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Recursive Data-based Prediction and Control of Product Quality for a Batch PMMA Reactor

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Abstract

In many batch processes, frequent process / feedstock disturbances and unavailability of on-line measurements make tight control of product quality very difficult. Motivated by this, we present a simple data-based method in which measurements of other process variables are related to the end product quality using a historical data base. The developed correlation model is used to make on-line predictions of the end quality, which can serve as a basis for adjusting the batch condition / time so that desired product quality may be achieved. This strategy is applied to a methyl methacrylate (MMA) polymerization process. Important end quality variables, the weight average molecular weight and the polydispersity, are predicted recursively based on the measurements of the reactor cooling rate. Subsequently, a shrinking-horizon model predictive control approach is used to manipulate the reaction temperature. The results in this study show much promise for the proposed data-based inferential control method.

1 Introduction

Batch operation is often the preferred choice for producing low volume / high value-added materials, including certain polymers, fine chemicals, bio-chemicals, semi-conductors, *etc.* In order to derive the maximum benefit from batch operations, product quality must be controlled tightly. Traditionally, engineers have attempted to achieve this indirectly by controlling some secondary variables, such as temperatures, pressures, and flow rates. However, with frequent feedstock variations, the policy of controlling operating variables over some fixed trajectories does not lead to consistent product qualities.

Statistical process control (SPC) method is helpful to combat this problem in some aspects [5]. In that paper, on-line measurements of process variables are used to detect various abnormalities. The SPC method, while effective for detecting abnormal batches early on, does not help reduce *normal* batch-to-batch variability.

In a recent paper by Yabuki and MacGregor [11], on-line as well as infrequent off-line measurements are used at some mid-course point to predict the final product quality. The correction move needed is then calculated and implemented if the predicted quality deviates significantly from the target. Joseph and Hanratty [4] proposed a similar approach that relies on neural network models. However, the assumption of known initial conditions restricts the applicability of this procedure. Russell *et al.*[7] recently proposed a method to predict and control the end quality using on-line process variable measurements on a recursive basis. As an extension, Chin *et al.*[1] developed a technique to conduct the quality control and tracking control simultaneously. In their technique, real-time feedback control and batch-to-batch learning control are combined for an improved result. The bottleneck for all these techniques lies in obtaining an accurate model.

In this paper, we examine the effectiveness of the method by Russell *et al.*[7] in controlling the product qualities for a PMMA process. Relevant secondary measurements are identified and their effectiveness in predicting the final product qualities in the presence of disturbances and noises are examined. Finally, the benefits from manipulating the reaction temperature based on the on-line predictions are demonstrated.

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2 Data-based Procedure Introduction

2.1 Formulation of On-line Quality Prediction

The main difficulty in quality control for batch processes stems from the fact that the operator has to rely upon secondary measurements to monitor and control the process since the measurements of the end product quality do not become available until the batch is finished. Therefore, for achieving tight quality control, the main issue is how to develop a model that enables an accurate prediction of the end quality based on the input and output measurements available *during* the batch. A general form of the end-quality predictor we consider is:

$$\hat{q}_{t_f|i} = f(\mathcal{Y}_i, \mathcal{U}) \tag{1}$$

$\hat{q}_{t_f|i}$ represents the end-quality predicted using $\mathcal{Y}_i$, the measurements collected up to the i-th sample time, as well as $\mathcal{U}$, the input trajectory for the entire batch. t_f is the total number of sample time steps during a whole batch and therefore represents the total batch time. The challenge is to identify this relationship from existing data and without a fundamental model .

To simplify the identification task, one may choose to develop a *linear* predictor that corresponds to the linearized form of the above general predictor with respect to some "nominal" (mean or reference) trajectories $\mathcal{Y}_i^0$, $\mathcal{U}^0$:

$$\hat{q}'_{t_f|i} = A\mathcal{Y}'_i + B\mathcal{U}' \tag{2}$$

where $\mathcal{Y}'_i = \mathcal{Y}_i - \mathcal{Y}_i^0$, *etc.* From here on, the superscript $\{\}'$ will be suppressed for the convenience of exposition.

In order to build the suggested empirical model for on-line quality prediction, certain problems associated with the nature of batch processes must be addressed. First, to detect quality deviations and make necessary corrections in time, we need to be able to predict the end-quality accurately based on partial batch information. Hence, the predictions are developed over the progression of a batch, preferably at a number of sample steps located in different phases of the operation. This may require several models to be developed, one for each sample time at which the prediction is desired. Alternatively, one may develop a single model that uses all the measurements collected during a whole batch, but in order to use such a model during a batch, one must somehow fill in the missing future measurements.

2.2 Recursive Prediction Procedure

This problem was addressed in Russell *et al* [7]. In their work, a statistically optimal linear recursive predictor of q_{t_f} is formulated based on a Kalman filter with state $\mathcal{Z} = [\mathcal{Y}^T q_{t_f}^T]^T$. The state of the Kalman filter consists of *all* the on-line measurements to be collected during a batch from $t = 0$ to $t = t_f$. Let us ignore the effect of the deterministic input $\mathcal{U}'$ for the moment. Then, the state-space model used for the filter design is:

$$\mathcal{Z}_{i+1} = \mathcal{Z}_i \tag{3}$$

$$y_i = \underbrace{[0 \cdots 0 \;\; I_{n_y} \;\; 0 \cdots 0]}_{C_i} \mathcal{Z}_i \tag{4}$$

C_i is a time-varying matrix that picks out from $\mathcal{Z}_i$ y_i, the measurements collected at the i-th sample step. The Kalman filter equations are given by:

$$\hat{\mathcal{Z}}_{i+1|i+1} = \hat{\mathcal{Z}}_{i|i} + K_{i+1}[y_{i+1} - C_{i+1}\hat{\mathcal{Z}}_{i|i}] \tag{5}$$

$$K_{i+1} = P_{i|i}C_{i+1}^T(C_{i+1}P_{i|i}C_{i+1}^T)^{-1} \tag{6}$$

$$P_{i+1|i+1} = (I - K_{i+1}C_{i+1})P_{i|i} \tag{7}$$

This Kalman filter is to be initialized with the covariance matrix calculated based on historical batch data ($P_{0|0} = \frac{1}{N}\sum_{i=1}^{N} \mathcal{Z}(i)\mathcal{Z}^T(i)$, where N is the number of batches used for modeling). As new measurements become available, the predictions of the quality variables are recursively upgraded based on the correlation between the measured states and the quality variables (given by the covariance matrix). Note that the quality predictions are simply the last n_q elements of the filter state estimate:

$$\hat{q}_{t_f|i} = [\; 0 \;\; \ldots \;\; 0 \;\; I_{n_q} \;]\hat{\mathcal{Z}}_{i|i} \tag{8}$$

Having developed the recursive predictor for the purely stochastic case, the effects of deterministic inputs can be added in a straightforward manner. First the input effects on the measurement and end quality can be modeled as $\mathcal{Z} = B_u\mathcal{U} + \tilde{\mathcal{Z}}$. Then the input effects are subtracted from the original data for $\mathcal{Z}$, leaving the residual data, $\tilde{\mathcal{Z}} = \mathcal{Z} - B_u\mathcal{U}$, that contain the correlation between $\mathcal{Y}$ and q_{t_f} that is irrespective of the deterministic input moves. The Kalman filter can be then formulated just as before.

2.3 Reducing Model Dimension

Another difficulty in developing the prediction model from historical data stems from the large

dimension of inputs and outputs and strong correlation that exist among them. This not only results in a high demand for computation and storage, but also makes the initial covariance matrix $P_{0|0}$ ill-conditioned and very difficult to identify. To overcome both the high dimensionality and the conditioning problem, multivariate statistical methods such as the principal component analysis (PCA) can be used to project the filter state $\tilde{\mathcal{Z}}$ onto a subspace of a much lower dimension to create a reduced-order state $\underline{\tilde{\mathcal{Z}}}$:

$$\underline{\tilde{\mathcal{Z}}} = P\tilde{\mathcal{Z}} = \begin{bmatrix} P_{\mathcal{Y}} & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \mathcal{Y} \\ q_{t_f} \end{bmatrix} \tag{9}$$

where $P_{\mathcal{Y}}$ is a matrix that projects $\mathcal{Y}$ to a lower dimensional space through PCA.

For the reduced-order filter design, the following model can be used:

$$\underline{\tilde{\mathcal{Z}}}_{i+1} = \underline{\tilde{\mathcal{Z}}}_i + \underline{b}_i u_i \tag{10}$$

$$y_i = \underline{C}_i \underline{\tilde{\mathcal{Z}}}_i + \epsilon_i \tag{11}$$

where $\underline{b}_i = Pb_i$ and b_i is the i^{th} column of the input matrix B_u. Note the followings: (1) In the above model, the effect of the deterministic input is entered recursively; hence, $\underline{\tilde{\mathcal{Z}}}_i$ contains the effect of the input $u_0, \cdots, u_{i-1}$. (2) A residual error term ϵ has been included in the measurement equation. This modification is necessary, because some information is inevitably lost in the process of projecting the state vector down to the lower-dimensional space.

A Kalman filter can be designed straightforwardly based on the above model. And, the quality prediction is given by:

$$\hat{q}_{t_f|i} = \begin{bmatrix} 0 & I_{n_q} \end{bmatrix} \left[\underline{\hat{\tilde{\mathcal{Z}}}}_{i|i} + [\underline{b}_i \cdots \underline{b}_{t_f-1}] \begin{bmatrix} u_i \\ \vdots \\ u_{t_f-1} \end{bmatrix} \right] \tag{12}$$

From a practical standpoint, it is convenient to divide the total batch cycle time into several different phases and then apply the control algorithm at the beginning of each phase. In addition, the dimension of control input can be reduced through some appropriate parameterization. That is, within each interval, the input trajectory may be parameterized with only a few parameters.

2.4 Data-based Quality Control

Having developed the on-line quality prediction, the future inputs calculation can now be formulated as a quadratic optimization problem,

$$\min_{\theta_i^+} \hat{q}_{t_f|i}^T \Lambda_q \hat{q}_{t_f|i} + [\mathcal{U}_i^+(\theta_i^+)]^T \Lambda_u \mathcal{U}_i^+(\theta_i^+) \tag{13}$$

where $\mathcal{U}_i^+$ represents the future input trajectory (with respect to the i-th sample step), which is parameterized through the vector θ_i^+. Λ_q and Λ_u are weighting matrices. Although all the future input moves are calculated, only the moves for the present phase are implemented and the rest are recomputed at the beginning of next phase. The number of input parameters calculated decreases as the batch proceeds, giving rise to the name "shrinking horizon control".

3 MMA Process Introduction

Methyl Methacrylate (MMA) is an important industrial material. Modeling and control of MMA batch polymerization system has received much attention. Most of the previous work ([10],[6],[2]) focus on the problem of tracking a pre-determined temperature profile and hence the control of end-quality could suffer when initial charge disturbances occur. Ellis et al.[3] implemented on-line estimation and control of molecular weight distribution on an experimental MMA solution polymerization system, based on a two-time scale EKF. But the fundamental model needed to design the EKF is generally very difficult and expensive to develop in practice. The data-based procedure adopted in this paper offers the advantage of easy implementation and should therefore be a viable alternative for industrial applications.

MMA polymerization is a typical free radical chain growth polymerization. It is also a diffusion-controlled reaction which exhibits gel effects and glass effects near the high conversion stage of batch. In this study, the model generated by Seth and Gupta [9] is selected for the simulation. This model overcomes some important shortcomings of other models that previously existed and has already been tested and found to be suitable for an industry use.

Solution polymerization with initial volume fraction of solvent $f_s^0 = 0.3$ is chosen for this study. The nominal operation is isothermal with reaction temperature, $T = 70^0C$. The relevant product quality in this process is characterized by the weight average molecular weight (Mw) and the polydispersity (Pd), which are critical for end-use polymer characteristics. The two major feed

disturbances are initiator charge fluctuation and monomer impurity. The initiator charge fluctuation is assumed to be in the range of ±10%, while the monomer impurity is simulated as the existence of inhibitors.

The reaction heat related information has been used to control batch polymerization reactor. One of the methods is using calorimetric state estimator to estimate the heat-release of reactor [8], which can be further used for control purposes. In this study, the cooling rate needed to maintain a constant temperature profile, is assumed to be measured every minute and used for the prediction of end quality. When a disturbance occurs, the heat generated from the polymerization reaction changes and results in a deviation of the cooling rate profile from the nominal trajectory. This information was found to be strongly correlated with the deviation of the end-quality variables and therefore useful for predicting the end-quality variables for control purposes.

In this paper, we also assumed that the reaction temperature was controlled perfectly through a low-level loop. Hence the reaction temperature was treated as an input variable that can be manipulated for control purposes, albeit within some constraints. The batch cycle time (6 hours) was divided into 5 intervals, which begin at 0, 50, 100, 150, and 250 minute marks respectively. The reactor temperature was assumed to be held constant within each interval. The data-based control procedure introduced earlier was used to calculate the reactor temperatures during these intervals.

4 Results

The very first step in applying the data-driven control procedure is the generation of data that can be used for the model-building. It is important to recognize that the prediction capabilities of data-based models are heavily dependent upon the nature of data supplied for building the model. The batch data should contain the effects of various disturbances as well as the potential input moves one may make for the purpose of control. This will allow the correlation (or the causal relationships) among the input moves, process output measurements, and final product quality to be captured in the model. In our simulation study, 60 batches of data were generated by randomly changing the initial charge and the reactor temperature values during each interval.

The first objective of the simulation study was to assess the prediction capability of the proposed recursive method. For this, another 20 batches with randomly varying disturbances were simulated. Figure 1 shows the results for one of the 20 test batches. Figures 1c-d show the trajectories for the measured variable (cooling rate) and the manipulated variable (reactor temperature) respectively. The peaks in Figure 1c indicates the effects of inputs (setpoint changes for the reaction temperature) at beginning of each control interval. Figure 1a–b give an indication of how the prediction from the recursive filter evolves throughout the batch as more and more measurements become available. As can be seen from the figures, the end-quality predictions eventually converge close to the actual values as more and more on-line measurements are taken in.

Since an accurate prediction of the end-quality at an early stage of reaction is the key to making the corrective adjustments needed to suppress the disturbance effects, the prediction capability was tested at various mid-points during a batch. Figure 2 plots the predictions at the 100 minute mark for the same 20 batches. The predictions are very good.

Since the recursive prediction adopted in this paper is based on on-line measurements, the accuracy of measurements should certainly affect the prediction capability. Several levels of measurement noises were added to test the sensitivity of the prediction. One tested case with an extremely high level of noises is illustrated in Figure 3. In Figure 3, the noise seems so large that it is difficult to discriminate the real signal (*i.e.*, the deviation from the nominal trajectory) from it. However, the predictions for the 20 batches still follow the right trend. This demonstrates the robustness of the recursive method with respect to measurement noises. The robustness is afforded by the use of the PCA method in constructing the correlation model.

The second objective of this simulation study was to assess the performance of the quality control strategy. At the beginning of each interval, future input parameters were calculated according to (13). To test the effectiveness of the control strategy, another 20 batches with randomly varying disturbances were simulated. The comparison between the operation with the data-based control

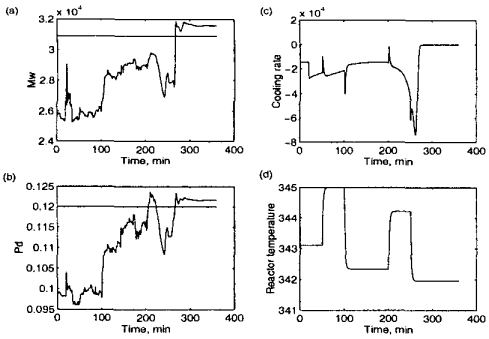

Figure 1: Measurement / input profiles and recursive predictions of end qualities for a typical batch

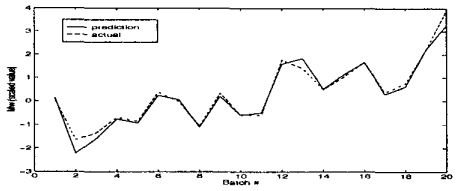

Figure 2: Prediction results for Mw at t=100 minute for the 20 tested batches

and the conventional isothermal operation is displayed in Figure 4. It shows that much tighter quality control can be achieved with the data-based control approach.

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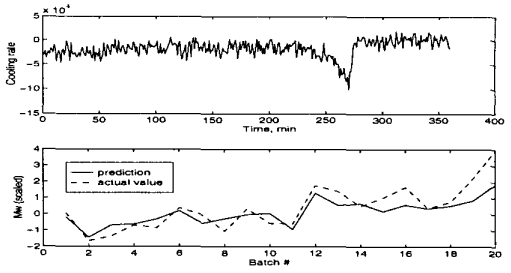

Figure 3: Prediction results for Mw for the 20 batches in the presence of strong measurement noises

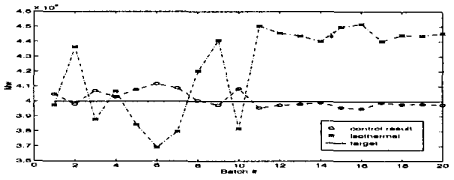

Figure 4: Comparison between operation with the data-based control and isothermal operation

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