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AQUASIM – A TOOL FOR SIMULATION AND DATA ANALYSIS OF AQUATIC SYSTEMS

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ABSTRACT

A survey over the capabilities of a new simulation and data analysis program for laboratory, technical and natural aquatic systems is given. In this program, the spatial configuration of a model system is represented by compartments, which are connected by links. The program allows the user to define an arbitrary number of substances to be modelled and it is extremely flexible in the formulation of transformation processes. It not only offers the possibility of performing simulations of the time evolution of the user-specified system, but it provides also methods for system identification (sensitivity analysis and automatic parameter estimation) and it allows us to estimate the uncertainty of calculated results. These features, together with the user-friendly interface, very much support scientist in analyzing their data. Three examples illustrate the capabilities of the program.

KEYWORDS

Mathematical Modelling; Simulation; Data Analysis; System Identification; Sensitivity Analysis; Parameter Estimation; Aquatic Systems; Environmental Modelling.

INTRODUCTION

The tremendous complexity of natural systems or of laboratory or technical systems involving natural components (such as microorganisms) makes it difficult to gain insight into basic mechanisms acting within the system out of measured data. Mathematical models can be helpful for such analyses because they allow exact calculation of the time evolution of a system with given interactions. Thus, comparisons of model calculations with measured data are an indirect test of hypotheses on the mechanisms within a system formulated with the aid of a model. Since mathematical models of natural systems require drastic simplifications of real processes, they usually contain empirical model parameters to be determined with experimental data. To account for these needs, computer programs implementing such models should not only be able to perform simulations, but also to judge the identifiability of model parameters, to estimate parameter values with the aid of given data and to estimate the uncertainty of calculated results.

Conventional simulation programs perform model calculations for a model selected by the programmer. Such a model can usually be adapted to the system investigated by the user by means of the choice of the values of model parameters or, in some cases, by a selection of a submodel from a given set (examples of such programs can be found e.g. in Ambrose and Barnwell, 1989). There are two main directions of improvement of the applicability of such models: To increase their predictive ability, model parameters may be estimated with the aid of expert systems (e.g. Barnwell et al., 1989; or Baffaut and Delleur, 1990) and esti-

mations of the uncertainty of model results can be performed (e.g. Brown, 1987); to make them more useful for scientific investigations, parameter identifiability analyses and parameter estimations are required (a review of uncertainty analysis and system identification techniques is given by Beck, 1987). The goal of the development of the program described in this report was to implement a tool which is much more flexible concerning model definitions specified by the user compared to most other programs, and which supports the user in identifying an adequate model of his system and in estimating the uncertainty of calculated results. Furthermore, the program should be easy to operate to encourage users to apply methods of system identification and uncertainty analysis in addition to model simulations. To account for the extremely problem dependent computational requirements and for the habits of the users, the program should be portable to various hardware platforms.

In this report, the program AQUASIM developed according to the requirements formulated above, is described. Three versions of the program exist: Two interactive versions offer a simple character-based interface and the native graphical user interface of the selected hardware platform, respectively. A command line version is designed to allow batch operation of long calculations. This description is illustrated with sketches of dialog boxes of the interactive version of the program using the graphical user interface. The exact appearance of these dialog boxes depends on the user interface of the selected hardware platform. In this paper, the main features of the program are briefly described and its utility is demonstrated with three examples. A detailed description of program handling and a list of supported hardware platforms is given in Reichert and Ruchti (1994).

MODEL DEFINITION AND EDITING

Many aquatic systems can be divided into zones with well defined transport processes in which spatial interactions are essential, but where the interactions with other zones are limited to a small number of well defined interfaces. Such zones are called compartments. The description of aquatic systems within AQUASIM is based on a division of the system into such compartments. Although the introduction of specific types of compartment limits the generality of the approach, it is advantageous because it allows the selection of efficient numerical algorithms according to the type of partial differential equation used to describe the transport process. Fig. 1 shows the types of compartment available in the actual version of the program. A *mixed reactor compartment* models a zone where concentration gradients can be neglected, a *biofilm reactor compartment* represents a mixed reactor on the wall of which a biofilm grows, and a *river section compartment* describes a reach of a river. The implementation of more types of compartments, e.g. for lakes or ground water aquifers, will extend the range of applicability of future versions of the program.

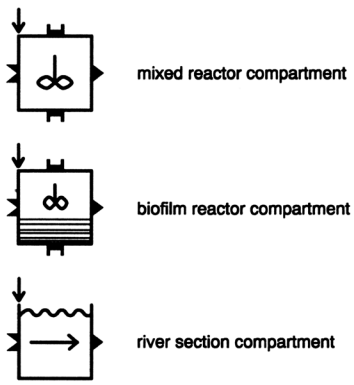

Fig. 1: Compartment types available in the actual version of AQUASIM.

The compartments can be combined to more complicated configurations with the aid of the links shown in Fig. 2. *Advective links* describe water and substance flow between compartments including bifurcations, substance separation and junctions. *Diffusive links* model membranes or other diffusive layers between compartments. Mass transfer coefficients and Henry coefficients (if one of the compartments represents a gas phase) can be specified for the substances penetrating the diffusive link. As indicated by the shape of the connections, there is a variety of possible spatial configurations with the elements shown in Figs. 1 and 2. Figs. 3 and 4 demonstrate two examples of spatial configurations of practical importance.

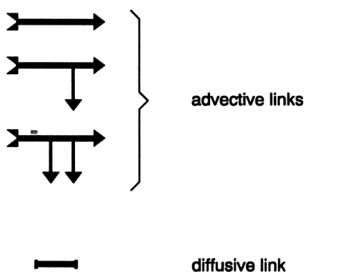

Fig. 2: Types of links available in AQUASIM.

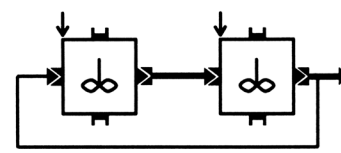

Fig. 3: Configuration representing a sewage treatment plant.

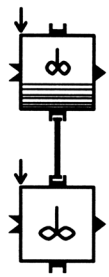

Fig. 4: Configuration representing a biofilm growing in a reactor on a diffusively permeable membrane.

In addition to the spatial configuration of an aquatic system described by compartments and links, the interactions within a system (e.g. biochemical processes) have to be represented by elements of the program. Since transformation processes in most cases are the main objects of investigation, their general formulation should be as universal as possible. To account for this requirement, two types of processes are distinguished. *Dynamic processes* are used to describe transformation processes, the dynamics of which are of importance on the time scale examined, whereas *equilibrium processes* are used to describe very fast processes, the effect of which can be approximated by the equilibrium concentrations of the affected substances.

For the definition of compartments, links and processes, a further element, the *variables*, representing substance concentrations, model parameters, growth rates, etc., is required for system formulation.

Fig. 5 reviews the mutual dependences of the subsystems of variables, processes, compartments and links that are caused by the need of variables for the definition of processes, compartments and links, by the availability of processes to be activated in compartments and by the availability of compartments for defining connecting links. This logical structure of an AQUASIM system shown in Fig. 5 makes it evident that the order of system definition is from variables to links. Therefore, this order will be used in the more detailed description of the subsystems in the following paragraphs.

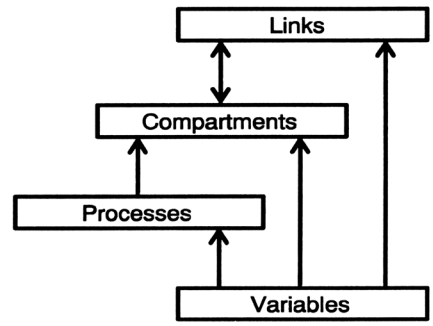

Fig. 5: Logical structure of AQUASIM systems consisting of four subsystems.

Variables

Variables form the base subsystem of model formulation (Fig. 5). They are characterized by the property of taking a possibly context-sensitive numerical value. As shown in Fig. 6, three categories of variables are distinguished.

The first category of variables, the *system variables*, represent quantities to be determined by the model or which have a predefined meaning in a compartment. The first type of system variables are *state variables* that describe properties of the water (usually concentrations of dissolved or suspended substances) or of a surface in contact with the water (usually mass or surface density of attached particles or of sessile microorganisms). State variables obtain their meaning indirectly by the transformation processes in which they are involved. This is in contrast to the second type of system variables, the *program variables*, which make a predefined quantity within a compartment available for use in the system of variables (e.g. time, space coordinates, water discharge, reactor volume, etc.).

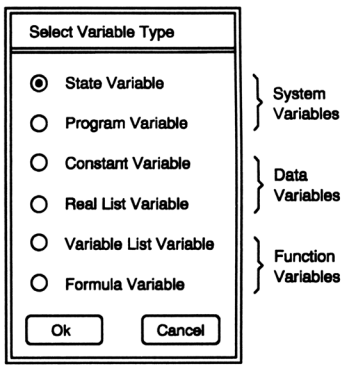

Fig. 6: Types and categories of variables available in AQUASIM.

The second category of variables are *data variables* used for making measured quantities available to the program. *Constant variables* describe single measured quantities, *real list variables* represent quantities measured as a series in function of another variable (e.g. time series or spatial profiles). Both types of data variables require not only the specification of a value but also an estimate of its uncertainty quantified by its standard deviation. Constant variables can be used as fit parameters, the value of which is estimated by the program with the aid of measured data. The interpolation technique for real list variables used in system definition can be selected to be linear interpolation, cubic spline interpolation or smoothing. Alternatively, the data pairs of real list variables can be used as target quantities for parameter estimations.

The third category of variables, the *function variables*, are used to build functional dependences needed for model formulation out of other variables. *Variable list variables* are similar to real list variables with the difference, that another variable corresponds to each value of the argument instead of a numerical value. This makes it possible to have more complicated dependences within the system of variables, such as multidimensional interpolation. As an example of a dialog box for the specification of variables, Fig. 7 shows the entry form for a variable list variable. As with each other variable, a variable list variable is identified by its name and additional documentation is possible by the description and the unit of the variable. The specific elements of a variable list variable are its argument (any other variable), the list of argument-variable pairs and the interpolation method. The second, but most versatile type of function variables are the *formula variables*. These variables allow new variables to be built as algebraic expressions of already defined variables using usual algebraic syntax including elementary functions and the possibility of logical branching with "if-then-else-endif" constructs.

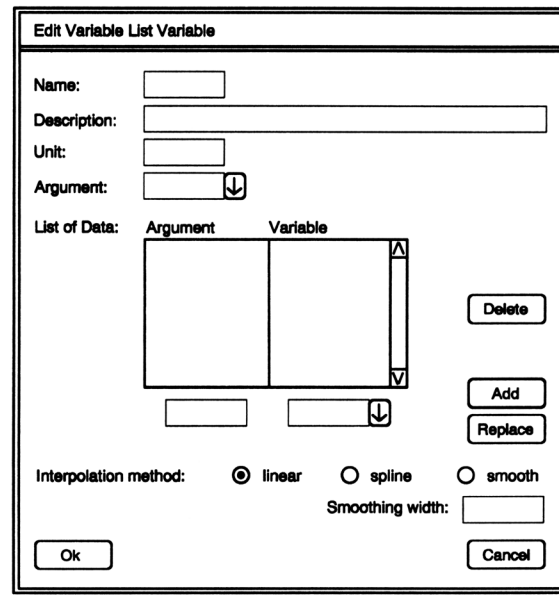

Fig. 7: Dialog box for defining a variable list variable.

Processes

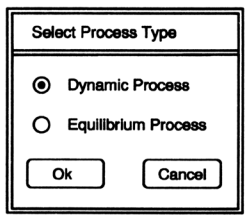

Fig. 8: Types of processes available in AQUASIM.

Fig. 8 shows the types of processes available in the program. Biochemical processes, which transform several substances in fixed stoichiometric ratios, are an important category of processes. This class of processes led to the structure of *dynamic processes* shown in Fig. 9, consisting of a process rate and a list of stoichiometric coefficients that give the factors with which the common process rate has to be multiplied to give the rates of change of the corresponding substances. This structure gives the user a maximum of flexibility for the formulation of dynamic processes (processes changing the concentration of a single substance can easily be formulated with this concept by using a single stoichiometric coefficient equal to one). *Equilibrium processes* are defined by an algebraic equation, the solution of which determines the value of the corresponding state variable.

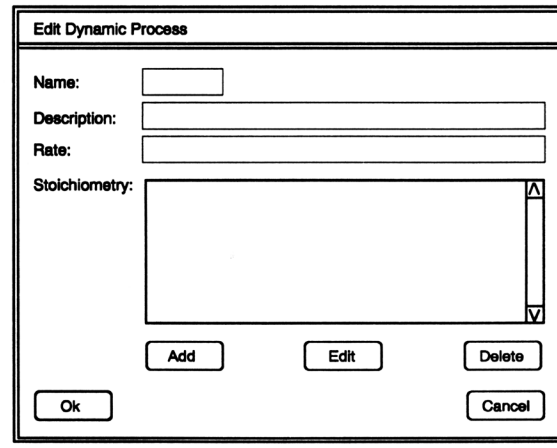

Fig. 9: Dialog box for defining a dynamic process.

Compartments

Fig. 10 shows the types of compartments available in the actual version of AQUASIM. A *mixed reactor compartment* models a zone, where concentration gradients can be neglected (e.g. a stirred laboratory

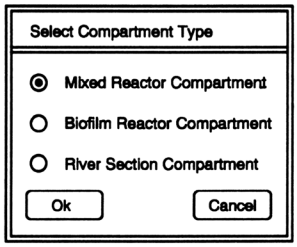

Fig. 10: Types of compartments available in the actual version of AQUASIM.

reactor, a mixed basin of a sewage treatment plant or a well mixed lake), a *biofilm reactor compartment* represents a mixed reactor on the wall of which a biofilm grows. The population dynamics of microorganisms and the concentration gradients of dissolved substances within this film are calculated according to the equations proposed by Gujer and Wanner (1989). A *river section compartment* describes hydraulics, transport and transformation of substances in a reach of a river. One-dimensional hydraulics is calculated according to the kinematic or the diffusive approximation to the St. Venant equations of open channel flow; transport and transformation are calculated with a set of advection-diffusion-reaction equations for all transported substances.

The first three lines of the dialog box for defining a mixed reactor compartment shown in Fig. 11 are common to all edit compartment dialog boxes: each compartment is identified by its name and an additional description can be given optionally. Then, the active state variables and processes have to be selected and input flow and initial conditions have to be specified. In the case of a mixed reactor compartment as shown in Fig. 11, additionally reactor volume or outflow (usually as a function of the actual reactor volume) has to be specified. Biofilm reactor compartments require additional information on particulate and dissolved substances, on biofilm properties and on numerical resolution. River section compartments need information on river geometry, friction, dispersion, on hydraulic controls bounding the section and on numerical resolution.

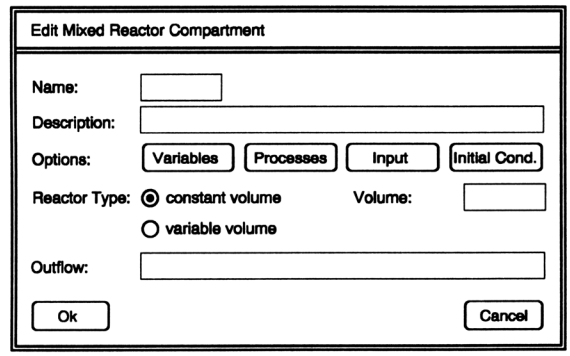

Fig. 11: Dialog box for defining a mixed reactor compartment.

Links

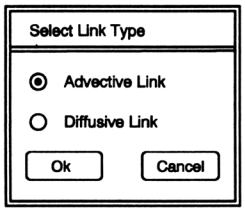

Fig. 12: Types of links considered in AQUASIM.

Fig. 12 shows the link types available for connecting the compartments. *Advective links*, the entry form of which is shown in Fig. 13, allow water and substance flow between compartments or out of the system to be modelled. These links also allow description of bifurcations, substance separation and junctions. *Diffusive links* model diffusive layers between compartments, e.g. membranes or molecular boundary layers. Due to the possibility of specifying Henry coefficients, diffusive links can model boundary layers not only between two water compartments but also between gas and water compartments (a mixed reactor compartment can be used to describe a reactor filled with gas as well as a reactor filled with water).

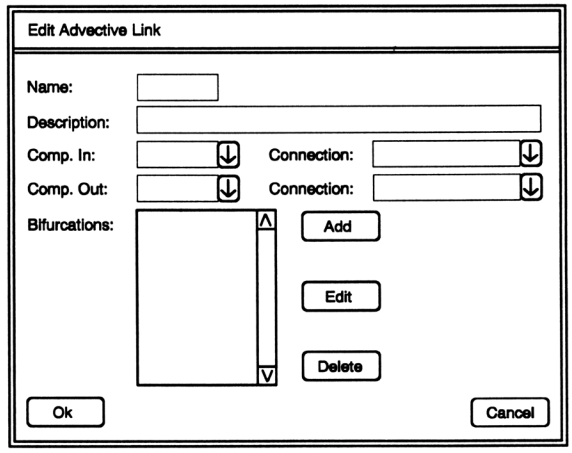

Fig. 13: Dialog box for defining an advective link.

SIMULATION AND DATA ANALYSIS

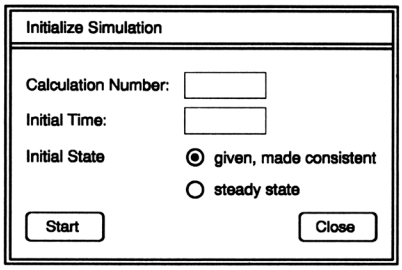

Fig. 14: Dialog box for initializing a simulation.

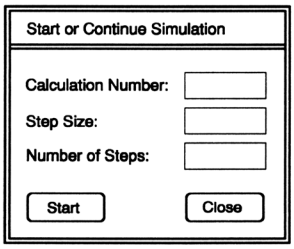

Fig. 15: Dialog box for starting a simulation.

For the model specified by the user as described in the previous section, it is possible to perform simulations, sensitivity analyses and parameter estimations.

Figs. 14 and 15 show the dialog boxes used for initializing and starting a *simulation*, respectively. Due to the eventual existence of algebraic equations resulting from boundary conditions or equilibrium processes, the initial state as given by the user may be inconsistent. Two possibilities of calculating a consistent initial condition are offered in the dialog box shown in Fig. 14: The first selection uses the initial state as given by the user with only the necessary corrections to make it consistent, whereas the second choice tries to find the steady state solution for the boundary conditions as given at the time of the initial state. Note that it depends on the model specified by the user, if such a steady state exists. As shown in Fig. 15, to start or continue a simulation, the step size and the number of steps have to be specified. This step size defines the resolution stored in the system file and available for plotting and printing results; it has, however, nothing to do with the step size used internally by the integration algorithm, which is determined according to the desired accuracy of the calculation. In both dialog boxes for simulations, a calculation number has to be specified. This is a non-negative integer which can be used to distinguish different calculations. Several calculations identified with their calculation numbers can be stored simultaneously. Since this number is available as a program variable, other variables may depend on the calculation number specified for the calculation. The advantage of such a dependence is discussed in more detail in the section concerning parameter estimations.

Sensitivity analysis allows us to calculate the absolute, relative or mixed sensitivity functions

$$\delta^{a,a}_{f,p} = \frac{\partial f}{\partial p}, \quad \delta^{r,a}_{f,p} = \frac{1}{f}\frac{\partial f}{\partial p}, \quad \delta^{a,r}_{f,p} = p\frac{\partial f}{\partial p}, \quad \delta^{r,r}_{f,p} = \frac{p}{f}\frac{\partial f}{\partial p},$$

of any variable, f, depending on any parameter, p. These sensitivity functions allow assessment of the identifiability of model parameters. Furthermore, the program allows the user to estimate the uncertainty of results and to detect major sources of uncertainty with the aid of linear estimations of the standard deviation, σ_f, of any variable, f, and of the contributions of all parameters to this uncertainty:

$$\sigma_f = \sqrt{\sum_i \left(\frac{\partial f}{\partial p_i}\right)^2 \sigma_{p_i}^2}, \qquad \delta^{err}_{f,p_i} = \frac{\partial f}{\partial p_i}\sigma_{p_i}.$$

Here p_i are the parameters, σ_{p_i} their standard deviations and the sum extends over all uncertain parameters.

As a last option, the user can perform *parameter estimations*. The parameters are estimated by minimizing the sum of the squares of the weighted deviations between measurements and calculation

$$\chi^2(p) = \sum_{i=1}^{n}\left(\frac{f_{meas,i} - f_i(p)}{\sigma_{meas,i}}\right)^2,$$

where $f_i(p)$ is any variable at a given time and location in a compartment as a function of the parameters p =

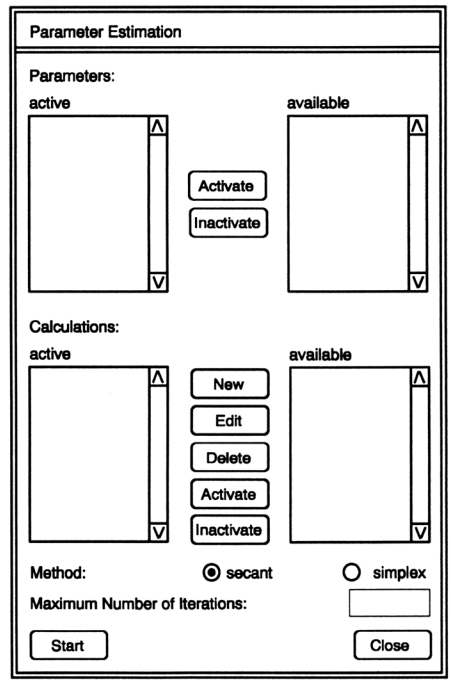

Fig. 16: Dialog box for defining and starting a parameter estimation.

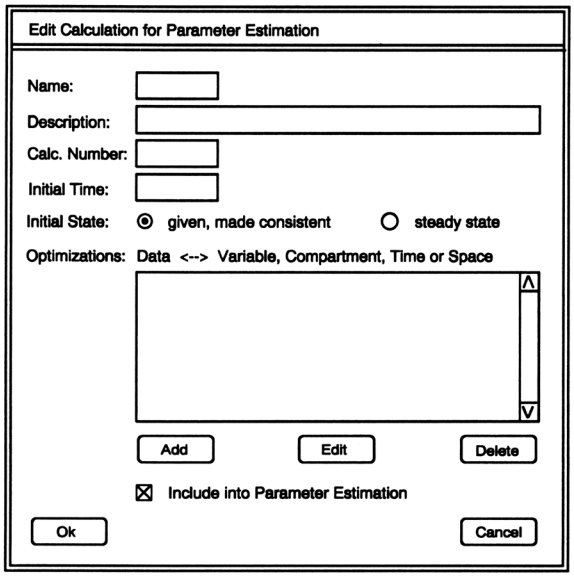

Fig. 17: Dialog box for defining a calculation for a parameter estimation.

$(p_1,...,p_m)$ and $f_{meas,i}$ and $\sigma_{meas,i}$ are values and standard deviations of measured quantities represented by real list variables. The sum extends over all variables, compartments, and calculations specified in the definition of the parameter estimation, and over all data pairs of the measured quantities involved. Fig. 16 shows the dialog box used for defining and starting a parameter estimation. The active parameters to be estimated have to be selected out of the available variables shown in the top right listbox. Several calculations defined in the dialog box shown in Fig. 17 can be specified. Each calculation requires a calculation number, a specification of the initial state similar to Fig. 14 and a series of definitions of target quantities for the fit. Each of those consists of a real list variable containing the measured data and of a variable, a compartment and a time or a space coordinate, where this variable has to be evaluated. As a last point shown in Fig. 16, the user can select the numerical method used for searching the minimum of χ^2 and the maximum number of iteration steps. Note, that a variable list variable with a list of constant variables and with the program variable "calculation number" as argument allows realization of calculation-specific parameters in addition to global parameters. This gives the user a lot of freedom in defining his fit problem.

VIEWING RESULTS

Graphical presentations of simulations and comparisons with measurements are important aids assisting data analysis. Fig. 18 shows the dialog box used for editing plot definitions. In a plot definition, different variables and sensitivity functions for several calculations can be added as curves to a common plot. After performing a calculation, such a plot definition can be used for displaying the results on the screen, for writing the results to a PostScript file which then can be submitted to a printer, or for listing the results to an ASCII file for external postprocessing.

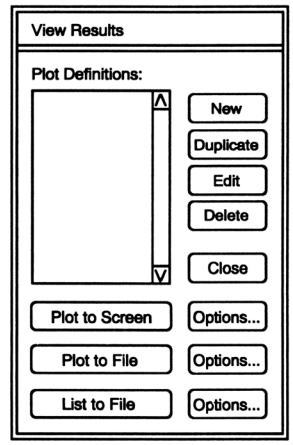

Fig. 18: Dialog box for editing plot definitions.

EXAMPLES

Three examples serve to demonstrate the capabilities of the program. The first example demonstrates the universality and flexibility of the formulation of biochemical processes by implementation of a simple activated sludge model for waste water treatment. The second example shows the calculation of spatial profiles of dissolved substances and of the microbial population in a biofilm. Finally, the third example discusses the utility of sensitivity analysis and parameter estimation with a simple model for gas exchange, primary production and respiration in a river.

Example 1: Activated Sludge Modelling of Waste Water Treatment

Gujer and Henze (1991) discuss several modeling levels of the activated sludge process for waste water treatment. All of these models are simplifications of the "activated sludge model no. 1" described by Henze et al. (1986). Both of these papers use the same notation for the formulation of biochemical processes: Such a process is defined by a process rate and a series of stoichiometric coefficients for all substances affected by

the process. The contribution of the process to the conversion rate of a substance is given as the product of the process rate with the stoichiometric coefficient of the substance. A biochemical process model can be written as a table which for each process contains one row. The columns are labelled with the substances considered in the model and contain the stoichiometric coefficients; the last column contains the process rates. Table 1 shows the simple process model for the activated sludge process as described in model B of Gujer and Henze (1991). Three processes are considered in this model: Heterotrophic growth consumes oxygen (S_O, gO/m^3) and dissolved substrate (S_S, gCOD/m^3) and produces heterotrophic biomass (X_H, gCOD/m^3). Lysis converts heterotrophic biomass into slowly biodegradable substrate (X_S, gCOD/m^3). Hydrolysis converts slowly biodegradable substrate into dissolved substrate. Process formulation uses the stoichiometric paramter Y_H and the kinetic parameters μ_H, K_S, $K_{O,H}$, b_H and K_X given in Gujer and Henze (1991). Each of the lines of the process model shown in Table 1 can be represented as a dynamic process of AQUASIM, which can be entered as shown in Fig. 9. The spatial configuration of the experiment is realized in AQUASIM with a mixed reactor compartment. Sludge recirculation is described by a bifurcation of an advective link leading back to the input of the reactor and transporting 85% of all particulate substances considered in the model. This configuration is similar to that shown in Fig. 3, but only with one compartment. Fig. 19 shows a comparison of measured oxygen uptake rates with a calculation using model B shown in Table 1. This is a reproduction of Fig. 3 of Gujer and Henze (1991) using AQUASIM. The feed of substrate between 2 and 14 hours causes a rapid increase of oxygen uptake due to heterotrophic growth. Because the available dissolved substrate after the stop of the feed at 14 hours rapidly reaches a lower dynamic equilibrium, the oxygen uptake rate is suddenly decreased. Between 14 and 24 hours the decrease of the oxygen uptake rate is much slower, because hydrolysis is now the rate limiting process.

TABLE 1: Activated sludge model B of Gujer and Henze (1991)

Process	S_O	S_S	X_H	X_S	Process Rate
Heterotrophic growth	$-\frac{1-Y_H}{Y_H}$	$-\frac{1}{Y_H}$	1		$\mu_H \frac{S_S}{K_S+S_S} \frac{S_O}{K_{O,H}+S_O} X_H$
Heterotrophic lysis			-1	1	$b_H X_H$
Hydrolysis		1		-1	$k_H \frac{X_S/X_H}{K_X+X_S/X_H} X_H$

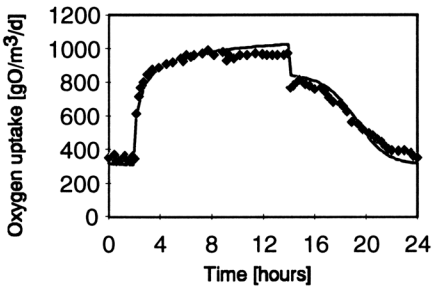

Fig. 19: Comparison of measured (Ekama and Marais, 1978; diamonds) and calculated oxygen uptake rate (full curve)

Example 2: Xylene Degradation and Microbial Population Dynamics in a Membrane-Bound Biofilm

This example demonstrates the calculation of spatial profiles of dissolved substances and of the microbial population in a biofilm according to the equations of Gujer and Wanner (1989). The analysis is based on an experiment described in Debus and Wanner (1992) and is published in Wanner et al. (1994). The biofilm was grown in an airtight reactor on a silicone tubing through which oxygen was supplied. The configuration shown in Fig. 4 was used to model the experimental system with AQUASIM. The mixed reactor compartment represents the gas phase inside the silicone tubing, the biofilm reactor compartment models the biofilm and the bulk water phase in the reactor and a diffusive link models diffusive mass flux between the two compartments. Fig. 20 shows spatial profiles of oxygen, of xylene and of the conversion rate of xylene. It is clearly shown that oxygen diffuses from the membrane-bound base into the film whereas the xylene flux is from the bulk fluid into the film. The conversion of xylene takes place in a narrow zone where both substances are available. As shown in Fig. 21, xylene conversion leads to growth of the heterotrophic population in the same active zone of the film. Near the membrane, where enough oxygen but no xylene is available, the heterotrophic population decreases due to endogenous decay; between the active zone and the biofilm-bulk fluid interface, the heterotrophic production is negative due to inactivation of heterotrophic bacteria to inert organic particles. All these processes, together with the advective shift of the population due to the expansion in the active zone in the film depth, lead to the heterotrophic profiles shown in Fig. 21.

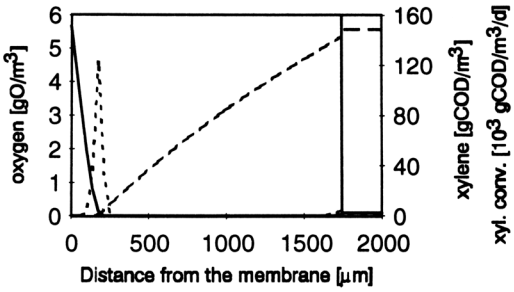

Fig. 20: Profiles of oxygen (solid), xylene (long dashes) and xylene conversion (short dashes) in the biofilm.

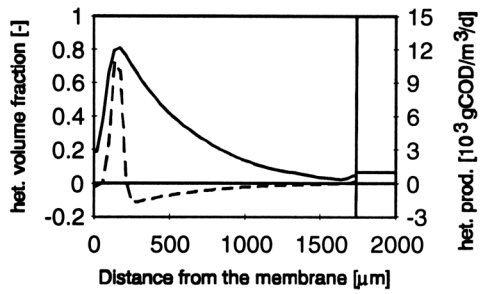

Fig. 21: Profiles of heterotrophic production (long dashes) and of heterotrophic volume fraction (solid) of the population in the biofilm.

Example 3: Data Analysis of Oxygen Time Series in a River

This example demonstrates the utility of the data analysis features of AQUASIM with an evaluation of oxygen time series in the river Glatt near Zürich, Switzerland. The river reach considered consists of a sequence of river sections with a slope of 0.7 % and a surface width of about 16 m, divided by cascades with heights between 1.35 m and 1.75 m. Discharge was about 3.5 m^3/s, water temperature about 20.5 °C. Oxygen concentration is influenced by total respiration, R, primary production, P, assumed to be proportional to global radiation impinging onto the river surface, and gas exchange at the cascades and within the river sections. The two parameters quantifying gas exchange are the gas exchange efficiency E at the cascades (relative reduction of the difference between actual concentration and oxygen saturation at the cascade) and the gas exchange coefficient K_2 within a river section (rate coefficient of reduction of the difference between actual concentration and oxygen saturation). The order of magnitude of these two parameters can be estimated to be $E \approx 0.6$ and $K_2 \approx 50\ d^{-1}$ by extrapolating the measurements of Cirpka et al. (1993) to another temperature (Committee on Sanitary Engineering Research, 1961). Using these gas exchange coefficients, an automatic parameter estimation with AQUASIM using the measured oxygen concentations yielded a respiration rate of $R \approx 27\ gO/m^2/d$ and a production rate of $P \approx 0.12\ (gO/m^2/d)/(W/m^2)$. The agreement of calculation and measurement for this set of parameters is shown in Fig. 22. To judge the simultaneous identifiability of the gas exchange parameters together with respiration and production, a sensitivity analysis of the oxygen concentrations with respect to E, K_2, R and P has been performed. Fig. 23 shows the relative sensitivity functions of oxygen with respect to these parameters. $\delta^{r,r}_{O_2,P}$ is zero during the night and positive during the day. $\delta^{r,r}_{O_2,R}$ is always negative, but somewhat smaller in magnitude during the day due to the larger oxygen concentrations. These differences in the behaviour of the sensitivity functions make the simultaneous estimation of P and R as shown in Fig. 22 possible (R is determined by the oxygen concentrations during the night, P is then adjusted to fit the oxygen concentrations during the day). Because the sensitivity functions of E and K_2 can approximately be constructed as a linear combination of those for P and R (see Fig. 23), it is not possible to estimate E and K_2 simultaneously with P and R out of the oxygen time series. To verify this conclusion, E and K_2 have been set to half of their original value and the parame-

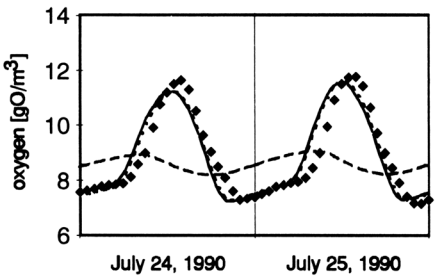

Fig. 22: Measured oxygen time series in a river (diamonds), first (solid) and second (dotted) calculation, and oxygen saturation (dashed).

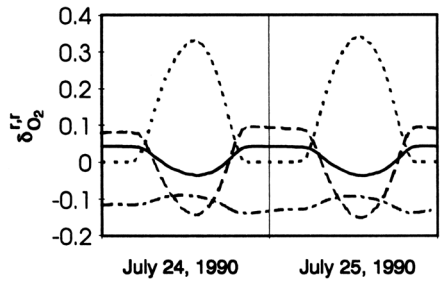

Fig. 23: Relative sensitivity functions of oxygen with respect to the parameters E (solid), K_2 (dashed), P (dotted) and R (dash-dotted).

ter estimation of P and R has been repeated. This fit yielded values of R ≈ 6.1 $gO/m^2/d$ and P ≈ 0.068 $(gO/m^2/d)/(W/m^2)$. As shown in Fig. 22, the corresponding oxygen curve for this set of parameters is not significantly different from the curve for the former parameter set. This clearly demonstrates the need to perform independent gas exchange measurements for the quantification of production and respiration in rivers.

CONCLUSIONS

The new simulation and data analysis program for aquatic systems described in this report includes more capabilities than most other such programs. It allows the user to compose the spatial configuration of an aquatic system out of different compartments and to specify freely the model of transformation processes. For such a user-defined model, the program offers the possibilities of performing simulations, sensitivity analyses, parameter estimations and uncertainty estimations. These features, together with the user-friendly interface, make the program a tool that considerably supports scientists in analyzing their data.

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