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A Step-wise sequential phase partition algorithm with limited batches for statistical modeling and online monitoring of multiphase batch processes

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Abstract: For batch processes, sufficient batches are in general required for statistical modeling and process monitoring. However, sometimes, it is difficult and may be impractical to conduct multiple cycles and wait until enough batches are available. Thus, how to derive reliable process information based on limited batches has been an important question. Starting from limited modeling batches, this article proposes a phase partition and process monitoring strategy for multiphase batch processes. First, a step-wise sequential phase partition algorithm is developed with limited batches where a generalized time-slice is constructed by combining several consecutive time-slices within a short time region to analyze changes of process characteristics. Multiple phases are thus identified in sequence along time direction which are described by different phase models. The feasibility and performance of the proposed method for online process monitoring are illustrated with experimental data from a typical multiphase batch process.

1. INTRODUCTION

Batch and semi-batch processes play a significant role in the processing of specialty chemical, semiconductor, food and biology industries for producing high-value-added products to meet today's rapidly changing market. Hence safety and reliability of batch and semi-batch process is focused on and proper process monitoring and diagnosis method is of great importance (Kourti et al. 1995, Kosanovich et al. 1996, Undey et al. 2002). Multivariate statistical methods such as Multi-way principle component analysis (MPCA) and Multi-way partial least square (MPLS) (Nomikos et al. (1994, 1995b), Wold et al. 1987) have been successfully used for batch processes. However, conventional MPCA and MPLS may be difficult to reveal changes of process characteristics along the time direction since they treat the entire batch data as a single object. it is also difficult for online application where unknown future data has to be estimated.

Considering that the multiplicity of operation phases is an inherent nature of many batch processes and each phase shows different process variable trajectories, operation modes and characteristics, it is better to develop phase-based models (Undey et al. 2002, Wold et al. 1987). Then each phase-based model can explain the local process behaviors, which effectively improve monitoring reliability and enhance process understanding. Kosanovich et al. (1994) and Dong et al. (1995) developed two MPCA (nonlinear MPCA) models to analyze the phase-specific nature of a two-phase jacketed exothermic batch chemical reactor, Lu et al. (2004) proposed a phase-based-sub-PCA modeling method. Since then, phase-based modeling methods (Zhao et al. 2007, 2008) have been widely developed to handle different problems in batch processes with multi-phase characteristics. However, they used clustering-based phase partition algorithm to get phase information, which did not take the time sequence of operation phases into consideration. So time segments with similar characteristics at different time may be mixed as a single phase, which makes the phase division results hard to explain and useless for process understanding. An automatic step-wise sequential phase partition (SSPP) algorithm (Zhao et al. 2013) was developed which can automatically determine phases in order along time direction in the batch process where enhanced process understanding and superior online monitoring performance have been demonstrated. However, as an empirical modeling method, it requires sufficient modeling batches to cover statistically sufficient batch-to-batch variations. This is relatively easy for batch processes with short duration and that are inexpensive to conduct many trial runs. However, for slow batch processes, such as bio-related processes, it takes very long time to complete a batch cycle. Also, for those batch processes which cost much to operate a batch cycle, it is uneconomic to conduct plenty of experiments. Therefore, it may be impractical to wait until sufficient batches are available. The insufficiency of modeling batches arouses difficulty for phase analysis and statistical modeling. Sometimes, although sufficient batches cannot be obtained, several batches are often available in practice. How to analyze phase nature, extract process information and develop monitoring models from limited batches (i.e. just several batches) are important issues, deserving significant attention.

To address the above problems, this article proposes a phase partition and process monitoring strategy for multiphase batch processes starting from limited batches. A step-wise sequential phase partition algorithm is developed with limited batches where a generalized time-slice is constructed by combining several consecutive time-slices within a short time region to analyze changes of process characteristics. After that, phase-based statistical models are developed with limited batches and used for online monitoring. The feasibility and performance of the proposed method for online process monitoring are illustrated with injection molding process. Although starting from limited batches, the proposed method can efficiently extract process information for statistical modeling and offer reliable fault

detection performance. Considering that it is common that sufficient batches cannot be guaranteed for some industrial processes, the proposed algorithm is significantly meaningful for fault detection in batch processes. From another viewpoint, the case with sufficient batches can be regarded as one extreme case of the concerned problem.

2. METHODOLOGY

In this section, a step-wise generalized time-slice-based sequential phase partition algorithm is developed to solve the problem of phase division based on insufficient batches; then phase-based monitoring system is developed where phase models and time-varying confidence limits are defined. For online monitoring application, the status of new samples can be supervised by adopting the corresponding phase models against the predefined confidence limits.

2.1 Data Arrangement with limited batches

In each batch run (batch index i = 1,2,…, I), assume that J process variables are measured online at k =1,2,…, K time instances throughout the operation cycle, forming each regular batch set, denoted as $\mathbf{X}(K \times J)$. In the present work, batches are of equal length without special declaration so that the specific time can be used as indicator for data processing. Here the batches are limited and the data collected from I batches are then arranged as a three way array $\underline{\mathbf{X}}(I \times J \times K)$. At each time, the time-slice can be separated as $\underline{\mathbf{X}}_k(I \times J)$ (k=1,2,…,K). For limited batches, information along batch direction is not sufficient, so the conventional time-slice which is composed of batches at each time fails to reveal the process characteristics as well as the batch-to-batch variations. To replace the "short" time-slices, a new data unit should be organized before statistical analysis.

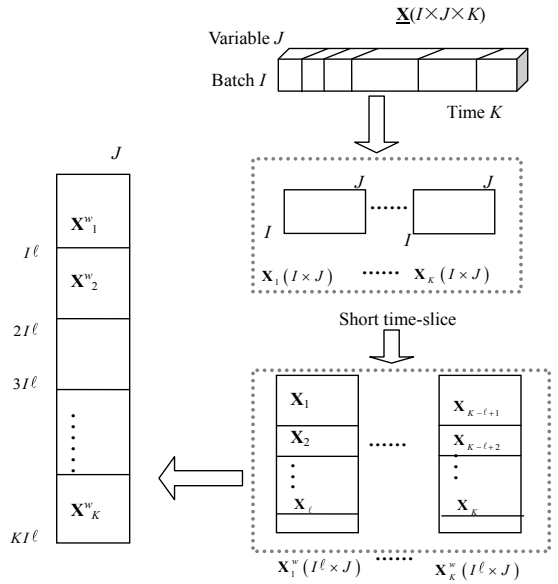


Fig. 1 Illustration of data arrangement for sufficient batches case and limited batches

As shown in Figure 1, several consecutive "short" time-slices are combined together to construct a "generalized" time-slice $\mathbf{X}^w_k(\ell I \times J)$ (k=1,2,…,K- ℓ +1). ℓ is the length of time region spanned by the generalized time-slice, so ℓI is the number of observations in each generalized time-slice. Without special declaration, "time-slice" means conventional time-slice which only covers batches at each time while "generalized time-slice" means the reorganized "time-slice" covering several conventional time-slices.

The time index is indicated by the specific process time corresponding to the middle time ($\ell/2$) of each generalized time-slice. For the time intervals before the first time index, they are all represented by the first generalized time-slice, for the time interval after the last time index, they are all represented by the last generalized time-slice. In this way, corresponding to each time, there is a generalized time-slice. For each generalized time-slice, process variables do not change significantly within such a short time, so the mean and standard deviation can be calculated as the normalization information which can be used to treat new samples. Thus the normalized generalized time-slice data matrix $\mathbf{X}^w_k(\ell I \times J)$ (k=1,2,…,K) at each time are prepared for the following phase analysis.

2.2. Phase Partition with Limited Batches

As mentioned above, generalized time-slices have been prepared. They are then analyzed for phase partition. The specific procedure is presented as follows:

Step 1. Data preparation

Arrange generalized time-slices from conventional time slices and input the normalized generalized time-slice data matrix $\mathbf{X}^w_k(\ell I \times J)$.

Step 2. Generalized time-slice based PCA modeling

Perform PCA algorithm on the normalized generalized time- slice data matrices and get the original models $\mathbf{X}^w_k = \mathbf{T}_k\mathbf{P}^{\mathrm{T}}_k + \mathbf{E}_k = \sum_{r=1}^{R_k} \mathbf{t}_{k,r}\mathbf{p}_{k,r} + \mathbf{E}_k$ (k = 1,2,…,K) where $\mathbf{T}_k$ and $\mathbf{P}_k$ are principal components(PCs) and corresponding principal loadings. R_k is the retained PCs which is determined to keep most of process variability (90% here). Then find the number of PCs that occurs most throughout the batch process and set it as the unified dimension of time-slice PCA models. Thus PCA models for each generalized time-slice have the same dimension.

Step 3. Confidence limit for time-slice model

Calculate the monitoring statistic value of squared prediction errors (*SPE*) of each PCA model, $SPE_{k,i} = \mathbf{e}^{\mathrm{T}}_{k,i}\mathbf{e}_{k,i}$; Then, confidence limit termed Ctr_k is determined by a weighted Chi-squared distribution (Lowry et al. 1995).

Step 4. Time-segment based PCA modeling

From the beginning of process, add next generalized time-slice to the former ones and variable-unfold them, $\mathbf{X}_{v,k}(\ell Ik \times J)$. Perform PCA on the rearranged matrix to get the time segment PCA model up to the current time k,

$\mathbf{X}_{v,k} = \mathbf{T}_{v,k}\mathbf{P}_{v,k}^{\mathrm{T}} + \mathbf{E}_{v,k} = \sum_{r=1}^{R_{v,k}} \mathbf{t}_{v,k,r}\mathbf{p}_{v,k,r} + \mathbf{E}_{v,k}$. Calculate *SPE* values for each generalized time-slice data matrix by using the time segment model $\mathbf{P}_{v,k}$. Then the confidence limit $Ctr_{v,k}$ is determined by a weighted Chi-squared distribution (Lowry et al. 1995).

Step 5. Compare model accuracy

Compare $Ctr_{v,k}$ with Ctr_k for each generalized time-slice within the concerned time region. If there exist consecutive three samples revealing $Ctr_{v,k} > \alpha * Ctr_k$, it means that the current generated time-slice has different variable correlations in comparison with the existing ones. The predefined parameter α called relaxing factor (Zhao et al. 2013) determines how much the time segment PCA model is permitted to be less representative than generalized time-slice model. Then the time slices before k^* are denoted as one sub-phase.

Step 6. Update data for recursive implementation

Remove the first sub-phase, then the remaining batch process data are employed as the new input data in the 4th step. Recursively repeat step 4~5 to determine the following sub-phases.

Using the above partition procedure, different phases are automatically identified in sequence along time direction to capture different operation statuses, which can guarantee similar characteristics within the same phase.

2.3 Sub-phase modeling with limited batches

The sub-phase data $\mathbf{X}_c(I\ell K_c \times J)$ are arranged by variable-wise unfolding the generalized time-slices $\underline{\mathbf{X}}_k^w(I\ell \times J)(k = 1, 2, ..., K_c)$ within the same phase *c*. Then PCA is performed on it and we can get the similar underlying characteristics in each phase:

$$\begin{aligned} \mathbf{X}_c &= \mathbf{T}_c\mathbf{P}_c^{\mathrm{T}} + \mathbf{E}_c = \sum_{r=1}^{R_c} \mathbf{t}_{c,r}\mathbf{p}_{c,r} + \mathbf{E}_c \\ \mathbf{T}_c &= \mathbf{X}_c\mathbf{P}_c \\ \mathbf{X}_c &= \mathbf{T}_c\mathbf{P}_c^{\mathrm{T}} = \mathbf{X}_c\mathbf{P}_c\mathbf{P}_c^{\mathrm{T}} \\ \mathbf{E}_c &= \mathbf{X}_c - \mathbf{X}_c \end{aligned} \tag{1}$$

where K_c is the duration of the current local time region c, $\mathbf{T}_c(I\ell K_c \times R_c)$ denote the principle components, $\mathbf{P}_c(J \times R_c)$ are the sub-phase loadings and they reveal the major variation directions in the current time region, R_c is the number of retained PCs to keep the most variations in each sub-phase. In this way, the systematic variation in $\mathbf{X}_c$ is described by $\mathbf{X}_c$, and the residuals $\mathbf{E}_c$ are deemed as noises.

The subspaces spanned by $\mathbf{P}_c(J \times R_c)$ and $\mathbf{E}_c$ are called systematic subspace and residual subspace respectively. In systematic subspace, monitoring statistic T^2 is calculated at each time, while in residual subspace we can get Q-statistic(*SPE*) from residuals at each time:

$$\begin{aligned} T_k^2 &= (\mathbf{t}_k - \bar{\mathbf{t}}_k)^{\mathrm{T}}\mathbf{S}_c^{-1}(\mathbf{t}_k - \bar{\mathbf{t}}_k) \\ SPE_k &= \mathbf{e}_k^{\mathrm{T}}\mathbf{e}_k \end{aligned} \tag{2}$$

where $\mathbf{t}_k(R_c \times 1)$ is the PC vector separated from $\mathbf{T}_c$, and $\bar{\mathbf{t}}_k$ is the mean vector of $\mathbf{T}_k(I \times R_c)$ which are separated from $\mathbf{T}_c$;. $\mathbf{T}_c$ represents the systematic variations in each sub-phase for training data. $\mathbf{S}_c$ denotes covariance matrixes for each phase $\mathbf{T}_c$. $\mathbf{e}_k(J \times 1)$ is the PCA residual vector which is obtained from the row vector in residual matrix $\mathbf{E}_c(I\ell K_c \times J)$.

In this work, data of time direction and batch direction are mixed at each time for generalized time-slice, whose variation of normal measurement samples do not follow a multivariate Gaussian distribution， so control limits cannot be determined by a F-distribution and a weighted chi-squared distribution(Lowry et al. 1995) respectively. Here, the confidence limits are defined empirically based on the modeling data. We arrange the values of each monitoring index in a descending order at each time and choose the values at 95% percentile of the sorted data. A coefficient is also used to relax the values and the enlarged values are defined as the control limits.

2.4 Online monitoring strategy

When new observing data $\mathbf{x}_{new}(J \times 1)$ is coming, it is first normalized by the mean and variance of corresponding time. Based on the monitoring system $\mathbf{P}_c$, the process status at each time can be checked by projecting the current measurements onto it:

$$\begin{aligned} \mathbf{t}_{new}^{\mathrm{T}} &= \mathbf{x}_{new}^{\mathrm{T}}\mathbf{P}_c \\ \mathbf{e}_{new}^{\mathrm{T}} &= \mathbf{x}_{new}^{\mathrm{T}} - \mathbf{t}_{new}^{\mathrm{T}}\mathbf{P}_c \end{aligned} \tag{3}$$

The new T^2 -statistic and new *SPE*-statistic are then calculated as:

$$\begin{aligned} T_{new}^2 &= (\mathbf{t}_{new} - \bar{\mathbf{t}}_k)^{\mathrm{T}}\mathbf{S}_c^{-1}(\mathbf{t}_{new} - \bar{\mathbf{t}}_k) \\ SPE_{new} &= \mathbf{e}_{new}^{\mathrm{T}}\mathbf{e}_{new} \end{aligned} \tag{4}$$

Process status is thus checked by continuously comparing the two monitoring statistics with predefined confidence limits.

Here, two evaluation indexes for the performance of monitoring system can be defined by calculating False Alarming Ratio (*FAR*) and Missing Alarming Ratio (*MAR*):

$$FAR = \frac{N_f}{N} \times 100\%, \quad MAR = \frac{N_m}{N} \times 100\% \tag{5}$$

where N is the total number of samples, *FAR* is used to evaluate the monitoring performance for normal case where if three consecutive samples go out of control, it is deem that false alarming is falsely issued and N_f is the occurrence number of those three consecutive samples. Similarly, *MAR* is utilized for evaluation of monitoring performance for fault case, if three consecutive samples stay well in confidence

limit for T^2-statistic or *SPE*-statistic, missing alarming is issued and N_m is the number of those issues.

In this work, how to better derive phase information and models from limited batches for online monitoring is focused on. Therefore, the performance of monitoring models developed from limited normal batches is the major concern. Here, batch-wise stepping model updating is simply used. Whenever one new normal batch is available, it is included into the modeling batches of normal case. Phases, data renormalization and monitoring models are then updated based on new information. With the supplementation of new normal batches, the time length of each generalized time-slice (ℓ) will decrease so that the generalized time-slice can more focus on the batch-wise variation.

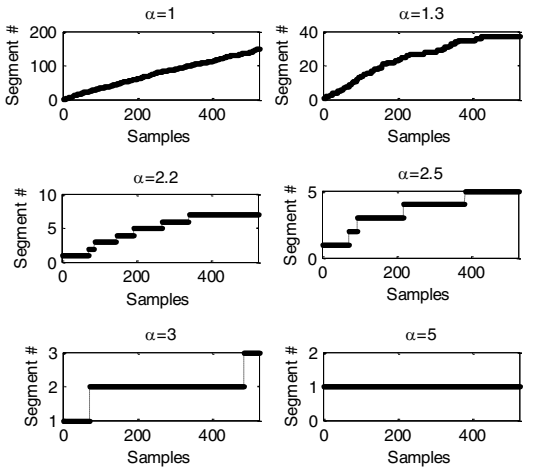
3. SIMULATION AND CASE STUDY

In this section, a typical multiphase batch process, the injection molding, is used to illustrate the performance of the proposed method. The effectiveness of the proposed algorithm is demonstrated compared with the SSPP algorithm with sufficient batches. Injection molding process, which is consisted of three major phases, is a typical multiphase batch process and has been widely used in previous work for process monitoring. Nine process variables are selected for modeling, six normal batch runs are conducted under normal operation conditions and are used to develop the PCA monitoring system. Besides, four types of fault are considered. All batches are unified to have even duration (526 samples in this experiment), which thus results in three-way $\underline{\mathbf{X}}(I \times 9 \times 526)$ where I denotes the number of batches for both normal and fault cases. Six normal batches are used for modeling and the other ten batches are utilized for model testing. For each fault case, ten batches are used for testing.

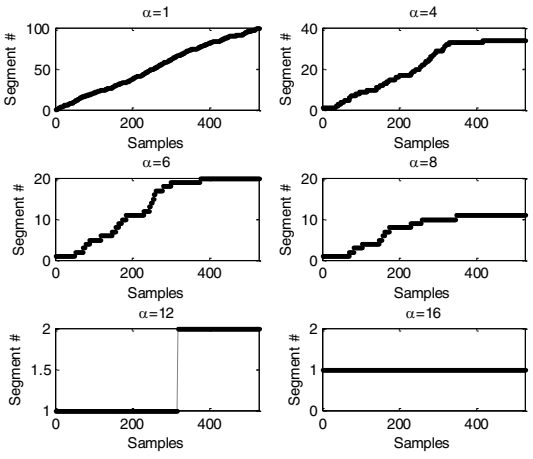
First, the training data $\underline{\mathbf{X}}(6 \times 9 \times 526)$ should be variable-wise unfolded; Then, generalized time-slice with the length of ℓ is determined to be four. Thus the actual length of generalized time-slice ℓI is about three times of the number of variables (Johnson et al. 2002). Subsequently, PCA is performed on each normal generalized time-slice data, the number of PCs for each generalized time-slice is determined to keep 90% variability. The unified PC number used for the proposed phase partition algorithm is three. The phase partition results are shown in Figure 2 for different values of parameter α in comparison with the results from SSPP algorithm which is used at the condition of sufficient batches. The relaxing factor α used in the proposed algorithm is comparatively larger than that of SSPP algorithm, what's more, a larger relaxing factor will result in fewer phases.

Although the proposed algorithm shows different phase division results from SSPP algorithm, they present similar convergence trend as α changes. Moreover, by using the proposed algorithm, the whole batch process is automatically partitioned into different time segments in time order based on limited batches, no extra post-processing has to be carried and division result is more directly and easy to understand, which is similar to the that of SSPP algorithm with sufficient batches.

Based on the phase partition result using the proposed algorithm, different PCA monitoring models are developed for each phase by variable-unfolding data matrices within the same affiliation, here the coefficient used to relax control limits is set to be two. Then online monitoring is carried on starting from the initial monitoring system. Table 1 presents the monitoring performance after updating regarding six values of α assessed by *FAR* for ten normal batches, the mean and mean absolute deviation (*MAD*) values of *FAR* index are calculated. Compared with T^2, *SPE* monitoring results are more seriously influenced by α. It is because that phase partition is implemented based on the evaluation of *SPE*. With α increases, it is noted that *SPE* results first decrease and then increase, and the monitoring performance has the same trend. Table 1 also shows the fault detection performance after model updating concerning six values of α. The results are evaluated by *MAR* for 40 fault batches (ten for each fault case). It is noted that *MAR* index indicates similar results with those by *FAR*.



(a)



(b)

Fig. 2 Phase partition results for IM process using (a) SSPP algorithm with sufficient batches (b) the proposed algorithm with limited batches

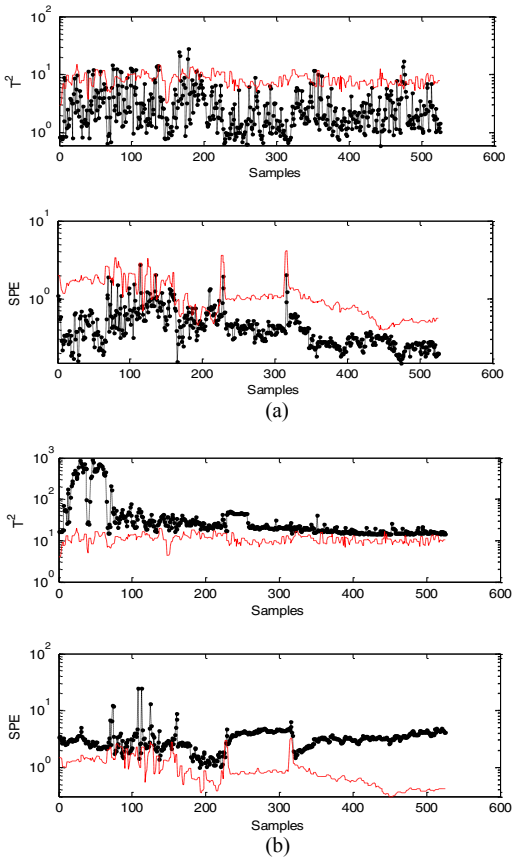


Fig. 3 Online monitoring results for (a) a normal batch (b) a fault batch using the proposed method before updating

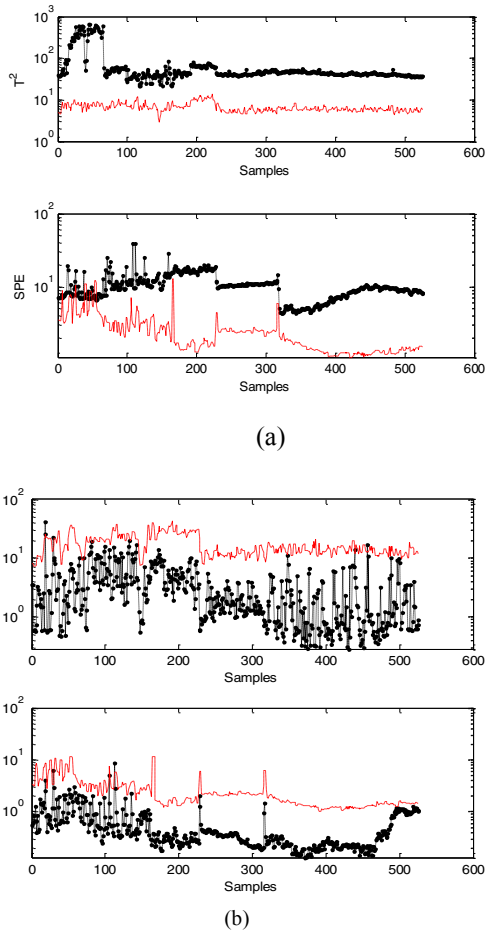


Fig. 4 Online monitoring results for (a) a normal batch (b) a fault batch using the proposed method after updating

Considering model accuracy and model complexity reflected by Figure 2 and Table 1, the value of α can be set to 8. Then as shown in Figure 3, without updating the monitoring model, the online monitoring results for one normal batch which is operated right after six normal batches and one fault batch are presented using the proposed algorithm with the parameter α=8. It is noted that no obvious false alarms are issued for normal case, indicating lower *FAR* values. For fault cases, there are no significant missing alarms for *SPE*. Reliability of the original monitoring model before updating is demonstrated by the above results.

Since the monitoring models are developed from limited normal batches, model updating may be needed as new normal batches are available whose process characteristics more or less different from those for model development. Figure 4 shows the online results for one normal case and one fault case after updating the monitoring model, where the value of α is also eight. It is noted that the updated model can better accommodate the normal variations and can better detect faults than initial monitoring models.

For the concerned normal case and four fault cases, the monitoring results are summarized in Table 2 for ten testing batches. The mean and mean absolute deviation of *FAR*% and *MAR*% are calculated. The proposed modeling method which is based on limited batches and batch-wise stepping model updating is compared with SSPP modeling method with sufficient batches. For comparison, with sufficient batches (30 batches here), phase partition and statistical models are also developed where generalized time-slices in fact converge to batch-wise observations at each time. For a fair comparison, best monitoring results are presented for each method with the parameter α=8 (for limited batches) and α=1.3 (for sufficient batches) respectively. From the results shown in Table 2, starting from limited batches and using stepping model updating, the values of *FAR* and *MAR* are generally lower than 8%. Hence, its monitoring performance is in general comparable with that using models developed from sufficient batches. The results show that for limited batches, the phase information can be effectively explored for model development and thus reliable online monitoring performance is obtained using the proposed algorithm.

4. CONCLUSION

In this work, a sequential phase partition algorithm and modeling method is proposed with limited batches to capture the time-varying process characteristics for multiphase batch process. By rearranging generalized time-slice as new analysis unit, changes of variable correlations are captured for phase partition. Then, based on the phase partition results, PCA monitoring system is set up for online monitoring. Simple stepping model updating is implemented to include new normal batch information and improve the monitoring performance. The case study on injection molding shows the

feasibility of the proposed method for both process understanding and online monitoring.

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Table 1 Monitoring performance regarding different α values (*FAR*% (*Mean* ± *MAD*) for normal case and *MAR*% (*Mean* ± *MAD*) for fault cases)

α		1	4	6	8	12	16
FAR%	T^2	3.00 ± 0.65	1.84 ± 0.67	1.95 ± 0.46	2.02 ± 0.52	1.54 ± 0.40	1.96 ± 0.42
	SPE	11.56 ± 10.89	8.02 ± 9.47	8.17 ± 9.35	7.95 ± 7.48	8.44 ± 9.57	10.68 ± 10.51
MAR%	T^2	2.28 ± 2.69	1.93 ± 2.38	1.85 ± 1.31	2.39 ± 1.72	1.92 ± 1.14	2.27 ± 2.94
	SPE	16.24 ± 25.69	11.96 ± 13.54	10.18 ± 12.56	7.78 ± 10.32	8.45 ± 10.03	9.39 ± 10.17

Table 2 Comparison of online monitoring performance (*FAR*% (*Mean* ± *MAD*) for normal case and *MAR*% (*Mean* ± *MAD*) for fault cases) for testing batches between two methods

Methods / Case	Limited batches $\alpha=8^a$		Sufficient batches $\alpha=1.3^b$	
	T^2	*SPE*	T^2	*SPE*
normal	1.58 ± 0.41	7.95 ± 7.48	1.50 ± 0.86	3.22 ± 4.12
fault	2.39 ± 1.72	7.78 ± 10.32	2.11 ± 1.23	2.15 ± 1.24

[a] It shows the best monitoring results for limited batches
[b] It shows the best monitoring results for sufficient batches