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Application of the PExSim package in identification of multi-dimensional model of a waste water treatment plant

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Marcin Stachura jest doktorantem w Instytucie Automatyki i Robotyki Politechniki Warszawskiej. Obszarem jego zainteresowań naukowych jest modelowanie i sterowanie wielowymiarowych procesów przemysłowych. Swoje prace prowadzi opierając się na przykładzie miejskiej oczyszczalni ścieków w Rzeszowie.

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Abstract

This paper presets a modern approach to the modelling of multi-dimensional industrial processes. A proposed methodology is focused on processes working in more or less complex technology environment and integrates different approaches for simulation of components of the investigated systems. It is realized in form of the elastic programmable software package. This kind of approach includes an application of mathematical models (derived from physical relations, parametric or others) implemented in a relevant software, that allows us to prepare simulations so as 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 a process dynamics with a satisfactory quality. Therefore, in this paper the problem of fitting physical models described by a set of ordinary differential equations is considered. This type of models have a set of unknown parameters that have to be estimated so as a model could properly mimic and predict the process. A tool for optimizing models prepared in the *PExSim* is described and its capabilities are presented. At last, an application of the *PExSim* in modelling of industrial processes and models optimization is presented with the help of an example of a waste water treatment process. Furthermore, some procedures of the complex models optimization are proposed. As the final result of an optimization a waste water treatment process model is achieved. Example results for selected concentrations of contamination in treated sludge are presented.

Keywords: *PExSim*, modelling, model optimization.

Zastosowanie pakietu PExSim do identyfikacji wielowymiarowego modelu oczyszczalni ścieków

Streszczenie

W artykule przedstawiono nowoczesne podejście do modelowania wielowymiarowych procesów przemysłowych oraz metod optymalizacji utworzonych modeli. W treści opisano narzędzia umożliwiające modelowanie oraz optymalizację wraz z przykładem ich zastosowania. Istotą prezentowanego podejścia jest możliwość elastycznego dostosowywania utworzonych pakietów programowych do potrzeb użytkownika.

Słowa kluczowe: *PExSim*, modelowanie, optymalizacja modeli.

1. Introduction

Simulation is a common approach used for investigation of industrial processes behaviours [1]. Almost all modern SCADA systems have some tools for the processes dynamics modelling, but often they are adopted to a platform used by this system and are not standard. Results of the simulation reveal different phenomena like, e.g. parasitic oscillations, response dead time and many others but the necessity of solving a problem with a predefined accuracy is in conflict with the possibility of real time operation and does not include the possibility of elastic introduction programs or procedures written in other standards. Therefore, during plant operation optimization, or even modernizing a technology, the application of advanced software supporting process optimization might be very useful. This kind of approach includes the application of mathematical models (derived from physical relations, parametric or others) implemented in the relevant software, that allows to prepare simulations so as to explore process behaviors in many situations, especially critical ones. The key issue of this type of approach is to prepare a model that would approximate the 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 the mathematical description. Therefore, in this paper a problem of fitting physical models described by a set of ordinary differential equations is considered. This type of models have a set of unknown parameters that have to be estimated so as a model could properly mimic and predict the process. Complex processes can have a large number of unknown parameters, so a proposal of approach to its estimation and a software tool that allows to perform necessary calculations is presented and discussed. Described software allows to select parameters that have to be estimated, optimization algorithms, limits and form of objective function and stop criterions.

The aim of this paper is therefore a presentation of an approach of systematic testing and optimizing of multi-dimensional models of industrial processes with the use of the ***PExSim*** (*Process Explorer and Simulator*) software, developed at the Institute of Automatic Control and Robotics of Warsaw University of Technology.

2. *PExSim* package

PExSim is open (this means it is designed as plug-in type software), freely configurable software similar to Matlab Simulink. The package has a form of menu-controlled software with different options for the choice of operators of processed signals, simple dynamic models of components and additional elements used for simulation of time signals or events with the possibility of visualization[1, 2].

With help of the ***PExSim***, it is possible to create complex signal transformations paths, Fig.1 More detailed description can be found in [3]. In the ***PExSim***, data processing algorithms are implemented as block schemes, called paths. Every path consists of function blocks, realizing different ways of signal processing. Proper connection of inputs and outputs of the blocks realizes intended flow of signals. Fig. 1 presents the structure of elements used for data processing.

Available, built-in block libraries are as follows: C/C++ Scripts, Controllers, Crisp Logic, Discrete Operations, Electric Components, Execution Control, Filtering, FIS Systems, Fuzzy Logic, Heat Exchange, Heuristic Tests, Hydraulic Elements, Incipient FDI, Linear Dynamic, Mathematic Operators, ***MITforRD*** Models, Nonlinear Dynamic, Nonlinear Elements, Parameters Optimization, Pneumatic Elements, Ports and Subsystems, Robotic Elements, Signal Routing, Sinks, Sources, Statistic Operators, Vector Library, Water-steam Dependencies, Waste Water Treatment Plant Elements. Furthermore, ***PExSim*** is a plug-in type software, that allows to construct new function blocks, designed by a user in the form of the available library. It is a big advantage, especially if investigated processes are individual adapted to investigated problem.

The simulation results can be observed in form of numbers exposed on top of each node of the simulated system, on multiple

time displays with the elastic configuration of colours, magnitude of responses and time marks on tangent axis.

The application of the identified model of the process dynamics determines a sampling interval for simulation. Then, all components of the simulated structure have to be processed with the same sampling interval.

3. Model optimization

A problem of optimization (minimization) can be defined as follows: to find a vector of real or integer variables within an allowed, finite set Ω_x [4] that achieve extreme value of some performance index. In a case of presented optimization problem it is equivalent to the estimation of unknown coefficients present in equations that describe the processes:

$$f(\hat{\mathbf{x}}) = \min_{x \in \Omega_{\mathbf{X}}} f(\mathbf{x}) \tag{1}$$

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

$$A : V \to V \tag{2}$$

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

In the ***PExSim*** the following algorithms were integrated:

- using a gradient of the objective function: *Conjugate Gradients* and *Variable Metric* method,
- not calculating an objective function gradient: *Hook – Jeeves'*, *Rosenbrock's*, *Simplex* (S) and *Powell's* method,
- global optimization algorithm: *Particle Swarm Optimization*,

Detailed descriptions of selected methods are available in [5, 6, 7]. For proper application of these algorithms, it is necessary to know: the sensitivity of a method for selection of a start point and the rate of convergence (interpreted as a number of function evaluations). According to [5, 7] , the least sensitive was Rosenbrock's method. Basically this method was slower than Hook – Jeeves' method, but almost always has yielded a satisfactory result. On the other hand, the fastest methods were the Conjugate Gradients and Variable Metric ones, which had to use objective function gradients.

The Powell's and Variable Metric Methods are sensitive to the starting point choice. In the case of an inadequate selection a convergence rate of them was approximately a quadratic one, so at the beginning it is slow, but nearly to a optimal solution could be quite fast. This behaviour can be explained by the processing manner: at the beginning, a search with unknown parameters is done with use of the orthogonal direction base. As the conjugate directions are well estimated, a proper search direction is set, and an efficiency of the optimization is increased.

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

The Particle Swarm Optimization (PSO) is a swarm intelligence based algorithm designed to find a solution to an optimization problem in the search space, or model and predict the social behavior in presence of objectives [8]. The Swarm is typically modeled by particles in the multidimensional space that have position and velocity. These particles fly through the hyperspace (i.e., $\Re^n$) and have two essential reasoning capabilities: their memory of their own best position and knowledge of the global or their neighborhood best. In a minimization optimization problem, the "best" simply means the position with the smallest objective value. Members of a swarm communicate good positions to each other and adjust their own position and velocity based on these good positions. So a particle has the following information to make a suitable change in its position and velocity:

- A global best that is known to all and immediately updated when a new best position is found by any particle in the swarm.
- Neighborhood best that the particle obtains by communicating with a subset of the swarm.
- The local best, which is the best solution that the particle has seen.

The particle position and velocity update equations in the simplest form that govern the PSO are given by [8]:

$$\mathbf{x}_i^{k+1} = \mathbf{x}_i^k + \omega \mathbf{v}_i^k + c_1 \mathbf{r}_1 \circ (\hat{\mathbf{x}}_i - \mathbf{x}_i^k) + c_2 \mathbf{r}_2 \circ (\hat{\mathbf{g}} - \mathbf{x}_i^k) \tag{3}$$

where: $\mathbf{x}_i$ – position of *i*-th particle, k – algorithm step, ω – interia constant, c_1, c_2 – convergence coefficients (cognitive and social), $\hat{\mathbf{x}}_i$ - best solution for *i-th* particle $\hat{\mathbf{g}}_i$ - global best solution.

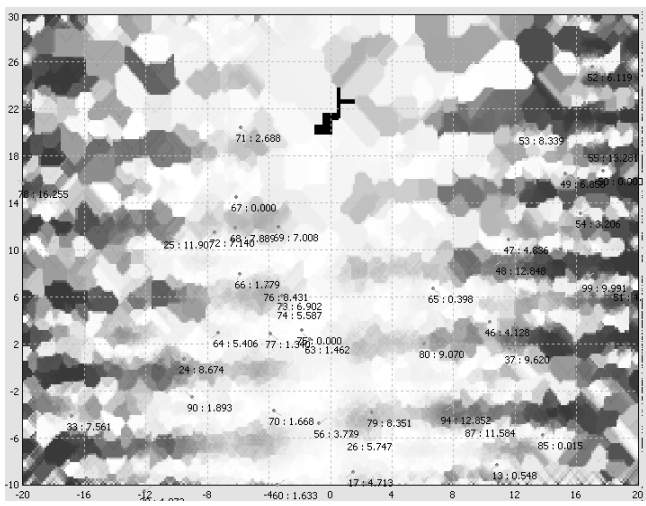

Fig. 1. An example of the PSO algorithm application. (the lighter colors mean the smaller value of the objective function)
Rys. 1. Przykład działania algorytmu PSO (jaśniejszym kolorom odpowiadają mniejsze wartości funkcji celu)

4. Application of the described optimization algorithms in the *PExSim*

Application of the above presented algorithms is currently implemented in stand alone overlay called ***PExSim Optimizer*** that in fact is a part of the ***PExSim*** package. The presented approach is focused on an issue of finding unknown parameters in mathematical descriptions so as to fit a model to a certain set of data obtained from the real process. In this way, it is possible to find a model that mimicks a real process with a satisfactory accuracy. The configurable objective function is a factor that tells about differences between a multi-dimensional process and its model, for example as:

$$f(\mathbf{x}) = \frac{1}{K} \sum_{k=1}^{K} \left(\sum_{n=1}^{N} \sqrt{\left[y_{m,n}(\mathbf{x},k) - y_{p,n}(\mathbf{x},k) \right]^2} + g(\mathrm{x},k) \right) \tag{4}$$

where: K – total number of performed simulation steps, k – current simulation step, N – number of process variables of a model and industrial process, $y_{m,n}$ – model n-th output value, $y_{p,n}$ – process n-th output value for selected parameters vector $\mathbf{x}$ in a discrete simulation step k, g – selected penalty function that is added when found solution is out of admissible set.

An example of the penalty function can be stated as:

$$g(\mathbf{x},k)=\sum_{n=1}^{N}\left[\left(\alpha^{(\mathbf{Ax}-\mathbf{H})\beta}+\chi^{(\mathbf{L}-\mathbf{Ax})\delta}\right)\right]_i \tag{5}$$

where **A** – coefficients matrix, **H** – vector of acceptable solutions, $\alpha, \beta, \chi, \delta$ – penalty function coefficients.

A methodology of optimizing industrial processes' can be described in the steps as follows:

- Preparation a model of the selected process in ***PExSim*** (this means selecting and connecting necessary blocks).
- Statement of a relevant objective function (for example the one that was presented above).
- Definition of a starting point $\boldsymbol{x}_0$ (if it is necessary) and an admissible set of solutions $\boldsymbol{\Omega}_x$.
- Selecting a stop criterion for the optimization algorithm.

At every step of optimization algorithms all of the above stated optimization parameters can be changed, so as to perform better and faster optimization process. For example, stop criterion or penalty function can be changed etc., with one exception: the problem dimensionality has to be fixed.

5. Example of application

Application of the ***PExSim*** in the modelling of industrial processes and models optimization will be presented with the use of an example of waste water treatment with use of a activated sludge process.

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 metabolized by the activated sludge, being partially or completely degraded and/or metabolized' [9]. The microorganisms growing in or on flocks are termed activated sludge or sludge biomass, and treatment process is accordingly known as an activated sludge process.

An activated sludge process applied in the considered WWTP consist of several phases of sewage treatment processes. It contains an introductory mechanic purification section, followed by the biological treatment and the 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 the crude sludge is mechanically filtered by a grit separator and then it is transferred to preliminary settling tank, to reduce mineral fixed components. The second stage is a biological treatment of sewage, to reduce nitrogen components by the activated sludge. At last is the second sedimentation process, in which some effects of biochemical processing (dead bacteria and heavy suspension) are divided from sewage flow by sedimentation and majority flow of the activated sludge is recovered to the biochemical phase of WWTP process.

A mathematical description of the biochemical processes, in this paper, is based on the ASM No. 1 model [10, 11, 12]. A main reason for this choice was actual structure of WWTP applied in Rzeszów. According to 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}, alkalinity molar units s_{ALK}.

For the approximation of the distributed character of the real process, each one of the elements was divided into many cells [11, 12], as shown in Fig.2, the structure of the preliminary settling tank.

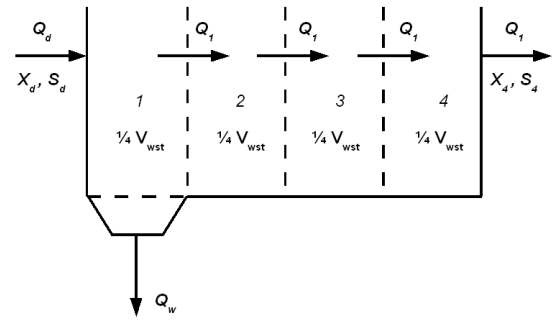

Fig. 2. Diagram of a cell model of the preliminary settling tank
Rys. 2. Schemat modelu osadnika wstępnego

The final model of the full scale waste water treatment plant consisted of:

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

Unknown parameters introduced in differential equations of he mathematical description of the WWTP processes, had to be evaluated to reduce possible differences between generated (by the model) process values and the 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, so for the effective study of a proper model an optimization technique was used.

Due to high number of the model parameters which were not precisely known and a limited number of recorded measurements, optimization of only a group of parameters was considered. These selected parameters were (for detailed description of selected parameters please refer [1, 4, 5, 6]):

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

All stoichiometric parameters, were set constant with default values taken from [13, 14,15, 16].

As an objective function a following formula was taken:

$$f(\mathbf{x})=\frac{1}{K}\sum_{k=1}^{K}\left[\sum_{i=1}^{n}\sqrt{\left(\frac{z_{M,i}(k)-z_{R,i}(k)}{z_{R,i}(k)}\right)^2}+\sum_{i=1}^{n}\exp\alpha\left(\frac{z_{M,i}(k)-z_{R,i}(k)}{z_{R,i}(k)}-0{,}5\right)\right] \tag{6}$$

where: K – total number of performer simulation steps, k - current simulation step, n – number of outputs, $z_{M,i}$ – *i-th* modelled output, $z_{R,i}$ – *i-th* measured output.

One of the crucial problems in the optimization of the multi-dimensional process models is the selection of a starting point for an optimization algorithm. The essential issue is a selection of starting points that would not lie close to the local minimum so as not to finish the optimization in that minimum. On the other hand application of stochastic algorithms (PSO might be an example) extends time of the optimization process. Therefore, the following approach was proposed:

- in the first step the *Particle Swarm Optimization* algorithm is started, with the assumed maximum steps number stop criterion. The basic aim of this step is to find a set of starting points that might lie close to local minima. One of these minimums is probably the global minimum.

- next, for every point found in the first step a fast algorithm (it means having a fast convergence) algorithm is started so as to find a minimum close to the selected starting point. The algorithm selectedn for this step was *Variable Metric* algorithm. An idea of this algorithm is based on the estimation of the conjugate directions of objective function minimization, starting from the following presented direction:

$$\mathbf{d}^{\mathbf{k}} = -\mathbf{V}_{\mathbf{K}} \nabla f(\mathbf{x}^{\mathbf{k}}) \tag{7}$$

where any selected matrix $\mathbf{V}_k$ in the sequential iterations approximates a matrix of second partial derivatives of a objective function in the following way:

$$V_{K+1} = V_K + \frac{s^k \rangle \langle s^k}{\langle s^k, y^k \rangle} - \frac{V_K y^k \rangle \langle V_K y^k}{\langle y^k, V_K y^k \rangle} \tag{8}$$

where: $\mathbf{s}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$, and $\mathbf{y}^k = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$.

- from all minimum found in that way the best point is chosen and an optimization is finished

A final result of an optimization is a waste water treatment process model. Example results for selected concentrations of the contamination in the treated sludge are presented below in graphic form. In this paper Total Nitrogen (N_T) and Biological Oxygen Demand (BOD_5)are presented as the most important outputs of the process and its model. Quality of the final model is quite good, and, moreover, the estimated values of its parameters are within admissible limits. It means that values of the stoichiometric and process kinetics parameters might be physically interpreted, and its values are close to literature ones.

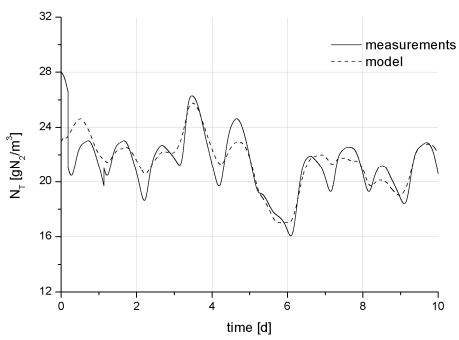

Fig. 3. Comparison of measured and modeled concentration of Total Nitrogen (N_T) in treated sludge

Rys. 3. Porównanie zmierzonego i modelowanego stężenia Azotu Ogólnego (N_T) w ściekach oczyszczonych

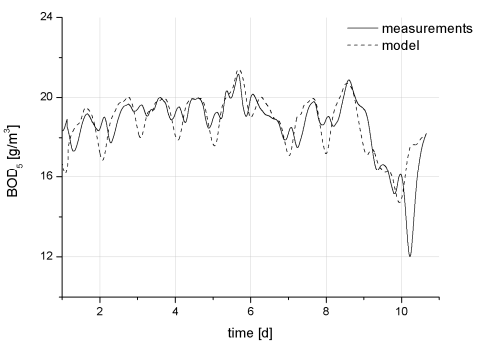

Fig. 4. Comparison of the measured and modeled Biological Oxygen Demand (BOD_5) in treated sludge

Rys. 4. Porównanie zmierzonego i modelowanego Biologicznego Zapotrzebowania Tlenu (BOD_5) w ściekach oczyszczonych

6. Summary

In this paper, a tool for the modelling of complex industrial processes was presented. Proposed software ***PExSim*** (*Process Explorer and Simulator*) is open, freely configurable software similar to Matlab Simulink. With the help of the ***PExSim***, it is possible to create complex signal transformation paths that are mimicking the real process. The application of the above described optimization is implemented by stand alone overlay called ***PExSim Optimizer*** that in fact is a part of the ***PExSim*** package. The presented approach is focused on an issue of estimation of unknown parameters in equations that describe a process.

The application of the proposed software tools was presented with the help of an example of the waste water treatment processes. The developed model of these processes had over 100 unknown parameters in differential equations. The proposed optimization approach yielded good results – performed model fits data recorded from the real plant with an acceptable quality and, what was crucial, estimated parameters had direct physical interpretation.

In summary, presented tools and methods might be very useful in the modelling and optimization of multi-dimensional industrial processes.

7. Acknowledgments

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Artykuł recenzowany