Instytut Badań Systemowych PAN

Raport IBS PAN/PMKiI/03/2001

Modelowanie matematyczne, symulacja komputerowa i identyfikacja miejskiej oczyszczalni ścieków

Pod redakcją Jana Studzińskiego i Lucyny Bogdan

Warszawa 2001

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W Raporcie przedstawiono trzy artykuły zawierające wyniki badań w zakresie modelowania, symulacji komputerowej, identyfikacji i sterowania procesów technicznych i technologicznych zachodzących w mechaniczno-biologicznej oczyszczalni ścieków. Badania były prowadzone w ramach projektu badawczego KBN pn. Optymalizacja i sterowanie procesu technologicznego w mechaniczno-biologicznej oczyszczalni ścieków na podstawie modeli matematycznych. Artykuły te, opublikowane w 2001 r., są następujące:

1. *Modellierung oekologischer Prozesse in Klaeranlagen (autorstwa J. Studzińskiego i J. Łomotowskiego), opublikowany w książce pt. Systemtheorie und Modellierung von Oekosystemen, w serii Umweltwissenschaften, wydanej przez Physica-Verlag w Heidelbergu pod redakcją A. Gnaucka*
2. *Komputerowe wspomaganie zarządzania komunalną oczyszczalnią ścieków (autorstwa J. Studzińskiego), prezentowany na konferencji pn. Komputerowe Systemy Wielodostępne KSW'2001, w Ciechocinku w br., opublikowany w książce pt. Rozwój i Zastosowania Technologii i Systemów Informatycznych, wydanej przez IBS PAN pod redakcją J. Studzińskiego, L. Drelichowskiego i O. Hryniewicza*
3. *Mathematical and neural network modelling of a wastewater treatment plant (autorstwa L. Bogdan, J. Łomotowskiego, Z. Nahorskiego, J. Studzińskiego i R. Szeteli), opublikowany w piśmie Archives of Control Sciences.*

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Mathematical and Neural Network Modelling of a Wastewater Treatment Plant

LUCYNA BOGDAN, JANUSZ ŁOMOTOWSKI, ZBIGNIEW NAHORSKI, JAN STUDZIŃSKI and RYSZARD SZETELA

Comparison of few methodologies of building models useful in wastewater treatment plant maintenance is performed. One is mathematical modelling of the activated sludge process. It consists of modellling of the basic vessels: primary clarifiers, aerator basins and secondary clarifiers, linked and partially looped, as well as equations describing the physical and biochemical transformations going on in the vessels: sedimentation in the clarifiers and biological processes changing the influent wastewater chemical composition. The models' parameters were estimated in two steps. In the first step the active volumes of the vessels were estimated from the experiment performed in the plant. In the second step, parameters known from the literature were used as the initial guess and then calibrated to fit the observations taken during normal plant operation.

Concerning other methodologies, results from the black box modelling of the performance of the plant with the neural network are given. The neural network and the time series models are also applied for prediction of the influent wastewater.

Key words: wastewater treatment, biochemical processes, modelling, parameter estimation, neural networks

1. Introduction

Conventional automation, with PID type controllers, has entered to the wastewater treatment plants since some time ago. Although it proved very useful in stabilizing different unit processes, in many cases it could not cope with the changing conditions caused by nonstationary inflow of the municipal wastewater with involved predominant diurnal periodicity.

Knowing mathematical equations describing transformations of wastewater components, it is possible to formulate a model of the overall treatment process. Models of this kind have been already built but their practical use in control of plants is still limited,

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because of a rather big complexity of the models and difficulty in obtaining satisfactory accuracy of prediction. However, these models, based on physical, chemical, and biological laws and principles, can be very useful in better understanding of the process itself and in its qualitative assessment. Moreover, it seems that more advanced applications of these models can be noticed. One of them is estimation of variables that are not possible to measure. Another is help in better manual control of the process, e. g. as a part of an expert system for process control.

The model presented in the first part of this paper goes in this direction. It has been prepared for the existing municipal wastewater treatment plant in Rzeszów, a town in southeast part of Poland, and calibrated to the measurements performed during an active experiment. The model belongs to the class known in the literature as the Activated Sludge Model No. 1 [17]. These kind of models describe wastewater processes with degradation of organic and nitrogen components only. The equations of the model presented in the paper form a subset of equations of a more general model presented in [32], chosen and modified to conform to the conditions of the Rzeszów plant.

This physically oriented model, although useful in many instances, is rather complicated and thus not very suitable for control and optimization. That is why simpler models have been proposed. Time series models, often with the recursive estimation of parameters, were used e. g. in [8, 19, 27, 28]. Carstensen [9] fitted AR models to transient processes occuring in the BIO-DENITRO and BIO-DENIPHO configurations to smooth the measurements. This smoothed sequence was further used to estimate the parameters of a physically oriented models. Separated stages of the BIO-DENITRO and BIO-DENIPHO processes considerably simplified the task.

Neural networks have been employed in [4, 15]. In the latter one it is combined with the fuzzy logic, see also [11,35], which was the third of proposed simplified methods of coping with the problem.

In this paper the time series and the neural network models are used to predict the inlet flow rate to the plant. Moreover, the neural network model is used for prediction of the quality of the effluent from the plant on the basis of measurements of different variables, both uncontrollable, in the influent, and controllable ones: the oxygen concentration in the aeration basin and the rate of recirculation flow in this basin.

2. Wastewater Treatment Plant in Rzeszów

The wastewater plant in Rzeszów is designed for treating 75 000 m^3/day of the wastewater coming from the part of Rzeszów town lying on the left bank of the Wisłok river. The town sewerage system is partly of the mixed type, as in the old town it is connected to the rainwater drainage. Apart from the domestic sanitary wastewater there are also industrial discharges, coming from 112 plants, among them pharmaceutical, food processing, big metal industry works, etc. The wastewater treatment plant consists of the inlet pumping station, grit chambers, two primary clarifiers, three parallel aeration basins and two secondary clarifiers. This is shown schematically in Fig. 1.

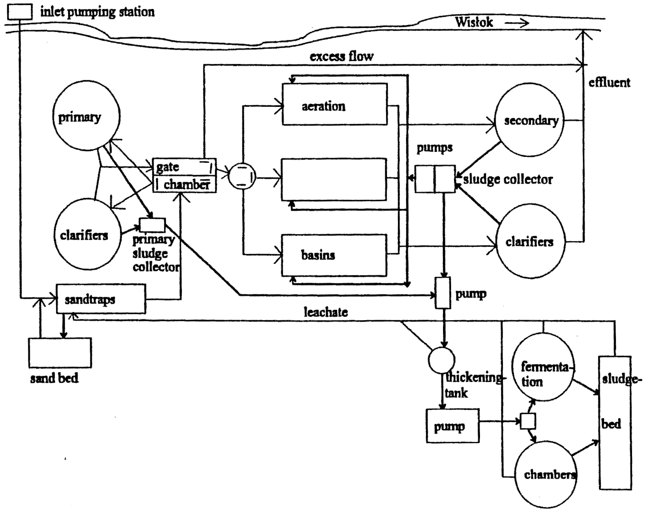

Figure 1. Water treatment plant in Rzeszów.

After removal of coarse solids by screening and degriting in the grit chambers the wastewater enters the primary clarifiers where settleable solids settle down while the rest of the wastewater flows to the activated sludge basins equipped with fine pore aeration system. The organic material is decomposed there biologically under aerobic conditions. The mixed liquor from the aeration tanks passes to the secondary clarifiers where the sludge is separated from the treated wastewater by means of gravitational settling of the sludge particles. Part of the sludge is recirculated to the inlet of the aeration basins while the excess sludge is removed from the process for further treatment.

Table 1 shows the treatment plant influent characteristics, as measured in 1994. On the basis of these data the wastewater can be classified as moderately loaded as far as nutrients (nitrogen, phosphorus) are concerned but heavily loaded in organic matter (high values of COD – the chemical oxygen demand, and BOD_5 – the five-day biochemical oxygen demand).

3. Prediction of the Plant Inlet Flow Rate

An important factor in operation of the wastewater plant is the inlet flow rate. Its basic component is of a cyclic form with predominant diurnal cycle. Moreover, the weekly cycle can be clearly seen in the flow rate diagram. They are connected with the periodic human activities in the area covered by the sewerage system. The flow rate depends also

Table 1. Influent loads at the Rzeszów plant in 1994.

	unit	min.	average	max.
Flow rate	m^3/d		35 000	
suspended solids	g/m^3	84.0	309.2	349.1
BOD5	gO_2/m^3	80.0	416.8	770.0
COD	gO_2/m^3	325.0	507.6	753.0
ammonia nitrogen	gN/m^3	14.0	28.3	40.0
total nitrogen	gN/m^3	29.0	52.9	81.0
total phosphorus	gP/m^3		15.1	
total sulphur	gS/m^3		94.2	

on the atmospheric conditions, like precipitation, melting of snow, etc., and dynamics of the sewerage system.

A possible approach to prediction of the plant inlet flow is the physically oriented mathematical modelling of the sewerage system. A successful application of this kind of approach depends on possibility of estimation of, usually many, unknown parameters of the system.

Another posibility is offered by the black box approach. This type of models enable prediction of the future values of the inlet flow rate on the basis of its past values as well as the past values of some variables which decide on the flow, like rainflow intensities in chosen locations of the sewerage area or the wastewater levels in the system, see e.g. [16]. As these kind of data were not available to us, we present here only results of prediction based on the past values of the inlet flow rate. Thus the model represents mainly the inertia of the sewerage system.

The data used were collected in the Rzeszów wastewater treatment plant in March and May 1996. The measurements were taken every 2 mins. and then averaged over one our, i.e. the average of 30 consecutive measurements formed one point of data which was then taken for further processing. This way 744 data from March and the same number from May were obtained. The former were used as the training sequence and the latter as the testing sequence.

Two methods were adopted. The first used a time series model, namely the autoregressive (AR) model, and the second a neural network. In both of them prediction was performed on the basis of five preceeding measurements. Thus the AR model had the form

$$y_n = a_1 y_{n-1} + a_2 y_{n-2} + \ldots + a_R y_{n-R} + e_n$$

with $R = 5$, where a_1 to a_5 are model parameters, and e_n, $n = 1,2,\ldots,N$ are the errors assumed to be independend and identically distributed stochastic variables with the distribution $\mathcal{N}(0,\sigma^2)$, where σ^2 is the unknown variance. Several methods of estimation of the parameters are known for this model. Out of them, the least squares method was used here. Tests of significance of the parameter estimates were done and all estimates were found significant.

A neural network consists of neurons. A neuron produces an output a from an input p using a weight w, a bias b and a transfer function F. Both w and b are adjustable. By adjusting w and b in all neurons, the network will be trained. That training can be done by various optimization methods, depending on network architecture, computer power and the criterion used. The neurons can be combined into a layer. A network contains of one layer or multiple layers. Here three layers were used: the input layer, the hidden layer, and the output layer. Each neuron on a layer is then connected through a weight matrix $w(i, j)$ to each neuron of the next layer. Each neuron sums up the weighted inputs and adds a bias. Depending on the form of the transfer function, linear or nonlinear neural models can be obtained. To determine the neural network the number of layers,

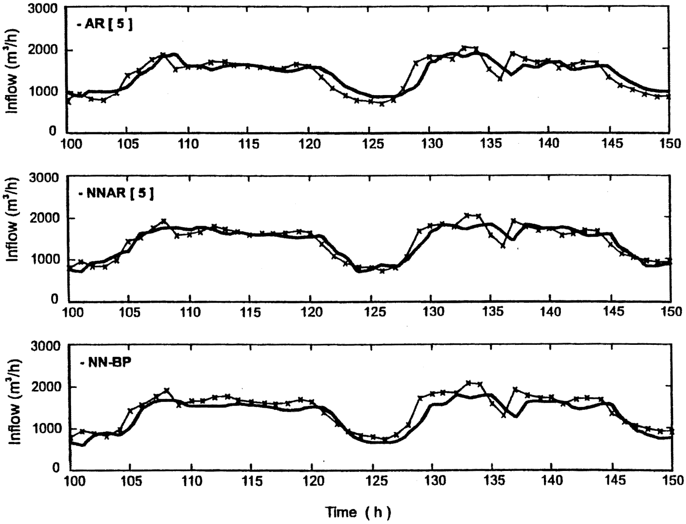

Figure 2. Fits of the models after the learning phase for the AR model (upper panel) and the two neural network models (middle and lower panels). The measurements are depicted with the crosses. The thick solid lines represent the outputs of the models.

the number of neurons on each layer and the values of parameters of each neuron have to be established. The latter are usually defined during the learning process which consists in adjusting the weight matrix and bias vector of each layer to fit the network output to the measurements. Sum of squared errors was used as the criterion and it was minimized using the Levenberg-Marquard method. The quality of the model was checked on the testing sequence. Two linear neural models were used: the NNAR model (neuronal net autoregressive model) had 5 neurons on the input layer, 7 neurons on the hidden layer and 1 neuron on the output layer, while the NNBP model (neuronal netback propagation model) had 5, 6 and 1 neurons, respectively. In both cases the data were normalized: for

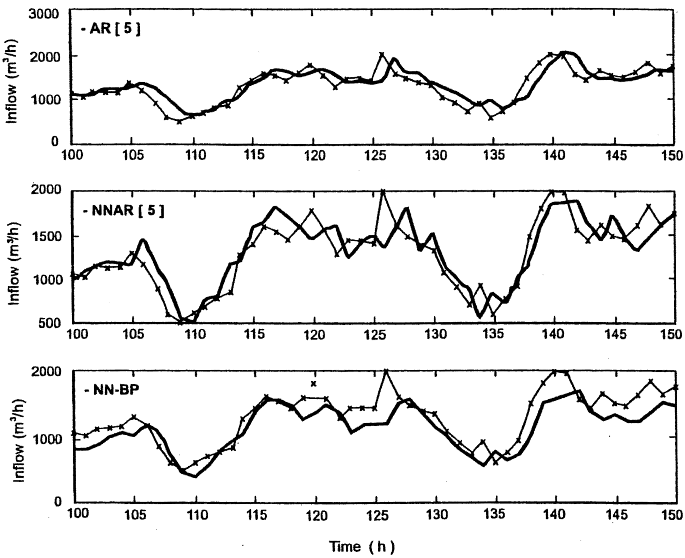

Figure 3. Fits of the models for the testing sequence for the AR model (upper panel) and the two neural network models (middle and lower panels). The crosses and the thick solid lines depict the measurements and the outputs of the models, respectively.

the NNAR model to form the zero mean and the unit variance series and for the NNBP model to the interval [0, 1]. In the NNAR model additionally pruning has been done, i.e. insignificant connections between neurons have been dropped.

Figures 2 and 3 show results from the learning and the testing phases. They present high similarity in the fits after the learning phase. In the testing phase the AR model gave a little more accurate fit. Yet for the practical reasons any of the models considered can be satisfactorily used for prediction purposes.

4. Hydrological Model

The hydrological model consists mainly of submodels of the basic vessels that may be treated as the ideally mixed tanks. There is only one unknown parameter in each submodel that is the vessel volume. Often only part of the vessel geometric volume is engaged in flow dynamics. It is called the active volume. It may differ significantly from the geometric one, as in the case discussed in the sequel. The main difficulty in estimating the active volume experimentally in the wastewater treatment process arises from the unsteady inflow to the plant during the day, as seen in Fig. 4. This is the reason why a mathematical model with variable parameters is proposed to describe the vessels.

Advantage of compensating for the variability of the parameters in flow systems before application of an identification procedure has been pointed out in [2], as resulting in much better simulation ability of the model and much smaller fluctuations of the estimated there residence time. The compensation used there was done by an appropriate resampling pattern. This idea can be as well used in our method, although ours works well also without resampling.

Variations of the inflow influence the volume of the liquid in the vessel. Typically, the excess liquid overflows through the vessel edges. Thus, higher inflow causes some raise of the liquid level. This phenomena will be discussed in the sequel. We start, however, with a simpler case, disregarding the changes in the volume.

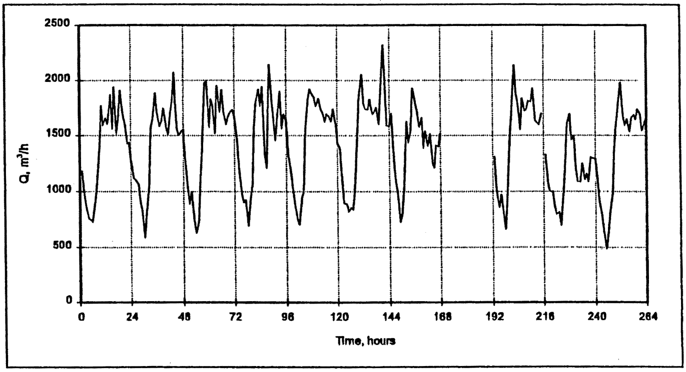

Figure 4. Influent flow rate to the plant.

4.1. Constant Vessel Volume

If a tracer is used in a measuring experiment, the balance of the tracer mass measured yields the equation

$$V\frac{dc(t)}{dt} = Q(t)[c_{in}(t) - c(t)] \tag{1}$$

where V is the active volume, $c(t)$ is the concentration of the tracer in the vessel and $c_{in}(t)$ its concentration in the influent, $Q(t)$ is the influent flow rate. This is the first order ordinary differential equation with a varying parameter.

Let us introduce a new variable [26]

$$\xi(t) = \int_0^t Q(\tau)d\tau$$

which is the amount of wastewater which has passed through the vessel from the beginning of observations. As $Q(t) > 0$, then there exists the inverse differentiable function

$t = g(\xi)$. Inserting it to (1) we get

$$V\frac{dc(\xi)}{d\xi}\frac{d\xi}{dt} = Q(\xi)[c_{in}(\xi) - c(\xi)]$$

where $c(\xi) = c(g(\xi))$ and similar for $c_{in}(\xi)$ and $Q(\xi)$. We have used here the same notation for the function $c(t)$ and for the superposition of functions $c(g(\xi))$ in order to simplify the consideration. But $d\xi/dt = Q(t)$, and therefore

$$V\frac{dc(\xi)}{d\xi} = c_{in}(\xi) - c(\xi) \tag{2}$$

Thus, when the lapse of time is measured in the passed liquid flow instead of time, then the vessel is described by the equation with a constant parameter.

When planing an active experiment it was found that the piecewise constant application of the tracer, $c_{in}(\xi) = c_{in}(\xi_{n-1})$ for $t_{n-1} \leqslant t < t_n$ where $\xi_{n-1} = \xi(t_{n-1})$, and t_{n-1}, t_n are the $(n-1)$th and nth observation time, respectively, would be technologically most suitable. In this case the equation (2) can be transformed to

$$c(\xi_n) = \frac{1}{V}\int_0^{\xi_n} e^{-\frac{\xi_n-\tau}{V}} c_{in}(\tau)d\tau = e^{-\frac{\Delta_n}{V}}c(\xi_{n-1}) + (1-e^{-\frac{\Delta_n}{V}})c_{in}(\xi_{n-1}) \tag{3}$$

where $\Delta_n = \xi_n - \xi_{n-1}$ is the observation interval.

The data used for estimation of the active volume V were gathered during the experiment in which chlorine ions were used as the tracer. This was achieved by adding salt (NaCl) to the vessel inflow. An optimal piecewise constant input for the constant observation interval was found to be periodic, with the period between $4V$ and $6V$ (depending on the value of Δ). The optimal observation interval was around V or $1.5V$ (two close optima), with a rather flat criterion function between and around them, see [25].

If the tracer concentration is observed with good accuracy, then the volume V can be estimated from the expression

$$\frac{c(\xi_n) - c_{in}(\xi_{n-1})}{c(\xi_{n-1}) - c_{in}(\xi_{n-1})} = e^{-\frac{\Delta_n}{V}},\ n = 1,2,...,N \tag{4}$$

The nonlinear least squares method can be used for this purpose.

For technological reasons it was not possible to measure concentrations of the chlorine ions at each inlet and outlet of the parallel vessels. Thus the respective sums of volumes for the two primary clarifiers, three aeration basins and two secondary clarifiers, respectively, have been estimated. Two estimation methods have been used: (i) linear least squares (LS) using equation (3), (ii) nonlinear least squares (NL) using equation (4). To use the LS method the signals $c(n)$ and $c_{in}(n)$ were interpolated to get constant values of $\Delta_n = \xi_n - \xi_{n-1} = \Delta$. This way the equation could be transformed to the form

Table 2. Estimates of the active volumes V of the vessels, in [m^3].

	primary clarifier	aeration basin	secondary clarifier	
			upper	lower
LS	5676	11246	4723	6303
NL	6283	12087	4612	6514
average of values above	5980	11667	4668	6408
geometric volumes	7820	13500	11060	
$\frac{\text{average}}{\text{geometric}}$ [%]	76,5	86,4	100	

$c(n) = ac(n-1) + bc_{in}(n-1)$ where $b = 1 - a$ and $a = exp(-\Delta/V)$ are constant parameters. A selection of the estimation results from [5] is presented in Table 2.

In the secondary clarifiers, see sketch on Fig. 5, the tracer output concentrations were measured both in the overflow and in the recirculated sludge outflow from the bottom of the clarifiers. Therefore, the total volume was divided into two zones: the upper zone V_g, attributed to the overflow, and the lower zone V_d, attributed to the recirculated sludge outflow. Both of them were estimated and the results obtained are shown in the right hand part of Table 2. For each estimation method the sum of both zone volumes is very close to the geometric volume of the clarifier.

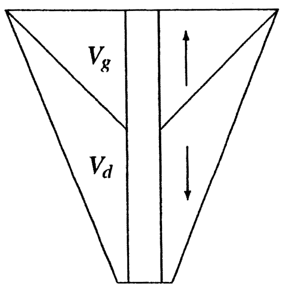

Figure 5. Sketch of the secondary clarifier

In the primary clarifiers only effluent tracer concentration was measured, as the slugde outflow is much smaller there. The active volume estimated is significantly smaller than the geometric volume. This can be connected with the sludge bed gathering in the bottom of the clarifiers. Few factors could also cause the active volume estimate of the aeration basins to be smaller than the geometric volume. Among them the dead parts of the basin volume and the air bubbles from the aeration are likely reasons.

4.2. Variable Vessel Volume

With the variable volume we have

$$V(t) = V_0[1 + \kappa(t)] \tag{5}$$

where V_0 is a constant (minimal, average) volume and $\kappa(t)$ is its variable fraction. The balance of the tracer mass involves now the following equation

$$\frac{d[V(t)c(t)]}{dt} = Q(t)c_{in}(t) - Q_{out}(t)c(t) \tag{6}$$

where $Q_{out}(t)$ is the outflow from the vessel which may be now different from the inflow $Q(t)$. The balance of the liquid in the vessel yields

$$\frac{dV(t)}{dt} = Q(t) - Q_{out}(t) \tag{7}$$

>From (6) and (7) we get

$$V(t)\frac{dc(t)}{dt} = -c(t)[Q(t) - Q_{out}(t)] + Q(t)c_{in}(t) - Q_{out}(t)c(t) = Q(t)[c_{in}(t) - c(t)]$$

which is similar to (1) but with two variable parameters $V(t)$ and $Q(t)$. Taking into account (5) we can, however, write

$$V_0\frac{dc(t)}{dt} = \frac{Q(t)}{1 + \kappa(t)}[c_{in}(t) - c(t)] \tag{8}$$

This way we reduced the problem mathematically to that from the previous subsection. Introducing now a new variable

$$\xi(t) = \int_{t_0}^{t} \frac{Q(\tau)}{1 + \kappa(\tau)} d\tau \tag{9}$$

we reduce the equation, as previously, to the constant parameter one

$$V_0\frac{dc(\xi)}{d\xi} = c_{in}(\xi) - c(\xi)$$

The variable ξ is now not merely the integrated flow, like before, but depends on the variable κ which includes some unknown yet variations of the volume, related to changes in the flow $Q(t)$. This relation depends on the construction of the vessel and is explained on an example below.

Let us consider a vessel whose upper part is a cylinder with the radius R. The upper edge of the cylinder has the saw-like shape, see Fig. 6. Denote by V_0 the volume of the liquid when it reaches the uppermost level with no outflow. Then $\kappa(t) \geqslant 0$. Assume that the geometrical dimensions of the edge are as on Fig. 7 where $h(t)$ is the variable height of the liquid level above the level of the lowest points of the saw. Then the outflow is

$$Q_{out}(t) = \begin{cases} Nvh^2(t)\tan\frac{\alpha}{2} & \text{if } \; 0 < Q_{out}(t) \leqslant \pi RHv \\ NvH^2\tan\frac{\alpha}{2} + 2\pi R[h(t) - H]v & \text{if } \; \pi RHv < Q_{out}(t) \end{cases} \tag{10}$$

where v is the velocity of the liquid normal to vessel edge surface, and N is the number of the outflow triangles around the whole edge. Because it holds

$$2NH\tan\frac{\alpha}{2} = 2\pi R$$

so, inserting N from the above to (10) yields

$$Q_{out}(t) = \begin{cases} \frac{\pi Rv}{H} h^2(t) & \text{if } \; 0 < Q_{out}(t) \leqslant \pi RHv \\ \pi Rv[2h(t) - H] & \text{if } \; \pi RHv < Q_{out}(t) \end{cases} \tag{11}$$

Two assumptions will be admitted:

1. change of the volume is slow, so that approximately $Q_{out}(t) \approx Q(t)$,
2. the velocity v is constant, independent of the liquid level.

Thus, the volume of the liquid in the vessel is

$$V(t) = V_0 + \pi R^2 h(t) =$$

$$= V_0 + \begin{cases} \sqrt{\frac{\pi R^3 H}{v} Q(t)} & \text{if } \; 0 < Q(t) \leqslant \pi RHv \\ \frac{R}{2}\left(\frac{Q(t)}{v} + \pi RH\right) & \text{if } \; \pi RHv < Q(t) \end{cases}$$

and finally

$$\kappa(t) = \begin{cases} \sqrt{\frac{\pi R^3 H}{vV_0^2} Q(t)} & \text{if } \; 0 < Q(t) \leqslant \pi RHv \\ \frac{R}{2V_0}\left(\frac{Q(t)}{v} + \pi RH\right) & \text{if } \; \pi RHv < Q(t) \end{cases} \tag{12}$$

In this case calculation of the variable ξ requires additional knowledge of the vessel characteristics as well as the unknown volume V_0. When necessary, as an approximation of V_0 the geometric volume can be used in the first iteration.

To test how much the disregard of variation of the liquid volume influences the distribution of the sampling times, as compared to the constant volume approximation, the flow rate data from the experiment described in the previous subsection have been used. The calculation gave κ in the range 0.015 - 0.025 and the estimate of the active volume slightly smaller than when using the approximation of the constant volume. The difference did not exceed 2,5% which is of the same order as errors of the statistical estimates. Taking into account difference in definitions of the active volumes in both cases (average volume versus minimal volume) which is of the order of 1%, one can conclude that the constant volume approximation gives sufficient precision of estimation although the volume estimator may be slightly biased, around 1% too high.

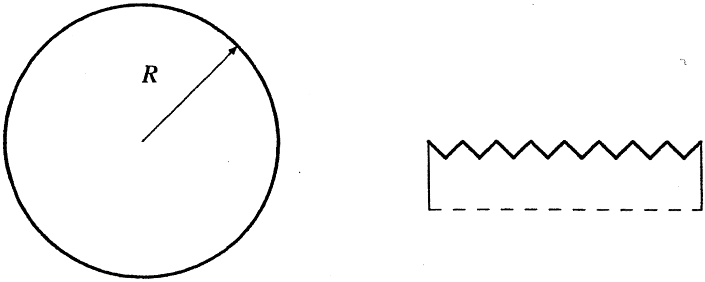

Figure 6. Shape of the upper part of the vessel

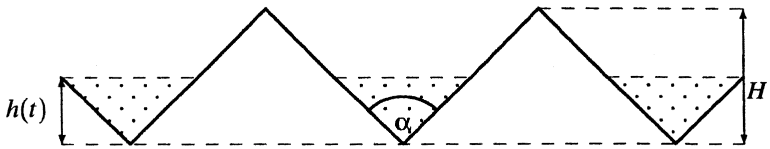

Figure 7. Geometrical dimensions of the vessel upper edge

5. Biological Processes

Various microorganisms take part in biological processes arising in the aeration basin, like bacteria, fungi, protozoa, etc. Out of them bacteria are most important for biochemical decomposition of the wastewater components. An integrated model of the wastewater biochemical transformations is rather complex, and will be not discussed here in full extent. More elaborated presentation of the biological part is presented in [6]. Full details of the model can be found in [32].

Different subprocesses can be distinguished in the wastewater purification process. Simple differential equations are typically applied to describe the changes in the concentrations of different media taking part in the transformations. The most important are:

- The first order kinetics

$$\frac{dx}{dt} = -kx$$

where x is the concentration of the medium and k is a constant,

- The Monod kinetics

$$\frac{dx}{dt} = \mu \frac{s}{k_s + s} x$$

where x is the concentration of the active biomass, s the concentration of a rate limiting nutrient or substrate, μ the maximum specific growth rate of the biomass, k_s a (half saturation) constant. If more than one limiting nutrient or substrate is involved, the product of the Monod expressions can be applied.

Introducing the yield

$$Y = -\frac{\Delta x}{\Delta s}$$

the corresponding rate of nutrient or substrate consumption is given by

$$\frac{ds}{dt} = -\frac{\mu}{Y} \frac{s}{k_s + s} x$$

The basic subprocesses arising during the wastewater treatment in the plant considered are the following.

Hydrolysis. In order to grow, bacteria need energy. Most of the activated sludge bacteria are heterotrophic ones, which use organics as carbon and energy source. The carbon has to be in readily biodegradable organic molecules, like acetic acid, methyl alcohol, ethyl alcohol, glucose, etc. The larger organic molecules (slowly biodegradable substrate) are transformed into smaller ones in a process called hydrolysis. This process is rather slow but starts already in the sewerage system. The rate of the hydrolysis is often described by a first order kinetic expression.

Biomass Growth and Decay. The growth of the biomass (organisms) is limited by availability of nutrients. The influence of a single limiting nutrient or substrate concentration on the growth rate can be described using Monod kinetics. Biomass decays due to endogenous metabolism, death, predation and lysis. This way the active biomass is transformed into slowly biodegradable substrate. The decay of biomass may be described as a first order equation. Decays of two kinds of bacteria are considered: the heterotrophic bacteria and the autotrophic bacteria. The decaying biomass contains also the inert fraction. The rest of the decaying biomass adds up to organic carbon and nitrogen.

Aerobic Removal of Organic Carbon. The conditions for the growth of the biomass depend on the dissolved oxygen and nitrate concentrations. If the dissolved oxygen concentration s_O is high (say $s_O > 0.5$ mg O_2/l), then the conditions are called *aerobic*. If the dissolved oxygen concentration is low, but there is a high nitrate concentration s_{NO}

(say $s_{NO} > 0.5$ mg N/l), then they are called the *anoxic* conditions. When both concentrations are small, then the conditions are *anaerobic*. Depending on the conditions, different bacteria genera may be predominant in the wastewater.

Under aerobic conditions, considered in this subsection, formation of a typical biomass compound $C_5H_7NO_2$ from a typical substrate average composition $C_{10}H_{19}O_3N$ is given by the following reaction

$$C_{10}H_{19}O_3N + 4.535O_2 + 0.593\,NH_4^+ = 2.035CO_2 + 4.814H_2O + 1.593C_5H_7NO_2 + 0.593H^+$$

The rate of this transformation depends on the availability of the substrate, oxygen and ammonia giving rise to an appropriate kinetics with three Monod factors.

The Nitrification Process. Nitrification is a two-step process in which ammonia is transformed into nitrite and subsequently into nitrate

$$NH_4^+ + 1.5O2\ NO_2^- + H_2O + 2H^+$$
$$NO_2^- + 0.5O2\ NO_3^-$$

Also this reaction arises in the aerobic conditions. The yield coefficient for nitrifying (autotrophic) bacteria is significantly smaller compared to those of heterotrophic bacteria. Taking into account assimilation process (building up the nitrogen in the biomass structure) and the yield coefficient, the following equation for the both phases of nitrification is obtained

$$1.013NH_4^+ + 0.063CO_2 + 1.937O_2 = NO_3^- + 0.975H_2O + 0.013C_5H_7NO_2 + 2.013H^+$$

All three components on the left hand side may be rate limiting but in practice only the ammonia and oxygen concentrations impose limitations. Thus the Monod kinetics contains two factors.

The Denitrification Process. Apart of the decomposition of organic material, during the denitrification process the heterotrophic bacteria transform nitrate into free nitrogen. This is done under anoxic conditions when the concentration of the nitrate in the wastewater is high while there is lack of oxygen. Heterotrophs use the nitrate as an electron acceptor. For a typical wastewater composition the reaction has the form

$$C_{10}H_{19}O_3N + 10NO_3^- = 9CO_2 + 2H_2O + 5N_2 + 10OH^- + NH_4HCO_3$$

Taking into account the biomass synthesis, it yields

$$C_{10}H_{19}O_3N + 3.272NO_3^- + 0.593NH_4^+ =$$
$$2.035CO_2 + 2.288H_2O + 1.636N_2 + 1.593C_5H_7NO_2 + 3.272OH^- + 0.593H^+$$

Heterotrophic bacteria use rather ammonia for growth and in its lack they can use nitrates. Therefore only two limiting concentrations will be used.

The processes mentioned above cause the wastewater alkalinity changes which is included in the model. The alkalinity may be also affected by chemical precipitation of the phosphorus. Phosphorus may be also removed from the wastes in the biological processes. The plant considered was not constructed for this purpose and therefore modelling of the related phenomena was not considered. Presentation of the this kind of model can be found in [18].

6. Wastewater Treatment Plant Model

A model of the basic treatment line consists of the models of primary clarifiers, aeration basins and secondary clarifiers, together with the appropriate connections between them, see Fig. 1. Two former vessels were modelled as the ideally mixed tanks, with the active volume estimates given in section 4, and with additional transformations going on in them. The biochemical transformations arising in the aeration basin were mentioned above. Here we concentrate on physical processes occurring in two other vessels and give overall view of the integrated model.

Primary Clarifiers. In the model the influent waste constituents were divided into different fractions gathered in two main groups. One is connected with the oxidation ability and the other with the contents of ammonia. The rest forms the suspended solids group.

Two measures of oxydation ability are mainly used. *Five day biochemical oxygen demand* (BOD_5) is defined as the mass of oxygen demand of a *Pseudomonas* culture over five days in a unit volume of the wastewater. *Chemical oxygen demand* (COD) is specified as the mass of oxygen required to completely oxidize the constituents of a unit volume of the wastewater. It is clear that BOD_5 is always smaller than COD.

Here we characterize the fractions of the wastewater in parts of COD and the total nitrogen N_{og}:

- COD fractions:

  - readily biodegradable fraction $s_s = 0.1608$ COD
  - slowly biodegradable fraction $x_s = 0.4384$ COD
  - dissolved inert fraction $s_I = 0.0451$ COD
  - suspended inert fraction $x_I = 0.3557$ COD

- nitrogen (N_{og}) fractions:

  - ammonia $s_{NH} = 0.7845$ N_{og}
  - dissolved organic nitrogen $s_{ND} = 0.0616$ N_{og}

- suspended organic nitrogen $x_{ND} = 0.1539\ N_{og}$

- suspended solids $z_m = 0.2927\ Z_{og}$,

where Z_{og} is the total suspension load. The fractions given above were identified from the measurements taken at the plant.

It is assumed that the dissolved fractions pass the primary clarifiers without any loss. A model describing the change of their concentration is that of an ideally mixed tank

$$V_p \frac{ds}{dt} = Q(s_{in} - s)$$

where V_p is the clarifiers active volume, Q is the flow, s_{in} is the concentration of the influent dissolved fraction and s is its concentration in the clarifiers.

The model for the suspended fraction includes, besides that of ideally mixed tank, also sedimentation of the suspension. The sedimentation rate is expressed as Ax^B where x is the concentration of the suspended fraction. The parameters A and B were estimated experimentally. Thus the model is

$$V_p \frac{dx}{dt} = Q(x_{in} - x) - V_p A x^B$$

where $x = x_s + x_l + z_m$. Because of sedimentation, the primary clarifiers reduce COD and nitrogen concentration of the wastewater.

Aeration Basins. Also the aeration basins were modelled as the ideally mixed tanks. The full model includes all transformations described in the previous section, as well as the change of the oxygen concentration and alkalinity of the wastewater. Flows from the primary clarifiers and the recirculated sludge from the secondary clarifiers mix together to form the input to the basins. The model includes the following processes:

- aerobic growth of heterotrophs with assimilation of nitrogen from NH_4^+
- aerobic growth of heterotrophs with assimilation of nitrogen from NO_3^-
- anoxic growth of heterotrophs with assimilation of nitrogen from NH_4^+
- anoxic growth of heterotrophs with assimilation of nitrogen from NO_3^-
- aerobic growth of autotrophs
- decay of heterotrophs
- decay of autotrophs
- ammonification of dissolved organic nitrogen
- hydrolysis

and transformations of the following components:

- organic readily biodegradable component
- dissolved inert organic component
- ammonia
- nitrate
- dissolved organic nitrogen
- dissolved oxygen
- alkalinity
- organic slowly biodegradable component
- inert organic component in suspension
- heterotrophic bacteria biomass
- autotrophic bacteria biomass
- inert organic component from decaying organisms
- organic component in suspension
- suspended minerals

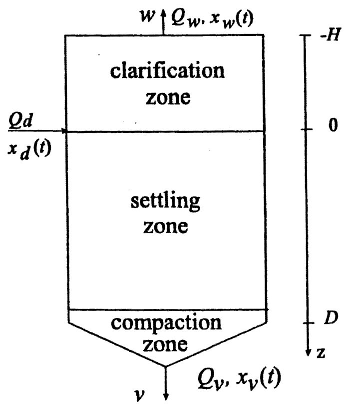

Figure 8. Secondary clarifier.

Secondary Clarifiers. The influent entering the secondary clarifiers from the aeration basins consists basically of flocculated bacteria and water. The most important phenomenon taking part in the secondary clarifiers is that of separation of these two components during the sedimentation process. Only this process is taken into account in the model. The secondary clarifier consists of two zones shown schematically on Fig. 8: the clarification zone and the settling zone. Sometimes also the compaction zone is distinguished at the very bottom part where the particles are compressed. There are two outlets from the clarifier. The effluent overflows the upper edge of the clarifier while the sludge leaves the clarifier at the bottom. There are then two currents connected with the outflows: the effluent current with the velocity w, predominant in the clarification (upper) zone, and the sludge current with the velocity v, predominant in the settling (lower) zone. Additionally, the gravitational force acting on solids enforces their move downwards. Its velocity u depends exponentially on the concentration of suspended solids x

$$u(x) = u_0 e^{-bx}$$

see [23]. Note that x is a function of both depth z of the clarifier and time t. The flux $q(x)$ of the suspended solids is then described by the following function (compare Fig. 8)

$$q(x) = \begin{cases} x[u(x)+v] & \text{for} \quad 0 < z \leqslant D \\ x[u(x)-w] & \text{for} \quad -H \leqslant z < 0 \end{cases}$$

The continuity equation is

$$\frac{\partial x}{\partial t} + \frac{\partial q}{\partial z} = 0$$

subject to the initial

$$x(z,0) = x_0(z), \quad -H \leqslant z \leqslant D$$

and a boundary (mass conservation at the inlet) condition

$$Q_d x_d(t) = P_0 x(0,t)[2u(x(0,t)) + v - w]$$

where x_d is the concentration of suspended solids in the influent, Q_d is the influent flow, P_0 is the cross-section of the clarifier at $z = 0$. To solve the above equations the model has been divided into 12 horizontal layers with components assumed homogeneous in each layer.

The model for the dissolved components lacks the flux $q(x)$ and reduces to an ideally mixed tank model for each layer.

7. Model Calibration

The simulation computer program WTPD [32] was used to implement the mathematical model at wastewater treatment plant in Rzeszów. High complexity of the model causes severe problems connected with identifiability of its parameters. This is related both to too large number of unmeasured states and parameters and to difficulties in unique estimation of the Monod kinetic parameters [20]. Moreover, available instrumentation and laboratory procedures are usually not adequate for verification of the details of such a complex model. It is also not clear whether normal operating varations of the input variables perturbe the process well enough to exite all its interesting dynamical modes.

A commonly used approach for estimation of the model parameters is a step by step procedure consisting in separation of different processes arising in the plant in the laboratory equipment to measure the relevant model parameters from wastewater samples taken from appropriate points of the plant [10, 14, 21]. Another approach is to use automatic estimation methods, see [1, 21] for examples of their early applications. Out of them the extended Kalman filter algorithm for recursive estimation of the states and parameters gained some popularity [3, 22, 24, 31]. It is usually combined with simplifications of the model either by exclusion of some processes, like e.g. denitrification, or by a physical insight, [22], or by linearization of the process, [13].

Yet experience from different wastewater plants show that some parameters are fairly constant in changing conditions and only a limited number of those exhibiting greater changes have to be adjusted for a specific plant. Coming from this observations the model was calibrated here using the human expert method, based on professional experience and expertise [21, 34]. Unknown parameter values were determined in a sequential procedure, after assuming default parameters values [32] as first estimates for the simulated plant performance calculations. Differences between predicted and observed output values were then noted, and step-wise adjustments in kinetic and stoichiometric parameter values were made based on the knowledge and experience of the authors. Such adjustments were continued until a reasonable match, as judged by the authors, was obtained between model predictions and actual observations. Because of the model overspecification, the least possible number of parameters necessary to obtain an acceptable fit was adjusted.

The experimental data used for the model calibration were collected during two weeks of the plant operation from 1995.10.23 to 1995.11.06. The collected data set consisted of concentrations of the basic components: suspended solids, suspended minerals, BOD_5, COD, ammonia nitrogen, total nitrogen, phosphate (PO_4) phosphorus, total phosphorus, dissolved oxygen and alkalinity, both in the influents and effluents (including sludge effluent) for the basic vessels: primary clarifiers, aeration basins and secondary clarifiers. These measurements were taken every 2 h at the inlet to the plant (168 samples) and once a day (from the sum of samples taken every 2 h with the volumes proportional to the flow rates, i.e. daily composite samples) in all plant inner points. Moreover, all corresponding flows were measured every 2 min.

The measurements at the inlet were averaged to get the average diurnal variations of the constituents, and normalized by dividing them by the daily means. Organic component was then calculated as the mean of COD and BOD_5 value, see Fig. 9, and nitrogen component as the mean of ammonia and total nitrogen, see Fig. 10.

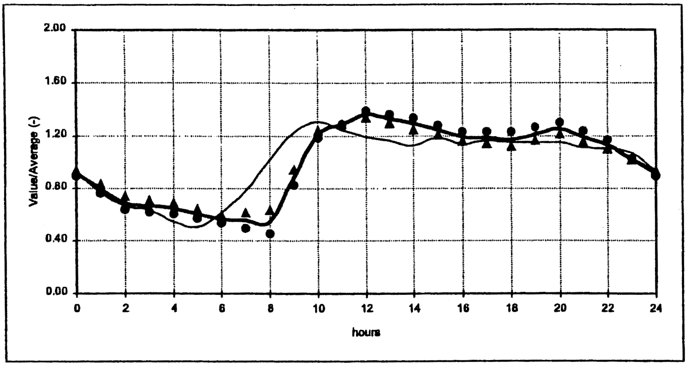

Figure 9. Normalised organic component diurnal variations in the influent as the mean of BOD_5 (•) and COD (△). Normalised flow rate drawn with the thin line.

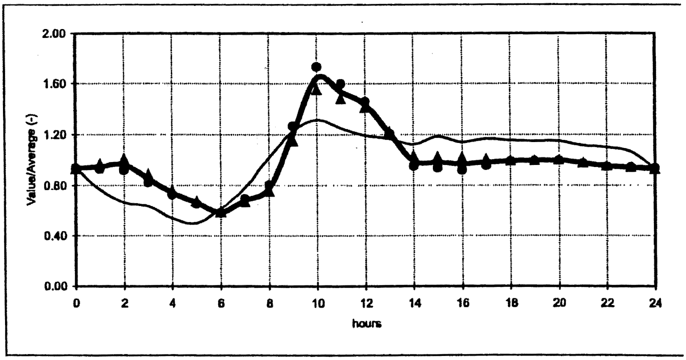

Figure 10. Normalized nitrogen diurnal variations in the influent as the mean of the NH_4 nitrogen (•) and the total nitrogen (△). Normalised flow rate drawn with the thin line.

Initial values of the model unknown parameters were taken from the literature [12, 14, 17, 36]. The average plant inlet values were put into the model to compute the stationary (repeated in each day) diurnal values of outlets from different vessels. These diurnal values were compared with the appropriate averaged values of measurements taken during the experiment. Then some parameter values taken from the literature were adjusted to get a satisfactory fit. Table 3 shows the results of fitting the primary clarifiers model, Tables 4 and 5 the aeration basins model, and Table 6 the secondary clarifier model. The error was measured as the difference between the model and the observation daily mean values, in percent.

As an immediate model application Figs. 11-12 present examples of variations of different unmeasurable components as simulated by the model from average day varia-

Table 3. Calibration results and model fit for primary clarifiers.

parameter	unit	calibration	literature [32]	
A	g/m^3d	$1.2\ 10^{-6}$	$1.2\ 10^{-6}$	
B		3.76	4.05	
parameter	unit	measurements	model	error [%]
suspended solids	g/m^3	163	162	0.6
suspended minerals	g/m^3	60	47	22
BOD_5	$g\ O_2/m^3$	186	188	1
COD	$g\ O_2/m^3$	448	451	0.7
ammonia	$g\ N/m^3$	29.3	26.3	10
total N	$g\ N/m^3$	39.3	32.0	19
alkalinity	val/m^3	8.3	7.9	5

Table 4. Calibration results for aeration basin.

parameter	unit	calibration	literature [14, 17, 36]
μ_h	d^{-1}	2.20	1.5 - 8
Y_h	g COD /g COD	0.67	0.67
k_s	$g\ COD/m^3$	10	5 - 30
k_{oh}	$g\ O_2/m^3$	0.1	0.1
k_x	g COD /g COD	0.03	0.02 - 0.05
k_h	g COD /g COD d	3.0	0.6 - 2.2
μ_a	d^{-1}	0.5	0.2 - 0.8
Y_a	g COD/ g N	0.15	0.15
k_{NH}	$g\ N/m^3$	1.0	1.0
k_{oa}	$g\ O_2/m^3$	0.5	0.5 - 1.0
f_p	-	0.08	0.08
b_h	d^{-1}	0.62	0.62
b_a	d^{-1}	0.05	0.05
i_{xb}	g N/g COD	0.086	0.086
i_{xp}	g N/g COD	0.06	0.06

tions at the plant inlet. These values were not observed directly but reconstructed from the model. For full results see [33].

The fit of the model is satisfactory, in many cases very good, of the order of few percents. Only in some cases the errors are bigger. The bigger errors in nitrogen fit seem to be caused by nonsatisfactory operation of the primary clarifiers during the measurement

Table 5. Fit of the aeration basin model.

parameter	unit	measurements	model	error [%]
biomass	g /m^3	3815	3890	2
sludge age	d	10.2	10.0	2
BOD_5	g O_2/m^3	18	18.3	2
COD	g $O2/m^3$	53	53.6	1
ammonia	g N/m^3	26.3	24.2	8
total N	g N/m^3	32.1	26.1	12
alkalinity	val/m^3	7.9	7.7	3

Table 6. Calibration results and model fit for secondary clarifiers.

parameter	unit	calibration	literature [12]	
u_0	m/d	187.2	187.2	
b	m^3/g	$6.23\ 10^{-4}$	$6.23\ 10^{-4}$	
p_f		0.00322	0.01088	
parameter	unit	measurements	model	error [%]
suspended solids	g /m^3	19	19	0
suspended minerals	g /m^3	14	7	50
BOD_5	g O_2/m^3	19	23	21
COD	g O_2/m^3	55	81	47
ammonia	g N/m^3	24.9	24.2	3
total N	g N/m^3	28.1	26.9	4
alkalinity	val/m^3	8.1	7.7	5
recirculated sludge	g /m^3	5719	6090	6

period. A worst fit of suspended minerals and organic material in the secondary clarifiers is connected either with the modelling, calibration or observation errors.

8. Neural Network Model

Unlike the case of difference or differential models, in neural networks the underlying equations of the process to be modelled are unknown. Thus only knowledge of input and output variables is required to model a process.

The wastewater treatment process is nonlinear and therefore a network which is capable to handle such nonlinearities was chosen. Namely, it was the feed-forward network with three layers (input - hidden - output) and with a nonlinear transfer functions. The

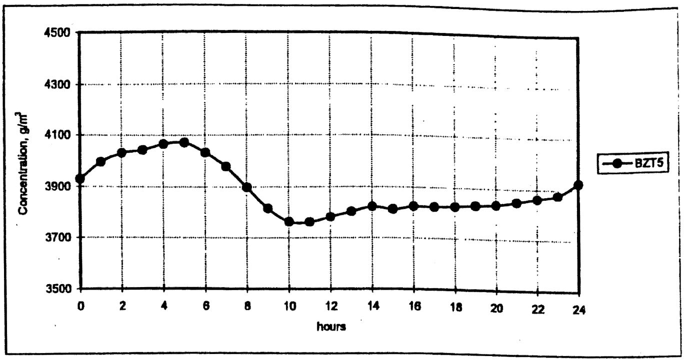

Figure 11. Simulated biomass concentration in the aeration basin.

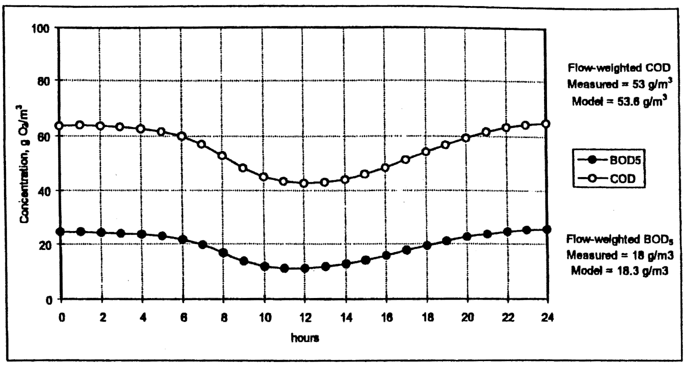

Figure 12. Simulated organic compounds concentration in the aeration basin.

transfer function of the first and the second layer was a sigmoid function

$$a_j = \frac{1}{1+\exp(-p_j - b_j)}$$

The transfer function of the third layer was linear

$$a_j = p_j + b_j$$

The data were collected over the first four months in 1997 in the wastewater treatment plant in Rzeszów. They consisted of 364 data sets, one data set per working shift, i.e. three sets per day. The data were presmoothed by a wavelet shrinkage method [14].

The data were measured in 4 different points of the plant (see Fig. 1):

1. the input to the plant,

2. the aeration basins,

3. the external recirculation system, and

4. the output of the plant,

where the following variables were measured:

- at the input to the plant: the wastewater inflow, BOD_5, nitrogen, ammonia and suspension concentrations,
- in the aeration basins: the oxygen and the activated sludge concentrations, and the activated sludge drop ability,
- in the external recirculation system: the recirculation flow and recirculated sludge concentration;
- at the output of the plant: BOD_5, nitrogen, ammonia and suspension concentrations.

The raw wastewater variables were treated as the uncontrollable input data, the oxygen concentration and the recirculation flow as the control variables and the rest of the variables measured as the output data.

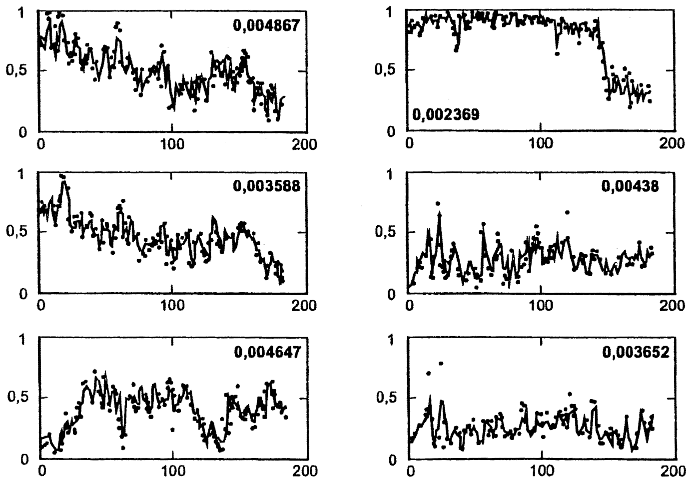

Figure 13. Results from training the network for six output parameters of the process model (points - the data, lines - the model).

For training the neural model all measured variables at the consecutive time t were inputed to the network while the outputs of the plant at time $t+T$ were compared with the outputs of the network. After having searched and tested for important or unimportant

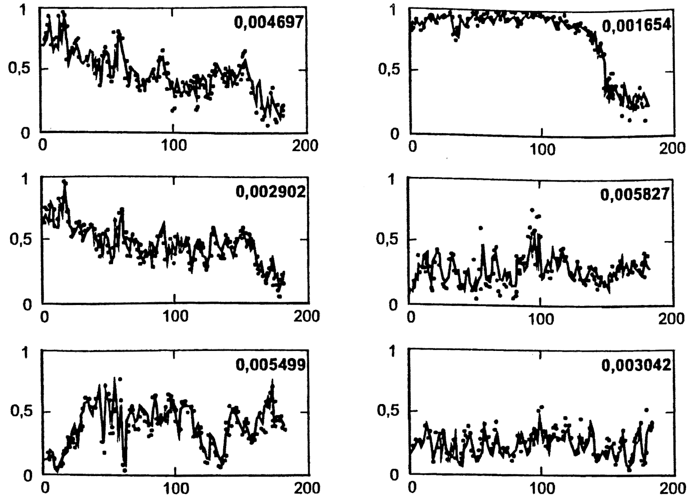

Figure 14. Results of testing the network for the same process parameters as in Fig. 13.

Table 7. Comparison of the residual sums of squares (SSE) in the learning and testing phases of the neural network model elaboration

variable	SSE	
	learning	testing
active sludge concentration	0.0049	0.0047
active sludge drop ability	0.0024	0.0017
recirculation sludge concentration	0.0036	0.0029
BOD_5	0.0044	0.0058
ammonia concentration	0.0046	0.0055
effluent suspensions	0.0037	0.0030

parameters of the process we finally arrived with the network of 12 neurons on the input layer, 6 neurons on the hidden layer, and 6 neurons on the output layer. The value of $T = 8$ h (i.e. one shift) was found to be optimal.

The fits of the neural model after the learning and the testing phases are depicted on Figs. 13 and 14 and summarized in Table 7.

9. Conclusions

In the paper modelling of the wastewater treatment plant in Rzeszów is presented. Two approaches were considered: the mathematical model of the physical processes taking part in the plant and the black box type neural network model. The consecutive stages in construction of the mathematical model consist of:

- formulation of ordinary differential equations and algebraic equations of the model on the basis of physical, chemical and biological mass conservation laws for each vessel,
- formulation of the hydrological models describing the dynamics of flows in the vessels,
- performance of an experiment in the plant to gather measurements necessary for estimation of the model unknown parameters,
- fitting the models to the measurements to obtain estimates of the parameters.

The basic vessels modelled were: a pair of the preliminary clarifiers (treated as one vessel), a triplet of the aeration basins (also treated as one vessel) and a pair of the secondary clarifiers (one vessel). The vessels are connected by pipes conveying influent or effluent liquids for each vessel. Only degradation of organic and nitrogen components was accomplished in the plant at the time when the experiment was carried out. Thus the model includes only equations describing chemical and biological transformations connected with these processes.

Estimation of parameters was performed in two steps. In the first step active volumes of the vessels were identified in the hydrological part of the model, describing flows of liquids only. For this, measurements from the active experiment in the plant were used with the chlorine ions applied as a tracer. The estimates of the active volumes were then used in the other equations of the model. The rest of their imprecisely known parameters were calibrated. For this, initial parameter estimates were first chosen within the ranges presented in the literature and then settled in step by step man-induced changes within the literature ranges, to obtain a satisfactory fit of the observed model states with the measurements done during the experiment. This step was rather burdensome and required a good intuition of the influence of different parameters on the model performance. Quite satisfactory fit obtained indicates that the model well describes the real wastewater clearance processes.

The neural network model is simpler to develop and much quicker in computations performed during the simulation stage. Thus it may be very useful for optimization purposes. A disadvantage of this kind of models lies in lack of their transparency, making impossible any physical interpretations of the neural network parameters. With this respect they are sensitive to changes in conditions in which they were trained and tested. Frequent adjustments may be needed to keep them relevant.

Thus, choice of the modelling approach depends very much on the purpose of their use. Although relative easiness in development of a neural network model favourably compares them at present with the burdensome physical models, it is our belief that with the growing knowledge of the processes and ways of their modelling the physical models will prove their superiority in the future.

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