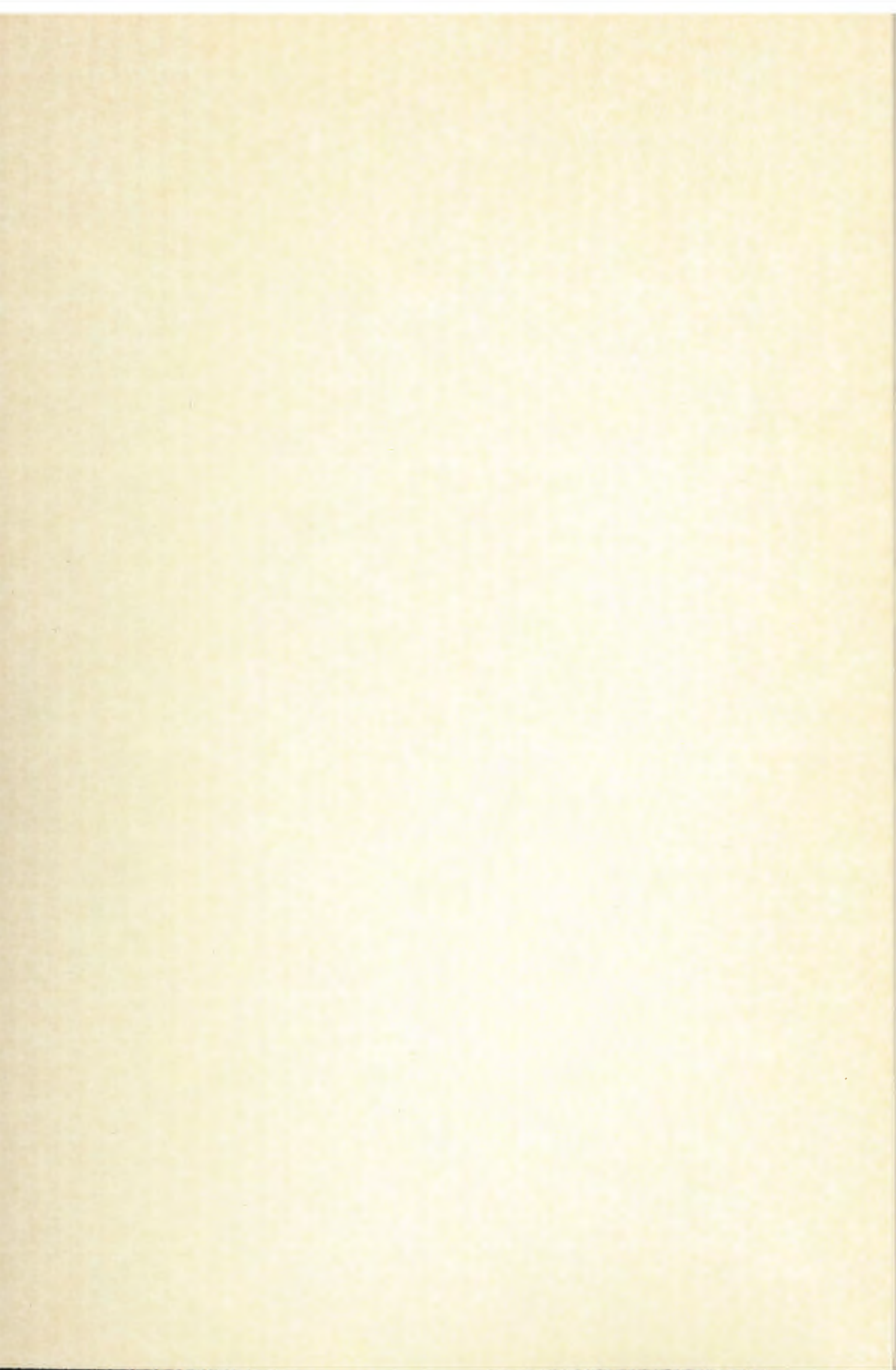




POLSKA AKADEMIA NAUK
Instytut Badań Systemowych

**WSPOMAGANIE INFORMATYCZNE
ROZWOJU
SPOŁECZNO-GOSPODARCZEGO
I OCHRONY ŚRODOWISKA**

Redakcja:
Jan Studziński
Ludostaw Drelichowski
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Książka wydana dzięki dotacji KOMITETU BADAŃ NAUKOWYCH

Książka zawiera wybór artykułów poświęconych omówieniu aktualnego stanu badań w kraju w zakresie rozwoju modeli, technik i systemów zarządzania oraz ich zastosowań w różnych dziedzinach gospodarki narodowej. Wyodrębnioną grupę stanowią artykuły omawiające aplikacyjne wyniki projektów badawczych i celowych KBN.

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ON THE USE OF COUPLED SOFTWARE TOOLS TO CONTROL WATER QUALITY IN SHALLOW LAKES

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The control of water quality of shallow lakes requires informatic tools of different time and space domains. Combining different simulators valuable water quality management tools are obtained. For this reason an eutrophication model (HavelMod) was coupled with the optimisation tool ISSOP within the MATLAB developing framework. Control strategies based on the limiting nutrient concept (elementary composition of phytoplankton) and threshold values of LAWA (German State Working Group on Water Quality) were used to compute optimal solutions. For model input a pre-treatment of time series by interpolation to generate equidistant data from sampled raw data is discussed.

Keywords: Eutrophication, shallow lakes, data processing, water quality modelling, ISSOP, HavelMod, MATLAB.

1. Introduction

Polluted water affects the functioning of freshwater ecosystems, various water uses and risk human health. Information on pollution levels are got by monitoring as well as laboratory experiments. The aim of water quality data analysis, modelling and simulation is an information mining process of the actual state, its spatio-temporal development and a forecast of its future development. In either case, support systems are necessary in order to screen the array of possible courses of anthropogenic actions. Therefore, water quality management requires decisions which are based on multiple contradictory goals, on different evaluation procedures and on distinguished valuation scales. Water quality management options are specified either in national and international regulations of river water quality or by effluent standards. But most often the management goals consist on suitable control schemes which present compromises between the available budget for environmental protection and an acceptable water quality.

On the other hand, water quality models are widespread used for water quality management. Then management decisions will be made on a scenario analysis. But only some simulation models include optimisation procedures to get optimal results (Cembrowicz 1988, Wierzbicki et al. 2000). For this reason new software tools consisting on combinations of different simulators have to be worked

out. The quality of such software developed is determined by non-functional properties (Pressman 2001). Three aspects of a software engineering must be considered: operation (correctness, reliability, usability, integrity, and efficiency), revision (maintainability, flexibility, testability) and transition (portability, reusability, interoperability). Within the first category functional properties are summarised. The second one circumscribes its ability to undergo changes, while the third one refers to its adaptability to new simulation environments. For simulation models the transition category is of great importance. On the one hand, the further development of data gathering techniques and the application of different methods of data pre-treatment may lead to modifications of an input interface of a simulation model. On the other hand, the use of model outputs for optimisation or prediction requires the application of new software tools or modifications of a model output interface.

To control the water quality of shallow lakes a modelling and optimisation framework for a sub-catchment of the Havel River was worked out. For this reason the *MATLAB* based eutrophication simulator *HavelMod* and the simulator *ISSOP* were coupled. In the paper first results of the coupled simulator are presented.

2. Coupling of simulators *HavelMod* and *ISSOP*

Water quality management of rivers requires decisions which are based on multiple contradictory goals, on different evaluation procedures and on distinguished valuation scales (Gnauck et al. 2002). Mostly they consist on scenario analyses based on results of water quality simulation models. To control the water quality of shallow lake area a modelling and optimisation framework for a subcatchment of the Havel River was worked out. For this reason the *MATLAB* based eutrophication simulator *HavelMod* and the simulator *ISSOP* were coupled.

2.1 The eutrophication simulator *HavelMod*

Eutrophication is characterised by an intensive increase of dissolved nutrients in a water body, by excessive growth of plants, mainly algae, and by restricted water uses due to anoxic water conditions as well as by odour problems. It refers to intensive man-made activities in the catchment. To forecast the eutrophication process in shallow lakes the simulator *HavelMod* was developed (Gnauck 1999). The model concept is given in (fig. 1). To simulate the changing water quality levels caused by internal pollution a submodel of phosphorus remobilisation from sediment was included. State variables are phytoplankton, zooplankton, orthophosphate phosphorus, ammonia nitrogen and nitrate nitrogen. The model itself consists on five differential equations (Gnauck et al. 2003). The time behaviour of physical water quality variables are modelled by sinusoidal functions according to Straškraba and Gnauck (1985).

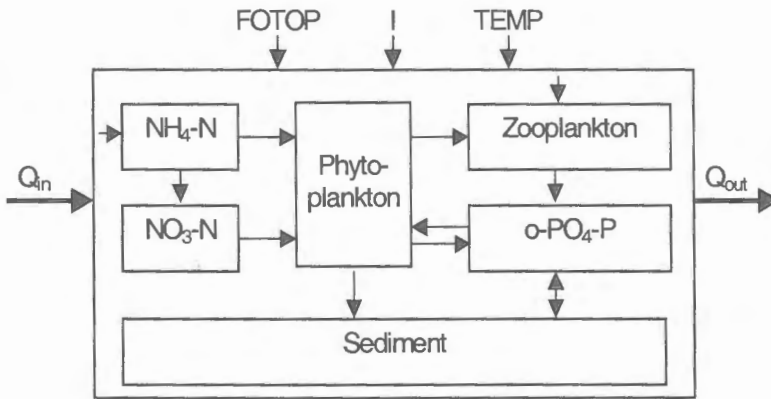


Figure 1. Concept of simulator *HavelMod*

Q_{in} and Q_{out} mean water inflow and outflow. External driving forces are photoperiod (FOTOP), solar radiation (I) and water temperature (TEMP).

2.2 The optimisation tool *ISSOP*

The management of complex systems containing a large number of state variables and parameters is only possible if their dynamic behaviour is well known or can be well estimated. To combine simulation and optimisation procedures for water quality management the software tool *ISSOP* was used (Krug 1997). Originally it was developed to support manufacturing, organisational and logistic processes. It includes an optimisation interface of *MATLAB* models (Wiedemann and Krug 2001). The *ISSOP* architecture of discrete optimisation methods used is given in fig. 2. Before starting an optimisation run each problem will be automatically transformed in the standard problem of optimisation (Krug 2002). The following optimisation methods are included: CENUM – component wise enumeration, DISOPT – a quasi-gradient method, EVOL – an evolutionary optimisation strategy, SIMCARLO – optimisation by Monte Carlo method, SIMGEN – optimisation by a genetic algorithm. Other optimisation procedures can be added by the developers of *ISSOP*.

The dialogue between external and internal models and optimisation methods is realised by the universal parameter interface. External static and dynamic models can be used without any restriction. Additionally *ISSOP* contains internal static and dynamic models of ordering, purchasing and manufacturing. On the lowest level of this architecture simulation models, goal functions and internal process models are given explicitly.

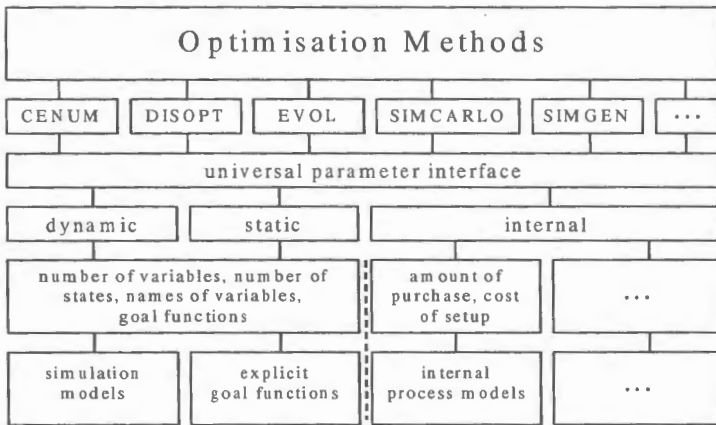


Figure 2. The ISSOP optimisation architecture

2.3 Coupling of *HavelMod* and ISSOP

Coupling the simulator *ISSOP* with another simulation system an open interface has to be used. The simulator *HavelMod* was carried out within the *MATLAB* environment. Fig. 3 shows the general structure of coupling. The input variables of the simulation system are denoted by $\alpha_1 x_1, \dots, \alpha_k x_k$, the outputs are symbolised by y_1, \dots, y_m , and the goal functions are represented by f_1, \dots, f_n with $f_i(M(\alpha_1 x_1, \dots, \alpha_k x_k)) = f_i(y_1, \dots, y_m)$ where $i = 1, \dots, n$. They will be optimised simultaneously. As goal functions f_i arbitrary continuous functions can be used. There are no restrictions for the goal. If $n > 1$, the goal functions f_1, \dots, f_n are aggregated to a weighted sum $S = \sum w_i f_i$. For the weighting factors w_i the condition $\sum |w_i| = 1$ is valid.

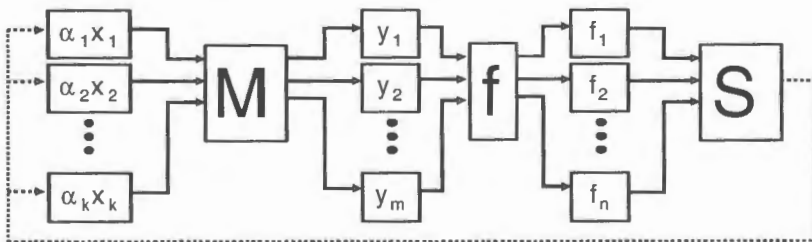


Figure 3. Coupling of *HavelMod* and ISSOP

The input variables of simulator *HavelMod* are denoted by x_1 (phytoplankton biomass), x_2 (orthophosphate phosphorus) and x_3 (nitrate nitrogen), and the output

variables y_1 , y_2 , and y_3 respectively. $M(\alpha_1x_1, \alpha_2x_2, \alpha_3x_3) = (y_1, y_2, y_3)$ denotes the system transfer function. Following goal functions are considered:

- phytoplankton biomass $f_1(t) = \sum_x \sum_t y_1(x, t) \rightarrow \min.$
- orthophosphate phosphorus $f_2(t) = \sum_x \sum_t y_2(x, t) \rightarrow \max.,$
- nitrate nitrogen $f_3(t) = \sum_x \sum_t y_3(x, t) \rightarrow \max.$

Corresponding to the input variables following restrictions are valid for the parameters α_1 , α_2 and α_3 : $\alpha_1 = 1$, α_2 and α_3 vary in the interval $[0,1]$. The information exchange between *ISSOP* and *MATLAB* is presented in fig. 4. *ISSOP* uses the model variables and target values as input data and gives optimised state variables back to the simulation system.

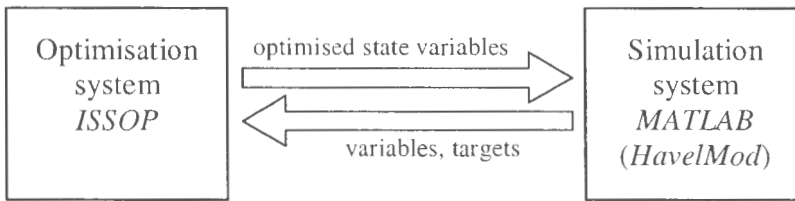


Figure 4. Information exchange between coupled simulators

3. Experimental area and data interpolation

Applying the coupled simulator on water quality problems of shallow lakes a stretch of the Lower Havel River between measuring points Hv0140 and Hv0180 was chosen (fig. 5). The River Havel belongs to the greatest tributaries on the right hand side of the River Elbe. It is strongly influenced by the River Spree. The length of the River Havel is about 325 km. It is characterised by a very small elevation difference between source (63 m above sea level) and mouth into the River Elbe (22 m above sea level). For low-flow situations a slope of the water level of 2 cm/km was observed. The watershed is characterised by shallow lakes, wetlands and marshy country, as well as by high evaporation rates. Only 25% of precipitation contributes to flow. Hydraulic works and banked-up water levels influence water flow and the intensity and kinetics of nutrient dynamics along the course of the river. The active sediment layer is given by 2 cm to 6 cm. For the water quality simulation framework the river basin of interest was divided into several segments of different length (fig. 5). Time series of water quality data from 1997 are taken into consideration as references, while time series from 1998 to 2002 with daily, weekly and two-weekly sampling intervals from different measuring points along the course of the river were used for modelling and parameterisation.

First, all data series were analysed by advanced statistical methods and time series analysis procedures to get qualitative and quantitative measures of the ecosystem state. All data series were sampled irregularly. That means they contain missing values and other irregularities.

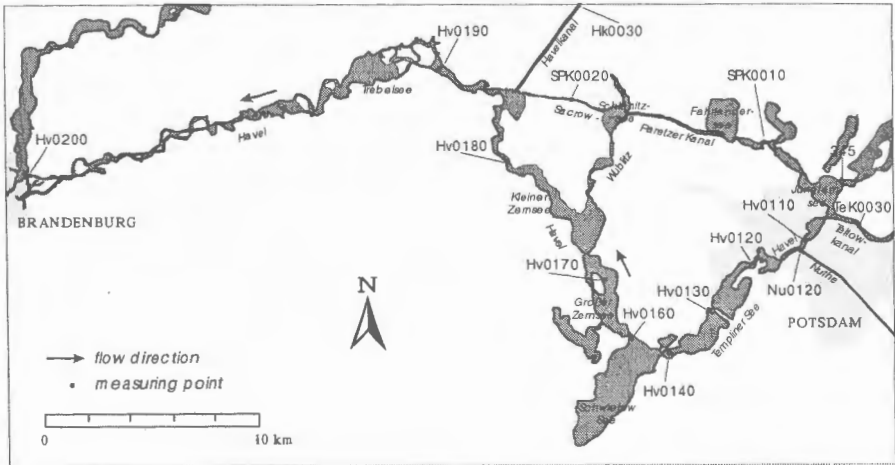


Figure 5. Experimental area of the Lower Havel River

Because *HavelMod* is working on a daily time scale irregular sampled data series affect the model output quality as well as optimisation results. Therefore, all data series were tested by four interpolation methods.

The procedure of pre-treatment of raw water quality data is shown in fig. 6.

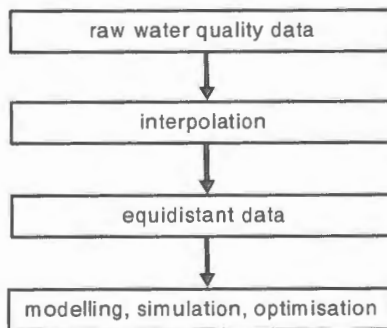


Figure 6. Pre treatment of water quality time series

In order to get time series with equidistant daily sampling intervals raw data series are interpolated by linear interpolation, nearest neighbour method, cubic

splines and cubic Hermite polynomials. The resulting data series are used as model input information for simulation and optimisation. For rivers with similar flow characteristics and water quality indicators mostly linear interpolation method has been proved the smallest standard error compared with (tab. 1).

Table 1. Interpolation algorithms used

Indicator	River Spree	River Havel
NH4-N	linear	linear
NO2-N	linear	linear
NO3-N	linear	linear
o-PO4-P	linear, spline, polynom	linear
chlorophyll-a	linear	linear

4. Results

To get weighting factors w_1 , w_2 and w_3 with $|w_1| + |w_2| + |w_3| = 1$ two control strategies are considered:

- (i) Weights according to the elementary composition of algal biomass (limiting nutrient concept)(cf. Uhlmann 1988, tab. 2).

Table 2. Normalised weights according to elementary composition

Variable	Quota CHA (%)	Normalised weight $ w_i $ (%)
CHA (mg/l)	100	90.5
o-PO4-P (mg/l)	1.27	1.1
NO3-N (mg/l)	9.22	8.4

The optimisation problem was solved by using gradient search method combined with MCM for $w_1 = 90.5\%$, $w_2 = -1.1\%$ and $w_3 = -8.4\%$ with the result $\alpha_2 = 0.01$ and $\alpha_3 = 0.90$. Optimised results according to the limiting nutrient concept are presented in fig. 7. As can be seen, an eutrophication control according to the limiting nutrient concept leads to a diminished phytoplankton maximum in late summer by optimised nitrate concentrations. No effect of optimised orthophosphate phosphorus concentration can be stated.

On the other hand, eutrophication control by weighting factors according to German States Working Group for Water Quality (LAWA 1998) (tab. 3) leads to nearly the same behaviour of phytoplankton biomass in spring but to smaller differences of phytoplankton maxima and to low nutrient concentrations in late summer (fig. 8).

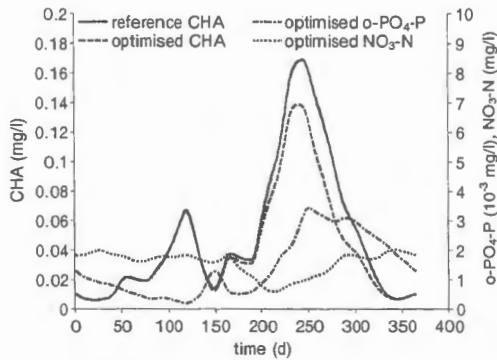


Figure 7. Control of phytoplankton biomass according to elementary composition

Table 3. Normalised LAWA weights

Variable	Target value (mg/l)	Reciprocal value (l/mg)	Normalised weight $ w_i $ (%)
CHA	0.08	12.5	42
o-PO ₄ -P	0.06	16.7	57
NO ₃ -N	3.7	0.27	1

Optimisation according to LAWA was done by weighting factors $w_1 = 42\%$, $w_2 = -57\%$ and $w_3 = -1\%$ with the result $\alpha_2 = 0.03$ and $\alpha_3 = 0.91$.

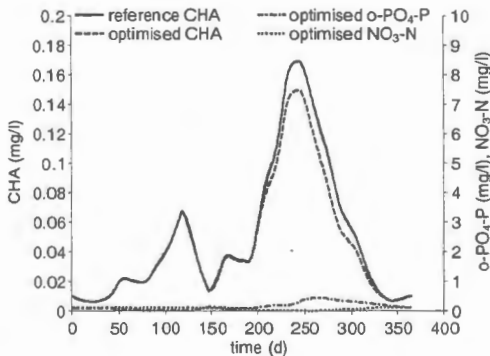


Figure 8. Control of phytoplankton biomass according to target values of LAWA

For the shallow lake area of the Lower Havel River following optimal averages of goal functions could be found:

Limiting nutrient concept: $f_1 = 44.991 \mu\text{g/l}$, $f_2 = 1.472 \mu\text{g/l}$, $f_3 = 1.54 \text{ mg/l}$,

LAWA concept: $f_1 = 48.762 \mu\text{g/l}$, $f_2 = 0.166 \mu\text{g/l}$, $f_3 = 0.08 \text{ mg/l}$.

As a result the LAWA concept leads to significant lower nutrient concentrations but to a slight increase of phytoplankton biomass. In opposite of that an eutrophication control according to the limiting nutrient concept results in lower phytoplankton concentrations but higher admissible nutrient inputs.

5. Conclusions

The use of combined simulation-optimisation procedures to manage the water quality of rivers, lakes and reservoirs is an approach promising more theoretical understanding of complicated natural processes and software engineering methods. Mostly, decisions are based on scenarios computed by water quality simulation models. A sustainable management to control freshwater ecosystems can only be achieved by using powerful informatic tools where simulation model and optimisation procedures are directly coupled. But some problems exist in formulating optimal management conditions which are most appropriate for rivers and lakes, and how far different goal functions are equivalent. In this context the study of goal functions can be seen as a study of mechanisms of land use changes in the catchment, rather than a study of water quality indicators as they are observable at a given instant of time, or at a given site and situation. Up to now, ecosystem risk has not been considered in the simulation models. Therefore, perspectives of development of informatic tools for water quality management on a river basin scale may be seen in combinations of water quality simulation models including risk, multi-objective optimisation procedures and visualisation tools.

Generally, freshwater system identification and model parameter estimation should be based on regular sampled or monitored data series. This prerequisite is mostly not fulfilled. Therefore, pre-treatment of data plays an important role to get valid simulation and optimisation results. Especially, filling of data gaps has to be regarded as a necessary task before applying a water quality model to solve management problems. Interpolation methods discussed in this paper lead to equidistant time series of water quality.

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