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A Novel Approach to Automated Mechanism Recognition based on Model Discrimination

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In this work, a model-based optimization framework is proposed which includes parameter identifiability and estimation, as well as an enhanced model discrimination step. For this purpose, a so-called Automated Mechanism Recognition (AMR) approach has been developed. It allows different models to perform in a collected set of measured data points. Each model stands for a diverse physical mechanism. Based on the developed framework, it is now possible to identify time points, i.e., time intervals where a certain model is valid or more appropriate. Thus, suitable control actions can be carried out in order to increase the process performance. By this means, a better process understanding can be obtained and undesired or even critical process states can be recognized. The application of AMR is demonstrated by means of case studies including a catalytic fixed bed reactor, a two-phase flow system and a biotechnical system.

1. Automated Mechanism Recognition

With the help of AMR, a measured data set is divided into intervals and for each interval the best model with its optimal parameter values is determined. The division into intervals is performed by another optimization step in which the best length for each interval (i.e. the best starting and end-time points or model switch points) is found. After the algorithm converged, it is possible to answer the question: during which time-scale, which model or mechanism prevails in the observed process? Thus, it can be used to determine which mechanism recently dominated the process. Another main task is to make the algorithm converge so fast as to be applied to online process control.

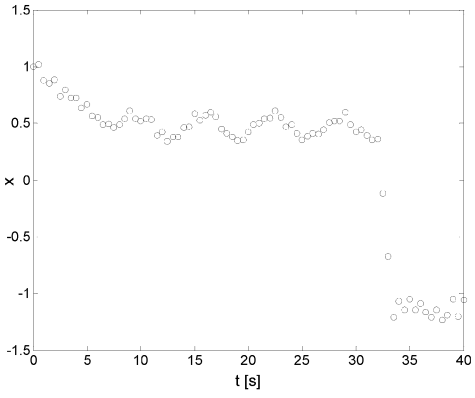

Figure 1:Example data set

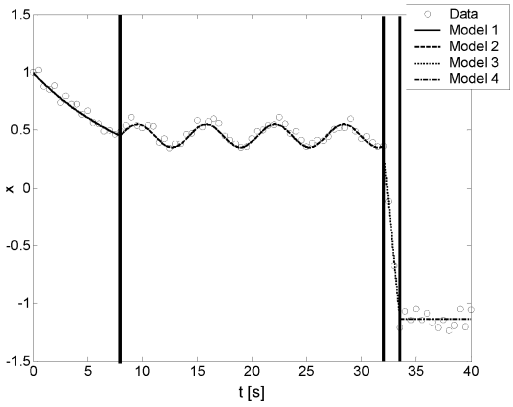

Figure 2: Results of the AMR optimization process

The aim of the AMR is first demonstrated based on a numerical example. Figure 1 shows a set of data points for the measured variable x for a time period of 40 seconds. Different dynamic behaviours can be recognized such as a exponential decrease (model 1), a sinus curve (model 2), a linear decrease (model 3) and steady state (model 4). Applying the AMR divides the data set into 4 intervals. For each interval the best model and its optimal parameter values are determined. The result is show in Figure 2. It is obvious that the approach to fit the data with only one of these models will have resulted in a lack of fit. Even the use of different models in equaly spaced intervals would not have produced a good fit.

The AMR is composed of three optimization steps (Fig.3). At first the parameters of the available models have to be estimated. Since this step is positioned in the inner loop, it has a great influence on the rate of the overall process. Nevertheless, it has to be reasonably accurate because this step decides whether a model is chosen or not.

The next step is the model discrimination. For each interval the available models are subjected to discrimination so that the best set of models is found. The next step includes the interval determination where the interval bounds are varied. The number of intervals per time period has to be specified for each problem. At the beginning it is assumed that this number is equal to the number of available models and, thus, giving each model the option to be active in one interval at least, as demonstrated in Figure 2. For a big set of models or short time periods (i.e. few data points per period) this assumption may result in low accuracy or slow convergence. The positions of the interval bound lines are subject to constrains. Each interval is supposed to have a lower and upper bound, and thus e.g. a next interval may not start before the last one.

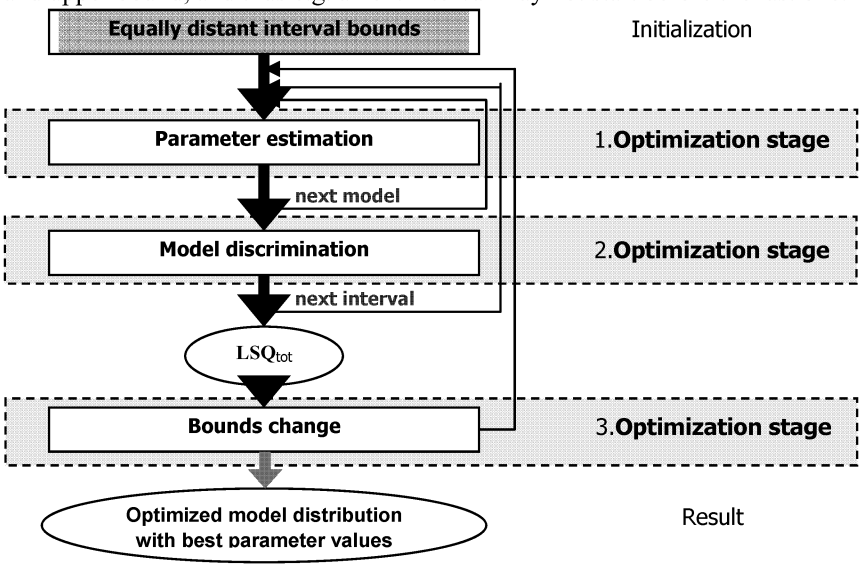

Figure 3: The AMR Optimization Framework

2. The optimization procedures

2.1 Parameter estimation

The first step of the AMR algorithm is a parameter estimation problem. The resulting optimization problem with a Maximum Likelihood objective function is defined as follows,

$$\min_{\mathbf{p}}\left[\sum_{i}^{NM}\sum_{k}^{NP}\frac{(y_{i,k}^{exp}-y_{i,k}^{cal})^2}{\sigma_{i,k}^2}\right] \tag{1}$$

$$\text{s.t.}\quad f_i(y_i^{cal},\dot{y}_i^{cal},\mathbf{p},\mathbf{u},t)=0$$

$$\mathbf{p}_l\le\mathbf{p}\le\mathbf{p}_u$$

This is the formulation for NM quantities which are measured at NP data points with the variance σ^2. The dynamic system described by the DAEs f_i (model equations) includes the parameters **p** and is influenced by the set values of **u**.

The fastest way to solve this problem depends on the type of the DAE system **f**. An agreement has to be found between accuracy and speed (Asprey 2003). For complex DAE systems the computation of the Jacobians might be time consuming. For those cases, good results were obtained by applying the Nelder-Mead Simplex algorithm (Largarias et al. 1998). However, if the Jacobians are available in a short time a Quasi Newton method is recommended.

2.2 Model discrimination

For model discrimination the smallest element of the vector containing the Least Squares (LSQ) of the models has to be found (Eq. 2). This is a straightforward procedure. The main challenge is the definition of the bounds and the dependencies of the model parameters. The results of the discrimination are only reliable when these are well defined in a physical sense.

$$\min_{\text{Model}}\mathbf{LSQ} \tag{2}$$

2.3 Change of interval bounds

In order to find the optimal intervals **I**, i.e. the model switch points (t_A and t_E respectively), the following optimization problem is formulated:.

$$\min_{t_A,t_E}[LSQ_{tot}(I_1,I_2,...)] \tag{3}$$

$$\text{s.t.}\quad I_m=f(t_{A_m},t_{E_m})$$

$$t_{A_{m+1}}=t_{E_m}$$

$$\mathbf{A}\cdot\mathbf{t}_{AE}\le\mathbf{0}$$

$$y(t_{E_m})=y(t_{A_{m+1}})$$

In this optimization problem there is linear equality and inequality constrains. This speaks against a stochastic optimization algorithm. However, since the objective function is highly discontinuous and nearly randomly distributed, gradient based optimization algorithms will fail. So for instance if the bound of two intervals moves between two data points, the value of the objective function is not changing (zero gradients). But when the bound crosses a point, the model distribution in all intervals may change resulting in a step up or down of the objective function. The problem can be reformulated as a mixed integer nonlinear optimization problem, but this makes it more difficult to apply it to data with changes in time step within. In this work, the stochastic algorithm approach: particle swarm optimization (PSO), published by Kennedy (Kennedy et al. 1995), is utilized. With a reliable set of initial particles a fast convergence can be reached. The PSO also handles easily high dimensions so that problems with a large number of intervals can be solved.

3. Case studies

3.1 Catalytic fixed bed reactor

In catalytic reactions several steps could influence the reaction rate (Fig. 4). First component **A** has to diffuse from the bulk flow towards the boundary layer (a).

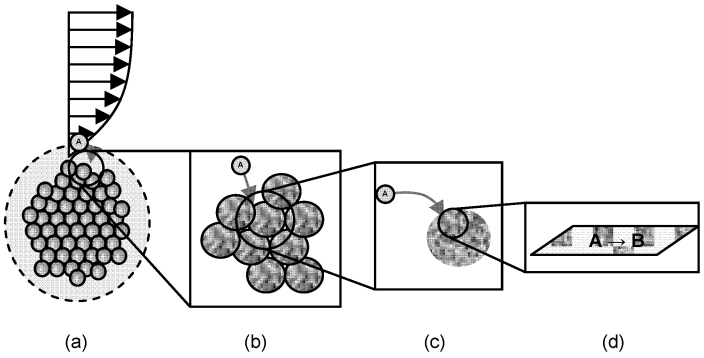

Figure 4:(a) External diffusion; (b) Internal diffusion; (c) Adsorption; (d)Reaction

Following this, it has to enter into the catalyst pores (b). Then it can be adsorbed on the catalytic surface (c) where the reaction takes place (d). These steps are followed by desorption and transport of the product B to the bulk flow. At steady state operation is common to work with a rate limiting step (RLS) assuming that only one step dominates the reaction resistance. In most cases this is the reaction step (d) (Fogler 2006). However, each step could be described with model equations, containing parameters to be estimated (e.g. Pinto 2007). Applying the AMR procedure, it is possible to identify process states in which other steps dominate the process. This may happen for example due to catalyst decay. With the knowledge of the actual problem a suitable counter measure can be initiated.

3.2 Two-phase flow in an horizontal absorber tube

The direct vaporisation of water in parabolic solar collectors is an interesting alternative to the actually used synthetic oil because it reduces significantly the investment costs, which are the main drawback in the application of solar farm power plants. The problem is that boiling crises could lead to a critical temperature profile in the absorber tubes, damaging or even destroying them. Some different flow patterns in horizontal tubes are shown in Figure 5.

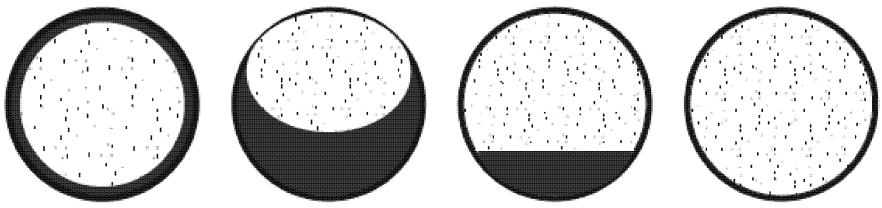

Figure 5: Flow patterns in horizontal absorber tubes

The third tube from left in Fig. 5 demonstrates the most dangerous state of the flow: the stratified flow. In the section where liquid covers the tube, the surface temperature is low, because a high convective boiling heat transfer takes place. At the dry surface the heat can not be removed so fast due to the boiling crisis. The temperature differences in the lower and the upper tube area produce tensions that can easily break the absorber.

However, here again the different flow patterns can be described with diverse models (e.g. Baehr 1998), and the AMR framework can be used to identify and avoid such critical process states before they take place.

3.3 Activated sludge membrane filtration

Activated sludge processes are an innovative alternative for waste water treatment plants. Micro-organisms in a biological reactor clean the contaminated feed water, which is then pumped through membrane units, holding back the whole biology. The main drawbacks for these new kinds of processes are the high energy consumption and the expensive cleaning effort. Both are result of the membrane fouling. It is state-of-the-art to drive the process by using heuristics. So the initiated countermeasures are independent of the actual situation on the membrane surface, producing the fouling effect. Figure 6 exemplifies some reasons for the flux reduction (i.e. fouling).

Based on the AMR approach the current situation on the membrane surface can be identified and the effect of fouling becomes quantifiable. Using these results a process optimization strategy is developed taking into account the actual needs for cleaning.

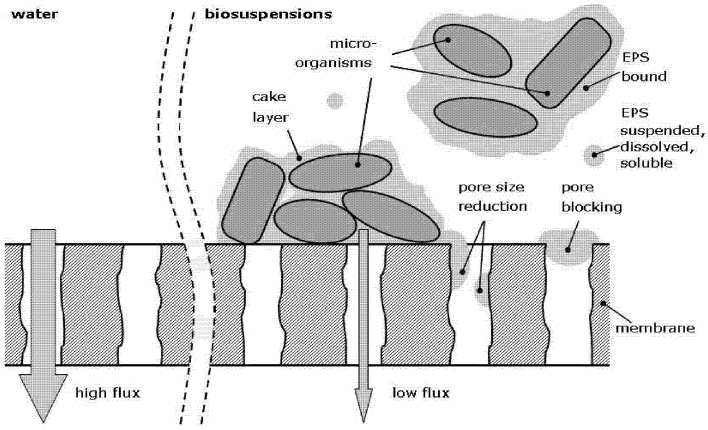

Figure 6: Effect on the membrane surface

4. Conclusions and future work

The results obtained demonstrated that there are variety of applications for the proposed new approach of AMR. Based on the case studies it could be shown that with AMR optimal control strategies can be developed in order to increase the process performance. The remaining challenge is to develop algorithms for the different stages in the AMR. Furthermore AMR is helpful in process modelling as it gives a better insight into dominant process mechanisms.

The entire procedure is being subject to a continuous development with the aim to increase convergence velocity and stability. Here recently developed mathematical methods and optimization algorithms have been integrated.

5. References

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