Optimal Experiment Design Techniques Integrated with Time-series Segmentation

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***Abstract*—Process models play important role in computer aided process engineering. Although the structure of these models is a priori known, model parameters should be estimated based on experiments. The accuracy of the estimated parameters largely depends on the information content of the experimental data presented to the parameter identification algorithm. Optimal Experiment Design (OED) can maximize the confidence on the model parameters. Considering that OED is an iterative process, it may happen that the designed experiment contains segments which are not or less useful for parameter identification. Using the tools of the OED there is the opportunity to qualify the segments of the time-series of different data sets. After the segmentation, it will be possible to choose the most appropriate segments for identification of each parameter, i.e. to determine the parameters as accurate as possible.**

Keywords: Optimal Experiment Design, Parameter Identification, Segmentation, Time Series

I. INTRODUCTION

Process models play important role in computer aided process engineering since most of advanced process monitoring, control, and optimization algorithms rely on the process model. Unfortunately, often some of the parameters of these models are not known a priori, so they must be estimated from experimental data. The accuracy of these parameters largely depends on the information content of the experimental data presented to the parameter identification algorithm [1].

1. Contribution

In this paper, the problem of creating identification algorithm is investigated. We present a new and intuitive segmentation based method, which makes possible to identify each parameter in the most appropriate time frame of the experimental data. With the help of this method, it becomes possible to reduce the number of experiments and at the same time reduce the time consumption of parameter estimation since a considered time segment is useless in a certain point of view, but from another aspect the same time series segment can be applicable to determine other parameters.

The rest of the paper is organized as follows. In Section 2, the previous works related to OED are reviewed. Section 3 and Section 4 present the theoretical background of our work, i.e. the applied segmentation method and classical OED, while Section 5 conducts our approach through a case study. Finally, we present our conclusions and suggestions for future work.

II. PREVIOUS WORK

Optimal Experiment Design (OED) can maximize the confidence on model parameters through optimization of the input profile of the system. For parameter identification of different dynamic systems and models, this approach has been already utilized in several studies [2–6]. OED uses an iterative algorithm where the optimal conditions of the experiments or the optimal input of the system depends on the current model, which parameters were estimated based on the result of the previously designed experiment. Consequently, experiment design and parameter estimation are solved iteratively, and both of them are based on nonlinear optimization of cost functions.

That means in practice, the applied nonlinear optimization algorithms have great influence on the whole procedure of OED, because for nonlinear dynamical models the design of the experiment is a difficult task. This problem is usually solved by several gradient-based methods e.g. nonlinear least squares method or sequential quadratic programming. Several gradient computation methods are described in [7]. In [8] extended maximum likelihood theory is applied for optimizing the experiment conditions.

III. SEGMENTATION

A univariate m-element time series, $x = [x(1),x(2),\ldots,x(m)]$, is a column vector, where $x(i)$ is the ith element. The ith segment of x is a set of consecutive time points, $S_i(a,b) = [x(a), x(a+1),\ldots, x(b)]$, while the c-segmentation of x is a partition of x to c non-overlapping segments, $S^c_x = [S_1(1,a), S_2(a+1,b), \ldots, S_c(k+1,m)]$. In other words, a c-segmentation splits x to c disjoint time intervals, where $1 \le a$ and $k \le m$.

The simplest but yet powerful segmentation technique for univariate time series is PAA. In this case, to reduce the m-length data from N, the time series are simply divided into N similar sized frames and each frame is represented by its mean value. Assuming that N is a factor of m, we get:

$$\underline{x}(i) = \frac{N}{m} \sum_{j=\frac{m}{N}(i-1)+1}^{\frac{m}{N}i} x(j), \tag{1}$$

where $\underline{x}(i)$ represents the ith PAA segment of x. Please note, PAA is not the most straightforward segmentation method but it is perfectly suits for our case study as it can be seen in Section 5.

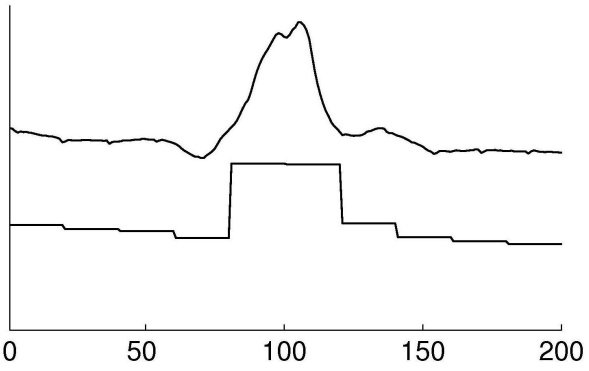

Figure 1. The original signal (top) and its PAA representation (bottom) using 10 segments

IV. CLASSICAL OPTIMAL EXPERIMENT DESIGN

The case study considered in this paper belongs to the following general class of process models:

$$\frac{dx(t)}{dt} = f(x(t),u(t),p) \tag{2}$$

$$y(t) = g(x(t)), \tag{3}$$

where u is the vector of the manipulated inputs, y is the vector of the output, x represents the state of the system and p denotes the model parameters. The p parameters are unknown and should be estimated using the data taken from experiments. The estimation of these parameters is based on the minimization of the square error between the output of the system and the output of the model:

$$\min_p \left[J_{mse}(u(t),p) = \frac{1}{t_{\exp}} \int_{t=0}^{t_{\exp}} (e^T(t) \cdot Q(t) \cdot e(t)) dt \right] \tag{4}$$

$$e(t) = \tilde{y}(u(t)) - y(u(t),p), \tag{5}$$

where $\tilde{y}(u(t))$ is the output of the system for a certain $u(t)$ input profile, and $y(u(t))$ is the output of the model for the same $u(t)$ input profile with p parameters. Q is a user supplied square weighting matrix that represents the variance measurement error. The basic element of the experiment design methodology is the Fisher information matrix F, which combines information on the output measurement error and the sensitivity of the model outputs y with respect to the model parameters:

$$F(p^0,u(t)) = \frac{1}{t_{\exp}} \int_{t=0}^{t_{\exp}} \left(\frac{\partial y}{\partial p}(u(t),p)_{p=p^0}\right)^T \cdot Q(t) \cdot \left(\frac{\partial y}{\partial p}(u(t),p)_{p=p^0}\right) dt \tag{6}$$

The sensitivities are calculated based on the partial derivatives of the model parameters. As the true parameters p^* are unknown during experiment design, the derivatives are calculated near to the so-called nominal parameters p^0, which can be given by some initial guess, extracted from literature or estimated from the previous experiments. The optimal design criterion aims the minimization of a scalar function of the F matrix. Several optimal criterion exist, we present D-optimal[1] and E-optimal[2] criterion suggested by Bernaerts et al. [1]:

$$J_D = \min_{u(t)}(\det(F)) \tag{7}$$

$$J_E = \min_{u(t)}\left(\frac{\lambda_{\max}}{\lambda_{\min}}\right) \tag{8}$$

If the p^0 nominal parameters are far from the p^* true parameters, convergence cannot be guaranteed after the first optimal design. So an iterative design scheme is needed to obtain convergence from p^0 to p^* (Fig. 2).

Both the parameter estimation and the experiment design steps of this iterative scheme represent a complex nonlinear optimization problem, hence the effectiveness of the applied optimization algorithms have great influence on the performance of the whole procedure. The classical solution is to use nonlinear least squares (NLS) algorithm for parameter estimation (4), and sequential quadratic programming (SQP) for the experiment design (8).

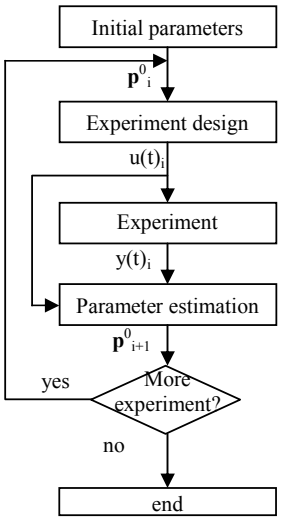

Figure 2. Scheme of the classical sequential design of experiments

V. APPLICATION EXAMPLE

1. Process description

The reactor what have been studied is a SISO (single input-single output) process, a continuously stirred tank reactor (CSTR) where a free radical polymerization reaction of methyl-metacrylate is considered using azobisisobutironitil (AIBN) as initiator, and toulene as solved. The aim of the process is to produce different kinds of product grades. The number-average molecular weight is used for qualifying the product and process state, and it can be influenced by the inlet initiator flow rate. When this assumption is considered, and the effect of the temperature is neglected, the multi input-multi output model could be reduced to a SISO process.

[1]Minimizes the determinant of the covariance matrix and thus minimizes the volume of the joint confidence region

[2]Minimizes the condition number of F, i.e. the ratio of the largest to the smallest eigenvalue of the Fisher matrix

Because of the isothermal assumption, a four-state model can be obtained [9].

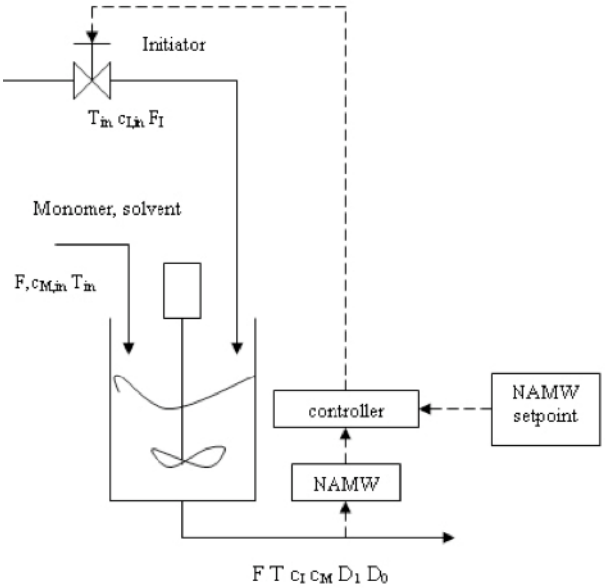

Figure 3. The configuration of SISO process

$$\frac{dC_m}{dt} = -(k_p + k_{fm})C_m P_0 + \frac{F(C_{m,in} - C_m)}{V} \quad (9)$$

$$\frac{dC_I}{dt} = -k_I C_I + \frac{F_I C_{I,in} - FC_I}{V} \quad (10)$$

$$\frac{dD_0}{dt} = (0.5k_{Tc} + k_{Td})P_0^{\,2} + k_{f_m} C_m P_0 - \frac{FD_0}{V} \quad (11)$$

$$\frac{dD_1}{dt} = M_m(k_p + k_{fm})P_0 C_m - \frac{FD_1}{V} \quad (12)$$

$$y = \frac{D_1}{D_0}, \quad (13)$$

where:

C_m – concentration of the monomer in the reactor

$C_{m,in}$ – monomer concentration in feed

C_I – initiator concentration in the reactor

$C_{I,in}$ – initiator concentration in feed

k_p, k_{fm}, k_I, k_{Tc}, k_T – kinetic parameters and

$$P_0 = \left[\frac{2f \cdot k_I C_I}{k_{Td} + k_{Tc}}\right]^{0.5} \quad (14)$$

D_0 is the zero order moment of the chain length distribution of the inactive polymer chain, which represents the length of inactive chains. D_1 is the first order moment of inactive polymer chains, which means the distribution of molecular weight of inactive chains. The number-average molecular weight, represented by y, cannot be measured, but it is calculated, as can be seen in the (13).

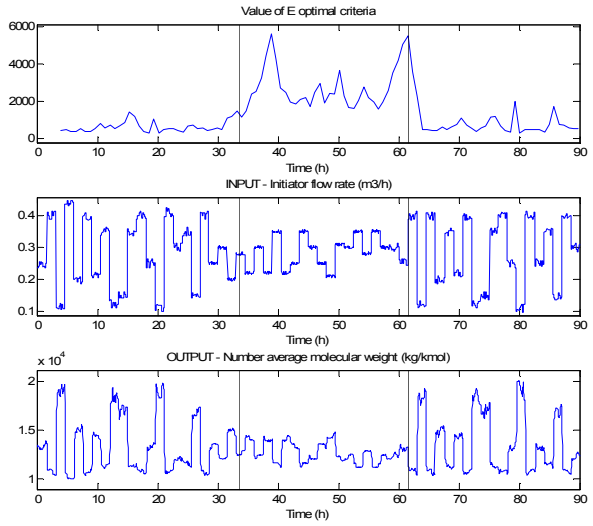

Figure 4. Segmentation of time series of E criteria and the segments of the experimental time series

2. *Example for using OED tools and segmentation*

This paper introduces the combination of OED tools and time series segmentation for support parameter identification through a case study of the previously presented polymerization reactor.

The model of the reactor is used as the operating plant and at the same the model also represents the process model that needs some of its parameters to be identified. Imagine that k_p and k_i kinetic parameters are not known properly and previously an experiment was carried out to determine the parameters.

Expression (8) was applied as the basis of extracting more information from these time series. It means that lower value the cost function E has, indirectly the considered time series segment is more and more appropriate for identification purposes. Directly the value of the E criteria can express the potential information content of the examined input signal segment regarded to the considered parameters. That is why important to examine the value of E optimal criteria as function of time over the period of the experiment.

Performing the presented PAA method for segmentation of time series of E – and indirectly throughout this the original experimental time series also – we have the possibility to separate the useful time series segments from the time series segments with less information content. The result of the segmentation is shown by Fig. 4.

As it can be seen, the experiment can be divided into 3 parts. The first and the last segments have lower E value than the middle one. This means that input signal of these segments have potentially more information content that the middle segment possess. That is why middle segment can be neglected during the process of parameter identification.

In Fig. 5 the result of the identification is presented. During identification, the first and last time series segments were applied. As it can be seen, the parameter fitting for the model was pretty successful since the output of the model is equal to the experimental data.

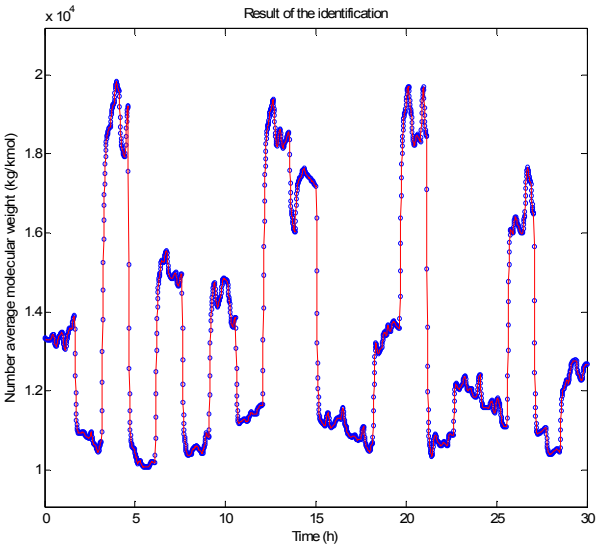

Figure 5. Result of the identification (circles – experimental data, full line – model output)

VI. CONCLUSION

Determination of model parameters of process models is a crucial issue since process models play important role in computer aided process engineering. That is why the aim of this paper was to introduce a new approach of applying the existing time series from the previous experiments throughout an example of a polymerization reactor. This approach combines the tools of Optimal Experiment Design (Fischer matrix based E and E optimal criteria) and time series segmentation to extract relevant information for parameter identification. The introduced case study expresses the applicability of this approach; however, our work is in the beginning of its way.

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