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Validation and Model Optimization for Waste Water Treatment Processes

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Abstract

In paper some procedures for calibration and optimization of waste water treatment plants models, based on model called ASM 1 were described and discussed. In performed studies data recorded in a plant in Resovia (south – eastern Poland) was taken into consideration. Calibration of a process was considered as a manual adaptation of the ASM 1 model to information obtained from investigated object, while optimization was an automatic investigation with use of computational optimization algorithms. In conclusions advantages and disadvantages of applied procedures were described.

1. Introduction

Application of mathematical models of the industrial processes is a common technique used for investigation of a system behavior in different operation conditions. Mathematical models might have different structure, can be described by of parametric model, neural network, set of state equations representing physical and chemical relations and others.

Physical models are usually described with use of differential equations derived from balance of energies, flows, torque, masses etc. where all parameters introduced in mathematical description have physical interpretation. A big advantage of such representation is direct help in explanation of a specific behavior of an investigated process, but on the other hand a calibration of a process model is not easy task, especially for multi – dimensional representations.

Implementation of biological nutrient removal in waste water treatment processes has been followed by many works concerned with modeling of an activated sludge process. Development of dynamic models of waste water treatment processes allows preparing precise models of considered waste water treatment plant (WWTP) [Henze and others 2000]. To implement these it is crucial to calibrate a chosen process model properly. In this paper calibration is understood as an adaptation of a model to set of information measured during special supervising experiment performed at investigated plant. Calibration might be performed as a manual process of adaptation realized by investigator based on his expert knowledge of process or automatic one with use of selected mathematical algorithms. The second mode will be called optimization. It is worth to underline, that there are surprisingly few references that contain details of the applied model calibration and optimization procedures. The aim of this paper is, therefore, to present a study concerned with validation of ASM 1 model for selected waste water treatment processes.

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2. Activated sludge technology applied in Resovia WWTP

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

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

2.1 Mathematical description of the WWTP process

A mathematical description of the biochemical processes is based on ASM No. 1 model. A main reason of choice of this type approach was a structure of WWTP used in Resovia plant. According to ASM-1 model, the following components are taken into consideration: inert particulate organic fraction 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}, alkalinity molar units s_{ALK}.

An activated sludge tank model was considered and investigated. For better approximation of the real process a tank model was divided into several sub-sections, so called “cells” as it is show at fig.1.

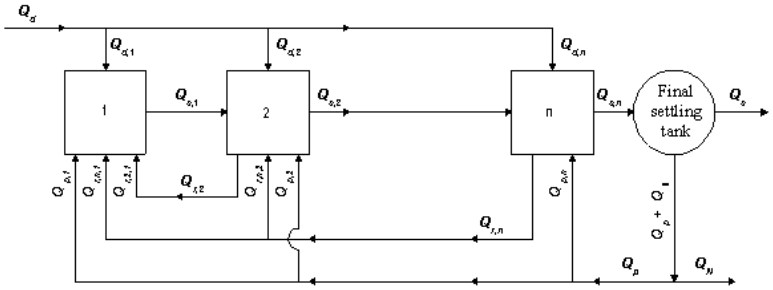

Fig. 1: Schema of cell model of activated sludge tank.

A mathematical description of each cell consists of systems of differential equations, that describes a dynamics of changes for above mentioned components. Model formulas have a general form [1][3]:

$$\frac{dc_i}{dt} = \frac{1}{V_{K,i}}\left(L_{d,c,i} - Q_{e,i}c_i\right) + R_{c,i} \qquad (1)$$

where: $L_{d,c,i}$ - total charge of the component c flowing to *i-th* cell [g/d], $V_{K,i}$ – active volume for section i of sludge tank [m^3], Q_e - sewage outlet flow intensity[m^3/d], c - concentration of a c component [g/ m^3], R_c - resultant rate of a processing of a c component [g/ m^3 d], i – cell number. In investigated model of active sludge tank 4 cells were considered. Concluding a calculation effort for above waste water treatment proc-

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ess – calibration and optimization process have investigated a system of 13 differential equations for each cell with variable number of coefficients from 3 to 7.

To apply the investigated model, as a useful tool, for system behavior analysis, values of coefficients used in description (1) have to be chosen correctly, so as the model could approximate a real process. In presented study a calibration and optimization procedures were described only for selected group of parameters. Finally a vector of unknown coefficients has consisted of 24 elements.

3. Model calibration

Unknown coefficients, approaching in differential equations of mathematical description, have to be estimated so as to fit specific information based on plant structure and process conditioning. Most easy approach is to use optimization methods to estimate unknown parameters. In the particular case of waste water treatment processes application of such methods is however not an easy problem due to dimensionality of a process. Hence, before starting an optimization of process equations a manual calibration of coefficients was performed. In the calibration procedures was based on an experience, knowledge of a technology and intuition of a researcher, who has performed calibration.

So as to make model calibration an easier task, only a limited group of parameters was taken into consideration. These selected coefficients were (for detailed description of selected parameters see notations used in available literature [Henze and others 2000, Studzinski 2004]): μ_H, μ_A, k_H, k_A, k_h, k_a, introduced in equations describing nitrification processes of WWTP plant. At calibration was assumed, that all stechiometric parameters, were constant with default values taken from available literature [Studzinski 2004]. Primary in investigated coefficients were describing rates of biochemical reactions. This selection allows fitting a model to obtained measurements, but due to fixed stechiometric values, values of the calibrated coefficients may differ from presented in literature [Studzinski 2004].

For systematization of problem, an influence of the calibrated coefficients on the process variables was investigated, in form of sensitivity functions of these coefficients to biochemical reactions rates R_i, e.g. Fig.2. It has given valuable clue for acceleration of calibration process at manual fitting of model coefficients.

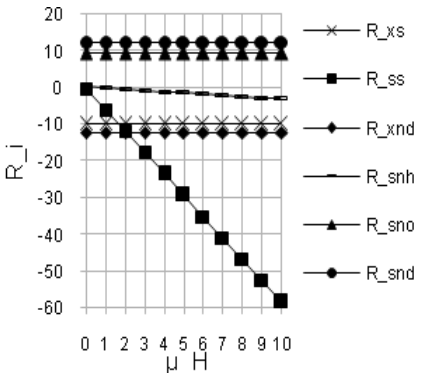

Fig. 2: Testing a sensitivity of influence of μ_H on biochemical reactions rate R_i.

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4. Model optimization

Problem of optimization (minimization) is: to find a vector of real or integer variables within an allowed, finite set Ω_x [Luenberger 1974]. In a case of optimization a WWTP model it is equivalent to estimation of unknown coefficients present in equations, that have described processes:

$$f(\hat{\mathrm{x}}) = \min_{x \in \Omega_X} f(\underline{\mathrm{x}}) \tag{2}$$

where: f – minimized objective function, $\underline{\mathrm{x}}$ – coefficients vector, $\hat{x}$ - optimal coefficients vector, $f : R^n \to R$ and Ω_X is the set of admissible solutions. Different iterative optimization algorithms are used. All algorithms are defined as a sequence of projections of the elements $\mathrm{x} \in \Omega_X$ onto a set Ω_X:

$$A : V \to V \tag{3}$$

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

Methods used for optimization in this paper were: *Hook-Jeeve's*, *Rosenbrock's, Powell's*, *Simplex* (by Nelder and Mead), *Conjugate Gradients* (by Polak and Riebery) and *Variable Metric* (by Davidon Fletcher and Powell). The first four of them did not use objective function gradient, while the last two had to estimate gradient vector. Detailed descriptions of selected methods are available in a literature [Findeisen and others 1977]. For proper application of optimization algorithms, there is necessary to know: sensitivity of method for selection of a start point and rate of convergence (interpreted as a number of function evaluations).

According to available literature [Finedisen, Szymanowski Wierzbicki 1977, Mathews 1992], the least sensitive from above mentioned methods, is Rosenbrock's method. Basically this method is slower than Hook – Jeeves' method, but in almost always yields satisfactory result. On the other hand, the fastest methods are Conjugate Gradients and Variable Metric, which have to use objective function gradients.

The Powell's and Variable Metric Methods are very sensible on starting point choice. In a case of not proper selection of starting point a convergence rate is approximately quadratic, so at beginning it is quite slow, but close to optimal solution can be quite fast. This behavior can be explained by fact, that at beginning of a search of unknown parameters it is done with use of orthogonal direction base. As the conjugate directions are well estimated, a proper search direction is set and an effectiveness of an optimization is increased.

Simplex method has very advantageous feature: a choice of starting point in areas of steep "valleys" did not effect in method speed decrease. This method has shown almost linear convergence rate, so consecutive accuracies are reached with the same speed. A disadvantage of this method is a strong sensitivity of shape of objective function. For starting points, that were in flat areas, quite close to optimal solution, this method is slower than other presented methods. Many evaluations of objective functions are done as a result of little differences of objective function between evaluated points.

4.1 Objective function

In a model of WWTP process, optimization task was determined as the objective function of the form:

$$f(x) = \frac{1}{K}\sum_{k=1}^{K}\left[\sum_{i=1}^{n}\sqrt{\left(\frac{z_{M,i} - z_{R,i}}{z_{R,i}}\right)^2} + \sum_{i=1}^{n}\exp\alpha\left(\frac{z_{M,i} - z_{R,i}}{z_{R,i}} - 0{,}5\right)\right] \tag{4}$$

where: $z_{M,i}$ – concentration of *i-th* component z calculated by the model, $z_{R,i}$ – measured concentration of z, α – exponential function factor, that prevents purely numerical determination of z (value α=30).

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Thanks to this type of objective function, a relative error between modeled and measured process variables were very small and added exponential part protects from decreasing process variables below half of measured values, even if an overall error of a model was not satisfactory.

4.2 Results of model optimization

As was mentioned, vector of unknown parameters was estimated with use of selected optimization algorithms, described above. In each task the optimal vector have consisted of 24 coefficients (4 cells, 6 parameters for each cell). Evaluated values of these coefficients, for selected cells, are presented at Table 1. Despite the Hook – Jeeves method evaluated the best objective function value, the evaluated coefficients were quite different from commented in literature [Henze and others 2000, Studzinski 2004]. It was not clear, if the evaluated parameters vector had any reasonable physical interpretation. Similar disadvantage has shown Rosenbrock's algorithm. The fastest algorithms were of gradient type – PR and BDF. However meanwhile optimization process, they might find some local minimum, without possibility to move out from this point (what have been pointed in beginning of this section). This case could take place in presented study, so gradient–type methods did not achieve the best solution.

Metodhod		Calibration	HJ	R	P	S	PR	BDF
f(x)		47,55	26,809	36,621	33,069	39,803	34,53	37,87
Cell No 1	μ_H	2,2	9,965	2,2	1,98	2,2	2,463	2,198
	μ_A	0,01	0,282	0	0,038	0,01	0,01	0,01
	k_H	0,62	0	0	0	0,62	0,002	0,619
	k_A	0,05	0,575	0	0	0,566	0,05	0,049
	k_h	2,7	10	2,7	3,796	2,7	3,322	2,703
	k_a	0,5	1	0	1	0,526	0,93	0,506
Cell No 4	μ_H	2	2,441	2,16	2,198	2,201	2,806	2,18
	μ_A	0,01	0,01	0,01	0,01	0,104	0,013	0,01
	k_H	0,62	0	0	0,055	0,629	0,12	0,619
	k_A	0,05	1	0,129	0,324	0,058	0,513	0,057
	k_h	2,7	2,671	2,66	2,735	2,701	3,482	2,718
	k_a	0,5	0,138	0,536	0,053	0,501	0,459	0,5

Tab. 1. Results of parameters optimization with use of applied optimization

where μ_H, ..., are notation used for presentation of model [Henze and others 2000]. Convergence of used algorithms at optimization of a WWTP model is presented at below figure:

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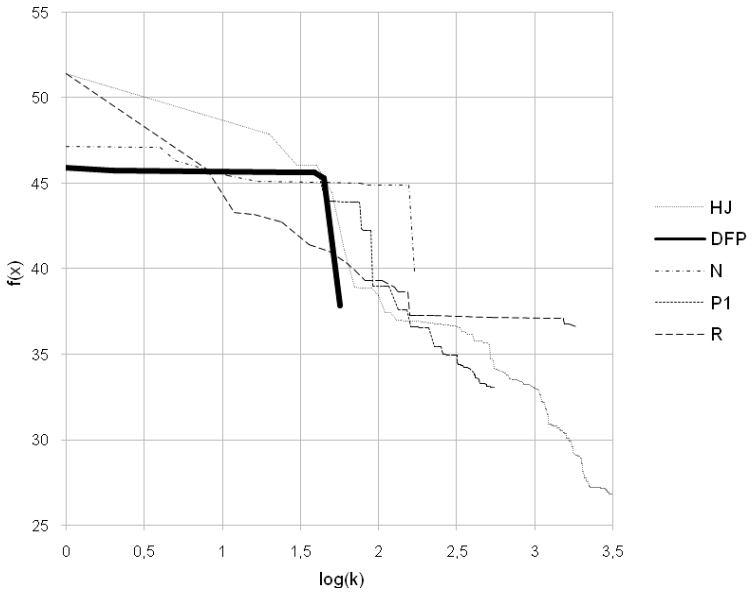

Fig. 5: Convergence rate of applied optimization algorithms.

By inspection of optimization problem for WWTP models, it was hardly possible to mark out the best method. Each of applied methods had some specific properties, described above. Most important in each case was a proper choice of starting point. However performed first calibration, should be o good recommendation of initial choice, the dimensionality of problem (one complete calculation of objective function has got over 50s of calculation time), together with observed local fixing of solutions, were most visible troubles at calculations. Probably some way for stochastic push out an algorithm without achieved minimum (alike stochastic annealing process) could solve this problem. The best approach, that might be proposed in this task was to use every of presented algorithms and next analysis of evaluated results. This technique is quite time–consuming, but provides some objectivity in proceedings It is also worth to consider, whether some other optimization algorithm would be not more useful (genetic for example).

4.3 Model verification

Below presented transients, of measured and modeled process variables enable comparison of developed WWTP models. For comparison of efficiency of applied optimization algorithms, transients of simulated outcome, form different optimized models are presented together, on common figures.

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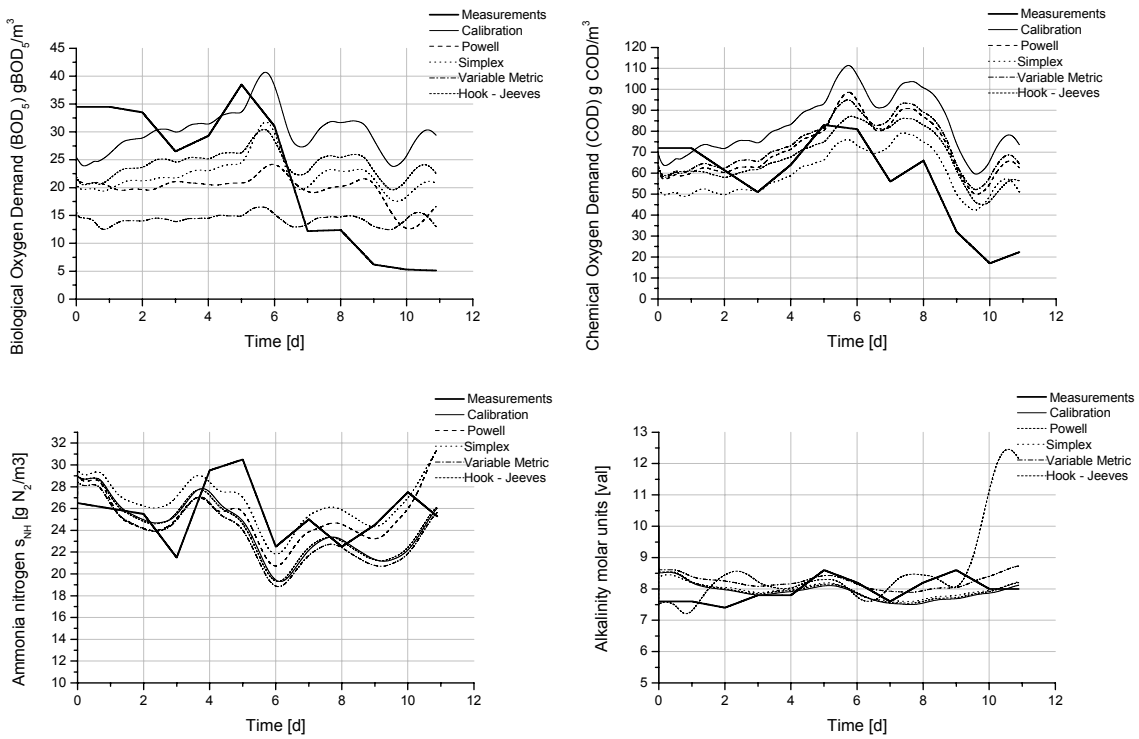

Fig. 6: Simulation transients for selected process variables in WWTP process model

Considering similar values of mean errors (between modeled and measured process variables) for different algorithms, it might be better to perform a visual comparison of results, fig.6, to distinguish a model (method) that recorded better dynamic behavior of investigated WWTP. In practical model application some numerical inaccuracy of a model might be accepted, on condition that a process dynamics would be mimicked properly. This kind of approach was considered during model calibration and optimization.

5. Conclusions

In this paper some approach to systematic fitting an ASM 1 model coefficients to measurements recorded on real WWTP plant in Resovia was presented and discussed. Any of ASM 1 models has a 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 modeling subsystem. At calibration phase some sensitivity functions were used. In this phase were assumed some stechiometric conditions for process operation. This phase of processing did not demand optimization of model coefficients, an expert knowledge of process was more suitable for proper choice of important impacts, however some confirming calculations were quite useful. Adaptation of the model to selected information, obtained from investigated WWTP plant was performed in next steps.

The first one was „hand-made" calibration. The aim of calibration was to manually estimate the unknown parameters, for easier guess of initial optimization point for differential balance equations that describe the WWTP process. At this stage the sensitivity analysis clearly has shown, that calibrated model was indeed sensitive on changes of the coefficients that had to be modified.

The second stage was an automatic optimization. In this stage different optimization algorithms that were most effective in presented optimization problem were marked out: Powell's conjugate directions

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method, conjugate gradients method and variable metric method. It is worth to underline, that starting point for each method was not random, but the one that was evaluated during calibration stage. This type of approach gives an opportunity to estimate parameters, that would not differ much from literature presented values and that would have acceptable physical interpretation.

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