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lApplication of non-linear dynamic optimization in advanced process control of product grade transitions of polymerization processes

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Abstract

One of the main characteristics of producing synthetic polymers is that the same process is used for the production of different kind of products (various molecular weights, compositions, etc.). Since the producers are forced to satisfy various demands of various costumers, frequent grade transitions are needed. These grade transitions are expected to be short and effective to avoid the production of so-called off-specification products. It became very popular to apply model predictive controllers (MPCs) to reduce the quantity of off-specification products, however most of them use linear models for prediction. Since polymerization reactions are highly non-linear, using linear models may cause significant difference between the response of the model and of the real plant and this can cause problems e.g. in predictive control. The difference appears mainly during grade transitions, hence it is important to tune the appropriate parameters of the regulators to realize the grade transitions as soon as possible. In this article a novel method – in the field of predictive control - is introduced for parameter tuning, although this method is well known in the field of experiment design. The statistical tools like design of experiments (DoE) permit the investigation of the process via simultaneous changing of factors' levels using reduced number of experimental runs. Through a case study the applicability of full factorial design is going to be examined. It will be proven that full factorial design is appropriate for finding the right tuning parameters of MPC controlled polymerization reactor. The aim of the case study is the reduction the time consumption of grade transitions, so applying the tools of design of experiments as a quasi-APC.

Keywords: experiment design, advanced process control, model predictive control, polymerization process

1. Introduction

The production of the synthetic polymers represents an important part of chemical industry. In this industrial segment a general practice is that one reactor is used for producing various products (with various molecular weights, compositions, etc.).
During transitions between products, off-specification products are produced. This product is generally worth less than the on-specification material (which fulfill all the commercial and quality requirements), therefore it is crucial to minimize its quantity. The on-specification product can be produced under varying circumstances and at varying operating points, which are more or less sound from an economical point of view, motivating the optimization of the production during production stages.

In these processes a large number of different grades are produced, and the transition times between the productions may be relatively long and costly in comparison with the total amount produced. The demand for reduction of the time and cost of grade transition inspires the researchers to find more innovative solutions (Flores-Tlacuahuac and Biegler, 2008, BenAmor et al., 2004) The optimization of complex operating processes generally begins with a detailed investigation of the process and its control system (Lee et al., 2004). It is important to know how information stored in databases can support the optimization of product transition strategies, and how hidden knowledge an be extracted from stored time-series, which can assure additional possibilities to reduce the amount of off-grade products. The optimization of product grade transition is a typical and highlighted task in process industry (McAuley and MacGregor, 1991).
Unfortunately, it is very difficult to find the right tuning parameters of the controllers in the whole operation range because of the nonlinearity of the polymerization process, and identified models (for MPCs) from input-output data are mostly linear. In the industrial practice commercial Advanced Process Control (APC) systems are installed to handle the problem of tuning parameters of the controllers. In the most of cases the the operation of these systems based on a linear cost function, which usually contains the cost of the production and the price of the raw materials and products. Obviously the goal of the application of APCs is to maximize the quantity of on-specification materials and at the same time minimize the cost of the production. Since these control systems are relatively expensive so limitedly accessible, in some cases the right parameters of the production (e.g. set-points, tuning parameters of controllers, valve positions) is determined experimentally using the intuition of engineers.
One of the common experimentation approaches is One-Variable-At-a-Time (OVAT) methodology, where one of the variables is varied while others are fixed. Such approach depends upon experience, guesswork and intuition for its success. On the contrary, the statistical tools like design of experiments (DoE) permit the investigation of the process via simultaneous changing of factors' levels using reduced number of experimental runs. Such approach plays an important role in designing and conducting experiments as well as analyzing and interpreting the obtained data. These tools present a collection of mathematical and statistical methods that are applicable for modeling and optimization analysis in which a response or several responses of interest are influenced by various designed variables (factors) (Farzaneh and Tootoonchi, 2009).
In this study the applicability of full factorial design is going to be examined through a case study. It will be proven that full factorial design is appropriate for finding the right tuning parameters of MPC controlled polymerization reactor. The aim of the case study is the reduction the time consumption of grade transitions, so applying the tools of design of experiments as a quasi-APC.
The paper is organized as follows: in Section 2 the theoretical background of the applied methodology is going to be presented. In section 3 the applied methodology will be discussed throughout an application example, which is followed by a conclusion.

2. Theoretical background and the applied methodology

The applied methodology can easily be inserted into the scheme of the classical experiment design steps:

I. As the first step the mean values of the parameters are determined. As the step of experiment design the matrix of factorized variables is constructed which practically contains the values of the factors in the different experiments.

II. In second step the experiments are carried out and the results of the experiments are saved.
III. In this step, the experiment with the best value of the objective function is chosen and the parameters of this experiment will be substituted into the mean values of initial parameters in the next iteration step/experiment. In this step it is necessary to determine the interval of variation based on the gradient of the fitted linear function estimated by regression based on the results of experiments.
The iteration is continued pre-determined times, because it is important to note that carrying out experiments is a time and cost demanding process.
Experimental-statistical tools permit to reduce the number of experimental runs and to investigate the interaction effects between the designed variables (factors). Therefore, this methodology was employed for optimization of the tuning parameters of linear model predictive controller. These variables are the value of prediction and control horizon and the move suppression coefficient. For statistical calculations the actual variables were coded according to Eq. (1).

$$x_i = \frac{z_i - z_i^0}{h_i} \qquad (i = 1 \ldots n) \tag{1}$$

where z denotes the current value of the designed variable, z^0 is the center point (mean) of the designed variable, h is the interval of variation, x is the coded level of the designed variable (dimensionless value) and n is the number of variables. Thus, each variable has two different coded levels (±1). The full factorial design is a set of experimental runs where each level of the designed variable is investigated at both levels (+1) and (−1) of all the other factors. It is an orthogonal design, which allows the estimation of a factor effect independently of all other effects.
Based on experimental design matrix the factorial models were developed to ascertain the relationship between responses and factor effects. According to this method, a response y is set as a functional relationship of the designed variables (factors) and for a full factorial design the effects of factors may be estimated by linear regression model:

$$y = b_0 + \sum_{i=1}^{n} b_i x_i \tag{2}$$

where y is the predictor of the response, b_0 , b_i are the regression coefficients.
In order to ascertain the regression coefficients of the factorial model, Eq. (2)., the linear regression method was employed. According to this method the least square estimations of the regression coefficients can be written:

$$\overline{b} = (\overline{\overline{x}}^T \overline{\overline{x}})^{-1} \overline{\overline{x}}^T \overline{y} \tag{3}$$

where b is the vector of regression coefficients, x is the matrix of the independent variables levels, y is the vector of the response (experimental values).
To realize the *Step III.* described in 2.1. section the interval of variation has to be determined, which is in this case study represented by Eq. (4):

$$h = \alpha \cdot grad(y) \tag{4}$$

where α constant, *grad(y)* is equal to the parameter values determined in Eq. (3).

3. Application example

In this case study the task is to realize a grade transition between two different kind of grades, called A and B. The main goal is to minimize the amount of the off-grade product, so reduce the grade transition time as much as possible. To qualify the success of this purpose the following linear cost function is applied:

$$E = P_{on-spec} \cdot Q_{on-spec} - P_{off-spec} \cdot Q_{off-spec} \tag{5}$$

The studied polymerization reactor is a SISO (single input-single output) process, a CSTR (Continously Stirred Tank Reactor) where a free radical polymerization reaction of methyl-metacrylate is considered using azobisisobutironitil (AIBN) as initiator, and toulene as solvent. 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, where the influenced (control) variable is the flow rate of inlet initiator. 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. Because of the isothermal assumption, a four-state model can be obtained. (Maner and Doyle, 1997)
As the next step, the model for MPC is chosen: a linear, step response SRM model was identified, since the designed MPC – a DMC controller – is based on it (Ricker, 1988). As a following step the DMC controller was installed to the reactor to realize the grade transition (Abonyi et al., 2000). Since the set point signal and all the operating parameters - except the tuning parameters of the controller - were pre-determined, the inputs of the controlled system were the value of prediction and control horizon (H_p and H_c), and move supression coefficient (Λ), since these are the main factors of the objective function of the DMC controller:

$$\min_{\Delta u(k+j)} \sum_{j=H_{p1}}^{H_{p2}} (w(k+j) - y(k+j))^2 + \lambda \sum_{j=1}^{H_c} \Delta u^2(k+j-1) \tag{6}$$

The output of the whole system was based on Eq. (5).
To determine the inputs of the system, the steps of classical design of experiments were applied. As Fig.1. shows execution, only 2 iteration steps were enough to reach the maximum value of the cost function (values are normalized).

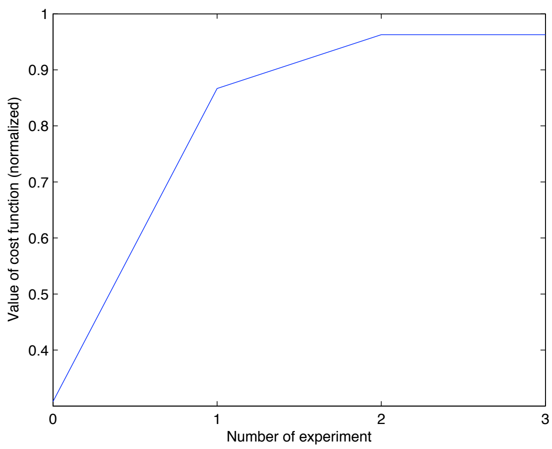

Figure 1. – Change in the value of the cost function during the experiments

To express the development in the production of on-specification products the performance of the controller with initial and tuned parameters have been compared, see Fig. 2. (values are normalized).

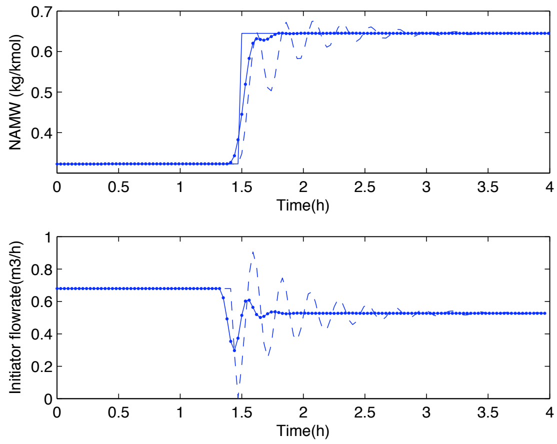

Figure 2. – Comparison of the grade transitions with initial parameters (dashed line) and with the experimentally determined parameters (dotted line)

As Fig. 2. shows, the time demand of the grade transition is significantly shortened. Although a badly tuned MPC is also capable of performing the grade transition, the optimization of tuning parameters is necessary, because in the optimized case the system produces on-spec product in the 91 % of the examined time horizon in contrast to the initial guess where this ratio is only 63 %. To have the opportunity to evaluate the result of the applied methodology, evolutionary strategy (ES) was used to optimize the examined parameters. Evolutionary strategy is a stochastic optimization algorithm that uses the model of natural selection (Madár and Abonyi, 2005). The advantage of ES is that it has proved to be successful in problems that are highly nonlinear and stochastic. Because of the nonlinearity of the polymerization process, this kind of optimization method is worth applying. Deterministic optimization algorithms, like sequential quadratic programming (SQP) have several drawbacks. Since H_p and H_c are discrete variables, it was not possible to use the SQP algorithm in MATLAB Optimization Toolbox successfully, hence ES was applied instead.

In this case study the result of ES and experiment design were almost the same as it is summarized in Table 1.

Table 1. Comparison of the experimentally tuned and the optimized (with ES) values

	H_p	H_c	λ (10^{10})	*Value of obj. fun.*	*On-spec time (%)*	*Function evaluated*
Evolution. strat.	6	3	0.95	0.985	91.79	58
Experiment des.	6	6	1.4	0.963	91.04	16

To sum up the experience of the case study, it can be stated that the method of experiment design is applicable as described in this paper. Although the optimal solution is not reached, its value can be estimated as Table 1 shows. One of the main advantage of this method that only few experiment are needed compared to the optimization method and almost the optimal solution is reached with significantly less effort.

4. Conclusion

In this study an optimization approach incorporating the factorial modeling and analysis approach was applied on optimization of product grade transition of a polymerization process. A full factorial design involving a reduced number of experimental runs to localize the optimal value of tuning parameters of a linear model predictive controller (DMC) which is attached to a benchmark polymerization example. To evaluate the obtained tuning parameters these are also optimized by using evolution strategy. The comparison of results shows that the tools of experiment design are successfully applicable in cases like this, since the solution is pretty close to the optimal solution determined by ES. The main benefits of using the introduced framework are the less number of necessary experiments and there is no need to possess the model of the operating system in contrast to the application of other optimization methods.

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