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APPLICATIONS OF INFORMATICS IN ENVIRONMENT ENGINEERING AND MEDICINE

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Jan Studzinski
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This book consist of the papers describing the applications of informatics in environment and health engineering and protection. Problems presented in the papers concern quality management of the surface waters and the atmosphere, application of the mathematical modeling in environmental engineering, and development of computer systems in health and environmental protection. In several papers results of the research projects financed by the Polish Ministry of Science and Information Society Technologies are presented.

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CHAPTER 1

Water and Air Quality Management

OPTIONS FOR EUTROPHICATION MANAGEMENT OF SHALLOW WATER BODIES

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The functioning of freshwater ecosystems and various water uses are affected by natural processes and anthropogenic activities in river basins. While natural pollution is mostly small the nutrient input due toman-made pollution force the eutrophication process. It is characterised by an increase of dissolved nutrient concentrations, by excessive growth of plant biomass, and by restricted water uses due to anoxic water conditions as well as by odour problems. Especially, internal pollution by nutrient remobilisation from sediments plays an important role in shallow water bodies. A sustainable management of such freshwater ecosystems can be achieved by using effective simulation models. To evaluate the eutrophication process a simulation framework was developed including the DO balance and phosphorus remobilisation from sediments. Combining an eutrophication simulator with an optimisation tool a valuable water quality management tool will be obtained. Control strategies based on the limiting nutrient concept and on target values of LAWA (German State Working Group on Water Quality) were used to compute optimal solutions. Results are presented for shallow river stretches and riverine lakes of the Lower Havel River.

Keywords: Water quality management, euthrophication, shallow water bodies, HavelMod, ISSOP.

1. Introduction

Basic information on pollution levels are got by monitoring and laboratory experiments as well as by data analysis and mathematical modelling. The aim of these procedures is an information mining on eutrophication or, more general, water quality levels. Water quality models are widespread used for managing eutrophication problems. Some eutrophication models contain optimisation procedures to get optimal results (Wierzbicki et al. 2000). Water quality management of freshwater ecosystems requires decisions which are based on multiple contradictory goals, on different evaluation procedures and on distinguished valuation scales. Problems of control and management of freshwater quality are inherently multi-objective in nature. Management options are specified either in trems of 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 freshwater quality. Therefore, support systems are necessary in order to screen the array of possible courses of anthropogenic actions.

To obtain optimal control options for eutrophication management of shallow water bodies a simulation and optimisation framework was developed. It consists on a MATLAB based eutrophication simulator *HavelMod* which is coupled with an optimisation tool *ISSOP* (Krug 1997, 2002). A first step of information mining was the detection of control mechanisms decsribing internal and external pollution by nutrients (Gnauck 1999a). Modern time series analysis methods (Mallat 1998; Gnauck 1999b) are used for process identification. Hoffmann (1999) developed a special process model describing the phosphorus remobilisation from sediment as a part of the eutrophication simulator *HavelMod* (Gnauck 1999a, Gnauck et al. 2002b). The coupling of *HavelMod* with *ISSOP* gives out optimised simulation results. Options for eutrophication management are discussed.

2. The Eutrophication Process

Eutrophication of freshwater ecosystems is characterised by an intensive increase of dissolved nutrients in water bodies, by excessive growth of green plants, mainly algae, by decreasing transparency, by anoxic conditions of deeper water layers, by loss of species diversity, by restricted water uses as well as by taste and odour problems (Uhlmann 1988, Schnoor 1996). Eutrophication refers to intensive man-made activities in river basins. Phosphorus together with carbon and nitrogen belongs to the essential nutrients for aquatic life. Artificially enhanced input of phosphorus and nitrogen into water bodies due to intensive use of mineral fertilizers on agricultural areas, or orthophosphate in laundry detergents, as well as intensive inputs of sewage effluents has led to exceptionally high loads of phosphorus and nitrogen into rivers and lakes. These man-made impacts have caused shifts from oligotrophic to eutrophic and hypertrophic freshwater ecosystems. Sediments have been accumulated nutrients over several decades so that they now function as internal sources. Compared with the amount of nutrients in the pelagic zone of eutrophic lakes, mostly the sediment content is considerable higher. Therefore, the eutrophication process is now more sustained by internal than by external sources.

The eutrophication process is stimulated by nutrient remobilisation from sediment supported by meteorological and hydrochemical conditions. Methane formation due to decay of organic material in sediments leads to an increase of nitrogen and phosphorus from pore water. Schettler (1995) stated out water temperature is one of the most important control variable. Fig. 1 shows details of Daubechies wavelet analysis between water temperature and phosphate phosphorus at level 5. Heating and cooling of the water is accompanied by an opposite event of phosphate phosphorus because of temperature dependencies of chemical reaction rates.

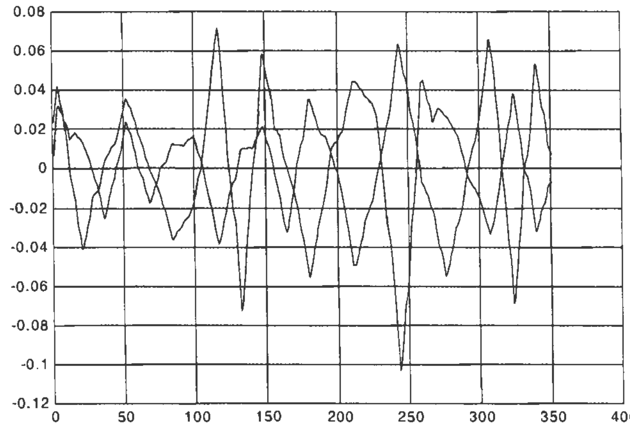


Figure 1. Details of Daubechies wavelet analysis of water temperature and phosphate phosphorus at level 5

Dead organic matter as algal biomass is mineralised by micro-organisms. This process needs electron acceptors which are supplied from the water column. They enter the sediment by molecular diffusion, convection, or bioturbation. The presence of electron acceptors in the water body, as dissolved oxygen, nitrate, iron (III), manganese (IV), sulphate, is a prerequisite for the remobilisation of nutrients from sediment. Nitrate and dissolved oxygen are major electron acceptors before iron is consumed. The order of consumption is determined by the Gibbs free energy gained in the reaction. In the case of aerobic conditions phosphate will be fixed in sediments. The dissolved inorganic phosphorus is bounded by $Fe(OH)_3$ or $Fe_3(PO_4)_2$. Anaerobic conditions and formation of hydrogen sulphide cause a destruction of the iron(III)phosphate and iron(III)hydroxide layer of the mud-water interface which prevents phosphorus remobilisation under aerobic conditions (Uhlmann 1975; Uhlmann und Horn 2001). The species iron(III)phosphate will be reduced to iron(II)phosphate under formation of iron sulphide. Phosphate is released into pore water and due to diffusion to the water column above sediment.

3. Informatic tools for eutrophication management

A modelling and optimisation framework for controlling the quality of shallow water bodies was worked out. It consists of a coupled simulation model and optimisation software tool.

3.1 The eutrophication simulator HavelMod

To simulate the eutrophication process in shallow water bodies a stationary 1D-model was developed. Fig. 2 shows the model concept.

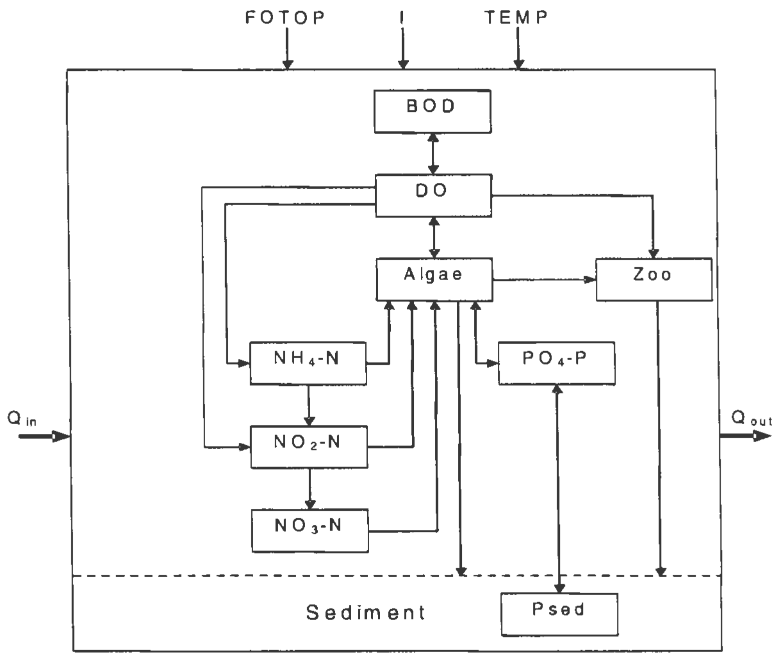


Figure 2. Conceptual model of the eutrophication simulator

Model state variables are given by the water quality indicators phytoplankton (algae), zooplankton (zoo), orthophosphate phosphorus (PO_4-P), ammonia nitrogen (NH_4-N), nitrite nitrogen (NO_2-N), nitrate nitrogen (NO_3-N) as well as by dissolved oxygen (DO) and biochemical oxygen demand (BOD). To cover the phosphorus remobilisation process from sediment a submodel (P_{sed}) was included in the phosphorus balance equation. Detailed descriptions of model equations, parameters, site constants and system specific parameters are presented by Gnauck et al. (2002b) and Gnauck et al. (2003). Q_{in} and Q_{out} describe the discharges into and out of the river segment or lake under consideration. External driving forces are photoperiod (FOTOP), solar radiation (I) and water temperature (TEMP). Model equations are given as follows:

Phytoplankton biomass A (mg CHA/l)

$$dA/dt = Q/V\cdot(A_{in} - A) + G - UA\cdot A\cdot f - FRZ\cdot Z\cdot A\cdot CR - RESP\cdot TEMP\cdot A$$

P-remobilisation from sediment

$$dPsed/dt = phi\cdot hs\cdot(-Dsp/(1-\log(phi^2))\cdot(P-(Psed/(hs\cdot phi)))/(hs/2) + \Theta\,(cpcrit - cpEA)/cpcrit\cdot KFe\cdot cp\cdot qp)$$

where $\Theta = 1$ if $cpEA \le cpcrit$ and $\Theta = 0$ otherwise

Phosphate phosphorus P (mg P/l)

$$dP/dt = Q/V\cdot(P_{in} - P) + FRZ\cdot A\cdot Z\cdot CR\cdot(\,(1 - AZP)\cdot KSA/(KSA+A)\,) + RESP\cdot TEMP\cdot A - G + (1/4)\cdot dPsed/dt$$

Ammonia nitrogen NH4-N (mg N/l)

$$dNH4/dt = Q/V\cdot(NH4_{in} - NH4) + B_3\cdot NORG_{in} - B_1\cdot NH4 - FA1\cdot FUP\cdot G$$

Nitrite nitrogen NO2-N (mg N/l)

$$dNO2/dt = Q/V\cdot(NO2_{in} - NO2) + B_1\cdot NH4 - B_2\cdot NO2$$

Nitrate nitrogen NO3-N (mg N/l)

$$dNO3/dt = Q/V\cdot(NO3_{in} - NO3) - (1-FUP)\cdot FA1\cdot G + B_2\cdot NO2$$

Zooplankton Z (mg C/l)

$$dZ/dt = Q/V\cdot(Z_{in} - Z) + FRZ\cdot A\cdot Z\cdot CR\cdot AZP\cdot C\cdot KSA/(KSA+A) - MORT\cdot TEMP\cdot Z$$

Dissolved oxygen DO (mg/l)

$$dDO/dt = Q/V\cdot(DO_{in} - DO) + K_2\cdot(DO_{sat} - DO) + (a_3\cdot G/A - a_4\cdot RESP\cdot TEMP)\cdot A - K_1\cdot BOD - K_4/zmix - a_5\cdot B_1\cdot NH4 - a_6\cdot B_2\cdot NO2 - a_7\cdot MORT\cdot TEMP\cdot Z$$

Biochemical oxygen demand BOD (mg(l)

$$dBOD/dt = Q/V\cdot(BOD_{in} - BOD) + K_1\cdot BOD - K_3\cdot BOD$$

According to Straškraba and Gnauck (1985) temperature dependencies of physical water quality variables are modelled by sinusoidal functions. Saturation concentration of DO is expressed by a third order polynomial (Thomann 1972).

3.2 The optimisation tool *ISSOP*

Krug (1997) developed a software tool *ISSOP* (integrated system for simulation and optimisation) 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 shown in fig. 3. The dialogue between external and internal models and optimisation methods is realised by the universal parameter interface.

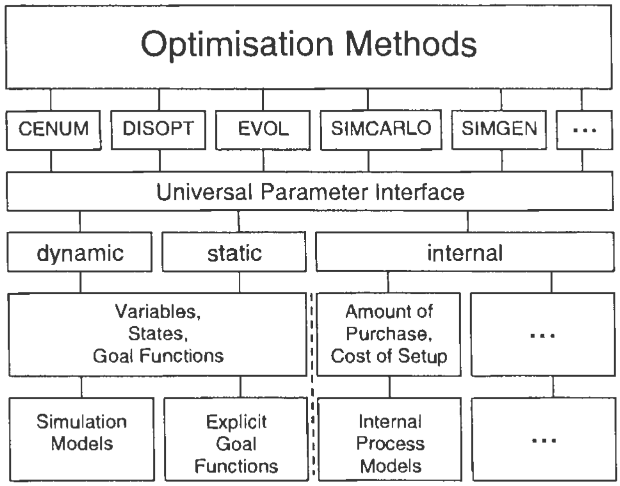


Figure 3. The *ISSOP* optimisation architecture

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*. Before starting an optimisation run each simulation problem is automatically transformed into the standard problem of optimisation (Krug 2002). On the lowest level of this architecture simulation models, goal functions and internal process models are given explicitly. External static and dynamic simulation models can be implemented without any restriction. Convexity of goal functions is not necessary.

3.3 Coupling of *HavelMod* and *ISSOP*

The eutrophication simulator *HavelMod* was carried out within the MATLAB environment. The coupling of *HavelMod* with the optimisation tool *ISSOP* was realised by using the universal open interface. The input variables of the simulation system are denoted by $\alpha_1 x_1,\dots,\ \alpha_k x_k$, outputs are symbolised by $y_1,\dots,y_m$ respectively. Goal functions are denoted 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, and arbitrary continuous functions can be used. They will be optimised simultaneously. If $n > 1$, the goal functions $f_1,\dots,f_n$ are aggregated to a weighted sum $S = \Sigma\ w_i f_i$ with $\Sigma|w_i| = 1$ and w_i are weighting factors. *ISSOP* uses the model variables and target values as input data and gives optimised state variables back to the simulation system.

4. Experimental area and basic simulations

For water quality simulations the river basin was divided into several segments of different length (fig. 4).

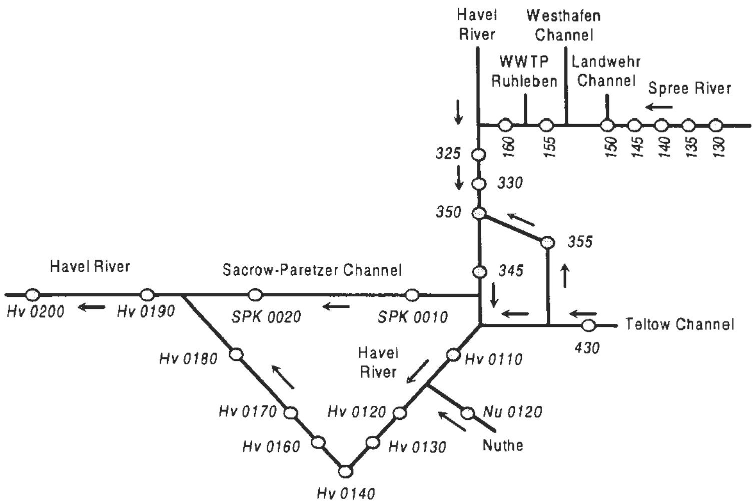


Figure 4. Scheme of the experimental area

The Havel River with its tributary Spree River belongs to the catchment of the Elbe River. Both rivers form a basin which is characterised by small elevation differences between source and mouth, by shallow lakes, wetlands and marshy country, as well as by high evaporation rates (Klose 1995; Kalbe 1997). Only 25% of precipitation contributes to flow. The experimental area is part of the Berlin/Potsdam region. Time series of water quality data from 1997 are taken into consideration as references, while time series from 1998 to 2002 from different measuring points along the course of the rivers were used for modelling and parameterisation. After validation procedures the eutrophication simulator *HavelMod* was used to carry out basic simulations for the rivers Spree and Havel.

Fig. 5 shows the results of simulation runs for phytoplankton, orthophosphate phosphorus and nitrate nitrogen.

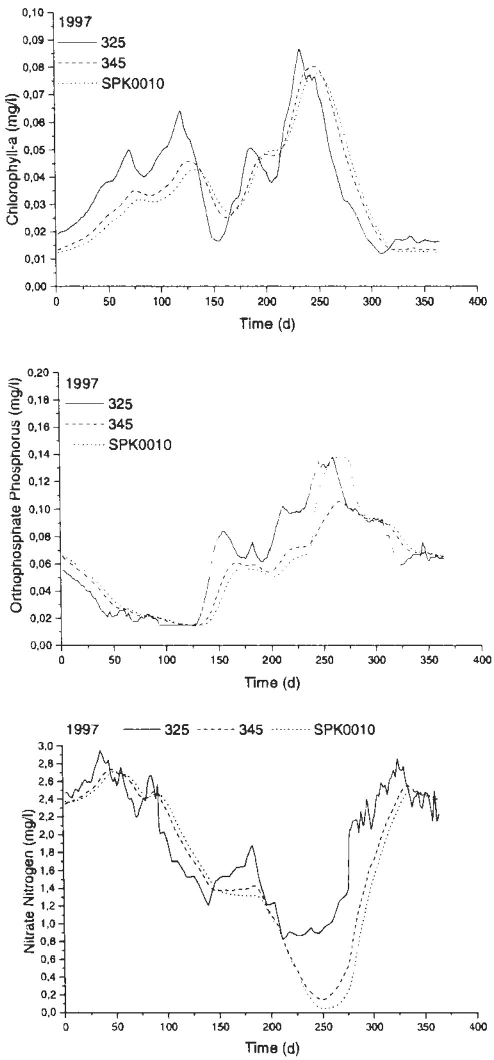


Figure 5. Basic simulation runs for the urbanised area of the river basin

The water quality of this river stretch is mainly influenced by the anthropogenic activities of the urbanised area of Berlin/Potsdam. The concentration levels vary strongly at monitoring station 325 as it can be seen from fig. 5. At the other stations concentration lines are more smoothed. Phytoplankton shows the typical behaviour for this region: A local maximum of phytoplankton is caused by diatoms in spring and a higher one in late summer by cyanobacteria. In accordance with this behaviour phosphate phosphorus is decreased in spring. The increase in late summer is caused by phopshorus remobilisation from sediment. On the other hand, the nitrogen compounds ammonia and nitrate show higher values in spring but lower values in late summer and fall. This overall behaviour is based on two different processes. The first process is known as nitrification (bacterial oxidation of ammonia to nitrate in two steps). The other one is referred to nitrate uptake by cyanbacteria. Increase of nitrogen content at the end of the year is caused by import processes from other river segments.

The concentration lines of important water quality indicators of the following river stretches up to the City of Brandenburg show smaller disturbances. This part of the river is more influenced by natural ecological processes with high retention times of the water body. These conditions lead to a high growth rate of phytoplankton but also to high decay rates of dead organic material. Especially in late summer and fall anoxic conditions on sediment surface hold. From fig. 6 can be seen a considerable higher the amount of soluble phosphorus at the end of the river stretch (Hv0200) under investigation.

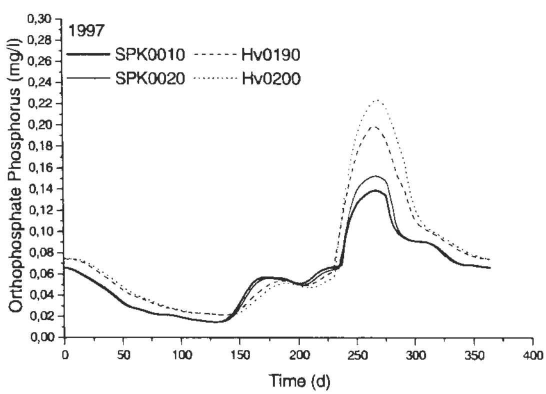
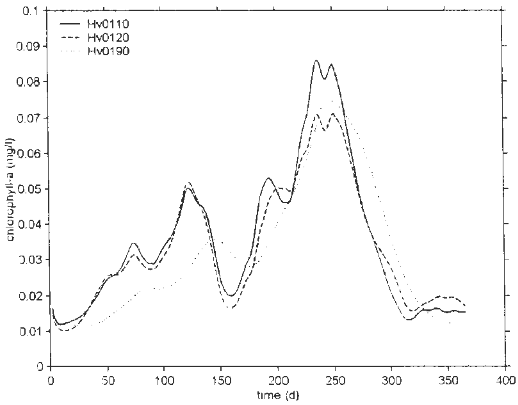


Figure 6. Basic simulation runs for orthophosphate phosphorus

Management options will then be obtained by scenario analyses with changing parameter values. Fig. 7 shows a result of a study concerning an enlargement of some river stretches of the River Havel (Gnauck et al. 2002a). Comparing the ecosystem state after river enlargement with the reference state from 1997 no better water quality can be expected. The biomass concentration levels are more or less the same.



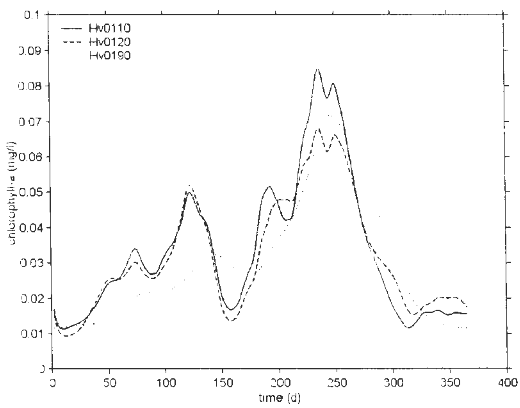


Figure 7. Comparison of basic simulation runs and scenarios

5. Optimisation runs

To get optimised management options the coupled simulator was used. In the case of *HavelMod* the input variables 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. $M(\alpha_1 x_1, \alpha_2 x_2, \alpha_3 x_3) = (y_1, y_2, y_3)$ denotes the system transfer function. 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].

Following goal functions are considered:

Phytoplankton biomass $f_1(t) = \Sigma_x \Sigma_t \, y_1(x, t) \rightarrow \min.$

Orthophosphate phosphorus $f_2(t) = \Sigma_x \Sigma_t \, y_2(x, t) \rightarrow \max.$

Nitrate nitrogen $f_3(t) = \Sigma_x \Sigma_t \, y_3(x, t) \rightarrow \max.$

Weighting factors w_1, w_2 and w_3 with $|w_1| + |w_2| + |w_3| = 1$ are derived from two management strategies:
(i) Weights according to limiting nutrient concept (LNC).
(ii) Weights according to LAWA concept (LAWA 1998).
Values are given in table 1.

Table 1. Normalised weights $|w_i|$ (%)

Variable	LNC	LAWA
CHA (mg/l)	90.5	42
o-PO4-P (mg/l)	1.1	57
NO3-N (mg/l)	8.4	1

In the case of LNC the optimisation problem was solved by using gradient search combined with MCM for w_1 = 90.5%, w_2 = -1.1% and w_3 = -8.4% and α_2 = 0.01 and α_3 = 0.90 while in the other case gradient search method was used only with weighting factors w_1 = 42%, w_2 = -57% and w_3 = -1% and α_2 = 0.03 and α_3 = 0.91.

Management options according to LNC lead to a diminished phytoplankton maximum in late summer by optimised nitrate concentrations as can be seen from fig. 8. No effect of optimised orthophosphate phosphorus concentration can be stated.

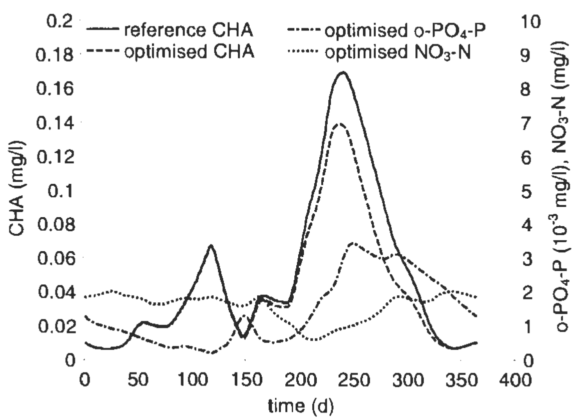


Figure 8. Management options for phytoplankton biomass according to LNC

On the other hand, management options according to LAWA regulations lead 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. 9).

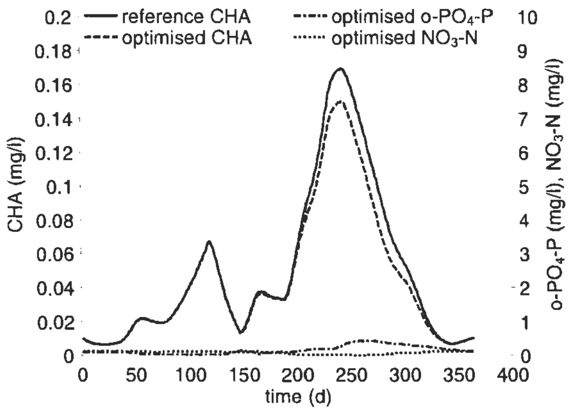


Figure 9. Management options according to target values of LAWA

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

LNC: $f_1 = 44.991$ µg/l, $f_2 = 1.472$ µg/l, $f_3 = 1.54$ mg/l,

LAWA: $f_1 = 48.762$ µg/l, $f_2 = 0.166$ µg/l, $f_3 = 0.08$ mg/l.

6. Conclusions

The use of combined simulation-optimisation procedures to manage the quality of freshwater ecosystems is an approach promising more theoretical understanding of complicated natural processes and software engineering methods. Mostly, management options 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. Some problems exist in formulating optimal management conditions which are most appropriate for freshwater ecosystems, and how far different goal functions are equivalent. The study of goal functions can be considered as a study of land use changes in the river basin. 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.

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APPLICATIONS OF INFORMATICS IN ENVIRONMENT ENGINEERING AND MEDICINE

The purpose of the present publication is to popularize applications of informatics in environment and health engineering and protection. Runned papers are thematically chosen from the works presented during the conference *Multiaccessible Computer Systems* (*Komputerowe Systemy Wielodostępne*) that has been organized by the Systems Research Institute and University of Technology and Agriculture of Bydgoszcz for several years in Ciechocinek. Problems described in the papers concern quality management of the surface waters and the atmosphere, application of the mathematical modelling in environmental engineering, and development of computer systems in health and environmental protection. In several papers results of the research projects financed by the Polish Ministry of Science and Information Society Technologies are presented.

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