Marcin STACHURA, Krzysztof JANISZOWSKI, Paweł WNUK
Warsaw University of Technology, Warsaw

THE APPLICATION OF *PExSim* IN THE OPTIMISATION OF THE MULTI–DIMENSIONAL PROCESS MODELS ON THE EXAMPLE OF ACTIVATED SLUDGE WASTEWATER TREATMENT

Key words

Simulation, modeling, optimization, wastewater treatment.

Summary

The application of mathematical models of industrial processes (derived from physical relations) implemented in relevant software, allows preparing simulations of such process models so as to explore industrial process behaviour in many situations, especially critical ones. The key issue of this type of approach is to prepare a model that would approximate a process dynamics with proper quality. In this paper the problem of fitting physical models, described by a set of ordinary differential equations, to a set of measured data is considered. This type of model has a set of unknown parameters that have to be estimated so the model could mimic and predict a process behaviour. In this paper, some procedures for the optimisation of modelling wastewater treatment plants, based on model called ASM 1 are described and discussed. In the performed studies, data recorded in a plant in Resovia (southeastern Poland) was used. The final result of the optimisation is the wastewater treatment process model. Results for selected concentrations of contamination in treated sludge are presented.

Introduction

In urban complexes a large amount of pollution is produced that might penetrate into natural environment. Crucial part of it is water pollution, so improving the quality of the water treatment is the key issue in environment protection. Nowadays, wastewater treatment processes proceed in mechanical and/or biological plants (WWTP), with use of activated sludge technology [1]. This process itself is rather expensive so, during plant work optimisation (so as to achieve proper parameters of the treated sludge), or even modernising a technology, application of advanced software supporting an optimisation process might be very useful [2]. This kind of approach includes the application of mathematical models (derived from physical relations, parametric or others) implemented in relevant software that allows the preparation of simulations to explore process behaviours in many situations, especially critical ones. The key issue of this type of approach is to prepare a model that would approximate process dynamics with satisfactory quality. For multi-dimensional processes, this dynamics is described by many differential equations, and then the basic task is to estimate correct values of corresponding coefficients introduced in a mathematical description. The aim of this paper is to present an approach of systematic testing and optimising of a multi-dimensional model based on an example of water treatment processes.

Computer models of an activated sludge process have been developed in Canada, Great Britain, Switzerland, Denmark, Belgium, and Germany [1]. Most of these models are software packages realised at the universities or research centres. The most important software is *GPS-X* from Canada, *STOAT* from Great Britain, and *AQUASIM* from Switzerland, but worth mentioning are also *EFOR* and *SIMBA* from Denmark, *WEST* from Belgium, and *ARASIM* and *SIMMON* from Germany [1]. However, none of the above mentioned software have been integrated with optimisation algorithms. In this paper, application of *PExSim* (*Process Explorer and Simulator*) software, developed at the Institute of Automatic Control and Robotics of the Warsaw University of Technology is considered.

1. Presentation of technology applied in test case – a WWTP in Rzeszow

The activated sludge process is defined in TGL 55032/04 as ‘biological sewage treatment in artificially aerated vessels, in which the organic constituents of the sewage are metabolised by the activated sludge, being partially or completely degraded and/or metabolised’ [3]. The microorganisms growing in or on flocks are termed “activated sludge” or “sludge biomass,” and the treatment process is accordingly known as an “activated sludge process.”

An activated sludge process, applied in the considered WWTP, constitutes several phases of the sewage treatment processes. It contains an introductory mechanic purification section, followed by biological treatment and a final sedimentation tank with recycling stream of activated sludge.

The technological process of the municipal WWTP can be divided into several sub-processes: At the beginning, crude sludge is mechanically filtered by a grit separator and then transferred to the preliminary settling tank, to reduce mineral fixed components (like sand). The second stage is a biological treatment of sewage, to reduce nitrogen components by activated sludge. Last is the second sedimentation process, where some of the effects of biochemical processing (dead bacteria and heavy suspension) are divided from sewage flow by sedimentation and the majority flow of activated sludge is recovered to biochemical phase of the WWTP process.

A completed sewage treatment plant of conventional design, which was explored in Rzeszow, comprises the various technical stages shown in Fig. 1.

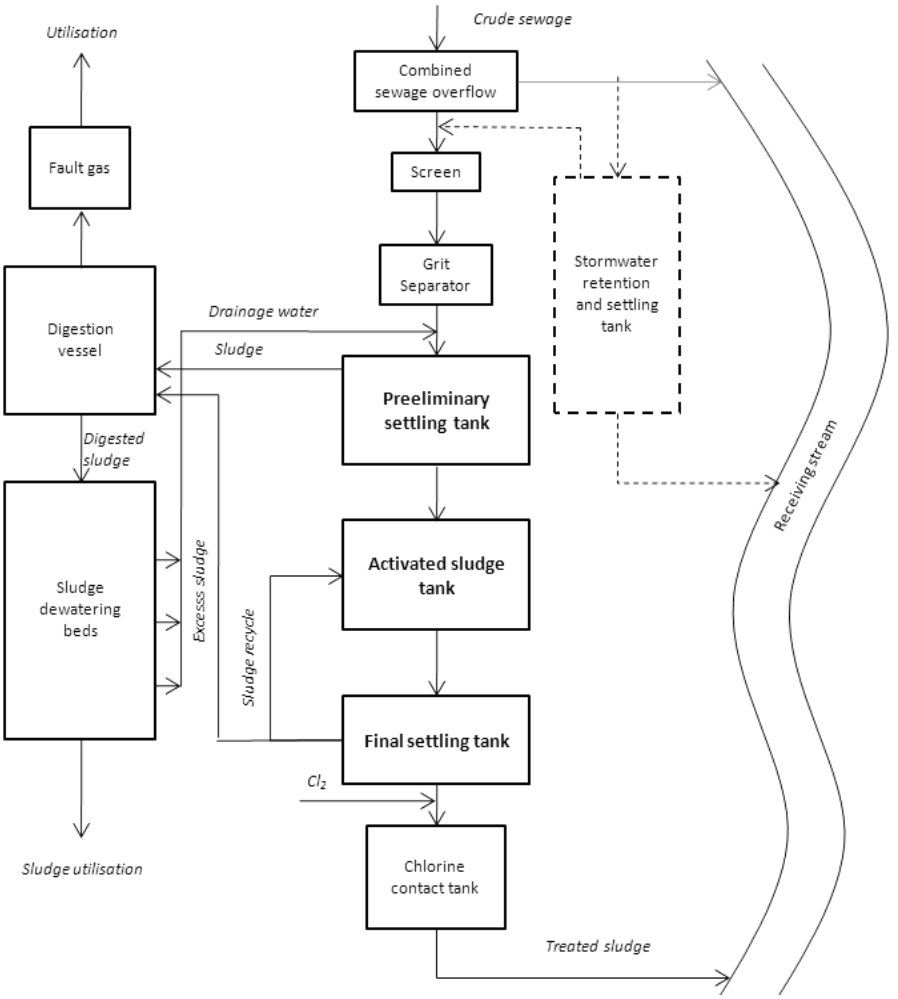

Fig. 1. Diagram showing the layout for WWTP used in Rzeszow

2. Short description of the investigated WWTP

In order to encourage engineers to use a modelling technique more extensively during the analysis of alternative wastewater treatment systems, in 1983, the *International Association on Water Quality* (*IAWQ*) appointed a task group to review models for suspended growth cultures and to produce one model capable of depicting the performance of wastewater treatment systems receiving both soluble and particulate substrates in which organic substrate removal, nitrification, and denitrification were all occurring. They completed their task in 1986, outlining the major features of the activated sludge model ASM No.1. It contains 8 processes and 13 components, both particulate and soluble [4–6]. The success of this project has resulted in that the *IAWQ* task group on mathematical modelling was reconstituted and asked to produce a consensus model ASM No.1, capable of mimicking the performance of systems, reproducing organic substrate removal, nitrification, denitrification, and phosphorous component removal. This was quite complicated task, because of the complexity of biological phosphorous removal and the evolving nature of understanding it. The report was released in 1995 and a model was called ASM No. 2 [4]. Alternatively, in 1999, a ASM No. 3 model was developed. It removes some deficiencies, which were observed during use of ASM No.1 model. In ASM No. 3, a new process was taken into consideration: accumulating organic compounds (substrates), where idea of decay and regeneration was replaced by intracellular respiration.

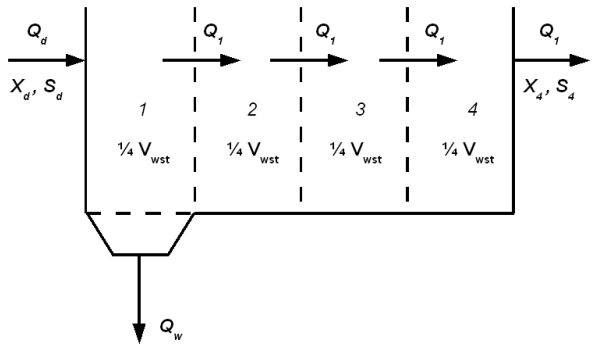

Fig. 2. Schema cell model of preliminary settling tank

A mathematical description of the biochemical processes, in this paper, is based on the ASM No. 1 model. The main reason of this choice was the actual structure of WWTP used in Rzeszow. According to the ASM No. 1 model, the following components are taken into consideration: inert particulate organic matter x_I, slowly biodegradable substrate x_S, active heterotrophic biomass x_{BH}, active autotrophic biomass x_{BA}, debris from biomass x_D, inert soluble organic

matter s_I, readily biodegradable substrate s_S, oxygen s_O, nitrate nitrogen s_{NO}, ammonia nitrogen s_{NH}, soluble biodegradable organic nitrogen s_{NS}, particulate biodegradable organic nitrogen x_{NS}, and alkalinity molar units s_{ALK}. In this research, three basic elements of modelling the plant are considered: the preliminary settling tank, the activated sludge tank, and the final settling tank.

For an approximation of distributed character of the real process of each of the elements was divided into many cells, as shown in Fig. 2, indicating the structure of preliminary settling tank.

A mathematical description of each element consists of a system of differential equations that describes the dynamics of the changes of the above mentioned components for each cell of the considered element. In other words, for each element (preliminary settling tank, activated sludge tank, final settling tank), there are different systems of equations for the same structure for each cell.

Preliminary settling tank model

A presentation of the oscillation of concentrations (of particulate and soluble components) consists of the following formulas [1, 5, 6]:

$$\frac{dx_i}{dt} = \frac{4}{V_{wst}}\left[Q_1\left(x_{i-1} - x_i\right) - \frac{k_{sed,i}x_i}{\overline{x}_i} \right] \tag{1}$$

$$\frac{ds_i}{dt} = \frac{4}{V_{wst}} Q_1\left(s_{i-1} - s_i\right) \tag{2}$$

where:

x – concentration of a particulate component [g/m^3],

s – concentration of a soluble component [g/m^3],

$\overline{x}$ – total concentration of particulate components [g/m^3],

Q_1 – inlet flow to first cell of the tank [m^3/d],

Q_w – crude sludge flow [m^3/d],

k_{sed} – sedimentation speed [g/d],

V_{wst} – active volume of corresponding tank [m^3/d].

Activated sludge chamber model

A dynamic representation for each component has a general form [4]:

$$\frac{dc_i}{dt} = \frac{1}{V_K}\left(L_d - Q_e c_i\right) + R_i \tag{3}$$

Table 1. Process kinetics and stoichiometry for carbon oxidation, nitrification and denitrification [4]

Component → i		1	2	3	4	5	6	7	8	9	10	11	Process Rate, ρ_j [$ML^{-3}T^{-1}$]
		S_I	S_S	X_I	X_S	X_H	X_A	X_P	S_O	S_{NO}	S_{NH}	S_{ND}	
j	Process ↓												
1	Aerobic growth of heterotrophs		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$		$\mu_H\left(\frac{S_s}{K_s+S_s}\right)\left(\frac{S_o}{K_s+S_s}\right)X_H$
2	Anoxic growth of heterotrophs		$-\frac{1}{Y_H}$			1				$-\frac{1-Y_H}{2{,}86\,Y_H}$	$-i_{XB}$		$\mu_H\left(\frac{S_s}{K_s+S_s}\right)\left(\frac{K_{OH}}{K_{OH}+S_o}\right)\left(\frac{S_{ND}}{K_{ND}+S_{ND}}\right)X_H$
3	Aerobic growth of autotrophs						1		$-\frac{4{,}57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$i_{XB}-\frac{1}{Y_A}$		$\mu_A\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_o}{K_{OA}+S_O}\right)X_H$
4	"Decay" of heterotrophs				$1-f_p$	-1		f_p					$b_H X_H$
5	"Decay" of autotrophs				$1-f_p$		-1	f_p					$b_A X_A$
6	Ammonification of soluble organic nitrogen										1	-1	$k_a S_{ND} X_H$
7	"Hydrolisis" of entrapped organics		1		-1								$k_h \frac{X_S / X_H}{K_x+(X_S / X_H)}\left[\left(\frac{S_s}{K_{OH}+S_s}\right)+\eta_h\left(\frac{K_{OH}}{K_{OH}+S_o}\right)\left(\frac{S_{ND}}{K_{ND}+S_{ND}}\right)\right]$
Observed Converdion Rates [$ML^{-3}T^{-1}$]		$R_i=\sum_j \nu_{ij}\rho_j$											
Stoichiometric Parameters: Heterotrofic yield: Y_H Autotrofic yield: Y_A Fractionof biomass yielding particulate products: f_p Mass N / Mass COD in biomass: i_{XB} Mass N / Mass COD in products from biomass: i_{XP}		Soluble inert organic matter	Readily biodegradable substrate	Particulate inert organic matter	Slowly biodegradable substrate	Active heterotrofic biomass	Active autotrophic biomass	Particulate products arising from biomass decay	Oxygen	Nitrate and nitrate nitrogen	Ammonia nitrogen	Soluble biodegradable organic nitrogen	**Kinetic Parameters:** Heterotrophic growth and decay: μ_H, K_S, K_{OH}, K_{NO}, b_H Autotrophic growth and decay: μ_A, K_{NH}, K_{OA}, b_A Correction factor for anoxic growth of heterotrophs: η_g Ammonification: k_a Hydrolisis: k_h, k_X Correction factor for anoxic hydrolisis: η_h

where:

L_d – the total charge of the *c* component flowing to considered cell [g/d(day)],
V_K – the volume of the activated sludge chamber [m^3],
Q_e – sewage outlet flow intensity [m^3/d],
c – the concentration of a *i-th* component [g/m^3],
R_i – the observed conversion rate of a *c* component change [g/m^{3}d].

Observed processes conversion rates are presented at Table 1 in a matrix format.

Final settling tank model

Processing in the final settling tank is a fundamental issue in the activated sludge process. It is based on the processes of thickening and clarifying, which determine the final concentration of a recycled sludge and a concentration of particulate components in the treated wastewater. Movement of particulate components is evoked by gravity force, which causes sedimentation with velocity *v* and a swage flow with velocity *u*, proportional to recalculated sludge flow.

Sedimentation velocity is the function of a sludge concentration and is represented by [1, 5, 6]:

$$v = v_0 e^{-BX} \tag{4}$$

where:

v – sedimentation velocity [m/d],
v_0 – velocity linear coefficient [m/d],
B – velocity exponential coefficient [m^3/g].

Balance equations of particulate components for layers (*j*) in the thickening zone are presented below:

$$\frac{dX_j}{dt} = \frac{1}{H_j}\left(G_{T,j+1} + G_{T,j}\right) \tag{5}$$

and corresponding balance equations for layers (*j*) in the clarifying zone [1, 5, 6]:

$$\frac{dX_j}{dt} = \frac{1}{V_j}\left[Q_e\left(X_{j-1,E} - X_{j,E}\right) + \left(G_{v,j+1} - G_{v,j}\right)A_{wt}\right] \tag{6}$$

where:

H_j – height of the *j*-th layer [m],
V_j – volume of the *j*-th layer [m^3],
X – concentration of the component,
Q – flow intensity [m^3/d],

G – flow stream,
u – related to sewage flow velocity,
T – related to total sewage velocity (u+v),
v – related to sedimentation velocity.

3. *PExSim* (Process Explorer and Simulator) software

PExSim is open (this means designed as plug-in type software), freely configurable software similar to *Matlab Simulink*. With the help of *PExSim*, it is possible to create complex signal transformations paths (Fig. 3). In the package are libraries of transform blocks consisting of basic math functions, a math

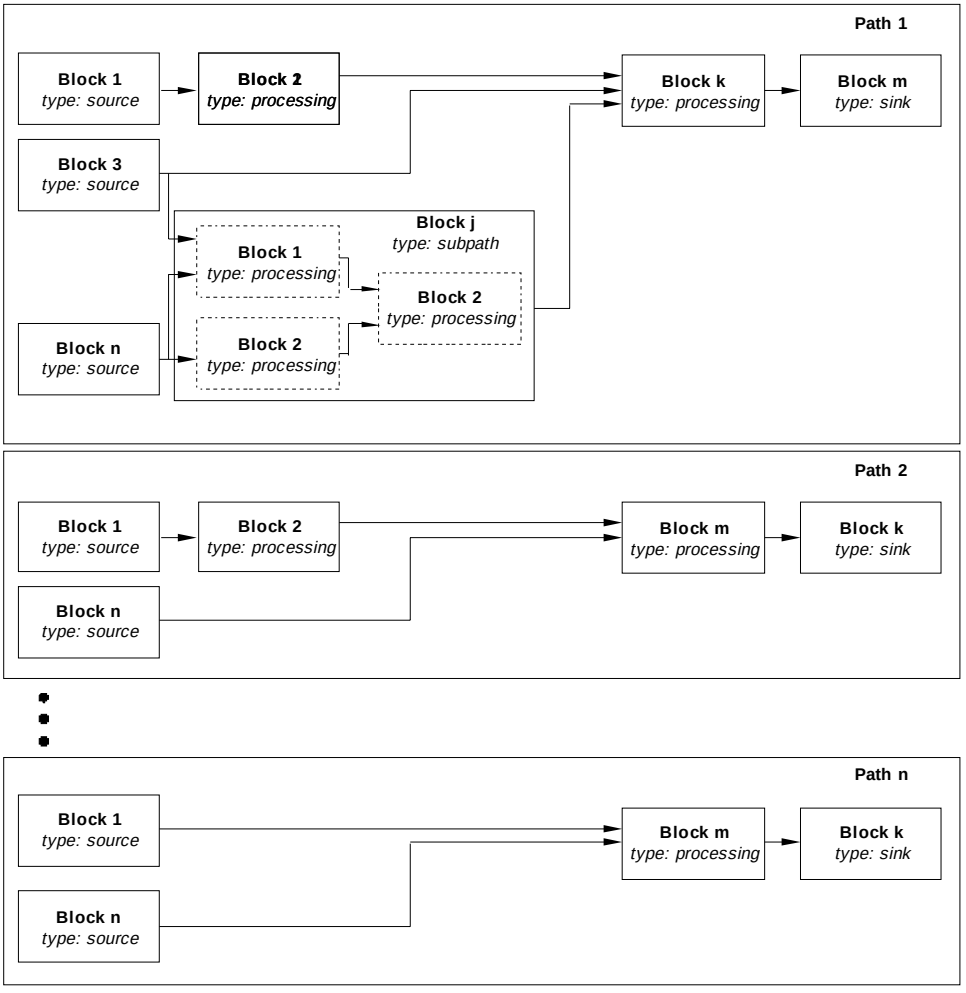

Fig. 3. Tree-type scheme of data processing paths`

parser, statistical and logical operators, and a set of specialised functions to design diagnostic tests algorithms [2]. There is also available a library used to simulate parametric models, identified with the use of the *MITforRD* package. A more detailed description can be found in [7]. In *PExSim*, data processing algorithms are realised as block schemes, called paths. Every path consists of function blocks, realising different ways of signal processing. Proper connection of inputs and outputs of the blocks realises the intended flow of signals. Fig. 3 presents a structure of the elements used for data processing.

As mentioned, *PExSim* is a plug-in type software that allows the construction of new function blocks, designed by a user in the form of an available library. It is a big advantage; especially if investigated process are individually adapted to the investigated problem, e.g. modelling a WWTP process. For the investigated case, such a special library was prepared. It was named *WWTP Elements* (*Wastewater Treatment Plant Elements*). The prepared blocks are as follows: preliminary settling tank cell, activated sludge tank cell, and final settling tank cell, and include the mathematical descriptions presented above (1) – (6). Using these function blocks, e.g., Fig.4, it is possible to build the WWTP structure configuration according to the ASM No. 1 model.

An activated sludge process model is quite complex – each element can be represented by a variable, without a strictly defined number of cells, so each of elements, shown on Fig. 1 is represented by a *subpath*, Fig. 5, composed of cells connected in series. According to literature [1, 5, 6], preliminary settling and activated sludge tanks were divided into 4 cells, while the final settling tank was divided into 8 cells (4 for the clarifying zone, 4 for the condensing zone).

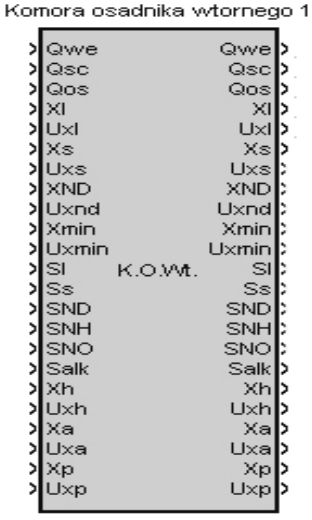

Fig. 4. Final settling tank layer

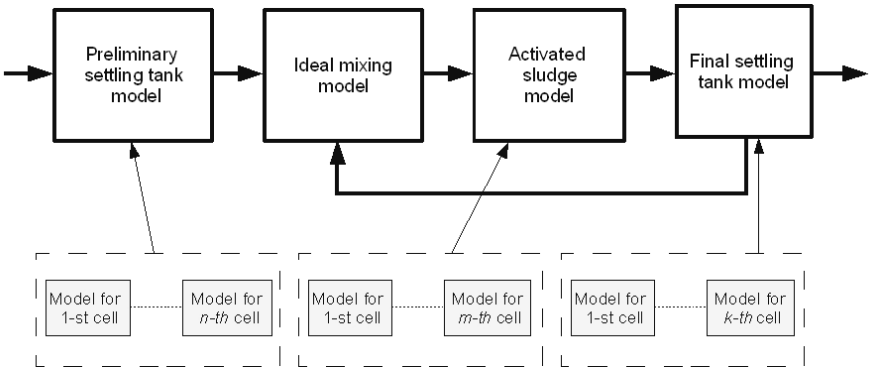

Fig. 5. Block system structure for WWTP

4. Problem formulation

The final model of the full scale wastewater treatment plant consists of the following:

- A system of 10 differential equations for each cell of the preliminary settling tank, and each equation for the particulate component had 2 parameters;
- A system of 13 differential equations for each cell of the activated sludge tank, where number of parameters was variable from 3 to 7; and,
- A system of 13 differential equations for each cell of the final settling tank, where each equation for particulate component had 2 parameters.

Unknown parameters, introduced in differential equations of the mathematical description of the WWTP processes, had to be evaluated to reduce possible differences between generated (by model) process values and recorded measurements. The developed model had over 100 unknown parameters in differential equations. A manual adaptation of all these parameters would be extremely time consuming; therefore, for an effective study of a proper model, an optimisation technique was used. An initial stage of the calibration of the model was also performed to evaluate a starting point for the optimisation procedures.

5. Calibration

Unknown coefficients used in the differential equations for mathematical description had to be estimated to fit specific information based on plant structure and process conditioning. The easiest approach was to use optimisation methods to estimate unknown parameters. In the particular case of wastewater treatment processes, the application of such methods is not an easy problem due to complexity of the process. Hence, before starting the optimisation of process

equations, a manual calibration of coefficients was performed. The calibration procedures were based on experience, knowledge of the technology, and the intuition of a researcher, who performed the calibration.

To make model calibration an easier task, only a limited group of parameters was taken into consideration. These selected coefficients were as follows (For a detailed description of selected parameters see notations used in available literature [1, 4, 8]): A, B are introduced in equations describing sedimentation process in preliminary settling tank; μ_H, μ_A, k_H, k_A, k_h, k_a, are introduced in equations describing nitrification processes; and, v_0, B are introduced in the final settling tank model.

During the activated sludge tank model calibration, it was assumed that all stoichiometric parameters were constant with default values taken from available literature [1, 8]. The primarily investigated coefficients were for describing the rates of biochemical reactions. This selection allowed fitting the model to obtained measurements; however, due to fixed stoichiometric values, the values of the calibrated coefficients may differ from those presented in literature [1, 8].

For the systematisation of a wastewater process model calibration problem, the influence of the calibrated coefficients on the process variables was investigated in the form of sensitivity functions. As an example, the influence of considered coefficients stated in an activated sludge tank mathematical description and the sensitivity functions of these coefficients to biochemical reaction rates R_i, are shown in Fig. 6. It has a given valuable clue for the acceleration of the calibration process during manual fitting of model coefficients.

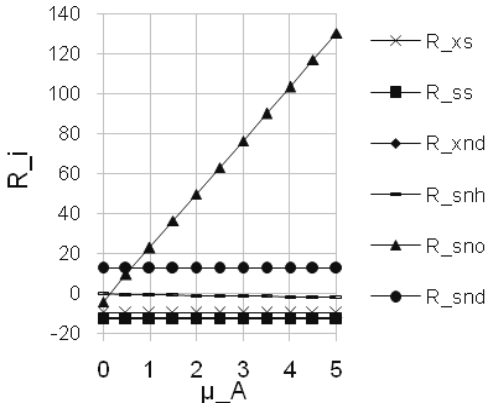

Fig. 6. Testing the sensitivity of the influence of μ_A on biochemical reaction rate R_i [8]

6. Optimisation of model parameters

The problem of optimisation (minimisation) can be defined as follows: To find a vector of real or integer variables within an allowed, finite set Ω_x [9], that achieve the extreme value of some performance index. In the case of the optimisation of a WWTP model, it is equivalent to the estimation of unknown coefficients present in equations that have described processes:

$$f(\hat{\mathrm{x}}) = \min_{x \in \Omega_X} f(\underline{\mathrm{x}}) \tag{7}$$

where:

$f : R^n \rightarrow R$ – minimised objective function,
$\underline{\mathrm{x}}$ – coefficients vector,
$\hat{x}$ – optimal coefficients vector,
Ω_X – set of admissible solutions.

Different iterative optimisation algorithms can be used. All optimisation algorithms are defined as a sequence of projections of the elements $x \in \Omega_X$ onto itself:

$$A : V \rightarrow V \tag{8}$$

and mean an association of a set $A(x) \subset V$ to each element $x \in V$.

In *PexSim*, the following algorithms were integrated:

- Not calculating an objective function gradient: *Hook–Jeeves'* (HJ), *Rosenbrock's* (R), *Simplex* (S) and *Powell's* (P) method; and,
- Using a gradient of objective function: *Conjugate Gradients* (PR) and *Variable Metric* method (DFP).

Detailed descriptions of selected methods are available in [10–12]. For proper application of these algorithms, it is necessary to know the following: the sensitivity of the method for the selection of a starting point and the rate of convergence (interpreted as a number of function evaluations). According to literature [10, 11], the least sensitive was Rosenbrock's method. Basically, this method was slower than Hook–Jeeves' method, but it almost always yields a satisfactory result. On the other hand, the fastest methods were Conjugate Gradients and Variable Metric, which had to use objective function gradients.

The Powell's and Variable Metric Methods were sensitive to the starting point choice. In a case of improper selection, a convergence rate of the values was approximately quadratic; therefore, at beginning was slow, but a close to optimal solution could be quite fast. This behaviour can be explained by processing manner. At the beginning, a search with unknown parameters was done with use of an orthogonal direction base. Since the conjugate directions

were well estimated, a proper search direction was set, and the efficiency of an optimisation was increased.

The Simplex method had very advantageous feature: the choice of starting point in areas of steep "valleys" did not effect in rate of method. This method has shown an almost linear convergence rate, so consecutive decrements of the objective function were reached with the same speed. A disadvantage of this method was the sensitivity of the shape of the objective function. For starting points that were in the flat area close to the optimal solution, this method was slower than other methods.

In the model of WWTP processes, the optimisation task was determined as the objective function of the form:

$$f(x) = \frac{1}{K}\sum_{k=1}^{K}\sum_{i=1}^{n}\sqrt{\left(\frac{z_{M,i} \quad z_{R,i}}{z_{R,i}}\right)^2} + \sum_{i=1}^{n}\exp\alpha \ \frac{z_{M,i} \quad z_{R,i}}{z_{R,i}} - 0{,}5 \tag{9}$$

where:

$z_{M,i}$ – concentration of *i-th* component *z* calculated by the model,
$z_{R,i}$ – measured concentration of *z*,
k – simulation step,
K – number of steps.

The investigated model was quite complex, and the only reliable information was the recorded measurements. Application of optimisation algorithms could push the solution into areas where most of the modelled variables were close to the measurements, but one of them was far from the recorded value. Therefore, the second term of expression (9) contained an exponential function factor that prevented purely numerical determination of *z* (value α = -30). The added exponential part protected the optimisation process from decreasing process variables below half of measured values, even if the overall error of the model (first part of equation (9)) was satisfactory.

7. Results of model optimisation

Due to quite large amount of imprecisely known model parameters and a limited number of recorded measurements, optimisation of only a group of parameters was considered. These selected parameters were as follows (for detailed description of selected parameters please refer to available literature [1, 4–6]):

- Parameters A, B stated in equations describing the primary settling tank model (6);
- Parameters μ_H, μ_A, k_H, k_A, k_h, k_a, stated in equations describing the nitrification process model; and,
- Parameters v_0, B stated in equation (4) of the sedimentation process in tanks.

All stoichiometric parameters were set as constant with default values taken from [1, 4–6, 8].

Examples of the application of different optimisation schemes and approaching problems of the discussion of obtained results are presented as an estimation of parameters for the activated sludge tank. The optimal vector has consisted of 24 coefficients (4 cells, 6 parameters for each cell). Evaluated values of these coefficients, for selected cells, are presented in Table 1. The Hook–Jeeves method achieved the best value of the objective function, and the estimated coefficients were quite different from those found in literature [1, 4]. It was not clear if the vectors of these parameters had any reasonable physical interpretation. A similar disadvantage has shown by Rosenbrock's algorithm. The fastest algorithms were of the gradient type – PR and DFP. However, during the optimisation process, they might find some local minimum, without the possibility of moving away from this point, which has been pointed out the beginning of this section. This case could take place in the presented study, so gradient–type methods did not achieved the best solution.

Convergence of the used algorithms at optimisation of a WWTP model is presented in Fig. 7, where the argument was a logarithm of the number of function calls.

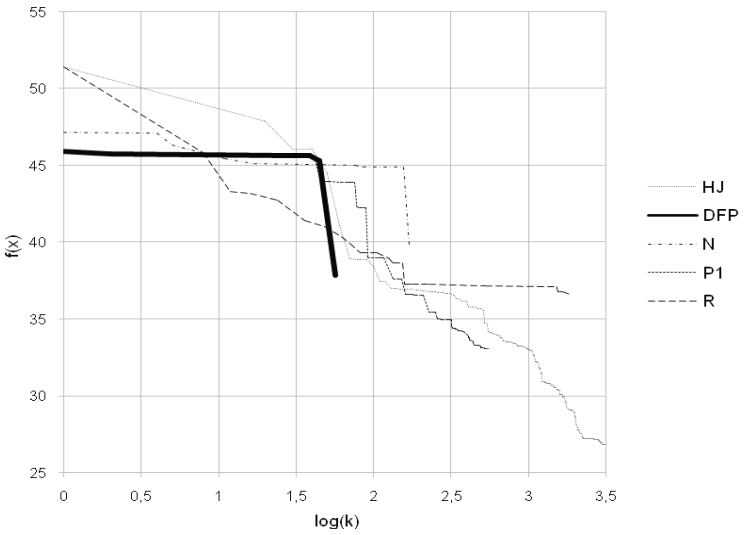

Fig. 7. Convergence rate of applied optimisation algorithms

An inspection of optimisation results did not give a clear answer to which of compared optimisation methods was the best. Each of the applied methods had

some specific properties, described above. Very important in each case was the proper choice of the starting point. However, the performed calibration (based on literature default values), should provide a good recommendation for the initial choice. The dimensionality of problem and the large amount of calculation (one complete calculation of objective function has got over 50 s of calculation time), together with the observed local fixing of solutions, were the most visible problems in the calculations. Probably, some means for stochastic rejection of an algorithm without an achieved minimum (alike the stochastic annealing process) could solve this problem. An important aspect of the investigation was the possibility of using different optimisation schemes; hence, a local achieved minimum by one approach could be verified by another optimisation method. Quite another approach, that might be effective, was a visual comparison of results determined by models obtained with the use of the mentioned method.

8. Model reduction

As was mentioned, the number of cells in each element of the WWTP was not precisely known. An initial choice of the number of cells for the primary sedimentation tank was 4 (same as in active sludge chamber), and 8 cells in secondary sedimentation tank was a subjective choice. Within model optimisation, a reduction of these values was considered. We investigated whether the number of cells in each element could be reduced for an increase in calculation speed and an reduction in the complexity of the sub-models. This problem was investigated during the optimisation process: applied algorithms might evaluate parameters values as close to zero (for linear dependencies) or less than zero (for exponential dependencies). This observation was an indication that model reduction was possible, because some of sludge processing was not active. After simplification of the structure, a comparison of errors observed of the modelled and measured process variables, both for the original and the reduced model, was made. If the reduced model gave the same accuracy as the original, the reduced model was accepted. In this study, the reduction of the preliminary settling tank model from 4 to 2 cells was made.

9. Model verification

In this section are presented some transients of measured and modelled process variables that enable the comparison of developed WWTP models (Fig. 8, Tab. 2). Comments are added on the measurements of the plotted data. The rough character of presented transients was a result of chemical analysis performed only once a day during all of the 2 weeks of experimental charge. Other plots (from estimated models) were calculated with a 2 minute simulation interval.

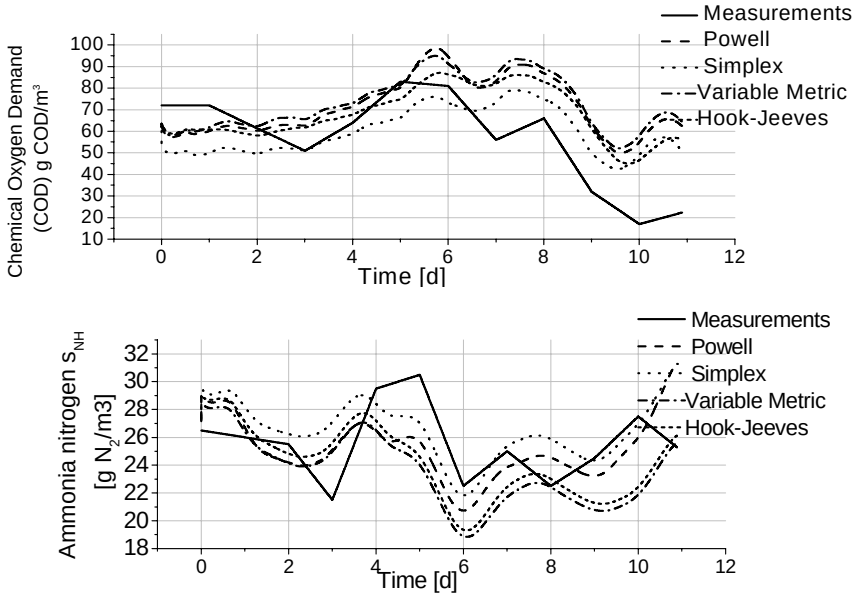

Fig. 8. Comparison of selected variables in WWTP process model

Table 2. Comparison of the models estimated with use of presented optimisation algorithms

$E(X_{BN})$						
Method:	HJ	R	P1	N	PR	DFP
BOD_5	0.264491	0.265901	0.260928	0.331709	0.298005	0.260950
COD	0.174580	0.210344	0.209315	0.169900	0.170604	0.222530
X_{min}	0.192439	0.192982	0.192695	0.194903	0.194856	0.193825
N_t	0.112574	0.097283	0.078922	0.153091	0.092085	0.134350
S_{NH}	0.063429	0.071742	0.065643	0.089977	0.066239	0.081508
S_{alk}	0.056086	0.044982	0.045841	0.045841	0.054114	0.045071
AVERAGE	0.143933	0.147206	0.142224	0.164237	0.145984	0.156372
$Var(X_{BN})$						
Method:	HJ	R	P1	N	PR	DFP
BOD_5	0.009512	0.014930	0.013971	0.029538	0.011107	0.019680
COD	0.016055	0.021818	0.022002	0.012766	0.017319	0.025780
X_{min}	0.033388	0.032991	0.033189	0.035020	0.034868	0.034336
N_t	0.003112	0.003939	0.001886	0.005144	0.003108	0.005252
S_{NH}	0.001840	0.001785	0.001939	0.003580	0.001672	0.002925
S_{alk}	0.016705	0.001290	0.001361	0.001361	0.001002	0.000967
AVERAGE	0.013435	0.012792	0.012391	0.014568	0.011513	0.014823

$E(X_{BN})$ – average error between modelled and measured process concentration values, *$Var(X_{BN})$* – error variation for considered algorithms: *HJ* – Hook-Jeeves, *R* – Rosenbrock, *P1* – conjugate directions (by Powell), *PR* – conjugate gradients (by Polak and Riebery), *DFP* – variable metric (by Davidon, Fletcher and Powell).

Conclusions

In this paper, an approach to a systematic fitting of ASM 1 model coefficients to measurements recorded on real a WWTP plant in Resovia was presented and discussed. All of the ASM 1 models have quite large number of coefficients, starting from unknown, proper division of each part of process into subsections (due to distributed character of described phenomena), up to number of unknown coefficients that describe each part of modelling subsystem.

The proposed flexible and modern software tool, called *PexSim*, allows easy preparation and optimisation of multidimensional process models. The modularity of this package gives an opportunity to investigate processes that are not well known, such as in the presented example. Implemented optimisation algorithms are ready to use in complex models of technologic installations.

Different optimisation algorithms that were the most effective in the presented optimisation problem were indicated as follows: Powell's conjugate direction method, the conjugate gradient method, and the variable metric method. It is worth highlighting that the starting point for each method was not random, but it was one that was evaluated during the calibration stage. This type of approach gives an opportunity to estimate parameters that would not differ much from the values presented in literature and that would have acceptable physical interpretation.

The research was made using the installation of municipal WWTP in Rzeszow, and partially sponsored by projects no. R11 001 01 and R01 012 02 of Polish Ministry of Science and Higher Education.

References

1. Studzinski J.: Identification, simulation and control of wastewater treatment plants. Systems Research Institute Publication, Warsaw, 2004 (in Polish).
2. Janiszowski K., Wnuk P.: PExSim – novel approach to the problem of the investigation of complex dynamic systems in industrial environment. Problemy Eksploatacji, 2006, 4, 17–35.
3. Grady L, Daigger G., Lim H.: Biological wastewater treatment. Marcel Dekker, New York 1999.
4. Henze M., Gujer W., Mino T., Loosdrecht M.: Activated sludge models. IWA Publishing, London 2000.
5. Bogdan L. i in.: Modelling and calibration of a municipal wastewater treatment process model. Systems Science, 2000, 2.
6. Bogdan L. i in.: Mathematic modelling of purification processes in mechanical – biological wastewater treatment plant. Gutenbaum J. (ed.): Automatyka-Sterowanie-Zarzadzanie. Systems Research Institute Publication, Warsaw, 2002 (in Polish).

7. Wnuk P.: Object identification in *AMandD* system. Pomiary-Automatyka-Kontrola, 2005 (in Polish).
8. Stachura M.: Modelling and optimization of selected wastewater treatment processes. Systems Research Institute Publication, Warsaw 2008 (in Polish).
9. Luenberger D.G.: Optimization by vector space methods. John Wiley and Sons, Inc, New York 1974.
10. Findeisen W., Szymanowski J., Wierzbicki A.: Theory and numerical examples of optimization methods, PWN, Warsaw, 1977 (in Polish).
11. Mathews J.: Numerical methods for mathematics. Science and Engineering. Prentice Hall, Upper Saddle River, 1992.
12. Press W., Teukolsky S., Vetterling W., Flannery B.: Numerical recipes in C. Cambridge University Press, Cambridge, 1992.

Reviewer:
Wojciech CHOLEWA

Zastosowanie pakietu *PExSim* w optymalizacji modeli procesów wielowymiarowych na przykładzie oczyszczania ścieków z osadem czynnym

Słowa kluczowe

Symulacja, modelowanie, optymalizacja, oczyszczanie ścieków miejskich.

Streszczenie

Zastosowanie matematycznych modeli procesów przemysłowych (wyprowadzonych ze zjawisk fizycznych), zaimplementowanych w odpowiednich algorytmach komputerowych, umożliwia prowadzenie symulacji modeli procesów. Badania takie mogą dać wiele cennych informacji na temat zachowania procesu w różnych sytuacjach, w szczególności w stanach krytycznych i awaryjnych. Podstawowym zagadnieniem w tego typu podejściu jest oszacowanie współczynników modelu, który w sposób zadowalający odzwierciedla proces przemysłowy. W niniejszym artykule przedstawiono zagadnienie dopasowania modelu, opisanego układem równań różniczkowych zwyczajnych, do danych uzyskanych z procesu. Dopasowanie modelu przeprowadzone zostało z użyciem algorytmów optymalizacji statycznej na przykładzie procesów oczyszczania cieków miejskich. Wykonane badania oparte są na danych zebranych z miejskiej oczyszczalni ścieków w Rzeszowie.