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Intra-Batch Evolution Based Process Monitoring for Multiphase Batch Processes

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Abstract: Batch-wise variations, called intra-batch evolution here, widely exist in batch processes. In this paper, intra-batch evolution is tracked and monitored for multiphase batch processes. First, a batch cycle is divided into multiple phases. Within each phase, sliding windows are constructed for analysis of intra-batch relative variations, based on which different process modes are separated in order along batch direction. Meanwhile, the part of variations with significant increases in new modes is separated from the other. Consequently, the original two monitoring subspaces are further divided into four subspaces, specifically, two parts which make contribution and no contribution to alarming T^2 monitoring statistic, the part responsible for the out-of-control *SPE* monitoring statistic and the left final residuals. The application to a typical multiphase batch process with intra-batch evolution, injection molding start-up process, illustrates the feasibility and performance of the proposed algorithm.

Keywords: Process monitoring, multiphase batch process, intra-batch evolution, relative variation.

1. INTRODUCTION

As an important type of industrial production, batch processes have been widely applied to fine chemical to obtain high-value-added products efficiently. Batch process safety has become a focus of research. Data-based statistical analysis techniques, such as multiway principal component analysis (MPCA) and multiway partial least squares (MPLS), are the popular tools to handle the three-dimensional data structure of batch processes (Nomikos et al. (1994, 1995a)), after which, different solutions were proposed (Wold et al. (1996), Westerhuis et al. (1998)).

The multiplicity of operation phases is an inherent nature of many batch processes, which requires special attention. Works have been done (Lu et al. (2004), Zhao C.H. et al. (2008, 2013a), Zhao L.P. et al. (2012, 2013)) for process monitoring and quality prediction focusing on multiphase characteristic of batch processes. Different statistical models were established to capture different characteristics of phases on the basis of such recognition that the underlying variable correlations are similar within the same phase.

Besides, batch-wise time-varying problem exists in batch processes due to various factors such as catalysis deactivation, sensor drifting, equipment aging and environment changes. Some techniques have been proposed to handle time-varying problem by model adaptation, such as consecutively updated MPCA (Lee D. et al. (2003), Lee J. et al. (2003)). The basic idea of these methods is to adjust the statistical monitoring model on-line continuously and directly. However, these methods barely evaluate the changes of monitoring models along batch direction, in which, models are in general updated arbitrarily following a certain frequency, leading to the increase of the chances of introducing disturbances. It is interesting to first analyze the change rules of batch-wise process variation and thus guide the model updating. The process variation along batch direction is called intra-batch evolution here. Different phases may have different batch-wise time-varying characteristics. Phase-based intra-batch evolution analysis can provide more information for process understanding and evolution monitoring.

In the present work, process evolution in successive batches is addressed for statistical modeling and online monitoring of multiphase batch processes. PCA is used as the basic statistical analysis tool to trace the intra-batch evolution. Considering multiphase characteristic, intra-batch evolution characteristics will be analyzed in each specific phase. Reference windows and sliding windows are constructed and new modes are judged when sliding windows present significant difference from reference windows. Multiple modes are thus separated along batch direction on the basis of analysis of relative changes (Zhao C.H. et al. (2013b)). Also, four subspaces are decomposed by checking between-mode relative changes, which are then modeled for online monitoring separately, revealing changes of different process variations. Analyzing the intra-batch evolution can help to better understand how a process changes along batch direction and separate different operation modes along batch direction. Meanwhile, between-mode relative analysis investigates the relationship of sequential modes and provides meaningful information for process monitoring.

The rest of this paper includes three parts: first, the proposed methodology is presented in Section 2, including the phase-based intra-batch evolution analysis, process modeling and online monitoring. In Section 3, the application to injection molding start-up process which has typical multiphase and intra-batch evolution nature is presented with result discussions. At last, the conclusion is drawn.

2. METHODOLOGY

2.1 Phase-Based Intra-Batch Evolution Analysis

The main idea of this section is to trace the process evolution along batch direction with the consideration of multiphase nature, including three steps: (1) phase division within each batch cycle, (2) intra-batch evolution analysis and (3) mode division along batch direction.

(1) Phase division within each batch cycle

Each batch cycle is divided into multiple phases in time direction by indicator variables determined by process knowledge. Process data is arranged as a three-way matrix $\underline{\mathbf{X}}(I \times J \times K)$, where I, J and K refer to the number of batches, process variables and time intervals. After phase division, process data of the cth phase is arranged as $\underline{\mathbf{X}}_c(I \times J \times K_c)$, where K_c refers to the number of time intervals within the cth phase, $c = 1, 2, ..., C$.

(2) Intra-batch evolution analysis

Reference windows and sliding windows covering different batches are constructed in batch direction. Relative changes of sliding windows to a reference window are analyzed in principal component subspace (PCS) and residual subspace (RS) of PCA system, respectively. The basic idea is that if the batches in a sliding window are operating in a different mode from the reference window, the monitoring models developed based on the reference window will fail to describe these batches. The specific procedure is listed as below.

(a) Building reference window and sliding window

First, construct a reference window $\underline{\mathbf{X}}_{c,r}(I_r \times J \times K_c)$ based on the first I_r batches in $\underline{\mathbf{X}}_c$ and obtain the two-dimensional data matrix after time-slice normalization and variable-unfolding, denoted as $\mathbf{X}_{c,r}(K_c I_r \times J)$.

Then, compose sliding windows. I_w represents the number of batches included in a sliding window. The moving step, L, indicates how many batches are passed from the current sliding window to the next. L should be less than I_w to make sure all batches are included in sliding window at least once. The process data within the cth phase of the wth sliding window, $\underline{\mathbf{X}}_{c,w}(I_w \times J \times K_c)$, are denoted as $\mathbf{X}_{c,w}(K_c I_w \times J)$, after time-slice normalization and variable-unfolding.

(b) Intra-batch evolution analysis

First apply PCA on the reference window $\mathbf{X}_{c,r}$:

$$\begin{aligned}\mathbf{X}_{c,r} &= \mathbf{T}_{c,r}\mathbf{P}_{c,r}^{\mathrm{T}} + \mathbf{E}_{c,r} = \mathbf{X}_{c,r}\mathbf{P}_{c,r}\mathbf{P}_{c,r}^{\mathrm{T}} + \mathbf{X}_{c,r}\mathbf{P}_{c,r}^{e}\mathbf{P}_{c,r}^{e\ \mathrm{T}} \\ &= \sum_{i=1}^{R_{c,r}} \mathbf{t}_{c,r,i}\mathbf{p}_{c,r,i}^{\mathrm{T}} + \sum_{j=1}^{R_{c,r}^{e}} \mathbf{X}_{c,r}\mathbf{p}_{c,r,j}^{e}\mathbf{p}_{c,r,j}^{e\ \mathrm{T}}\end{aligned} \tag{1}$$

where $\mathbf{T}_{c,r}\left(K_c I_r \times R_{c,r}\right)$ and $\mathbf{P}_{c,r}\left(J \times R_{c,r}\right)$ are principal components (PCs) and the corresponding principal loadings in PCS; $\mathbf{E}_{c,r}\left(K_c I_r \times J\right)$ and $\mathbf{P}_{c,r}^{e}\left(J \times R_{c,r}\right)$ are PCA residuals and the corresponding residual loadings. $R_{c,r}$ is the number of retained PCs determined by cumulative explained variance rate. $R_{c,r}^{e}$ is the number of retained directions in RS, $R_{c,r}^{e} = J - R_{c,r}$.

Then, to analyze relative variations of the sliding window to reference window, project $\mathbf{X}_{c,w}$ onto $\mathbf{P}_{c,r}$ and $\mathbf{P}_{c,r}^{e}$,

$$\begin{aligned}\mathbf{X}_{c,w} &= \mathbf{T}_{c,w}\mathbf{P}_{c,r}^{\mathrm{T}} + \mathbf{E}_{c,w} = \mathbf{X}_{c,w}\mathbf{P}_{c,r}\mathbf{P}_{c,r}^{\mathrm{T}} + \mathbf{X}_{c,w}\mathbf{P}_{c,r}^{e}\mathbf{P}_{c,r}^{e\ \mathrm{T}} \\ &= \sum_{i=1}^{R_{c,r}} \mathbf{t}_{c,w,i}\mathbf{p}_{c,r,i}^{\mathrm{T}} + \sum_{j=1}^{R_{c,r}^{e}} \mathbf{X}_{c,w}\mathbf{p}_{c,r,j}^{e}\mathbf{p}_{c,r,j}^{e\ \mathrm{T}}\end{aligned} \tag{2}$$

where $\mathbf{T}_{c,w}\left(K_c I_w \times R_{c,r}\right)$ and $\mathbf{E}_{c,w}\left(K_c I_w \times J\right)$ are PCs and PCA residuals for data in the sliding window.

If the process characteristics in two windows are similar with each other, the sliding window can share the monitoring model of reference window with no out-of-control monitoring statistics. If variations along some monitoring directions have increased in the sliding window, the calculated monitoring statistics may be too large and go out of control. The part of increased variations is separated from the other by relevant analysis (Zhao C.H. et al. (2013b)). Consequently, four subspaces are decomposed from the original PCS and RS, which explain variations as evaluated by indexes $Ratio_{c,w,i} = \dfrac{\mathrm{var}\left(\mathbf{T}_{c,w}(:,i)\right)}{\mathrm{var}\left(\mathbf{T}_{c,r}(:,i)\right)}\left(i = 1, 2, ..., R_{c,r}\right)$ and $\Delta_{c,w,i} = \left\|\mathbf{X}_{c,w}\mathbf{p}_{c,r,i}^{e}\mathbf{p}_{c,r,i}^{e\ \mathrm{T}}\right\|^2 - \left\|\mathbf{X}_{c,r}\mathbf{p}_{c,r,i}^{e}\mathbf{p}_{c,r,i}^{e\ \mathrm{T}}\right\|^2 \left(i = 1, 2, ..., R_{c,r}^{e}\right)$, where $\| \ \|$ denotes the Euclidean length. Specifically, in PCS, $\bar{\mathbf{X}}_{c,w,f}$ and $\bar{\mathbf{X}}_{c,w,o}$, captured by $\mathbf{P}_{c,w,f}$ and $\mathbf{P}_{c,w,o}$, respectively, represent two parts which make contribution and no contribution to alarming T^2 monitoring statistic. In RS, $\bar{\mathbf{X}}_{c,w,f}^{e}$, captured by $\mathbf{P}_{c,w,f}^{e}$, is the part responsible for the out-of-control *SPE* monitoring statistic in monitoring. The left after explanation of $\mathbf{P}_{c,w,f}$, $\mathbf{P}_{c,w,o}$, and $\mathbf{P}_{c,w,f}^{e}$ are the final residuals.

(3) Mode division along batch direction

Along batch direction, a series of sliding windows can be obtained for the analysis of intra-batch evolution. How to identify new mode is the major concern. In this work, the indexes $Ratio_{c,w,i}$ and $\Delta_{c,w,i}$ defined for relative analysis are used to measure the intra-batch evolution, and thresholds for the two indexes are defined. It is important to note that the thresholds reflect the compromise between model accuracy and model complexity. In general, the value of thresholds can be determined regarding their influences on the resulting modeling and monitoring performance. When a sliding window is detected having either of the indexes $Ratio_{c,w,i}$

and $\Delta_{c,w,i}$ exceeds the thresholds, a new mode is identified and new reference window is constructed. Then compare the following sliding windows with the new reference window. This procedure will repeat until all batches have been classified into different modes. Finally, the successive batches are divided into totally M modes ($m = 1,2,...,M$).

2.2 Intra-Batch-Evolution-Traced Process Modeling

In this section, monitoring system is established and different monitoring statistics are calculated for the current mode in phase c by projecting data onto different subspaces.

For the first reference mode, two-subspace monitoring models are developed:

$$\begin{aligned} \mathbf{T}_{c,tr} &= \mathbf{X}_{c,tr}\mathbf{P}_{c,tr} \\ \mathbf{E}_{c,tr} &= \mathbf{X}_{c,tr}\mathbf{P}^e_{c,tr}\mathbf{P}^{e\ \mathrm{T}}_{c,tr} \end{aligned} \tag{3}$$

where $\mathbf{T}_{c,tr}$ are the systematic scores and $\mathbf{E}_{c,tr}$ are the residuals corresponding to two different monitoring subspaces spanned by $\mathbf{P}_{c,tr}$ and $\mathbf{P}^e_{c,tr}$, respectively.

Then, the traditional monitoring statistics are calculated:

$$\begin{aligned} T_{c,tr,i}{}^2 &= (\mathbf{t}_{c,tr,i} - \bar{\mathbf{t}}_{c,tr})^{\mathrm{T}}\mathbf{\Sigma}_{c,tr}{}^{-1}(\mathbf{t}_{c,tr,i} - \bar{\mathbf{t}}_{c,tr}) \\ SPE_{c,tr,i} &= \mathbf{e}_{c,tr,i}{}^{\mathrm{T}}\mathbf{e}_{c,tr,i} \end{aligned} \tag{4}$$

where subscript i denotes the ith batch, $\bar{\mathbf{t}}_{c,tr}$ denotes the mean vector calculated from $\mathbf{T}_{c,tr}$ which is zero due to the data pre-processing at each time, and $\mathbf{\Sigma}_{c,tr}$ is a diagonal matrix with elements being the variance of each PC in scores $\mathbf{T}_{c,tr}$.

For the other modes, four-subspace monitoring models are developed based on relative analysis:

$$\begin{aligned} \mathbf{T}_{c,v,f} &= \mathbf{X}_{c,v}\mathbf{P}_{c,v,f} \\ \mathbf{T}_{c,v,o} &= \mathbf{X}_{c,v}\mathbf{P}_{c,v,o} \\ \mathbf{T}^e_{c,v,f} &= \mathbf{X}_{c,v}\mathbf{P}^e_{c,v,f} \\ \mathbf{E}^f_{c,v} &= \mathbf{X}_{c,v}\mathbf{P}^e_{c,tr}\mathbf{P}^{e\ \mathrm{T}}_{c,tr} - \mathbf{X}_{c,v}\mathbf{P}^e_{c,v,f}\mathbf{P}^{e\ \mathrm{T}}_{c,v,f} \end{aligned} \tag{5}$$

where $\mathbf{T}_{c,v,f}$, $\mathbf{T}_{c,v,o}$, and $\mathbf{T}^e_{c,v,f}$ are the scores in subspace spanned by $\mathbf{P}_{c,v,f}$, $\mathbf{P}_{c,v,o}$, and $\mathbf{P}^e_{c,v,f}$, respectively; $\mathbf{E}^f_{c,v}$ are the final residuals. They represent different types of relative changes in each mode in comparison with reference mode.

The relative analysis based monitoring statistics are:

$$\begin{aligned} T_{c,v,f,i}{}^2 &= (\mathbf{t}_{c,v,f,i} - \bar{\mathbf{t}}_{c,v,f})^{\mathrm{T}}\mathbf{\Sigma}_{c,v,f}{}^{-1}(\mathbf{t}_{c,v,f,i} - \bar{\mathbf{t}}_{c,v,f}) \\ T_{c,v,o,i}{}^2 &= (\mathbf{t}_{c,v,o,i} - \bar{\mathbf{t}}_{c,v,o})^{\mathrm{T}}\mathbf{\Sigma}_{c,v,o}{}^{-1}(\mathbf{t}_{c,v,o,i} - \bar{\mathbf{t}}_{c,v,o}) \\ T^e_{c,v,f,i}{}^2 &= (\mathbf{t}^e_{c,v,f,i} - \bar{\mathbf{t}}^e_{c,v,f})^{\mathrm{T}}\mathbf{\Sigma}^e_{c,v,f}{}^{-1}(\mathbf{t}^e_{c,v,f,i} - \bar{\mathbf{t}}^e_{c,v,f}) \\ SPE^f_{c,v,i} &= \mathbf{e}^{f\ \mathrm{T}}_{c,v,i}\mathbf{e}^f_{c,v,i} \end{aligned} \tag{6}$$

where $\bar{\mathbf{t}}_{c,v,f}$, $\bar{\mathbf{t}}_{c,v,o}$, and $\bar{\mathbf{t}}^e_{c,v,f}$ denote the mean vectors calculated from $\mathbf{T}_{c,v,f}$, $\mathbf{T}_{c,v,o}$, and $\mathbf{T}^e_{c,v,f}$, respectively, which are all zero vectors due to the data pre-processing at each time. $\mathbf{\Sigma}_{c,v,f}$, $\mathbf{\Sigma}_{c,v,o}$, and $\mathbf{\Sigma}^e_{c,v,f}$ are diagonal matrices with elements being the variance of each PC in scores $\mathbf{T}_{c,v,f}$, $\mathbf{T}_{c,v,o}$, and $\mathbf{T}^e_{c,v,f}$, respectively.

The control limits in the systematic subspace for each mode are defined by the F-distribution with α as the significance factor (Nomikos et al. (1995b)) and in the residual subspace, the representative confidence limit of SPE for each mode can be approximated by a weighted Chi-squared distribution (Lowry et al. (1995)).

2.3 Online Monitoring

Based on the above procedure, characteristics of M modes are captured by M models. When a new observation at the kth time interval of the cth phase, $\mathbf{x}_{c,new,k}(J \times 1)$, is available, if the mode index m is known, $\mathbf{x}_{c,new,k}$ is first pre-processed using the data normalization information from the mth mode. According to time indication, the phase c can be decided.

Then, adopt the mth monitoring model and calculate the statistics. For the first mode, $\mathbf{x}_{c,new,k}$ is then projected onto the traditional two-subspace monitoring system and the monitoring statistics are calculated as below:

$$\begin{aligned} \mathbf{t}_{tr,new}{}^{\mathrm{T}} &= \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}_{c,tr} \\ \mathbf{e}_{tr,new}{}^{\mathrm{T}} &= \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}^e_{c,tr}\mathbf{P}^{e\ \mathrm{T}}_{c,tr} \end{aligned} \tag{7}$$

$$\begin{aligned} T_{tr,new}{}^2 &= (\mathbf{t}_{tr,new} - \bar{\mathbf{t}}_{c,tr})^{\mathrm{T}}\mathbf{\Sigma}_{c,tr}{}^{-1}(\mathbf{t}_{tr,new} - \bar{\mathbf{t}}_{c,tr}) \\ SPE_{tr,new} &= \mathbf{e}_{tr,new}{}^{\mathrm{T}}\mathbf{e}_{tr,new} \end{aligned} \tag{8}$$

For the other modes after the first one, the relative analysis based monitoring is applied:

$$\begin{aligned} \mathbf{t}_{v,f,new}{}^{\mathrm{T}} &= \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}_{c,v,f} \\ \mathbf{t}_{v,o,new}{}^{\mathrm{T}} &= \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}_{c,v,o} \\ \mathbf{t}^e_{v,f,new}{}^{\mathrm{T}} &= \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}^e_{c,v,f}\mathbf{P}^{e\ \mathrm{T}}_{c,v,f} \\ \mathbf{e}^{f\ \mathrm{T}}_{v,new} &= \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}^e_{c,tr}\mathbf{P}^{e\ \mathrm{T}}_{c,tr} - \mathbf{x}_{c,new,k}{}^{\mathrm{T}}\mathbf{P}^e_{c,v,f}\mathbf{P}^{e\ \mathrm{T}}_{c,v,f} \end{aligned} \tag{9}$$

$$\begin{aligned} T_{v,f,new}{}^2 &= (\mathbf{t}_{v,f,new} - \bar{\mathbf{t}}_{c,v,f})^{\mathrm{T}}\mathbf{\Sigma}_{c,v,f}{}^{-1}(\mathbf{t}_{v,f,new} - \bar{\mathbf{t}}_{c,v,f}) \\ T_{v,o,new}{}^2 &= (\mathbf{t}_{v,o,new} - \bar{\mathbf{t}}_{c,v,o})^{\mathrm{T}}\mathbf{\Sigma}_{c,v,o}{}^{-1}(\mathbf{t}_{v,o,new} - \bar{\mathbf{t}}_{c,v,o}) \\ T^e_{v,f,new}{}^2 &= (\mathbf{t}^e_{v,f,new} - \bar{\mathbf{t}}^e_{c,v,f})^{\mathrm{T}}\mathbf{\Sigma}^e_{c,v,f}{}^{-1}(\mathbf{t}^e_{v,f,new} - \bar{\mathbf{t}}^e_{c,v,f}) \\ SPE^f_{v,new} &= \mathbf{e}^{f\ \mathrm{T}}_{v,new}\mathbf{e}^f_{v,new} \end{aligned} \tag{10}$$

Compare the monitoring statistics with the predefined confidence limits. If all monitoring statistics stay well within control limits, the current sample can be deemed to be normal. If any monitoring statistic exceeds control limits, there may be two situations: one is that the process is in a fault, and the other one is that the process is in the mode next to the current mode. To distinguish these two situations, where the mode index m is obtained should be considered. First, if m is identified from the current phase within the current batch, then, the observation should be detected as a fault because all observations from the same phase within a batch must belong to the same mode. Second, if m is identified from the corresponding phase within the previous batch or batches, that is, the process has already developed to the mth mode, then the monitoring model for the (m+1)th mode, should be applied. If the new statistics stay within control limits, it means the process (the current batch) has developed to the (m+1)th mode and the (m+1)th monitoring model should be applied. If any statistic exceeds control limits, the process is in a fault. It should be noted the monitoring models built in this work are in a certain order and a normal process will obey the intra-batch process evolution by fitting the model sequence. If the model sequence cannot be fitted, the process is identified as an abnormality.

If there is no mode information, set m=1 and pre-process $\mathbf{x}_{c,new,k}$ using the corresponding normalization information. Then, adopt the mth monitoring model and calculate the corresponding statistics. If all statistics stay well within control limits, the current sample belongs to this mode and can be deemed to be normal. If any statistic exceeds control limits, set m=m+1, and repeat the procedures above until all the statistics of one mode stay within control limits. If no mode can be identified until m exceeds M, a fault is detected.

3. ILLUSTRATION AND DISCUSSION

3.1 Process Description

A typical injection molding process consists of three major operation phases, injection of molten plastic into the mold, packing-holding of the material under pressure, and cooling of the plastic in the mold before ejection. Concurrent to cooling, plastication takes place to prepare polymer melt for next cycle.

In this work, injection molding start-up is selected to illustrate the proposed algorithm. The process starts with the barrel being heated to the temperature close to the requirement of the normal operation. Then, the process begins to operate the first a few batches to establish the steady state. During the start-up, process variables will drift and process characteristics are varying. All key process conditions can be online measured by their corresponding transducers. The material used in this work is high-density polyethylene (HDPE). The injection velocity is set at 20 mm/s and the packing-holding time is fixed to be 3s. Totally 95 batches are obtained within which 85 batches are used as training batches to build multiple monitoring models for different modes and 10 batches are used as test batches.

3.2 Phase-Based Intra-Batch Evolution Analysis

First, using indicator variables, each batch can be divided into four phases. Screw velocity and SV1 opening are chosen to be indicator variables based on process knowledge.

Second, the injection molding start-up process is separated into several modes. The results of intra-batch evolution analysis for the four phases are shown in Fig. 1 (a) to (d), respectively. In Fig. 1 (a), the injection phase is divided into five modes, and the 5th mode last more batches than the other modes. Similarly, in Fig.1 (b) to (d), the other three phases are divided into several modes, and the last modes contain more batches than others. It can be concluded that all phases evolve fast in the former half of the process and slow in the latter half. Therefore, it is necessary to build more monitoring models for the former half than the latter half.

After dividing the start-up process into several modes, corresponding models are built for process monitoring.

3.3 Online Monitoring

Several batches randomly chosen from the injection molding start-up process are put into online testing, respectively.

For one test batch, first, it is assumed no prior mode information is obtained, so the monitoring models are adopted from m=1 one by one to locate each phase in one mode and identify the right monitoring model. The four-subspace monitoring results using models of the previous modes for the four phases are shown in Fig. 2 (a) to (d). Dashed lines refer to the 95% control limits; dotted solid lines refer to the statistic values. For each phase, one or more statistic values exceed control limits, revealing that the phases do not match these models.

The final monitoring results for this batch are shown in Fig. 3 (a) to (d). The statistics stay well within control limits within the first three phases, so this batch is judged to be normal. It should be noticed in Fig. 3 (d), during the fourth phase, the mode is judged by the first 25 samples after which one big disturbance is detected by T_o^2 and SPE^f. Thus, this disturbance comes from the major systematic variability which makes no contribution to the intra-batch evolution. By diagnosis, this disturbance is caused by the injection cylinder pressure which varies badly during cooling phase. Since the injection cylinder pressure is the key manipulated process variable and is well controlled to avoid variation, the analysis result is consistent with the practical situation.

False alarm rate (FAR) of the proposed method and the traditional method are observed for four phases to evaluate the performance of online monitoring. Similar results are obtained for these phases. Here, due to the space limitation, only the FAR for injection phase are listed in Table 1. The FAR values represent an average monitoring performance of a series of batches. Both methods provide FAR around 5%, which is reasonable according to the 95% control limits. Further, the mean FAR of the two methods are compared by the paired T-test (α =0.05). The proposed method has similar performance to traditional method as plotted in Fig. 4. It can be concluded that the proposed method shows satisfied performance compared with the traditional method, but the analysis in four subspaces is more specific than the traditional.

4. CONCLUSIONS

In this work, a phase-based intra-batch-evolution-traced statistical modeling and online monitoring strategy is proposed for multiphase batch processes. A process with a series of batches is divided into several sequential modes by intra-batch evolution analysis. Meanwhile, multiphase nature of intra-batch evolution is addressed. Consequently, the intra-batch evolution can be well tracked and monitored, providing enhanced process understanding. The case study demonstrates the performance of the proposed algorithm.

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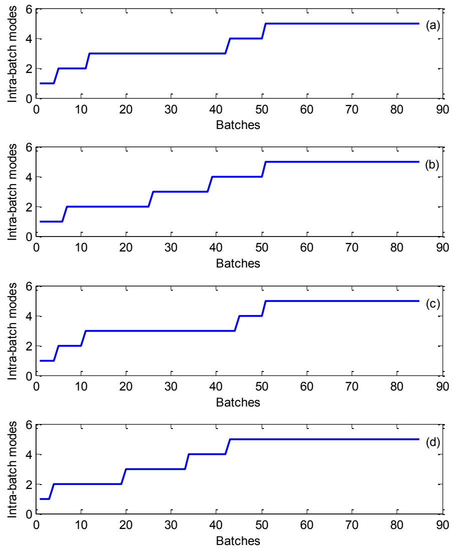
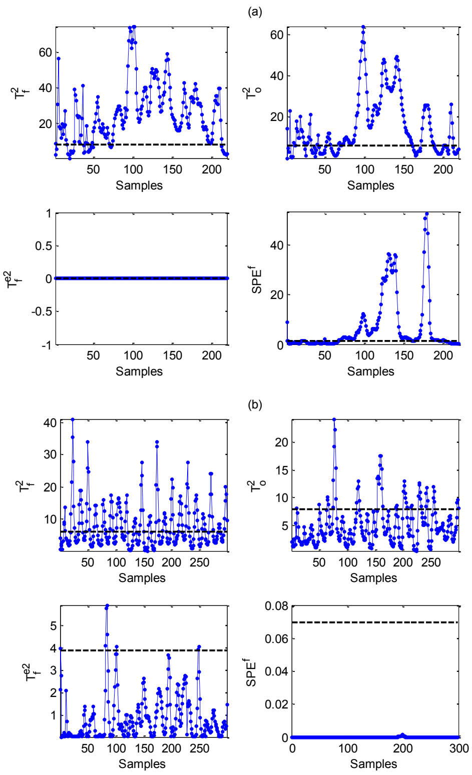


Fig. 1. The intra-batch evolution analysis results for four main phases: (a) injection, (b) packing-holding, (c) plastication, and (d) cooling.



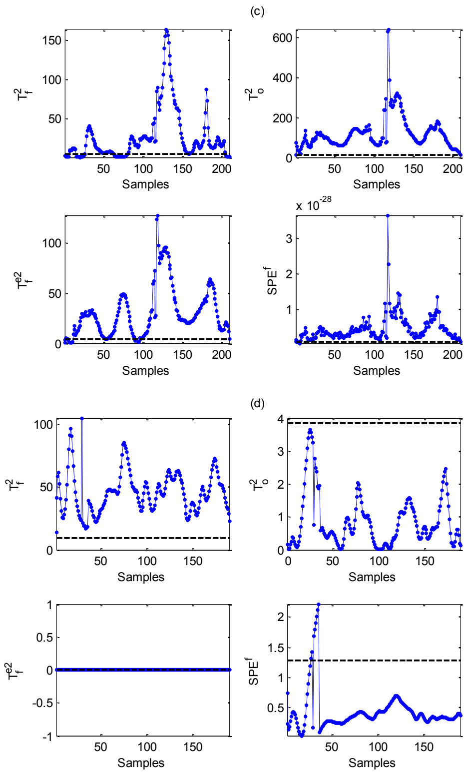
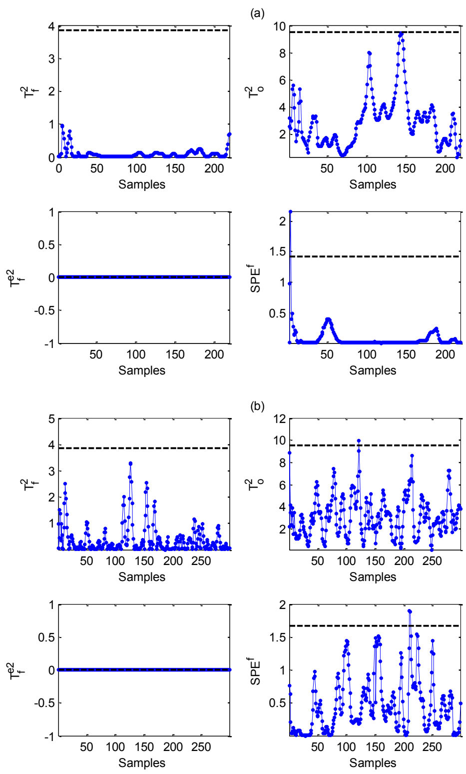


Fig. 2. The monitoring results of one test batch by the models of the previous modes for four phases: (a) injection, (b) packing-holding, (c) plastication, and (d) cooling.



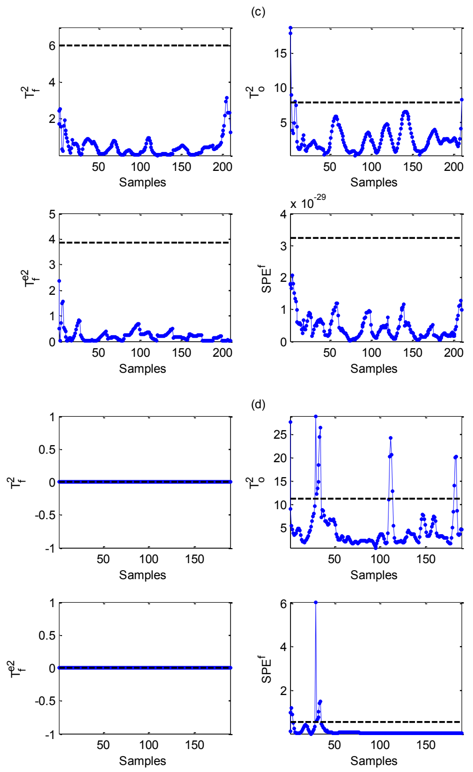


Fig. 3. The online monitoring results of one test batch by the models of the current modes for four phases: (a) injection, (b) packing-holding, (c) plastication, and (d) cooling.

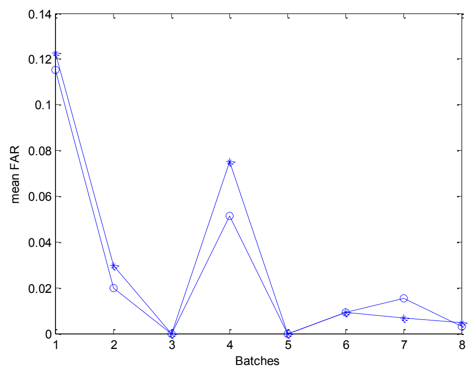


Fig. 4. The mean *FAR* of corresponding statistics using the proposed method (marked by circles) compared with the traditional method (marked by stars) for injection phase.

Table 1. The *FAR* (*Mean*±*MAD*[1]) using the proposed method compared with the traditional method (10^{-2})

Statistic / Batch	Traditional		The proposed method			
	T^2	SPE	T_f^2	T_o^2	T_f^{e2}	SPE^f
Training batches	3.15± 4.13	0.51± 0.86	3.76± 5.74	3.14± 3.97	NaN	0.65± 1.08
Test batches	5.91± 6.93	0.28± 0.43	2.84± 4.26	4.72± 5.14	NaN	0.45± 0.68

[1]*MAD*: mean absolute deviation, which is calculated as $\frac{1}{I}\left(\sum_{q=1}^{N}\left|Z_q - \frac{1}{I}\sum_{i=1}^{I} Z_i\right|\right)$ where *Z* denotes the values of *FAR* index for different batches. *I* is the number of training batches or test batches. Mean is calculated to evaluate the batch-wise "average" monitoring performance for each monitoring statistic; *MAD* can evaluate the batch-wise variability of monitoring performance for each monitoring statistic.

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