Multivariate Statistical Process Monitoring of Batch-to-Batch Startups

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In batch processes, multivariate statistical process monitoring (MSPM) plays an important role for ensuring process safety. However, despite many methods proposed, few of them can be applied to batch-to-batch startups. The reason is that, during the startup stage, process data are usually nonstationary and nonidentically distributed from batch to batch. In this article, the trajectory signal of each process variable is decomposed into a series of components corresponding to different frequencies, by adopting a nonparametric signal decomposition technique named ensemble empirical mode decomposition. Then, through instantaneous frequency calculation, these components can be divided into two groups. The first group reflects the long-term trend between batches, which extracts the batch-wise nonstationary drift information. The second group corresponds to the short-term intrabatch variations. The variable trajectory signals reconstructed from the latter fulfills the requirements of conventional MSPM. The feasibility of the proposed method is illustrated using an injection molding process. © 2015 American Institute of Chemical Engineers *AIChE J*, 61: 3719–3727, 2015
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Introduction

In industrial manufacturing, batch processes are widely applied for manufacturing low volume and high value-added products. To ensure product quality and process safety, many multivariate statistical process monitoring (MSPM) methods have been developed for fault detection of batch processes.[1,2] The most famous method among them is multiway principal component analysis (MPCA),[3,4] which unfolds three-way batch process data into a two-way matrix and then generates monitoring statistics based on principal component analysis (PCA). MPCA relies on a basic assumption that the process data measured at the same sampling interval in different batches are independent and identically distributed (IID). Most other batch process monitoring methods are based on the same assumption as MPCA, such as adaptive hierarchical PCA,[5] phase-based sub-PCA,[6] batch dynamic PCA,[7] Gaussian mixture model,[8,9] mixture discriminant monitoring,[10] and so forth. However, such assumption may not be held for the data collected from batch process startups.

Batch processes are generally divided into two stages: batch-to-batch startup and steady-state production. Here, in contrast to that in continuous processes, a different definition of steady state is prescribed in the context of batch processes. A batch process is considered in batch-to-batch steady state, when the variable trajectories follow a stable pattern with random noise, provided that the process is in normal operation.[11] On the contrary, the operations in startups have different characteristics. In the engineering viewpoint, the batch-to-batch startup refers to an operational period after starting the machine, during which the properties of incoming materials and the machine conditions have not been stabilized. As a result, the products manufactured during such stage usually do not have consistent and reliable quality. Meanwhile, during batch-to-batch startups, the data series collected at each sampling time point in different batches are nonstationary and not IID, making the conventional MSPM methods unsuitable.

Although consistent and reliable products are only manufactured in steady-state batch operation, effective fault detection in startups is still desired, as abnormalities occurring in this stage could increase the startup time and the number of unacceptable products or lead to safety problems. However, relatively few research efforts have been devoted to such issue. In 2001, Wurl et al.[12] proposed to identify the batches in startup using a partial least squares (PLS) model. In their method, product characteristics should be obtained from samples through offline laboratory analysis. In addition, historical steady-state operation data are also required. Later, Aguado et al.[11] developed an MPCA-based method for steady state identification (SSID) of batch processes. Their method also relies on the completeness of historical data. In 2009, an online batch process SSID method was proposed by Yao et al.,[13] which is based on the information of variable

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correlation and Mahalanobis distance. Most recently, Huang and Yao[14] provided improved results by signal decomposition. Nevertheless, none of the aforementioned methods are for statistical fault detection. To avoid the assumption of batch independency in process monitoring, several methods have been developed, such as the lifted state space model[15] and the modified MPCA model that incorporates information from prior batches into model building.[16] In recent years, a two-dimensional dynamic PCA (2-D-DPCA) method was proposed,[17–19] which models batch process dynamics in both within-batch and batch-to-batch time directions by integrating the PCA technique and the 2-D autoregressive structure. However, these methods are applicable only when the batch-wise dynamics are stationary and not suited for monitoring batch process startups.

In this article, a nonparametric signal processing method called ensemble empirical mode decomposition (EEMD)[20] is adopted to decompose the trajectory signal of each batch process variable into a finite number of intrinsic mode functions (IMFs) and a monotonic residue. These IMFs reflect the characteristics of the trajectory signals at different frequencies. According to the instantaneous frequency information, the IMFs and the residue can be divided into two groups: one corresponding to the long-term trend from batch to batch, and the other corresponding to the short-term variations that consist of intrabatch dynamics, disturbances, and measurement noise. The nonstationary drift between batches is described by the former, while the variable trajectories reconstructed from the latter follow a stable pattern as long as the batches in startup are in normal operation. Therefore, monitoring of batch process startups can be conducted on the short-term variations.

The organization of this article is as follows. In Nonparametric Decomposition of Variable Trajectory Signals Section, the nonparametric decomposition of variable trajectory signals is introduced. Then, the way of instantaneous frequency calculation is presented in Identification of Long-Term Trend and Short-Term Variations Section, together with the identification of long-term trend and short-term variations. MSPM Based on Reconstructed Variable Trajectories Section describes the MSPM modeling based on the short-term variations, taking MPCA for instance. In Application Results Section, the proposed method is implemented on an injection molding process for both Phase I and Phase II monitoring, verifying the effectiveness of the proposed method. Finally, conclusions are drawn in Conclusions Section.

Nonparametric Decomposition of Variable Trajectory Signals

In batch process startups, the batch-to-batch nonstationary features contained in each variable trajectory are characterized by a long-term trend. If such trend can be eliminated from the trajectory signals, the remaining values at each sampling time point are approximately IID between batches and hence, can be monitored with conventional MSPM methods. Therefore, it is important to choose a proper signal decomposition method. Here, EEMD is adopted for its nonparametric nature and flexibility in handling signals of different types.

EEMD is an improved version of empirical mode decomposition (EMD)[21] which is an adaptive time-frequency data analysis method. Through a sifting process, EMD separates a time series signal into several IMFs corresponding to different frequencies, together with a residue of mean trend. By design, an IMF is a function satisfying the following two requirements. First, both the upper and lower envelopes of an IMF are symmetric with respect to zero. Second, in each IMF, the number of extremes and the number of zero-crossings are equal or differ at most by one. Mathematically, IMFs are approximately monocomponent and orthogonal to each other.

Different from other conventional signal decomposition methods, such as Fourier transform and wavelet analysis, EMD is a nonparametric method, which means that it makes no prior assumption with respect to the signal composition. Therefore, the wavelet basis, which is critical in wavelet analysis, is not required in EMD. Such characteristic is desired in the decomposition of nonstationary and nonlinear signals, for example, variable trajectory signals in batch process startups.

Denote a variable trajectory signal as y, where t-th sample in y is represented by $y(t)$. For an observation measured at the k-th sampling time point in the i-th batch, $t=(i-1)\times K+k$, where K is the total number of observations in each batch. The sifting process searching for the IMFs is summarized as follows.

1. Choose $\varepsilon>0$ and initialize the sifting process by setting $n=m=1$ and $f_{1,1}=y$.
2. Calculate the upper and lower envelopes $f_{n,m,\mathrm{upper}}$ and $f_{n,m,\mathrm{lower}}$, together with the local average $l_{n,m}=(f_{n,m,\mathrm{lower}}+f_{n,m,\mathrm{upper}})/2$.
3. If $||l_{n,m}||<\varepsilon$, set $f_n=f_{n,m}$. Otherwise, set $f_{n,m+1}=f_{n,m}-l_{n,m}$, increase m by 1, and then go back to Step 2.
4. Let $f_{n+1,1}=f_{n,1}-f_n$. If there is no more than one extremum in $f_{n+1,1}$, then set $r=f_{n+1,1}$ and stop the sifting process. Otherwise, increase n by 1, reset m to 1, and go back to Step 2.

In the above process, f_n is the n-th IMF and r is the residue. Thus, the original variable trajectory signal y is decomposed from high frequency to low frequency automatically, which can be expressed as

$$y(t)=\sum_{n=1}^{N}f_n(t)+r(t) \tag{1}$$

where N is the total number of IMFs. More details about EMD can be found in the references.[21,22]

A major shortcoming of EMD is that it is not suited to handling intermittent signals, because intermittency often causes mode mixing in the EMD results. In such cases, a single IMF may be made up of components of widely disparate frequencies, or signals with a similar time scale may be decomposed into different IMFs. When EMD is applied to variable trajectory signals of batch processes, mode mixing may occur, as the intermittency phenomenon is frequently observed at the joint point of two successive batches or the switch point between two operation phases. Therefore, EEMD should be conducted instead.

EEMD can be regarded as a noise-assisted EMD method,[20] which defines a "true" IMF as the average of the corresponding IMFs obtained via an ensemble of trials. In each trial, EMD is performed on a signal consisting of the original signal plus a white noise series of finite amplitude. The procedure of EEMD is illustrated graphically in Figure 1.

Identification of Long-Term Trend and Short-Term Variations

After applying EEMD to a variable trajectory signal, the next step is to identify the long-term trend and the short-term variations based on the decomposition results. It should be noted that the trend information may be contained not only in the final residue r but also in a number of low-frequency

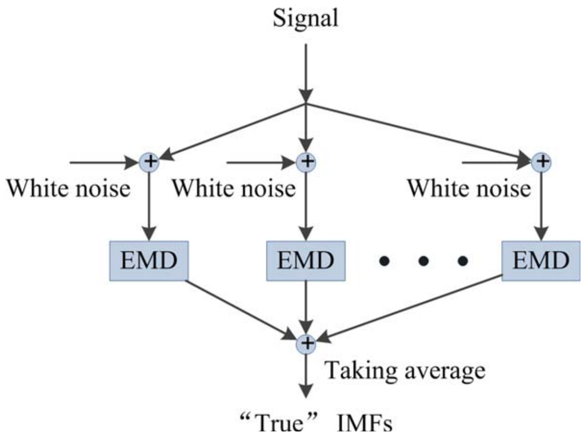

Figure 1. Illustration of EEMD procedure.

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IMFs. The basic idea is that the period of the long-term trend should be larger than the batch length. In other words, the frequency of the long-term trend should be lower than that of batch production, as frequency is the multiplicative inverse of period. Therefore, it is important to find a way to estimate the frequency of each IMF obtained via EEMD.

As an IMF may be nonlinear and nonstationary, it may not be characterized by a single frequency value. Instead, the generalized zero-crossing (GZC) approach[23] is adopted in this article to calculate the instantaneous frequencies for each IMF, whose concept is described below

Using the extrema and zero-crossing points, the instantaneous frequency of each point on a waveform can be estimated in the following way. First, one period can be approximated by the time spans between two consecutive maxima (or minima) or two consecutive up (or down) zero-crossings enclosing the point under consideration. In this way, totally four different estimates of the period can be obtained, denoted as T_1^1, T_1^2, T_1^3, and T_1^4, respectively. Second, the time spans between two consecutive extrema or two consecutive zero-crossings can be used to approximate a half period enclosing the concerned point. Therefore, there are two different estimates of the half period, called T_2^1 and T_2^2. Third, a quarter period can be approximated by the time spans between an extremum point and the next zero-crossing point, or between a zero-crossing point and the next extremum point. Only a single estimate of the quarter period enclosing the considered point is achieved in such way, denoted as T_4. In summary, for each point on an IMF, there are totally seven estimated values for the period, which are T_1^1, T_1^2, T_1^3, T_1^4, $2T_2^1$, $2T_2^2$, and $4T_4$, respectively. Accordingly, the instantaneous frequency is calculated as

$$\omega=\frac{1}{7}\left\{\frac{1}{4T_4}+\frac{1}{2T_2^1}+\frac{1}{2T_2^2}+\frac{1}{T_1^1}+\frac{1}{T_1^2}+\frac{1}{T_1^3}+\frac{1}{T_1^4}\right\} \tag{2}$$

Then, the average frequency of an IMF can be calculated by averaging all instantaneous frequencies at different points. If the value of the average frequency is smaller than $1/T$, where $T=K\tau$ is the batch length and τ is the sampling interval, the corresponding IMF is identified as mainly reflecting the long-term trend from batch to batch. Otherwise, the IMF is considered as only containing the intrabatch short-term variations.

MSPM Based on Reconstructed Variable Trajectories

After dividing the IMFs into two groups as described in Identification of Long-Term Trend and Short-Term Variations Section, the variable trajectory with the long-term trend eliminated can be reconstructed as

$$x(t)=\sum_{n=1}^{H} f_n(t) \tag{3}$$

where H represents the total number of IMFs related to the short-term variations, and f_n are the corresponding IMFs, $n=1, 2, \ldots, H$. As the batch-wise nonstationary information has been removed from the reconstructed variable trajectories, $x(t)$ of all process variables can be monitored based on the conventional MSPM models designed for batch processes, such as MPCA, sub-PCA, and so on. Here, the procedure of MSPM modeling is illustrated using MPCA.

Without loss of generality, suppose that there are totally J process variables, and the number of batches to analyze is I. The reconstructed trajectories $x_j(t)$ of all process variable can be reorganized into a two-way data matrix $\mathbf{X}$, where $j=1, 2, \ldots, J$

$$\mathbf{X}=\begin{bmatrix} x_1(1) & x_2(1) & \cdots & x_J(1) & \cdots & x_1(K) & x_2(K) & \cdots & x_J(K) \\ x_1(K+1) & x_2(K+1) & \cdots & x_J(K+1) & \cdots & x_1(2K) & x_2(2K) & \cdots & x_J(2K) \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ x_1((I-1)K+1) & x_2((I-1)K+1) & \cdots & x_J((I-1)K+1) & \cdots & x_1(IK) & x_2(IK) & \cdots & x_J(IK) \end{bmatrix} \tag{4}$$

the size of which is $I \times JT$. Thus, each row of $\mathbf{X}$ corresponds to the variable trajectories in a single batch. Then, this matrix is normalized by conducting autoscaling which combines centering and variance-scaling. Centering shifts the mean of each column to zero, while variance-scaling standardizes each column by its standard deviation. In doing so, all columns in the matrix have mean zero and unit variance.

In the next step, the normalized matrix $\mathbf{X}$ is decomposed by conducting PCA

$$\mathbf{X}=\sum_{m=1}^{JK}\mathbf{t}_m\mathbf{p}_m^T=\sum_{m=1}^{A}\mathbf{t}_m\mathbf{p}_m^T+\sum_{m=A+1}^{JK}\mathbf{t}_m\mathbf{p}_m^T=\mathbf{T}\mathbf{P}^T+\mathbf{E} \tag{5}$$

where $\mathbf{t}_m(I\times 1)$ are orthogonal principal component (PC) vectors, and $\mathbf{p}_m(JK\times 1)$ are orthonormal loading vectors transforming the

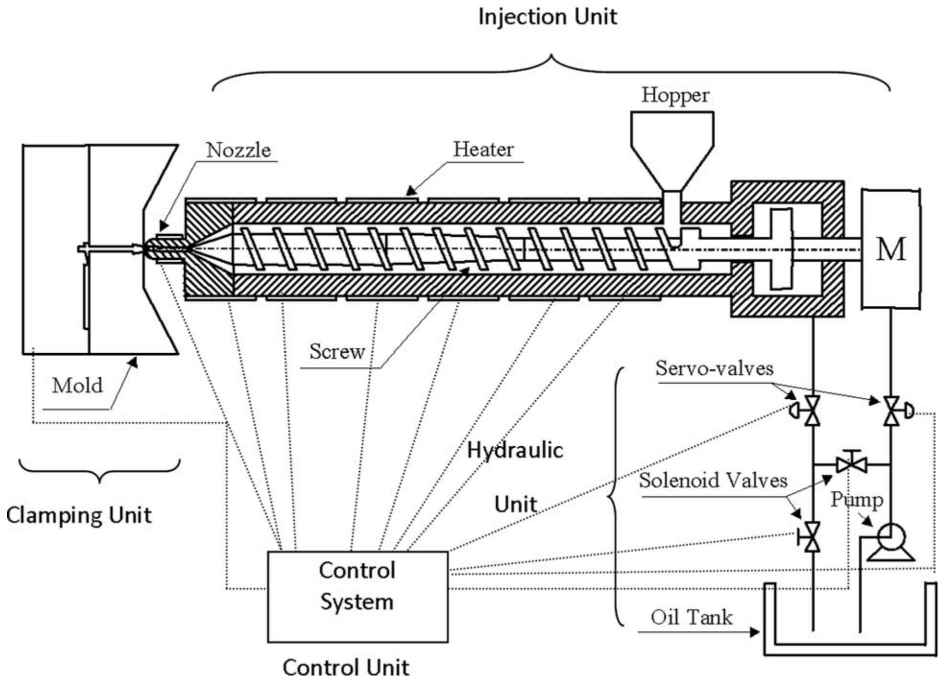

Figure 2. Schematic of reciprocating screw injection molding machine.

original variables into PCs, $\mathbf{T}(I \times A)$ is the score matrix, $\mathbf{P}(JK \times A)$ is the loading matrix, $\mathbf{E}(I \times JK)$ is called the residual matrix, and A is the number of PCs retained in the score space. Algebraically, $||\mathbf{t}_m||$ is equal to the m-th largest eigenvalue λ_m of the matrix $\mathbf{\Sigma} = \mathbf{X}^T\mathbf{X}$, and $\mathbf{p}_m$ is the corresponding eigenvector.

Usually, MSPM can be divided into two phases. In Phase I, the data used in modeling is analyzed. Any abnormal patterns leading the drive the process out of control should be detected. In this phase, for each row $\mathbf{x}_i^T$ ($i = 1,2, \ldots, I$) in $\mathbf{X}$, the corresponding scores $\widehat{\mathbf{t}}_i^T$ and residuals $\mathbf{e}_i^T$ can be described in the following way

$$\widehat{\mathbf{t}}_i^T = \mathbf{x}_i^T \mathbf{P} \tag{6}$$

$$\mathbf{e}_i^T = \mathbf{x}_i^T (\mathbf{I} - \mathbf{P}\mathbf{P}^T) \tag{7}$$

Accordingly, the monitoring statistics Hotelling-T^2 and squared prediction error (SPE) can be derived as

$$T_i^2 = \widehat{\mathbf{t}}_i^T \mathbf{S} \widehat{\mathbf{t}}_i \tag{8}$$

$$\text{SPE} = \mathbf{e}_i^T \mathbf{e}_i \tag{9}$$

where $\mathbf{S} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_A)$. T^2 measures the distance between each batch and the center of normal operation region, while SPE measures the model fitness. Taking the assumption that the data in $\mathbf{X}$ obey a multivariate normal distribution, the control limits of T^2 can be computed based on an F-distribution

$$T_{\text{lim},\alpha}^2 = \frac{A(I-1)}{I-A} F_{A,I-A,\alpha} \tag{10}$$

where α is the significant level, and $F_{A,n-A,\alpha}$ is the critical value of F distribution with significant level of α and degrees of freedom of A and $n-A$. Under the same assumption, the control limits of SPE can be calculated as

$$\text{SPE}_{\text{lim},\alpha} = \theta_1 \left(\frac{C_\alpha \sqrt{2\theta_2 h_0^2}}{\theta_1} + 1 + \frac{\theta_2 h_0 (h_0 - 1)}{\theta_1^2} \right)^{\frac{1}{h_0}} \tag{11}$$

where $\theta_i = \sum_{j=A+1}^{JK} \lambda_j^i$ $(i = 1, 2, 3)$, $h_0 = 1 - \frac{2\theta_1\theta_3}{3\theta_2^2}$, and C_α is the critical value of normal distribution corresponding to significant level of α. If either T^2 or SPE is outside the corresponding control limit, a fault is detected.

In Phase II, the major goal is to monitor process data not involved in the training set. For each new batch, T^2 and SPE can be calculated in a similar way to that described in Eqs. 6–9. Then, the fault detection results can be achieved by comparing the monitoring statistics to the control limits.

Application Results

Injection molding process

In polymer processing, injection molding, which usually uses a screw-type plunger to inject melted plastic material into a mold cavity to produce products with a shape conforming to the mold contour, is a typical batch process. Figure 2 shows a schematic of a reciprocating screw injection molding machine. Thanks to its flexibility, injection molding has been widely used in manufacturing high quality plastic parts with complex shapes.

Each batch of injection molding consists of several sequential operation phases, causing the nonlinear and dynamic behavior in variable trajectories within each single batch. After mold closing at the beginning of each batch, the screw moves forward, filling the melted plastic into the mold cavity. Then, the process operation switched to the next phase, that is, packing-holding. In this phase, the material shrinkage due to cooling and solidification is compensated by packing additional melt into the mold at a high pressure. Once the gate between the mold cavity and the nozzle is frozen, the

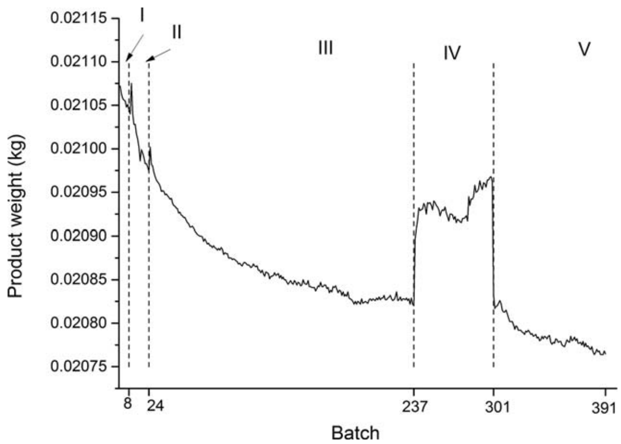

Figure 3. Product weight measured at the end of each batch.

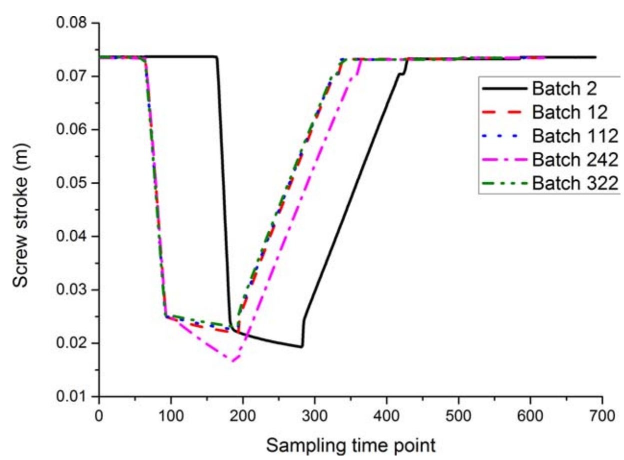

Figure 4. Variable trajectories of screw stroke.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

plastication phase starts. During this phase, the mold cavity is isolated from the injection unit and cooled down by heat exchange with cooling water. In the meantime, the screw rotates, plasticating the plastic in the barrel by the shear heating and conveying the achieved melt to the nozzle. Usually, cooling takes longer than plastication. Finally, the molded part is pushed out of the mold cavity by the ejector pins, when the mold opens at the end of each batch.

In the batch-wise direction, injection molding process also comprise two stages, that is, batch-to-batch startup stage and steady-state operation. During startups, significant interbatch nonstationary and nonlinear trend exist due to unstable material properties and adjustments of machine settings, hindering the utilization of traditional MSPM methods. A number of MSPM methods have been proposed for fault detection of the injection molding process, for example.[9,10,24–26] In process modeling and monitoring, these methods take various process characteristics into consideration, such as multiple operation phases, uneven batch durations, unlabeled process data, and so forth. However, while the batch-to-batch steady-state operation is well treated, the problem of fault detection in the startup stage is seldom concerned.

Data description

In this case study, the data were collected from 391 batches in the startup stage of an injection molding process, which involve four process variables: screw stroke, back pressure, injection velocity, and nozzle temperature.

According to the process engineer who conducted the experiment, these data can be divided into several parts. Part I includes batches 1–8, during which the machine was just started. The engineer kept adjusting the set points of barrel temperatures, packing pressure, and so forth, to achieve a satisfactory operation. Such adjustments were made based on the engineer's experience, while the trial set points of each process variable varied from each other significantly. Batches 9–24 can be regarded as Part II. During these batches, the process was operated manually. In the meantime, the process parameters were slightly adjusted. Then, in batches 25–237 (Part III), the process was operated automatically according to the determined parameters. In batch 238, the flow rate of the cooling water was increased due to an incorrect operation of the water valve. Then, in batch 281, the flow rate was raised again. The batches with abnormal cooling, that is, batches 238–301, are tagged as belonging to Part IV. The setting of the cooling water flow rate returned to its original value in batch 302. Therefore, the batches in Part V, that is, batches 302–391, had the same settings as batches 25–237.

Figure 3 shows the product weight of each batch, which is an indication of the changes in the process behavior. Overall, a decreasing trend in product weight can be observed. The reason is as below. During the startup stage, the material in the barrel was gradually heated from the room temperature to a desired temperature. Consequently, the density of the melted plastic decreased with the rising temperature, leading to less plastic (in weight) injected into the mold cavity. Hence, the product weight decreased from batch to batch in general. In the first 24 batches, large variations are noticed, which were caused by the parameter adjustments made by the process engineer. Then, in batches 25–237, corresponding to normal operation, the product weight became lower and lower gradually, indicating the existence of the nonstationary trend in the process startup. After the occurrence of the fault in the cooling water flow rate, the product weight increased in a sudden, due to the change in the density of the melt. Once the process returned to normal, a downward step change was observed in the product weight.

The laboratory analysis of product quality can only be achieved at the end of each batch and is usually time and labor consuming. In addition, it may not clearly reveal all the process characteristics. For example, in Figure 3, the difference between the first 24 batches and the following batches in normal operation is not very significant. Therefore, it is desired to realize process monitoring based on the trajectory information of process variables. However, as shown in Figures 4–7, the interbatch repeatability during startup is very poor, indicating that the batch-wise nonstationary trend also exists in variable trajectories. This hinders the implementation of conventional MSPM methods. In such situation, the proposed monitoring method is more appropriate.

Phase I and phase II monitoring

Figures 4–7 plot the variable trajectories along the sampling time points within each batch. For conducting signal decomposition, the trajectory signal of each variable was reorganized into a single data vector along a single time direction by connecting the successive batches side by side. Taking the screw stroke for example, Figure 8 shows the rearranged variable trajectory. For illustrating the feasibility of the proposed method,

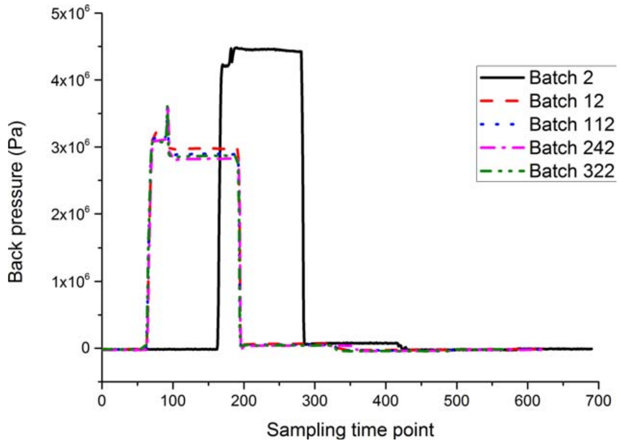

Figure 5. Variable trajectories of back pressure.

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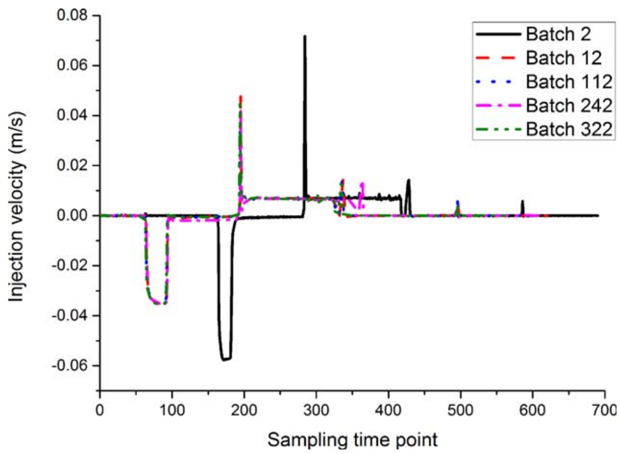

Figure 6. Variable trajectories of injection velocity.

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the total data set was divided into two parts. Batches 1–280 served as the training data, which were utilized in Phase I modeling and monitoring. Batches 281–391 were used as the test data in Phase II, which would be monitored according to

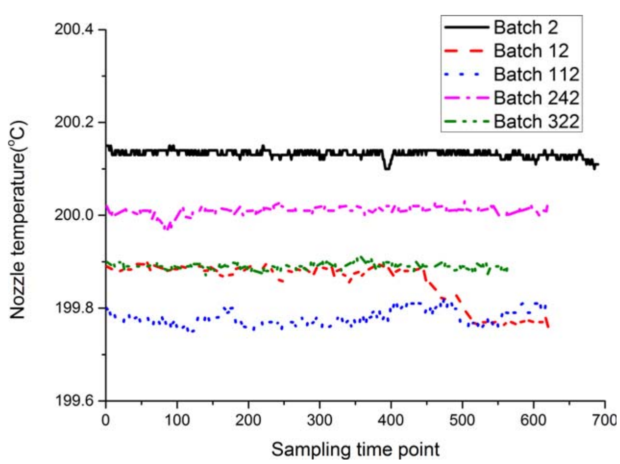

Figure 7. Variable trajectories of nozzle temperature.

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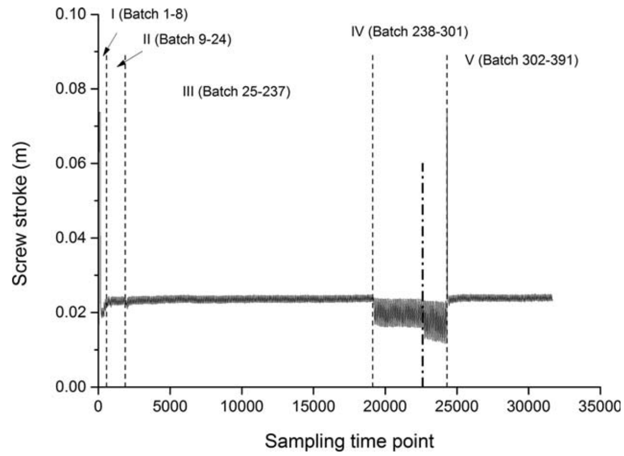

Figure 8. Rearranged trajectory signal of screw stroke.

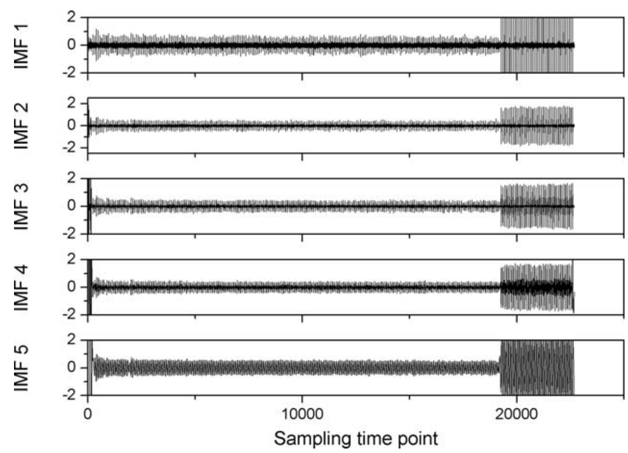

Figure 9. EEMD results of the trajectory signal of screw stroke in the training dataset: components corresponding to short-term variations.

the control limits derived in Phase I. The dot-dash line in Figure 8 indicates the division between the two subsets.

For eliminating the long-term nonstationary trend between batches, EEMD was conducted on both the training and test data. For illustration, Figures 9 and10 present the decomposition results of the trajectory signal of screw stroke in the training dataset. In both the figures, the resulted components including IMFs and residue are arranged in a descending order of signal frequencies. Then, by applying the GZC method described in Identification of Long-Term Trend and Short-Term Variations Section, the average frequency of each IMF was calculated and compared with the frequency of batch production. Through such comparison, the first five IMFs in Figure 9 were identified as representing the short-term variations, while the remaining IMFs and residue plotted in Figure 10 were categorized as containing the information of the long-term trend. Consequently, the short-term and long-term signals were reconstructed by summing all the components in the corresponding categories, as shown in Figure 11. The variable trajectory in the test dataset was decomposed and reconstructed in a similar way. The reconstructed subsignals of screw stroke in are plotted in Figure 12. Other process variables were processed following the same procedure.

In the next step, the reconstructed training data representing the short-term variations were subjected to MPCA for Phase I

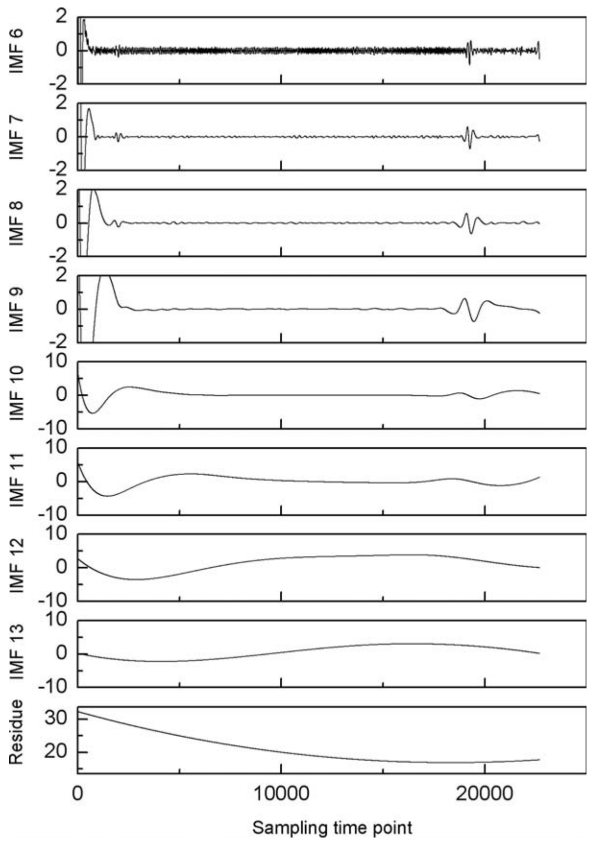

Figure 10. EEMD results of the trajectory signal of screw stroke in the training dataset: components corresponding to long-term trend.

monitoring. Before modeling, the problem of uneven batch durations should be solved. Various solutions to such problem have been suggested by researchers. The simplest method for variable trajectory synchronization is to cut the batches to the minimum length.[27] Other methods include missing data estimation,[28] utilization of indicator variable,[29] dynamic time warping,[30] and so forth. Trajectory synchronization is not the focus of this article. Hence, the minimum length method was adopted for its simplicity. Then, all the training batches were used in MPCA modeling, from which the T^2 and SPE control charts were derived. In the control charts shown in Figure 13,

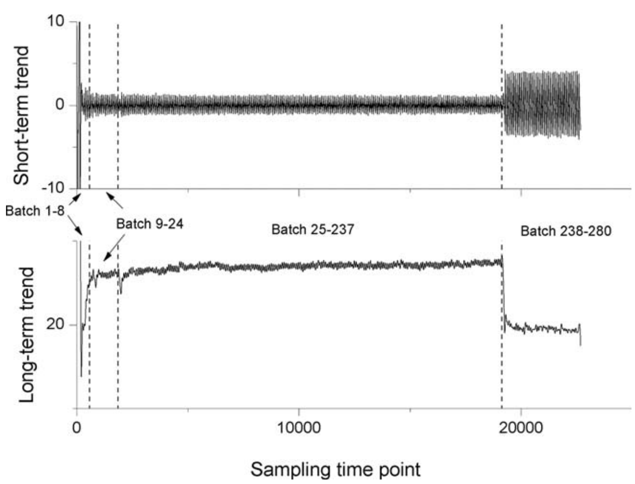

Figure 11. Reconstructed signals of screw stroke in the training dataset.

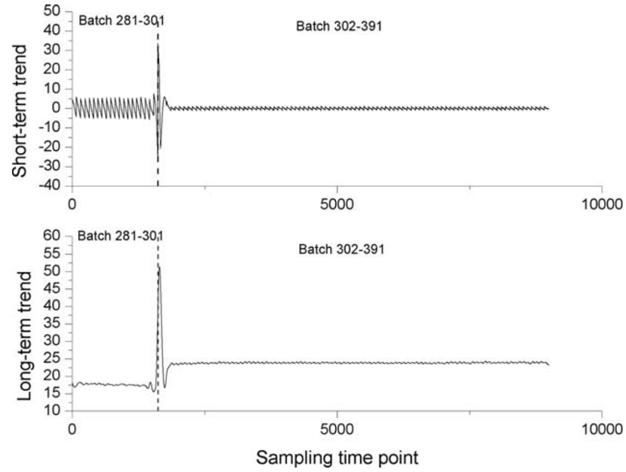

Figure 12. Reconstructed signals of screw stroke in the test dataset.

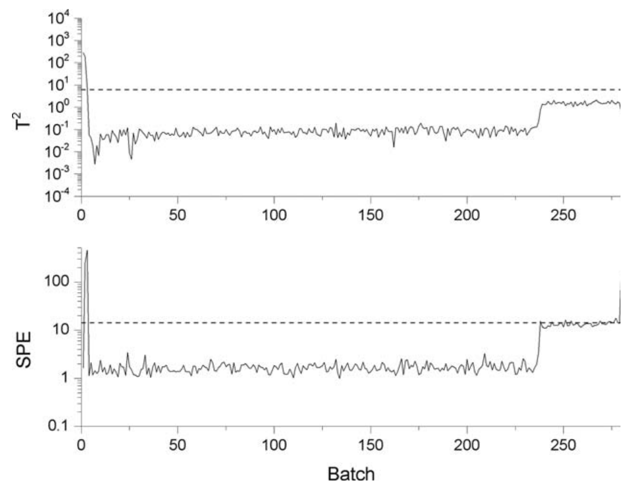

Figure 13. Phase I monitoring: first round.

it is observed that the first three batches are outside the 95% control limits (the dash lines) of both T^2 and SPE. In addition, the last 43 batches, that is, batch 238–280, are also close to or even outside the control limits. Especially, batch 280 is significantly out of control. Therefore, batches 1–3 and 280 were deleted from the training dataset before the second round

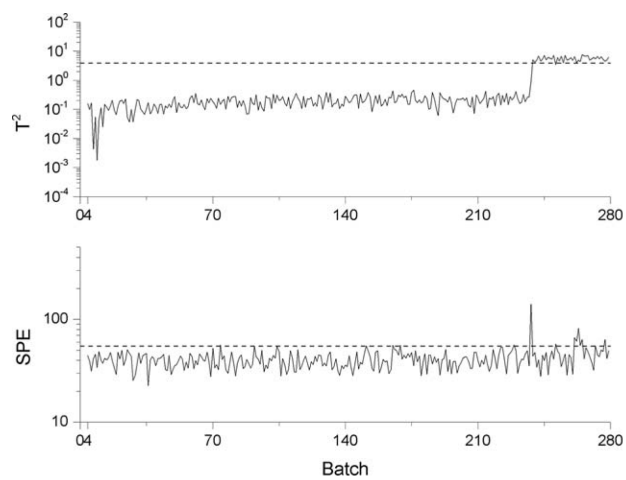

Figure 14. Phase I monitoring: second round.

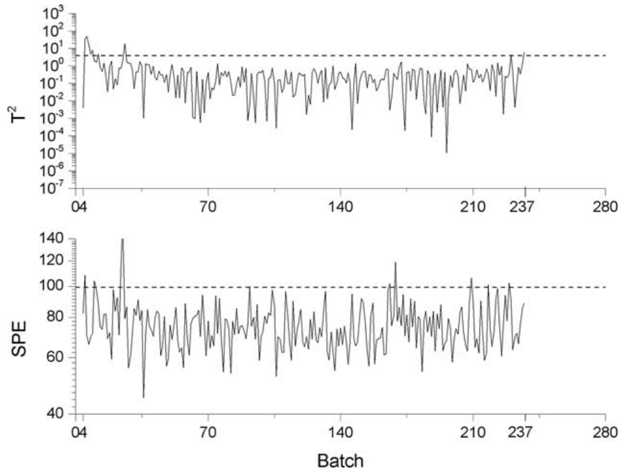

Figure 15. Phase I monitoring: third round.

modeling. The MPCA model based on the remaining 276 batches resulted in the control charts shown in Figure 14. Obviously, all the batches after and including batch 238 are out of control. These batches were then removed from the training set. The third round modeling provided the control charts in Figure 15, in which batches 5–8 were detected as abnormal. Consequently, only batches 9–237 were utilized in the fourth round modeling. Figure 16 shows that most of these batches are under the control limits, except that some batches before batch 24 behave like outliers. Such procedure is called control-and-adjustment in the textbooks, for example,[31] which is a standard procedure in Phase I monitoring.

The Phase I monitoring results are in accordance with the understanding of the process. As introduced in previous, the process engineer frequently adjusted the process parameters during batches 1–8. Therefore, the behavior of these batches was different from that of the following ones. Batches 238–280 suffered from the abnormal flow rate of the cooling water. It is desired that the control charts are able to detect such fault. In addition, batches 9–27 were under manual operation, during which the process engineer adjusted the process parameters occasionally. This is the reason why several outliers occur before batch 24. Batches 28–237 were under normal automatic control. The control charts well reflect such process characteristics, and are not influenced by the nonstationary trend between batches.

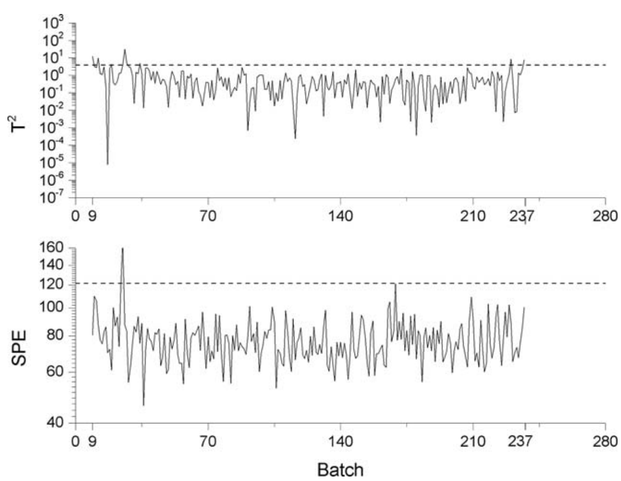

Figure 16. Phase I monitoring: fourth round.

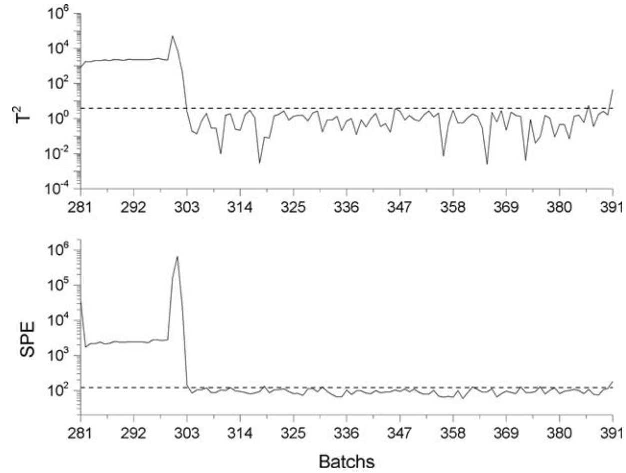

Figure 17. Phase II monitoring.

The MPCA model built in the fourth round was applied to Phase II for monitoring the test data. The monitoring results are shown in Figure 17. In the control charts, batches 281–303 are outside the control limits, while the following batches are in control. Such results agree with the information provided by the process engineer. Moreover, it is indicated that, although the flow rate of the cooling water was restored to its original setting in batch 302, the process spent two more batches for recovery from the fault.

For comparison, the conventional MPCA method, that is, MPCA without EEMD preprocessing, was also implemented. In Phase I monitoring, the same control-and-adjustment steps were followed. After three rounds of modeling, only batches 43–232 were identified as normal batches, while the other batches were regarded as abnormal. Such results diverged from the process understanding, and involved false alarms. Then, batches 43–232 were used to train the MPCA model for Phase II monitoring. The monitoring results are shown in Figure 18. It is observed that almost all the following batches, that is, batches 281–391, are outside the control limit and considered as faulty batches, although batches 301–391 were actually in normal operation. The reason why the conventional MPCA led to significant false alarms is that the nonstationary drift between batches breaks the premise of the classical statistical monitoring.

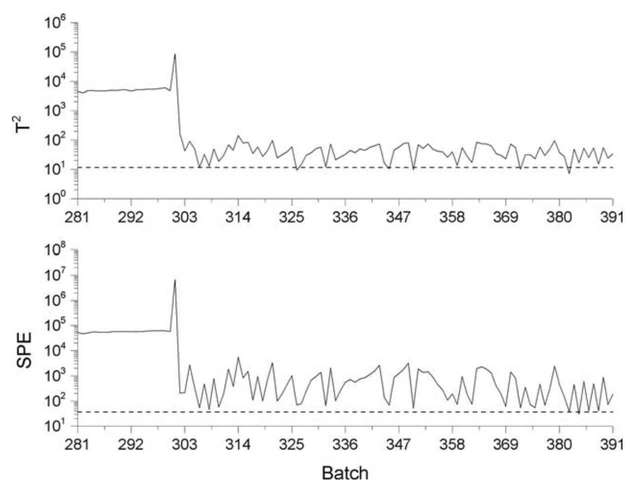

Figure 18. Phase II monitoring based on conventional MPCA.

Conclusions

Fault detection in batch-to-batch startups is an interesting but difficult problem in statistical batch process monitoring. The major difficulty lies in the treatment of nonstationary trend between batches. In this article, we propose to decompose each variable trajectory signal into a series of components corresponding to different frequencies. Such decomposition is achieved by adopting a nonparametric method named EEMD. Then, the long-term trend and the short-term variation signals can be identified via the calculation of instantaneous frequencies. By eliminating the long-term trend from the trajectory signal of each process variable, the remaining part of the process data obeys the statistical requirements of the conventional MSPM methods. Hence, monitoring of batch process startups becomes possible. We hope that the method proposed in this article provides a new angle for studying the batch startups monitoring problem.

To conclude this article, we would like to mention several possible future research topics in the related area. First, the method proposed in this article is mainly for offline monitoring. To monitor batch-to-batch startups in real time, one should first solve the problem of online signal decomposition. As EEMD is a purely nonparametric method that is empirical, it provides no model for online decomposition. Second, in this article, batch process monitoring is applied to the reconstructed trajectory signals that are based on the decomposition components corresponding to the short-term variations, while the long-term trend is simply discarded. However, as shown in Figures 11 and 12, the long-term trend may also contain certain information related to process faults. How to make use of such information remains a question. Third, it is possible to perform MSPM to each level of the EEMD components instead of the reconstructed trajectory signals. In doing so, more fault diagnosis information may be revealed.

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