Theses of the doctoral (PhD) dissertation

APPLICATION OF A PRIORI KNOWLEDGE IN CHEMICAL PROCESS ENGINEERING

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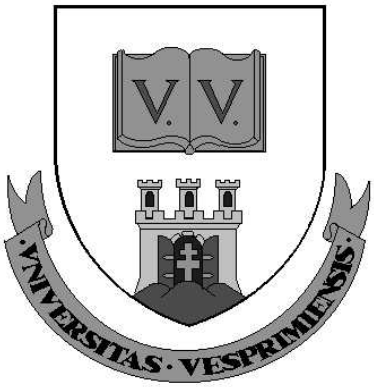

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2005

1. INTRODUCTION AND AIM OF THE WORK

Modeling, control and optimization of chemical processes are dynamically developing areas of process engineering. While these areas have great importance for chemical industry, there are several unsolved problems tied to them. It is due to that the information can be usually obtained from different sources, and handling together the pieces of knowledge of different nature often proves to be the bottleneck in the application of conventional process engineering and computational methods.

The aim of present thesis work was to develop new computational methods that are able to use information and models of different nature and different scope. Hence, the main question of this work was how one can improve the conventional process engineering methods by combining several types of information. The main objective of this thesis work was the development and realization new methods and algorithms for this purpose.

2. EXPERIMENTAL METHODS AND TOOLS

Present doctoral dissertation primarily contributes to modeling, control and optimization of chemical processes, especially of chemical reactors. Hence, during development of new results, I utilized the simulation and modeling techniques that are widely used in the process engineering.

The dissertation includes several simulation examples, e.g. a continuous stirred tank reactor, a batch fermentation reactor, and a continuous polymerization reactor. The dynamic models of these processes were taken from the literature. The simulations and models were realized in MATLAB software environment.

3. NEW SCIENTIFIC RESULTS

Before the presentation of new scientific results, I should note that the link among the theses is not a specific task but rather a problem class. So unlike most conventional doctoral works, the theses are relatively independent form each other.

1. Solving of multi- and conflicting-objective process optimization problems by interactive optimization procedure

Process optimization problems often lead to multi-objective problems where optimization goals are non-commensurable and they are in conflict with each other. In such cases, the common approach, namely the application of a quantitative cost-function, may be very difficult or pointless. For these problems, I developed a method that handles these problems by introducing a human user into the evaluation procedure. Namely, I propose a method that uses the expert knowledge directly in the optimization procedure. This approach has been applied successfully in computer graphics and engineering construction design, but it has not been used for chemical process engineering problems so far. During the development of the algorithm, I adopted this approach to typical process engineering problems. I illustrated that the proposed tool offers a more flexible way to make a compromise among different goals than the conventional optimization methods do. The practical usefulness of the framework was demonstrated through two application examples: tuning of a multi-input multi-output controller and optimization of a fermentation process.

2. Improvement of data driven identification of model structures and model orders by orthogonal least squares method

The data-driven model structure identification based on genetic programming is a quite new, but more and more popular technique in the scientific literature. I recognized that genetic programming tends to identify too complex models, especially when measurement noise is present, and most of the published works pay little attention to this problem. As a solution, I developed a new method that eliminates the negligible terms from linear-in-parameters models during the identification process based on orthogonal least squares method. I demonstrated that if the orthogonal least squares method is used, it results in more transparent models than without using it. The new method is also useful for identification of model order. The developed method was tested on model order identification problems of chemical reactors.

3. Improvement of data-driven identification of kinetic parameters by application of *a priori* knowledge

In many practical situations, the involvement of laboratory and industrial experiments are expensive and time consuming and accurate measurements cannot be made. This problem results in a small number of data points that are often noisy and obtained at irregular time intervals. Hence, data smoothing and re-sampling are often required to reduce the effect of measurement noise and irregular time intervals. Typically, an interpolation method is used for this purpose, e.g. cubic spline interpolation, but the disadvantage of the common interpolation methods is that they can not utilize any *a priori* information. Hence, I developed a new cubic spline

interpolation approach which utilizes *a priori* knowledge, e.g. material balance, or *prior* information about the measured properties. I demonstrated through the investigation of a simulated and an industrial chemical reactor that the new method improves the accuracy of the data-driven estimation of kinetic parameters.

4. Nonlinear controller design by hybrid *a priori* and *a posteriori* modeling

The critical point of nonlinear controller design is the *a priori* modeling of the controlled system. In practice, the effectiveness of nonlinear controllers is limited due to the uncertainties in model parameters, e.g. kinetic parameters, and in model structure. To cope with this problem, I developed a hybrid model which combines the *a priori* and *a posteriori* modeling in such a way that the uncertain part of the *a priori* model is replaced by an artificial neural network model. The advantage of this hybrid model compared to a complete *a priori* model is that it is much less sensitive to the model uncertainty. This was demonstrated by the nonlinear control of a simulated continuous stirred tank reactor.

4. PUBLICATIONS OF THE AUTHOR RELATED TO THE THESIS

Articles in international journals:

J. Madár, J. Abonyi, H. Roubus, F. Szeifert, Incorporating Prior Knowledge in Cubic Spline Approximation - Application to the Identification of Reaction Kinetic Models, *Industrial and Engineering Chemistry Research*, vol. 42. no. 17., pp. 4043-4049, 2003.

J. Madár, F. Szeifert, L. Nagy, T. Chován, J. Abonyi, Tendency Model-based Improvement of the Slave Loop in Cascade Temperature Control of Batch Process

Units, *Special Issue of Computers & Chemical Engineering*, vol. 28., pp. 737-744, 2004.

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J. Madár, J. Abonyi, B. Balaskó, F. Szeifert, Interactive Evolutionary Computation in Process Engineering, *Computers and Chemical Engineering*, vol. 29(7), pp. 1591-1597, 2005.

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Article in Hungarian journal:

J. Madár, J. Abonyi, F. Szeifert, New Approaches to the Identification of Semi-mechanistic Process Models, *Acta Agraria Kaposváriensis*, vol. 8(3), pp. 205-218, 2004.

Book chapters:

J. Abonyi, J. Madár, F. Szeifert, Combining First Principles Models and Neural Networks for Generic Model Control, in *Soft Computing in Industrial Applications - Recent Advances*, pp.111-122, Springer Engineering Series, 2001.

J. Madar, J. Abonyi, Evolutionary Algorithms, Chapter 2.10. in *Instrument Engineers' Handbook, 4th Edition, Volume 2 - Process Control*, editor: B. Liptak, 2005.

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Madár J., Abonyi J., Szeifert F., Dinamikus rendszerek identifikációja genetikus programozással, *31. Műszaki Kémiai Napok, Veszprém*, 2003.

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J. Madár, J. Abonyi, F. Szeifert, Application of Neumann's Machine of Self-Reproduction - Evolution and Artificial life in Process Engineering, *Proceedings of the International Conference in Memoriam John von Neumann*, *Budapest*, 2003.

J. Abonyi, J. Madár, F. Szeifert, Priori knowledge in Process Modelling and Optimization, *CAPE Forum*, *Veszprém*, 2004.

J. Madár, J. Abonyi, F. Szeifert, Population Based Algorithms for Batch Process Development, *32. Műszaki Kémiai Napok, Veszprém*, 2004.

J. Madár, J. Abonyi and F. Szeifert, Genetic Programming for System Identification, *Proceedings of Intelligent Systems Design and Applications*, *Budapest*, 2004.