8th International IFAC Symposium on
Dynamics and Control of Process Systems
Preprints Vol.2, June 6-8, 2007, Cancún, Mexico

BATCH PROCESS MODELING BASED ON PROCESS SIMILARITY

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Abstract: In batch process, operating conditions change to meet the requirements of market and customers. For different combinations of operating conditions, data based modeling process has to be repeated for the development of a new prediction model, if common process characteristics are ignored. Obviously, this is inefficient and uneconomical. Effective using and extraction of certain common process behaviors and characteristics can allow fewer numbers of experiments for the development of new process model, resulting in savings of time, cost and efforts. With this as the key objective, a modeling method is proposed for batch process modeling in this paper.

Keywords: base model, modeling, batch process, similarity, DOE.

1. INTRODUCTION

Batch processes, including injection molding, semi-conductor processing, fermentation, pharmacy, food industry and most bioprocesses, become increasingly preferred choice in chemical industry, to produce high value-added products to meet the rapidly changing market. This circumstance leads to a boom of quality-related activities such as 6 σ campaign and transition in a production system. The production of better quality products is based on a reliable and prompt prediction of product quality. In general, product quality is measured offline and quality measurement is a costly, cumbersome, and time-consuming practice. Therefore, it is important to develop a quality prediction method, allowing us to "measure" product quality in a fast, economical, efficient and accurate way.

Quality prediction is often based on a model built between process conditions and quality variables. In other words, it is a kind of regression problems in nature, aiming to find a relationship between a set of X-variables (process conditions) and one or several response variables Y (quality properties). Generally, the quality prediction models can be built mechanistically and empirically. A mechanistic model, built on the first-principle or prior process knowledge, has a better extension than empirical model. It, however, is difficult to develop such a model, due to process high dimensionality, complexity and batch-to-batch variation, and also due to limited product-to-market time.

In a batch process, operating conditions frequently change to meet requirements of market or customer. In other words, different specifications of product from the same family are produced by changing the recipe from first (or old) process to a second (or new) process. These processes might be of different sizes, process conditions and configurations, or with different equipments, though their intrinsic physical principles are the same. To rapidly and online predict the product quality, it is requisite to develop quality model which aims to find a relation between process conditions and response variable(s). Traditional data-driven approaches, including artificial neural networks (ANNs), fuzzy logic model (FLM), partial least squares (PLS) and support vector machines (SVMs), require a large number of experimental data to build these models (Lee, et al., 2005; Li, et al., 2004; Lu, et al., 2005). A practical problem is how to apply/modify the existing black-box model to new process where the process conditions have changed. For clarification, the existing model describing the old process is called a base model and model to be developed for new process is hereafter called new

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model. Changes in process conditions and environment may make the existing base model invalid for quality prediction. A possible solution to this model problem is to re-conduct the experiments, re-measure samples and build a new model for the new process. To obtain the similar model prediction precision as the base model, a same large number of data are required for the development. Obviously, this is inefficient, time-consuming and uneconomical, and this is particularly problematic for batch processes with expensive material and/or a long cycle.

As we know, despite that operating conditions may be different for different batch processes, certain process behaviors and characteristics remain common under these conditions. For example, in injection molding, when materials are processed into different specifications of product, or with different molds, process conditions, such as barrel temperature, packing pressure, injection velocity have similar impacts on the molded part qualities. In more general cases, making products from the same family, these similar processes might be of different sizes and configurations; they are all based on the similar physical principles and follow a certain similar process behavior. These characteristics, to a degree, should have been built in the data-driven model, i.e., the base model already. Obviously, extraction and utilization of these common process behaviors and characteristics, and taking advantage of the existing base model, can allow fewer data to be required for developing new process model, as shown in Fig. 1.

While there is a tremendous literature available for building model for batch process for quality prediction and optimization, to the best knowledge of the authors, there is little work published on the data-based model migration for batch process with aim of reducing number of experimental data. There exist a few literatures on the subject of model migration/transfer, but requiring the knowledge of the first principle or process mechanism. For example, hybrid models, which combine prior knowledge or first-principle and traditional data-driven methods, have been proposed for chemical process (Van Lith et al., 2003). Jaeckle et al. (2000) took advantage of information on existing mechanistic model of plant A to find the corresponding process conditions needed to manufacture the new product in plant B. The objective of that paper is to predict the process conditions for new plant rather than building new model. Multivariate calibration model is used for extracting chemical information from spectroscopic signals. The changes in spectral variations, due to different instrument characteristics or environmental factors, may render the original calibration model invalid for prediction in the new system. Feundale et al. (2002) reviewed various methods for transfer of calibration model to avoid time-consuming full-recalibration by taking advantage of the existing model. Most of calibration models are linear and one-dimensional; such methods are not suitable for batch process modeling.

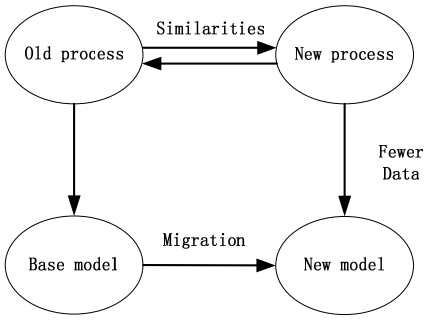

Fig. 1. Development of new model.

In this paper, we would like:

(a) To arose the attention and interest of the community for this important modeling work of batch processes.
(b) To state the problem and its challenges.
(c) To give an exemplary solution to a simple problem case.

The development requirements of new model based on a base model is that:

1. Use fewer training data to build new model than that required to build base model if two models with similar prediction ability, or
2. Build new model with higher prediction ability than that of the base model, if using equal or nearly equal number of training data.

With such a problem, we define it as “Batch Process Modeling Based on Process Similarity”, or BPMBPS. This work can be divided into the following a few steps: (a) information extraction from the base model, (b) design of experiment, (c) assessment of the similarities or differences between the new process and the old process, (d) model migration and verification of new model, as shown in Fig. 2.

The remainder of the paper is so organized. Section 2 presents the key requirements and challenges for each major step in the BPMBPS. Section 3 outlines several possible cases of differences between the new process and old process. Section 4, presents an exemplary solution to a simple difference case where input and output slope/bias correction could be used for the model migration. Section 5 gives an illustrative example application. Finally, some conclusions and remarks are given in Section 6.

2. REQUIREMENTS AND MAJOR CHALLENGES

The key requirements and challenges for “Batch Process Modeling Based on Process Similarity” can be summarized as follows:

2.1 Information extraction from base model.

Despite it has been developed with input-output data alone, base model, as pointed in the introduction, should contain a certain key process characteristic. Information could be extracted to assist the

understanding of old process and to guide the design of experiment for the new process. For example, with the base model, we could find which process condition (or factor) has significant influence on response variable; whether the influence on response is linear or nonlinear or not, if nonlinear, what kind of nonlinearity and monotonicity it is. The information such as these will be helpful for plan the experiments on the new process.

2.2 Design of experiment.

Traditionally, training data for modeling are collected through statistical design of experiment (DOE). Generally, without process information, an experimental program begins with a screening design only considering two levels for each factor, followed by an augmented experiment to develop a more accurate model (Montgomery, 2001). Conventional DOE approaches require the training data to be evenly distributed in input space, which apply equivalent weight on each data. With the availability of a base model, even spacing of input space is often on longer necessary and economical. Therefore, the key challenge of this step is how to develop and identify a guided new DOE method from the base model.

2.3 Assessment of difference.

With collection of data from the new process, analysis of experimental results can be conducted to first verify whether the base model is still valid for new process. If not, the analysis should be continued to find if the new experiments have captured key features of new process. The analysis should focus on where and how difference exists. With difference assessed, different migration strategies should be applied. A good experimentation should be on a sequential or hierarchical basis, so continually learning in an iterative process should take place to avoid conducting a single unnecessarily large number of experiments at the beginning. Therefore, DOE step is repeated if necessary, as shown in Fig. 2.

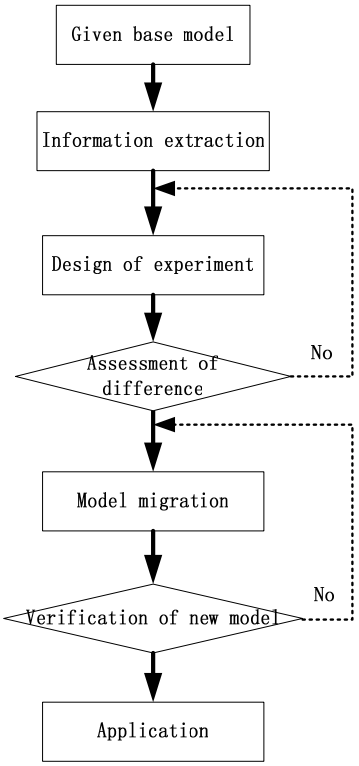

Fig. 2. Flow chart for developing new model based on process similarity.

2.4 Model migration and verification.

Different model updating and/or migration algorithms should be developed for the migration of the model to new process. This procedure should retain characteristics common to the old process, remove information relation that are no longer valid for new process and add, modify or update the new information evolved in new process. During this procedure, criteria should be developed to evaluate the migration performance of new model. This procedure can be repeated until the requirements are satisfied.

3. POSSIBLE CASES OF DIFFERENCE

In reality, there exist many causes that render the original model invalid. There are many different ways of assessing the difference between the original model and the new process. In this first attempt, we divide the difference in terms of difference complexity.

3.1 Simple difference - Shift and scale difference.

The simplest process difference is new process is just a shift and scale of the old process. The shift and scale difference occurs not only in output(s), but also in input(s). The traditional scale up analysis in the dimensionless group may be helpful to this class of problem, but it has been limited mostly to first principle model. This paper presents a possible solution to this class of problems.

3.2 Difference is less complex than the process itself.

Due to the changes in process dynamic behavior, new process can not be simply described by shift and scale of old process. However, process difference exhibits a relatively simple trend, and this can be corrected by a correction model.

3.3 The complex difference.

In certain cases, complexity of difference between two processes is more complex than the process itself. This is a true challenge case. In this case, it maybe possible that it is easier to build a new model rather than focus on model migration. The focus of this paper is on process with a certain similarity. So this case is not within the focus of the research.

4. EXEMPLARY SOLUTION TO A SIMPLE CASE

With the simplest case, new process is the shift and scale of old process, a systemic procedure is developed to demonstrate the concept of model migration to reduce experiments. The procedure begins with the given base model, followed by DOE guided by the information extracted from the base model. With collection of new data, experimental data analysis is conducted to determine the type of difference, and a slope/bias correction on base model is conducted to develop the new model. Since the given example is a simple difference case, not all steps involved in the Fig. 2 are necessary.

4.1 Process information extraction.

Base model is a good representative of old process and it consists of a lot of process information. This information can be used to guide DOE design on new process. In a particular process, different factors (inputs) have different impacts on response variable (output). To determine how much does the response variable change when each factor is changed, the main effect of each factor is introduced. The main effect of a factor is defined as the change in response produced by a change in the level of the factor. We use the generic notation y_i to denote the observation for the i^{th} experimental run. For example, to measure the average effect of a factor, say A, computer the difference between the average y_i value of all observations in the experiment at the high (+) level of A and the average y_i value of all observations in the experiment at the low (-) level of A. This difference is called the main effect of A, as shown in equation (1). Generally, A+ and A- are used to represent the high and low levels of A, respectively, (Wu, 2000).

$$ME(A) = \bar{y}(A+) - \bar{y}(A-) \tag{1}$$

4.2 Design of experiment (DOE).

To efficiently determine the new process' behavior with sparse influential and critical data points, the cluster estimation method, developed by Chiu (1994), is used. The procedure begins with discretization of input (x)-output (y) space ($z = [x^T; y]$) into N points on base model. Each data point is considered as a potential cluster center and a measure of the potential of data point z_i is defined as:

$$P_i = \sum_{j=1}^{N} e^{-\frac{4}{r^2}\|z_i - z_j\|^2} \qquad i, j = [1, N] \tag{2}$$

where P_i represents the potential of the i^{th} data point, N denotes the number of data points and r is effective radius, defining a neighborhood. Thus, the measure of potential for a data point is a function of its distances to all other data points. The closer a data point is to a candidate cluster center, the more it contributes to the potential of it. The traditional subtractive clustering uses a uniform radius for each dimension of input-output space. As we known, each input variable has different impact on output. In order to better describe the key features of process, a non-uniform effective radius based for measure of the potential of data point z_i is revised:

$$\begin{aligned} P_i &= \sum_{j=1}^{N} e^{-\frac{4\|z_i - z_j\|^2}{r^2}} \\ &= \sum_{j=1}^{N} e^{-4\left(\frac{\|z_{i,1} - z_{j,1}\|^2}{r_1^2} + \frac{\|z_{i,2} - z_{j,2}\|^2}{r_2^2} + \cdots \frac{\|z_{i,m+1} - z_{j,m+1}\|^2}{r_{m+1}^2}\right)} \\ &= \sum_{j=1}^{N} e^{-4\sum_{k=1}^{m+1}\frac{\|z_{i,k} - z_{j,k}\|^2}{r_k^2}} \end{aligned} \tag{3}$$

where k denotes the dimension of input-output space and m denotes the input space. Selection of effective radii is based on the input impact on output, larger the impact, smaller the radius. Thus, effective space of each center is changed from hyper-sphere to hyper-ellipsoid. Estimation of input impact can be done by calculating the main effect of each input variable (Wu, 2000).

By properly setting the effective radius of each dimension, the number and locations of cluster centers are found. Detailed literature survey about how to find the cluster centers can be found in Chiu (1994). Each cluster center is in essence a prototypical data point that exemplifies a characteristic behavior of the old process. Naturally, new experiments are conducted at each cluster center and describe the behavior of new process.

4.3 Slope/Bias correction.

In a simple case, new process is a shift and scale of the old process. Thus, new model can be obtained through a slope/bias correction of base model. This correction involves input and output correction. Given the base model of any form:

$$Y_{base} = f(X_{base}) \tag{4}$$

where X_{base} and Y_{base} are the inputs and outputs of base model, respectively, and f is any nonlinear function to describe the old process. If there only exists a shift and scale in input space, inputs of new process X_{new} should be transformed into those of old process X_{base} by a slope and bias correction, as shown in equation (5):

$$X_{base} = S_I \times X_{new} + B_I \tag{5}$$

where S_I and B_I denote scale and shift of old process in input space, respectively. Thus, new model is changed into:

$$Y_{new} = f(S_I \times X_{new} + B_I) \tag{6}$$

More generally, shift and scale occur in not only input space but also output, thus, new model is changed into equation (7), as shown in the Fig. 3:

$$Y_{new} = S_O \times f(S_I \times X_{new} + B_I) + B_O \tag{7}$$

where S_O and B_O represent scale and shift of old process in output space, respectively. Estimation of above parameters can be obtained by optimizing the following equations together with the training data from new process,

$$\text{Min } J(S_O, B_O, S_I, B_I) = \varepsilon\varepsilon^T$$
$$s.t.\ \varepsilon_i = y_i - \left\{S_O \times f(S_I \times X_{new,i} + B_I) + B_O\right\} \quad (8)$$

where, y_i is i^{th} training data on new process and ε denotes the predicted error between the true value and predicted value from base model. We should note that all identified shift and scale parameters are vectors determined by the dimension of input and output space.

5. APPLICATION

The performance of the proposed methodology was evaluated on injection molding with different molds. Injection molding, an important polymer processing technique, makes different shapes and types of products with different polymer materials and molds. The quality of product is the results of different combination of material property, mold and part geometry and processing conditions. This quality can be roughly divided into dimensional property, surface property and mechanical or optical property. For simplicity, dimensional property, such as width of injection-molded part is selected as the product quality in this project.

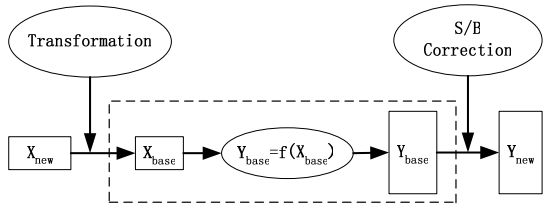

Fig. 3. Slope and bias correction.

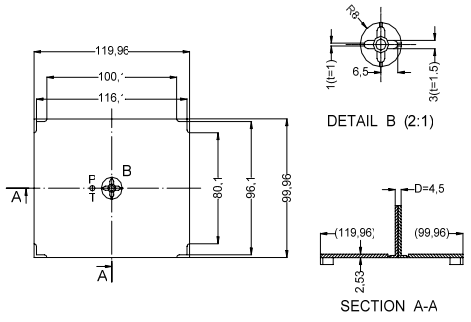

Fig. 4. Mold I with flat cavity.

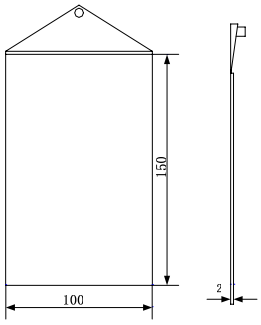

Fig. 5. Mold II with fan gate.

In order to illustrate the proposed method, the experiments were performed on an 88 tons Chen Hsong reciprocating-screw injection molding machine, model number JM88MKIII, with two different molds. Process with mold I and II are considered as the old process and new process, respectively. The two mold geometries are shown in Fig. 4 and Fig. 5. In order to focus on the mold influence on product quality, the same material, high-density polyethylene (HDPE) is used in these two processes. In the analysis, three process variables, including packing pressure, injection velocity and barrel temperature are chosen to describe part quality, as they have relative significant effect on part dimension. To build the base model, a full factorial design with 27 experimental runs is conducted, each factor with three levels, as shown in Table 1. An analysis of variance, ANOVA, is made on experimental data and a polynomial regression model is built as the base model with the mean squared errors (MSE) 3.51%.

Table 1 Factors and levels for full factorial design

Factor	Level		
	1	2	3
Packing pressure (bar)	150	300	450
Injection velocity (mm/s)	8	24	32
Barrel temperature (^{o}C)	180	200	220

With the base model, following our proposed procedure of in Fig. 2, a design of experiment (DOE) is conducted for new process (i.e., mold II). Calculation of main effect of each factor shows that packing pressure has significant impact on the part quality, and injection velocity and barrel temperature have relatively less significant but similar impact on the part quality. Therefore, the three effective radii for clustering estimation are selected as following equation shown:

$$[r_1, r_2, r_3] = [0.5, 0.9, 0.8] \quad (9)$$

Then, 1000 (10×10×10) generated data points from the base model are clustered to stand for experiment condition for the new process. Clustering results indicate that eight experiments should be conducted on the new process. These new experiments can not be directly conducted on new process before initial transformation of inputs, as each process variable has different operating ranges due to change of mold. We should note that, this kind of input transformation is different to slope/bias correction of inputs. An output slope/bias correction is conducted by using first four new experimental data. The verification of new model shows that the MSE of corrected model is equal to 3.84%, larger than that of base model. To further improve performance of new model, an input slope/bias correction is included based on previous corrected model by using eight new experimental

data. The verification result of new model shows a lower MSE 2.98%, comparable to that of base model. Table 2 shows prediction results with and without correction. The second column, shows significant prediction error with the results predicted from the model without migration, i.e. the original model. The other three columns show that prediction results from the corrected model are quite close to the actual value.

Table 2 Slope and bias correction results

No.	Base model	Correction in output	Correction in input and output	Actual value
1	116.95	97.62	97.60	97.57
2	117.11	97.79	97.79	97.68
3	116.84	97.53	97.47	97.42
4	117.15	97.90	97.85	98.02
5	116.48	97.02	97.04	97.06
6	117.16	97.89	97.85	97.86
7	117.52	98.33	98.29	98.27
8	116.75	97.43	97.38	97.32

6. CONCLUSIONS

Developing an accurate process model for complex batch process is generally a difficult and expensive task. In this paper, we outline a model migration method by taking advantage of a base model developed for an old process, using limited number of experiments. A systematic approach, including information extraction from a base model, design of experiment, analysis of difference, and model migration has been proposed. A solution to simple case has been developed, and the application to injection molding shows that the proposed method is effective.

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