Process Monitoring and Steady State Identification for Start-up Process of Batch Processes

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Abstract. Inter-batch evolution widely exists in the start-up process of batch processes, and different operation phases exhibit significantly different behaviors, so multiple models are necessary both along the batch direction and the time direction. In this work, reference windows and sliding windows are constructed within each phase for analysis of inter-batch evolution. Through analyzing two indexes, Ratio and \( \Delta \), the process is divided into different operating states. Different models are constructed for these states. In addition, a PCA similarity factor and the Mahalanobis distances between batch trajectories are used for online steady-state identification (SSID). The application to a typical multiphase batch process with inter-batch evolution, injection molding start-up process, illustrates the feasibility and performance of the proposed algorithm.

Introduction

Batch processes are widely applied in industry and operation safety of batch process has drawn people’s attentions. Multiway principal component analysis (MPCA) [1] was first proposed for batch process monitoring considering the three-dimensional matrix structure of batch process data. Multi-phase characteristic is another significant feature of batch processes. Some works [2,3] have been done focusing on multi-phase characteristic. Generally, different models were established to monitor different phases. Besides, process variation exists in batch processes due to various factors [4]. The process variation in the batch direction throughout the whole operation leads to different process states with different process characteristics. Some techniques have been proposed to handle process variations by model adaptation [5]. However, these methods barely evaluate the changes of monitoring models along the batch direction, in which, models are in general updated arbitrarily, increasing the chance of introducing disturbances into the process model. Also, there are multistate methods proposed to build different models for different states [6]. But the process variation along the batch direction may be too slow and continuous to be divided into several states.

Most batch processes have two operation periods: batch-to-batch start-up and steady-state operation. The batch operations in start-up are unsteady and cannot guarantee the satisfied products with consistent qualities. Usually, the durations of the start-up periods are unknown and varied from one process to another. Therefore, an efficient method is desired for the online identification of the operation states of batch processes which can indicate the product qualities. Based on the characteristic of batch processes, cross-correlations exist between process variables. Meanwhile, the variable trajectories are dynamic with certain magnitudes. Therefore, the batch process steady
state can be identified from two aspects: (1) the variable correlation structures remain stable from batch to batch; (2) the magnitudes of variable trajectories are similar between batches. There are different types of existing methods developed by the researchers and the industry for SSID [7].

Therefore, in this work, the inter-batch evolution along successive batches is addressed for statistical modeling and online monitoring of multiphase batch processes. To analyze the inter-batch evolution, reference windows and sliding windows are constructed including several batches to judge new states when sliding windows present significant difference from the reference window. Multiple states are thus separated along the batch direction. PCA is used as the basic statistical analysis tool to monitor those process states obtained. The problem of batch process online SSID is solved by dealing with the changes in both variable correlation structures and trajectory magnitudes. The proposed method for SSID can be applied to each single batch in PCA modeling. Therefore, this method is more suitable for online steady state detection. Besides, all of work will be done in each specific phase considering that multiphase characteristic is a major nature of many batch processes.

Methodology

A. Inter-batch Evolution Analysis

Within each phase, reference windows and sliding windows are constructed and analyzed along the batch direction. If new batches in a sliding window belong to a different state from the reference window, the original monitoring models developed based on the reference window will cause out-of-control monitoring statistics. The details are introduced below.

After phase division, process data of the $c$th phase is arranged as $X_c(I \times J \times K_c)$, where $K_c$ refers to the number of time intervals within the $c$th phase.

First, construct a reference window $X_{c,r}(I \times J \times K_c)$ based on the first $I_r$ batches in $X_c$, then time slices in $X_{c,r}$ are normalized to have zero mean and unit variance, and comprise the two-dimensional data matrix by unfolding preserving the variable dimension, which is denoted as $X_{c,r}(K_c I_r \times J)$.

Then, compose sliding windows. First, the length of sliding windows along the batch direction, $I_w$, is to be determined. Then, the moving step of sliding windows, $L$, which indicates how many batches are passed for the next sliding window relative to the previous sliding window, is determined. So the first sliding window starts from the $(L+1)$th batch. $L$ should be less than $I_w$ to make sure all batches would be included in one sliding window at least once. The process data within the $c$th phase of the $w$th sliding window is denoted as $X_{c,w}(I_w \times J \times K_c)$, where $w = 1, 2, \ldots, W$. Time slices in $X_{c,w}$ are normalized, and the data matrix obtained after unfolding preserving the variable dimension is denoted as $X_{c,w}(K_c I_w \times J)$, similarly to the reference window.

Apply PCA on the reference window $X_{c,r}(K_c I_r \times J)$:
\[ \hat{\mathbf{X}}_{c,r} = \mathbf{T}_{c,r} \mathbf{P}_{c,r}^{T} + \mathbf{E}_{c,r} = \mathbf{X}_{c,r} \mathbf{P}_{c,r}^{T} + \mathbf{X}_{c,r} \mathbf{P}_{c,r}^{e} \mathbf{P}_{c,r}^{e T} \]

\[ = \sum_{i=1}^{R_{c}} \mathbf{t}_{c,i} \mathbf{P}_{c,i}^{T} + \sum_{j=1}^{R_{c}} \mathbf{X}_{c,r} \mathbf{P}_{c,j}^{e} \mathbf{P}_{c,j}^{e T} . \]  

Project the sliding window, \( \mathbf{X}_{c,w} (K_c I_w \times J) \), onto \( \mathbf{P}_{c,r} \) and \( \mathbf{P}_{c,re} \) obtained in Eq. (1),

\[ \hat{\mathbf{X}}_{c,w} = \mathbf{T}_{c,w} \mathbf{P}_{c,w}^{T} + \mathbf{E}_{c,w} = \mathbf{X}_{c,w} \mathbf{P}_{c,w}^{T} + \mathbf{X}_{c,w} \mathbf{P}_{c,w}^{e} \mathbf{P}_{c,w}^{e T} \]

\[ = \sum_{i=1}^{R_{c}} \mathbf{t}_{c,w,i} \mathbf{P}_{c,i}^{T} + \sum_{j=1}^{R_{c}} \mathbf{X}_{c,w} \mathbf{P}_{c,j}^{e} \mathbf{P}_{c,j}^{e T} . \]

Inter-batch evolution analysis is conducted by relative analysis from the reference window to each sliding window in PCs and residuals of PCA monitoring, respectively.

(i) In PC Subspace: Define the ratio of variation between the PCs of reference window and sliding window as:

\[ \text{Ratio}_{c,w,i} = \frac{\text{var}(\mathbf{T}_{c,w}(:,i))}{\text{var}(\mathbf{T}_{c,r}(:,i))} \quad (i=1,2,...,R_{c,r}) . \]  

(ii) In Residual Subspace: The variation difference between reference window and sliding window in monitoring residual subspace is defined as:

\[ \Delta_{c,w,i} = \frac{\| \mathbf{X}_{c,w} \mathbf{P}_{c,w}^{e} \mathbf{P}_{c,w}^{e T} \|^2 - \| \mathbf{X}_{c,r} \mathbf{P}_{c,r}^{e} \mathbf{P}_{c,r}^{e T} \|^2}{\| \mathbf{X}_{c,r} \mathbf{P}_{c,r}^{e} \mathbf{P}_{c,r}^{e T} \|^2} . \]  

In this work, the indexes \( \text{Ratio}_{c,w,i} \) and \( \Delta_{c,w,i} \) defined for relative analysis are used to measure the inter-batch evolution, and thresholds for the two indexes, \( \text{Ratio}_{c} \) and \( \Delta_{c} \), are defined within the phase \( c \).

B. Online Monitoring

After the whole process is divided into \( M \) states, \( M \) monitoring models are built (state index \( m \), \( 1 \leq m \leq M \)), and the newly acquired observations are monitored online. If any monitoring statistic exceeds the control limits, it means that the current process is with larger variations exceeding the normal region defined by the current monitoring model.

C. Batch-to-batch Steady State Identification

To achieve a better online SSID for batch processes, it is necessary to develop a method which can model the process with limited history data. At the same time, this method should be able to compress the high-dimensional batch process data to a small number of indicators to reflect the state change.

(i) Detection of Variable Correlation Changes. In \( \mathbf{X}(I \times J \times K) \), each horizontal slice \( \mathbf{X}_{i}(K \times J) \) \( (i=1,2,...,I) \) is a two-dimensional data matrix corresponding to the data from the \( i \)th batch. These batch data matrices are then normalized. Then, PCA is adopted to decompose the normalized matrices.

The formula of the similarity between two PCA models is as below:
The value of \( \cos \theta_{jj} \) can be calculated as

\[
\cos \theta_{jj} = \frac{P_1(:, j) \cdot P_2(:, j)}{\|P_1(:, j)\| \|P_2(:, j)\|} = P_1(:, j) \cdot P_2(:, j).
\]

In online SSID for batch processes, we calculate the similarities between a referenced model and the batch PCA models in sequence as

\[
SIM_i = S_{PCA}^{paired} (P_i, S_i, P, S) . \quad (i=2,3,...).
\]

(ii) Detection of Trajectory Magnitude Changes. The Mahalanobis distances between the following batches and the first batch are computed as follows:

\[
\Phi_i = \sqrt{(x_i - \bar{x}_i)^T \Sigma_i^{-1} (x_i - \bar{x}_i)} .
\]

If no trend is detected in \( SIM_i \) and \( \Phi_i \), the process is at steady state.

Illustration and Discussion

A. Online Monitoring

Fig. 1(a) and (b) shows the change of \( \text{Ratio}_{c,w,i} \) and \( \Delta_{c,w,i} \) with the sliding windows sliding down in the injection phase when the thresholds \( \text{Ratio}_c \) and \( \Delta_c \) are set to 1.5 and 1.3. When either of the indexes exceeds the thresholds, the remaining sliding windows are analyzed with new reference window, therefore the indexes can return to the threshold below after exceeding the thresholds every time. As can be seen from Fig. 1, the indexes of the 3rd, 5th, and 9th sliding windows exceed the threshold, thus three new states are recognized. The whole process is divided into four operating states taking into account the initial state. Fig. 2 shows the results of the operating state division of the injection phase.

After the injection molding start-up process is divided into different states, corresponding models are then built for process monitoring.

For one typical test batch, it is assumed no prior state information is obtained, so the monitoring models are adopted from \( m=1 \) one by one to locate each phase of this batch in one state and identify the right monitoring model. The monitoring models for different phases are identified separately. The corresponding 99\% control limits of monitoring statistics are also calculated. Fig. 3 to 5 show the monitoring results for one of the typical test batches during the injection phase.

The statistic values obviously exceed the control limits as shown in Fig. 3 and 4, while stay well within the control limits in Fig. 5, revealing that this batch belongs to the third state within the injection phase. There is a peak which obviously exceeds the control limits at the end of \( SPE \) statistic of the third phase, because the segment is a transition between the injection phase and the packing-holding phase, which is normal noise and does not affect the normal operation of the injection molding process.

A faulty test batch is traced and monitored in a same procedure. As shown in Fig. 6, the statistic values obviously exceed the control limits when the test batch monitored...
with a model established in the first state. The results of other three states are similar to it, revealing that this batch does not belong to any states. Therefore this test batch is identified as a faulty batch.

In conclusion, the proposed monitoring strategy can clearly and correctly monitor the injection molding start-up process.

B. Online Steady State Identification

The Mahalanobis distances between the first batch and the following batches are plotted in Fig. 7(a), while Fig. 7(b) shows the SSID results based on the distance information. With Mahalanobis distances, the start-up period is detected to finish in batch 73. All measurement data used in this detection can be easily obtained online.

The values of the PCA similarities between the first batch and the following batches are plotted in Fig. 8(a), while Fig. 8(b) shows the SSID results based on the variable correlation information. With correlation structures, the start-up period is detected to finish in batch 63.
It can be seen from the Fig. 7 and 8 that the $R$ values calculated based on the variable correlation structure is significantly smaller than calculated based on the trajectory amplitude and undergo less batches to achieve steady state. This means that, during the injection molding start-up, the batch-to-batch differences are mainly caused by the drifts in variables, while the variable cross-correlations have less influence.

**Conclusion**

In this work, an online start-up process monitoring strategy based on inter-batch evolution analysis and an online SSID based on correlation structures and trajectory magnitudes are proposed for multiphase batch processes. First, reference windows and sliding windows are built for inter-batch evolution analysis, dividing the whole start-up process into different operating states, and different models are established based on PCA. Then an SSID method is developed to better online identify the operation states of batch processes. This method extracts both correlation structure information and variable trajectory magnitude information, using the paired PCA similarity factor and the Mahalanobis distance, respectively. The case study on injection molding start-up process demonstrates the reliable performance of the monitoring algorithm.

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**References**


