ways: a regret methodology based approach and direct Monte Carlo simulation (Somlyódy et al, 1994). In a regret matrix alternative decisions are compared against various scenario realizations; in this way the consequences of possible design errors are estimated. Designs with large regrets are risky and therefore less preferred.

Direct Monte Carlo simulation allows to test one particular decision against uncertainty generated in statistical fashion, in this case, in parameter space. Statistical parameters such as mean and variance can be computed from the resulting distribution. Based on this information, a judgement of performance of the decision in uncertain conditions can be formulated (Somlyódy et al, 1994).

3. DESERT V. 1.0

3.1 Extensions to the DESERT 0.5

There were several deficiencies in the previous version of DESERT. One of them was simplified hydraulics which limited application only to rivers or channels with relatively quiet stationary flows. Another drawback was the predefined, rigid structure of water quality model, in which user could not change the number of state variables, number of parameters, reaction schemes and so on. Changes were allowed only to the input data. Finally, the previous version of DESERT was written in conventional C programming language. As a result architectural design of software was limited by the procedural approach, which does not provide for easy extensibility

and reusability of code. Therefore, it is unlikely that the code of the previous version of DESERT could be maintained by someone outside of the original design team.

These problems were addressed in the next version of DESERT. The main design idea was to achieve flexibility in model formulation and data management, which would allow application of the software to virtually any river catchment, however specific the problem might be. The source code is easily managed and enhanced due to object-oriented design and C++ scalability.

The overall scheme of DESERT 1.0 is outlined in Figure 2. The subsequent sections describe individual modules in more detail.

3.2 Target software and hardware

It was important for the software to operate on widely available personal computers (PCs) in an inexpensive setting. At the same time a windowing system is very desirable since it allows attractive graphical display and easy interaction between the programs which is important for the integration of software elements. Our choice fell to the Microsoft Windows operating platform. Its use makes the system relatively cheap as compared to workstation software and hardware. The system scales to the significant resources of modern PCs, and its more powerful extension (Microsoft Windows NT) runs also on the workstation level computers.

Object oriented design ensured a high degree of reusability and ease code maintenance. As much as possible the standard C++ agreements on source code are supported and compatibility with requirements of ANSI C++ is maintained. The only exception is calls of Microsoft Windows API library functions which are not part of the ANSI standard library functions. They are separated in specific libraries, where all the user interface support code resides.

3.3 Data management

DESERT 1.0 uses a standardized format for input data sets. Data structure is flexible and can incorporate virtually any set used for water quality modelling. For instance, time dependent data referring to a river location are specified in accordance with the following guidelines. The four predefined fields contain:

1. Unique identifier of record or group of records;
2. Date (in standard dBase style);
3. Time (as character field HH:MM);
4. Time interval (numeric).

Reserved field names are specified in configuration file. All other numeric fields will be treated by data manager as input data, with field names serving as series identifiers. The rest of the character, logical and date fields are treated as comments.

3.4 Hydraulics

In general, hydraulical models are based on universal physical principles like mass continuity and momentum conservation, which are generic and applicable to any river system. However, there are several possible formulations of hydraulic models based on different approximations and assumptions. Suitability of any particular hydraulic model depends on assumptions and hypothesis lying at the basis of a given model. The software incorporates several hydraulic models, each of them oriented to handle a specific problem. The range of these models was designed to cover the whole scope of hydrological problems in a river basin. In our case, since the software is oriented primarily towards water quality management, the level of complexity of hydrological models should be limited. For dynamical situations (non-stationary in time), the diffusion wave approximation (Antontsev et al, 1986) strikes a good balance between complexity, accuracy and computation speed:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q^+(x, t) \quad (5)$$

$$\frac{\partial z}{\partial x} = -\frac{Q|Q|}{K^2} \quad (6)$$

where:

z - water elevation,

q⁺ - water discharges source along the river stretch.

3.5 Water quality modeling

Selection of a proper water quality model for a given problem (Figure 1) is a difficult problem, because, as a rule, the models contain much empirical or semi-empirical process description (hydrochemical, hydrobiological etc.) For any given process, several alternative formulations are usually available. For instance, the light limitation factor for algae growth can be expressed by at least ten formulations, most of which are very similar and differ only in details. During the process of modelling water quality, an expert uses past experience, experimental data, simulation and intuition to establish the main processes and select their description, discarding in the meantime many unsuitable formulations. This process can hardly be formalized. From the software point of view the modelling procedure can be illustrated by a diagramm in Figure 4.

As a rule, a model is formulated as a set of ordinary or partial differential equations, which describe relevant physical and chemical processes. After that the modeller must code the model in a some computer language such as FORTRAN, C or PASCAL. The next stage is building an executable module with the help of tools like compilers, linkers, librarians, etc. The process is very slow and prone to errors. Most often, the process is iterative since after evaluation of results corrections may be needed to the programming script or model formulation.

Another possibility is to use an interpreting language like BASIC thereby avoiding the phases of compile and link. Flexibility in model definition is significantly higher than in a compiling language but, unfortunately, the simulation speed is rather slow. In DESERT 1.0, a balanced approach was chosen: the model-independent parts of the code are compiled, but reaction schemes are interpreted during computation.

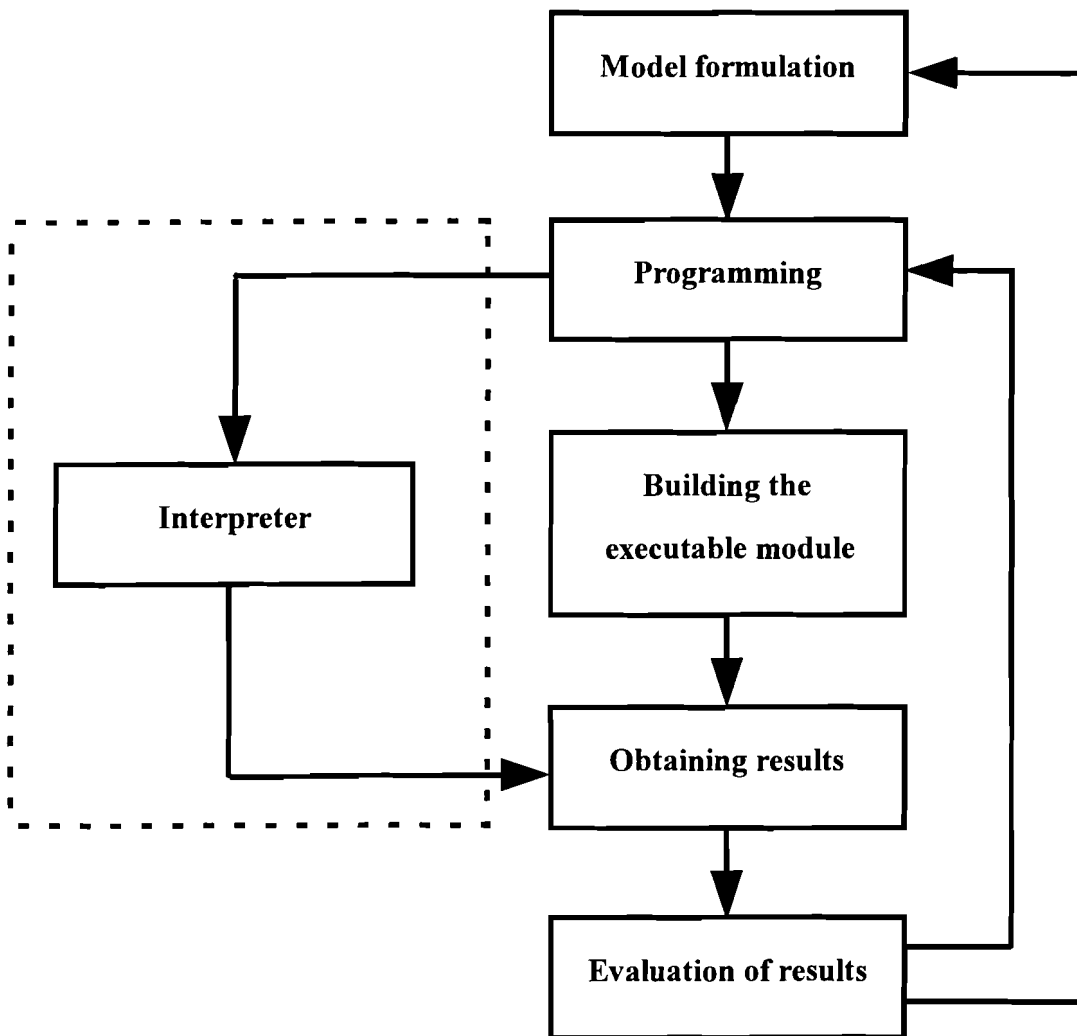


Figure 4. Conventional modelling procedure

The model independent part of a water quality process is defined by a law of mass conservation expressed as a transport equation. As a rule, all water quality constituents use one and the same transport equation in the following form:

$$\frac{\partial(A \cdot C^i)}{\partial t} + \frac{\partial(Q \cdot C^i)}{\partial x} = q^+(x, t) \cdot C_i^+(x, t) + F_i(x, t, C_1, C_2, \dots, C_i, \dots, C_N) \quad (7)$$

$i=1, \dots, N$

where:

- C_i - water quality constituent (state variable),
- N - number of state variables,
- C_i^+ - concentration of i -th water quality constituent in source water discharges,
- F_i - function that express the reactions scheme in which involved i -th state variable.

The simulation problem is thus decomposed into two subproblems:

1. a generic part (transport equation) - computed using precompiled instructions;
2. a specific part (reactions scheme): a set of functions F_i ($i=1,\dots,N$) - computed using interpreted commands.

For “on-line” specification of the reactions schemes, a model description language “MODUS” has been developed (Appendix 1). There is no explicit limit on the number of state variables. For each state variable a reaction scheme has to be provided, which is defined in an easy-to-understand fashion with BASIC type instructions.

3.5 Data transfer unit

The data transfer unit was rewritten in order to handle any OLE server application, not only Microsoft Excel. Now the user can choose any desktop application for spreadsheet or chart processing. Data transfer is initiated by a statement of MODUS language **plot**, so any data on any variable of the model can be transferred to a server application.

3.6 Example

The following is an example of use of the DESERT software for simulation and calibration of a simple water quality model. For this example, a data set from the upper part of the Sió catchment in Hungary (near Lake Balaton) was used.

The model formulation (see Listing 1) defines one state variable (component bod, standing for biological oxygen demand) which is subject to exponential decay. The calibration procedure is based on a Hornberger-Spear-Young algorithm, which involves a Monte-Carlo procedure in the parameter space (parameter k in this case is the rate of exponential decay). Figures 5 and 6 show DESERT user screen during calibration and simulation. The peaks in concentrations occur at the location of the sources of effluent.

```

#this is a comment line
# number of seconds in a day
DAYSEC=86400.0
# A22 is the field name for BOD measurements in the data set (National Hungarian Water
#Quality Monitoring Program)
var A22
#declaration of the state variable
component bod=A22
#process description
equation bod=-k*bod
# random variable used in calibration process as a coefficient
random k0[min=0.0, max=5.0/DAYSEC, type=uniform]
#instruction to compare measurements with simulation for the state variable
calibrate bod[window=0.3, reject=0]
# run the program 100 times and store the results
init 100

```

Listing 1. The statements in model formulation language of DESERT which define calibration procedure of exponential decay rate for one state variable.

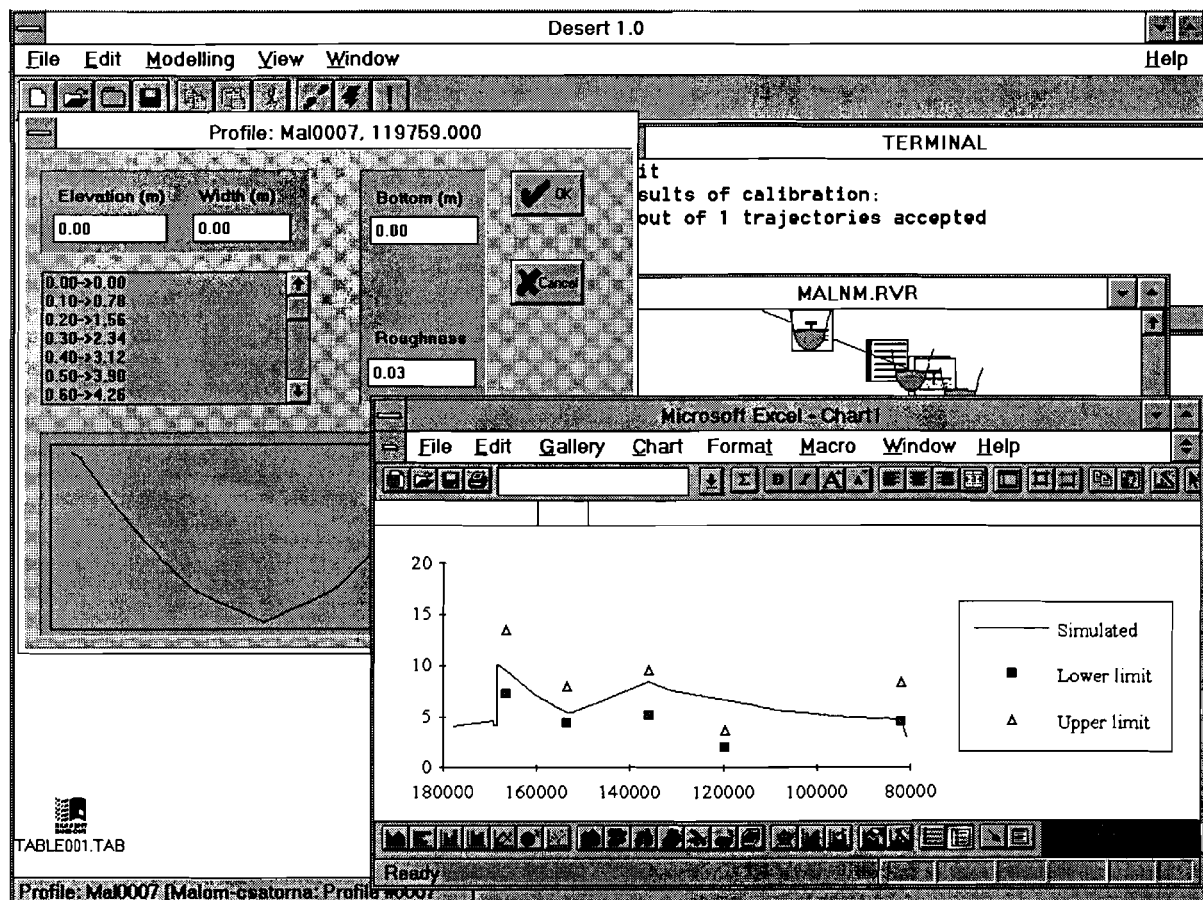


Figure 5. Calibration procedure for rate of exponential decay (see Listing 1).

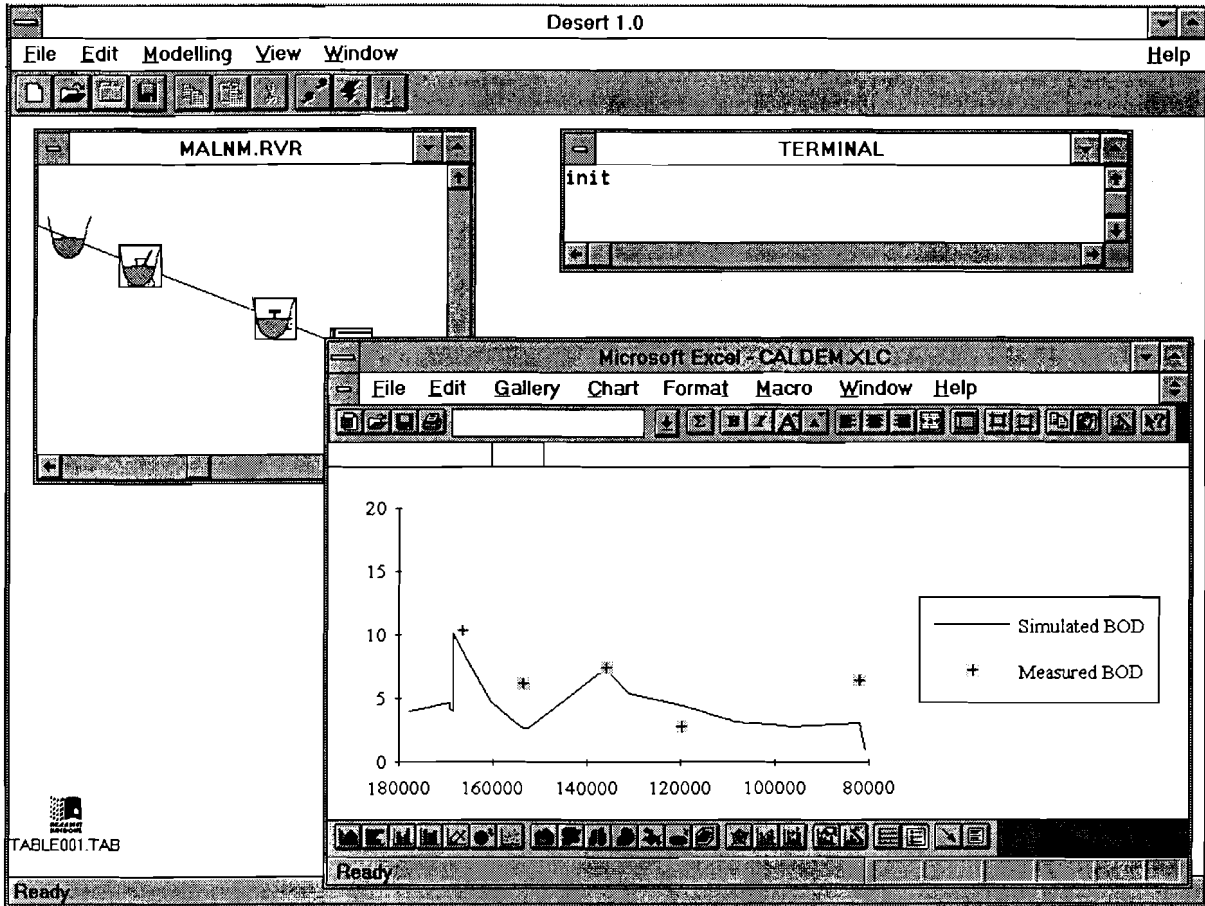


Figure 6. Simulation of exponential decay with calibrated parameter.

4. CONCLUSIONS

DESERT version 1.0 has all the necessary elements for a water quality assessment and planning on a river basin scale. It can be used for waste water allocation studies, to aid monitoring programs, in a river basin authority or an environmental inspectorate to develop and check emission control policies and as an aid in regional standard setting. Its ease of use and versatility makes it especially suitable for water quality experts, decision makers and environmental engineers. Several predefined model formulations are available with the software, so even the use of the input language is not required. For a more advanced user, who can formulate and test water quality models, DESERT is an indispensable tool for testing model structure, uncertainty analysis, calibration, validation and other modelling related activities.

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APPENDIX 1. KEY WORDS OF “MODUS” MODEL DEFINITION LANGUAGE

- **variable** *<identifier>*
Defines and initializes a variable with name *<identifier>*, searching databases for data series.
For instance, the statement
variable BOD
means that the system has to try to allocate BOD as a variable over all river stretches, using measured values in input data set.
- **let** *<identifier>* = *<expression>*
Assignment to a variable *<identifier>* a value determined by *<expression>*.
- **component** *<identifier>* = *<expression>*
Defines a state variable with name *<identifier>* computed using a common transport equation, where boundary conditions determined using *<expression>*.
- **solution** *<identifier>* = *<expression>*
Defines a state variable with name *<identifier>*, that should be computed using an analytical solution. Boundary conditions are to be determined using *<expression>*.
- **equation** *<identifier>* = *<expression>*
Defines a reaction scheme for a state variable *<identifier>*. When *<identifier>* was defined as solution, *<expression>* defines analytical solution for *<identifier>*.
- **init** *<expression>*
command to calculate (process) initial values for variables of the model, using steady state approximation for state variables; *<expression>* defines number of repeats.
- **step** *<expression>*
command to perform one time step of the model; *<expression>* defines number of repeats.
- **run**
command to perform continuous simulation until stopped by user or end of input data.
- **plot** *<identifier>*
Command to add variable/component with name *<identifier>* to the list of variables to plot using OLE libraries.
- **calibrate** *<identifier>* [*<calibration parameters>*]
Defines a state variable *<identifier>* to be used in parameter calibration.
- **random** *<identifier>* [*<distribution parameters>*]
Defines variable *<identifier>* as random parameter sampled from a specified distribution.
- **print** *<expression>*
prints the expression.