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Between-Mode Quality Analysis Based Multimode Batch Process Quality Prediction

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ABSTRACT: In batch processes, multiple process modes usually exist because operation conditions frequently change to satisfy different market requirements. Besides multiple modes, the multiplicity of operation phases within each batch is an inherent nature of many batch processes. Different between-batch modes and different within-batch phases may exhibit significantly different underlying behaviors and have different effects on the final product quality. Therefore, for better quality predictions, the multimode and multiphase problem should be addressed. In this work, based on between-mode quality analysis, prediction strategy is developed for multiphase batch processes with multiple operation modes. First, each batch cycle is divided into multiple phases. Then within each phase, for different modes comprised of different batches, different quality regression models are constructed. Also, between-mode quality analysis is conducted to judge the relationship between the new mode and the historical modes in the mode library, regarding whether a new model is necessary to update the mode library. In the between-mode analysis, a novel model for the new mode is built by a simple linear combination of historical modes, which is then compared with the model obtained by complete remodeling for the new mode. Online quality prediction for the new mode is conducted using the selected model. The proposed algorithm is applied to a typical multiphase batch process with multiple operation modes, an injection molding process, to illustrate the feasibility.

1. INTRODUCTION

As one important type of production, batch processes are widely applied in industry. To maintain the manufacture of higher-value-added products in batch processes, operation safety and consistent product quality have become a focus of research.[1−5] Due to the complicated characteristics of batch processes, it is difficult to build a first-principles model within a limited time period. On the other hand, the development of computers and sensors make it possible to obtain abundant process data covering much process information. Therefore, data-based multivariate statistical method, such as multiway principal component analysis (MPCA)[6] and multiway partial least-squares (MPLS) analysis[7] were proposed for batch process monitoring. These methods handle the three-dimensional data structure of the batch process, which is a significant feature of batch processes. However, it is difficult for them to reveal the changes of process correlations along the time direction since the entire batch data were taken as a single object. Also, it is difficult for online application since the whole new batch data are not available up to the concerned time so that the unknown future values have to be estimated.

Multiphase is a significant feature of batch processes. A series of phases comprises a batch cycle since multiple operation steps are included in each batch cycle, and each phase has its own characteristic, which requires special attention for multiphase batch process monitoring and quality analysis. Many works[8−19] have been done about batch process monitoring and quality analysis focusing on multiphase characteristic of batch processes since the 1990s. The basic idea is to establish different statistical models to capture different characteristics of different phases on the basis of such recognition that the underlying variable correlations are similar within the same phase while different across phases. Some extensions were investigated on the basis of phase characteristics for online process monitoring and quality analysis, such as transitions between neighboring phases[14−16] and uneven-duration problems.[17−19]

Besides multiphase characteristics, a multimode problem exists in batch processes due to various factors, such as change of production, the feedstock, manufacturing strategies, operation conditions, and the external environment. Especially, productions and operation conditions may often change to satisfy the fast changing market requirement, leading to operation mode changing frequently during production. If statistical models for process monitoring and quality prediction are only built for one operation mode, when a new operation mode happens, the models will mismatch the new mode and provide inaccurate analysis results. Therefore, the multimode problem has drawn people's attention, and possible solutions include two main directions: (1) building a hierarchical model which includes a common model part to cover the common characteristic for all operation modes and a specific model part to cover specific characteristics for different modes;[20−23] (2) building specific models for specific operation modes respectively, either based on a mode library[24−26] or adaptive

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model updating.[27,28] To focus on specific characteristics of each mode and extract as much information as possible from each mode, the method based on a mode library in the second direction is preferred for offline analysis. However, most of the methods based on a mode library are proposed for process monitoring whereas few are proposed for quality analysis, even though quality analysis can provide as much valuable information as process monitoring for normal production in batch processes.[11,13,16] Moreover, these mode-library methods build different models for different modes separately without any analysis or judgment of the relationship of those modes. As new modes happen one after another, all new modes have to be saved and then the mode library becomes bigger and bigger. This may cause a heavy burden on data saving, and the use of a mode library may be inefficient. Thus, the analysis of the between-mode relationship of one mode to other modes is necessary to judge if a mode is informative enough to be saved, which, however, has been barely investigated. Especially, for quality analysis, challenging problems need to be investigated. For example, does one mode have the same quality prediction information as that for another mode? Can the quality regression information from one mode be substituted by that from other modes? The answers to these problems may help significantly in understanding the process and maintaining normal production for multimode processes.

Therefore, it is desired to investigate a proper quality prediction method on the basis of the between-mode relationships for different modes within multiphase batch processes. The basic motivation of this work is to judge the value of one new mode for quality prediction to see if the mode library needs to be updated. If the new mode shares quality-related information with the historical modes, there is no need to include this mode into the mode library and the space could be saved for other valuable modes. According to the between-mode relationship between this new mode and the historical modes, a new process mode can be classified as interpolation or extrapolation of those historical process modes. That is, if the mode information on the new mode can be substituted by the information on the historical modes, this new mode is deemed to be an interpolation of the historical modes; otherwise, this mode is an extrapolation. Thus, the main objective of this work is to classify the new mode based on between-mode relationship analysis and provide information for quality prediction as well as mode library updating, which is a novel idea of quality analysis for multimode batch processes. First, a batch cycle is divided into multiple phases. Within each phase, different quality regression models are constructed for the historical modes in the mode library. For the new mode, on one hand, a quality regression model is built purely based on the process variables and the quality variable of this mode. On the other hand, another quality regression model is built based on not only the process variables and quality variable of this mode but also those of the historical modes in the mode library. Then, the performances of the two regression models for the new mode are compared to determine the appropriate model to be applied for this new mode and to judge if the mode library needs to be updated to include the new mode. This analysis is conducted for each phase of the batch cycle for quality prediction. The quality analysis from the perspective of the between-mode relationship inspires the idea of extracting between-mode process information from the historical modes for the new mode, which breaks the traditional idea of treating different process modes separately. Moreover, the model comparison and selection can guarantee the accuracy of the algorithm for quality prediction, and meanwhile the mode-library update is conducted on the basis of necessity rather than blindly embracing all new coming modes.

The rest of this work includes four parts: first, the basic algorithm of PLS modeling based on time slices for three-dimensional data of batch processes is briefly revisited in section 2. Then the proposed method is presented in section 3, including the phase-based single-mode quality regression modeling, between-mode quality regression modeling, model comparison and selection, and online quality prediction. In section 4, the application of the proposed method to a typical multiphase batch process is presented and discussions are conducted based on the illustration results. At last, the conclusion is drawn.

2. PLS MODELING BASED ON TIME SLICES

Batch process data are usually collected as a three-dimensional matrix $\underline{\mathbf{X}}(I \times J_x \times K)$, where I refers to the number of batches, J_x refers to the number of process variables, and K refers to the sample times within each batch. The measurement values of J_y final quality variables in I batches are summarized into a matrix $\underline{\mathbf{Y}}(I \times J_y)$. The variables are first centered and scaled across the batches. After that, the process data and the final qualities are denoted as $\mathbf{X}(I \times J_x \times K)$ and $\mathbf{Y}(I \times J_y)$. The measurement values of all J_x variables at the sampling interval k (k = 1, ..., K) are stored in $\mathbf{X}_k(I \times J_x)$, which is called the kth time slice of $\mathbf{X}$. After splitting $\mathbf{X}(I \times J_x \times K)$ into time slices $\mathbf{X}_k(I \times J_x)$, k = 1, ..., K, as shown in Figure 1, the correlation between the process variables and the quality variables at time interval k can be extracted from matrices $\mathbf{X}_k$ and $\mathbf{Y}$. By applying PLS, time-slice PLS models are achieved as follows:[11]

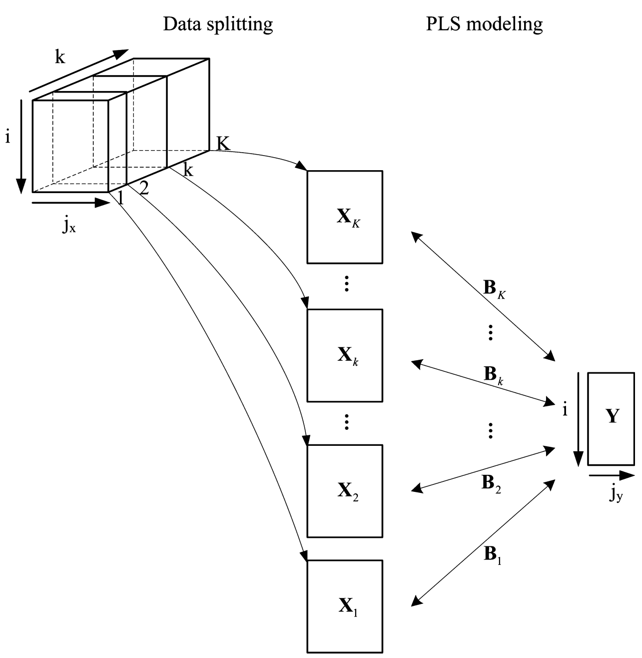

Figure 1. Illustration of PLS modeling based on time slices.

$$\mathbf{X}_k = \mathbf{T}_k\mathbf{P}_k^{\mathrm{T}} + \mathbf{E}_k \tag{1}$$

$$\mathbf{Y} = \mathbf{U}_k\mathbf{Q}_k^{\mathrm{T}} + \mathbf{F}_k \tag{2}$$

The preceding model can be written in regression form as

$$\hat{\mathbf{Y}}_k = \mathbf{X}_k \mathbf{B}_k \quad (3)$$

where $\mathbf{T}_k$ and $\mathbf{U}_k$ are the score matrices, $\mathbf{P}_k$ and $\mathbf{Q}_k$ are the loading matrices, $\mathbf{E}_k$ and $\mathbf{F}_k$ are the residual matrices, and $\mathbf{B}_k$ is the regression parameter matrix with $k = 1, 2, ..., K$. When a single quality variable $\mathbf{y}(I \times 1)$ is considered, the regression model can be simplified as

$$\hat{\mathbf{y}}_k = \mathbf{X}_k \boldsymbol{\beta}_k \quad (4)$$

where $\boldsymbol{\beta}_k$ is the regression parameter, $k = 1, 2 ,..., K$. In the rest of this work, without special introductions, the single quality variable is considered.

To be clear, the time-slice PLS modeling introduced here is indeed utilized to predict the quality obtained only at the end of each batch although the quality predictions are obtained online. The online quality predictions are obtained utilizing the regression relationship between the online process variables and the final quality, of which the basic idea has been proposed and improved in previous works.[11,13,16] In this work, a novel between-mode quality regression method will be proposed based on the time-slice PLS modeling for quality analysis and prediction of multimode multiphase batch processes.

3. METHODOLOGY

Considering the between-mode relationship between the new mode and the historical modes, a new operation mode can be classified as interpolation or extrapolation of the historical modes in the mode library. To achieve this, two models are built for the new mode: the model built purely based on the new mode and the model built based on the new mode together with the historical modes. Then, quality prediction performances of these two models are compared, and the model with the better performance is chosen as the model applied in online quality prediction for the new mode.

3.1. Phase-Based Single-Mode Quality Regression Modeling. In this section, single-mode regression models for the historical modes in the mode library as well as the new mode are established under the multiphase characteristic. The framework of this section is shown in Figure 2, including two steps: (1) phase division and (2) regression modeling for single mode. For concision, in Figure 2, only the time direction (k) and the batch direction (i) of the process data are shown for the illustration of the methodology, and the variable direction (j) is not shown. As shown in Figure 2, after phase division, within each phase, the relationship between process variables and the quality of each single mode among the historical modes as well as the new mode is analyzed and characterized by a regression model. The details are introduced as follows.

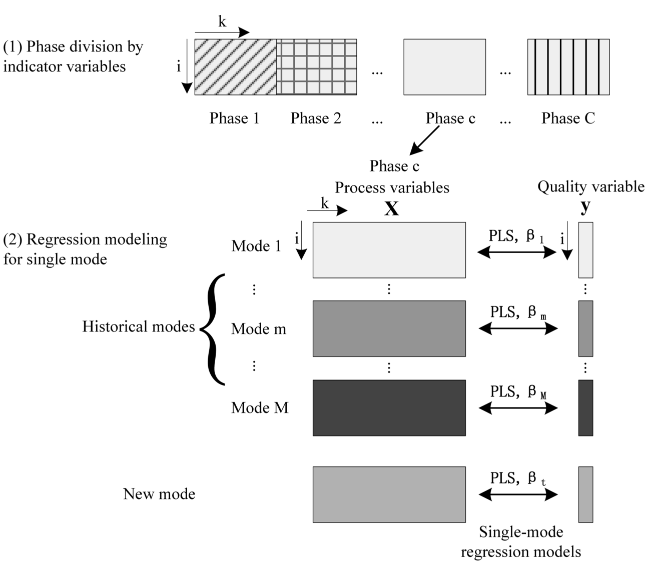

Figure 2. Illustration of phase-based single-mode quality regression modeling.

3.1.1. Phase Division. In phase division, the whole process is divided into multiple phases by indicator variables. The knowledge of a concrete process may be necessary to decide the indicator variables. Although the phases divided by indicator variables may have minor characteristic variation within phases,[19] in this work, to focus on the between-mode quality analysis, the characteristics along the time direction within each phase are assumed to be constant. Besides, it is assumed the batches considered have even durations for the phases within batch cycles as well as the whole batch cycles.

3.1.2. Regression Modeling for Single Mode. Within each phase obtained after phase division, regression models for each single mode among the historical modes as well as the new mode are built in this step. The number of the batches belonging to one mode should be at least twice the number of the process variables to obtain credible statistical analysis results.

First, for each single mode among the historical modes, regression models are built between process variables within phase c, $\mathbf{X}_{m,k}(I_m \times J_x)$, $k = 1, 2, ..., k_c$, and quality $\mathbf{y}_m(I_m \times 1)$ according to eqs 1−4, which have been normalized to have zero mean and unit variance, and the regression parameter $\boldsymbol{\beta}_{m,k}$ belonging to the kth time-slice PLS model is obtained,

$$\hat{\mathbf{y}}_{m,k} = \mathbf{X}_{m,k} \boldsymbol{\beta}_{m,k} \quad (5)$$

where m is the subscript for the historical modes in the mode library, $m = 1, 2, ..., M$.

PLS modeling based on time-slice matrices focuses only on the information at each sampling interval. According to the multiphase characteristic that the process characteristics of time intervals within the same phase are similar, average regression information in each phase is utilized in the prediction model. Considering the phase c, the average regression parameter from time-slice prediction models is used to represent the regression parameter of the prediction model for the whole phase:

$$\boldsymbol{\beta}_{m,c} = \frac{1}{K_c} \sum_{k=1}^{K_c} \boldsymbol{\beta}_{m,k} \quad (6)$$

where $\boldsymbol{\beta}_{m,c}$ is the regression parameter vector of the whole phase c and K_c is the number of the time intervals of the phase c, $k = 1, 2, ..., K_c$. Then the quality prediction for each time interval is obtained,

$$\hat{\mathbf{y}}_{m,c,k} = \mathbf{X}_{m,k} \boldsymbol{\beta}_{m,c} \quad (7)$$

To be clear, c is the subscript for phase c, $c = 1, 2, ...,$ C. Since the following analysis is based on phase division and takes phase c for example, to avoid overuse, subscript c is only used to describe the variables which represent the average characteristic of a whole phase (e.g., $\boldsymbol{\beta}_{m,c}$) or are obtained from those variables representing the average characteristic of a whole phase (e.g., $\hat{\mathbf{y}}_{m,c,k}$), whereas the other variables are not labeled by subscript c although they also belong to phase c (e.g., $\boldsymbol{\beta}_{m,k}$ or $\mathbf{X}_{m,k}$). Besides, to focus on the between-mode quality analysis, the problem of transitions between phases for quality prediction is not

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analyzed in this work, of which detailed analysis can be found in ref 16.

For the new mode with normalized process variables within phase c, $\mathbf{X}_{t,k}(I_t \times J_x)$, $k = 1, 2, ..., K_c$, and quality $\mathbf{y}_t(I_t \times 1)$, the same strategy as before is adopted and similar equations are obtained,

$$\hat{\mathbf{y}}_{t,k} = \mathbf{X}_{t,k}\boldsymbol{\beta}_{t,k} \tag{8}$$

$$\boldsymbol{\beta}_{t,c} = \frac{1}{K_c}\sum_{k=1}^{K_c}\boldsymbol{\beta}_{t,k} \tag{9}$$

$$\hat{\mathbf{y}}_{t,c,k} = \mathbf{X}_{t,k}\boldsymbol{\beta}_{t,c} \tag{10}$$

where t is the subscript for the new mode which is the target of this investigation.

3.2. Between-Mode Quality Regression Modeling. After building models representing the quality-related information on each mode, in this section, by analyzing the regression relationship between process variables and the quality of the new mode through the regression models of the historical modes, a novel between-mode quality regression model is built for the new mode. The model is built on the basis of not only the new mode but also the historical modes in the mode library. The framework of this section is shown in Figure 3, where, like Figure 2, only the time direction (k) and the batch direction (i) of the process data are shown for concision.

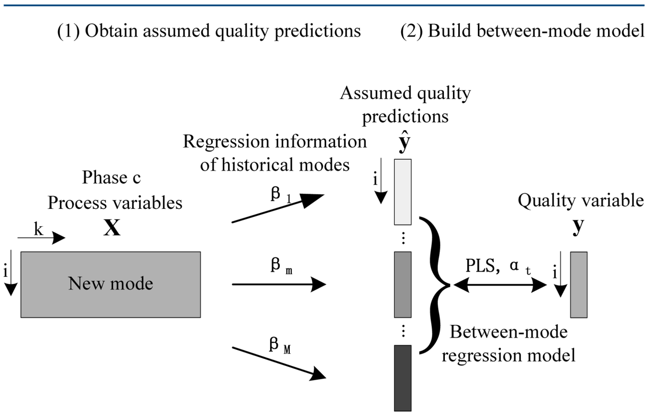

Figure 3. Illustration of between-mode quality regression modeling.

As shown in Figure 3, first, (1) the regression models of the historical modes are used to get a series of assumed quality predictions for the new mode, and then (2) the regression relationship between these assumed predictions and the real quality of the new mode is extracted by the between-mode model. These two steps establish the relationship between the new mode and the historical modes, where the useful information (if any) from the historical modes can be obtained and applied in quality regression for the new mode.

The details of between-mode regression modeling are introduced as follows.

For the new mode with normalized process variables within phase c, $\mathbf{X}_{t,k}$, and quality $\mathbf{y}_t$, process variables are first applied to the regression models obtained for the historical modes by eq 5 to get the assumed quality predictions,

$$\hat{\mathbf{y}}_{t,m,k} = \mathbf{X}_{t,k}\boldsymbol{\beta}_{m,k} \tag{11}$$

where t is the subscript for the new mode, m is the subscript for the historical modes in the mode library, $m = 1, 2, ..., M$. It should be noted that $\hat{\mathbf{y}}_{t,m,k}$ are called assumed quality predictions because $\hat{\mathbf{y}}_{t,m,k}$ are not quality predictions in the traditional concept. The regression models of the historical modes, $\boldsymbol{\beta}_{m,k}$, are not the actual regression model for the new mode, and when process variables of the new mode, $\mathbf{X}_{t,k}$, are applied to $\boldsymbol{\beta}_{m,k}$, there is an underlying assumption that $\mathbf{X}_{t,k}$ can be regressed by $\boldsymbol{\beta}_{m,k}$. Here, obtaining assumed quality predictions links the new mode variables to the historical modes, and whether each historical mode is valuable in the between-mode relationship will be further measured by the regression parameter in the next step.

Then, all these assumed predictions of the historical modes can comprise a new matrix $\mathbf{Z}_{t,k}(I_t \times M)$, $\mathbf{Z}_{t,k} = [\hat{\mathbf{y}}_{t,1,k},...,\hat{\mathbf{y}}_{t,m,k},...,\hat{\mathbf{y}}_{t,M,k}]$. Time-slice PLS regression models are built between $\mathbf{Z}_{t,k}$ and $\mathbf{y}_t$ by the same principle in eq 1 through eq 4, and novel predictions are obtained,

$$\hat{\mathbf{y}}^*_{t,k} = \mathbf{Z}_{t,k}\boldsymbol{\alpha}_{t,k} \tag{12}$$

where * indicates this new regression relationship of the new mode based on between-mode relationship analysis and $\boldsymbol{\alpha}_{t,k}$ is the regression parameter vector belonging to the kth time-slice PLS model, $k = 1, 2, ..., K_c$. By $\boldsymbol{\alpha}_{t,k}$, the relationship between each historical mode and the new mode is represented in quality prediction.

For a phase c, similar to $\boldsymbol{\beta}_{m,c}$, the average regression parameter of these time-slice prediction models is used to represent the regression parameter of the prediction model for the whole phase c:

$$\boldsymbol{\alpha}_{t,c} = \frac{1}{K_c}\sum_{k=1}^{K_c}\boldsymbol{\alpha}_{t,k} \tag{13}$$

where K_c is the number of the time intervals within phase c. Then the perditions, $\hat{\mathbf{y}}^*_{t,c,k}$, based on the regression parameter of the whole phase, $\boldsymbol{\alpha}_{t,c}$, are obtained,

$$\hat{\mathbf{y}}^*_{t,c,k} = \mathbf{Z}_{t,k}\boldsymbol{\alpha}_{t,c} \tag{14}$$

According to eq 8 through eq 10 and eq 11 through eq 14, two kinds of models are built and two quality predictions for the new mode can be obtained. One is on the basis of purely the new mode, and the other one is on the basis of the new mode together with the historical modes. To be clear, these two models are called "single-mode model" and "between-mode model" in the rest of this work, respectively. Both the single-mode model and between-mode model should be trained by enough batches within each mode, and the basic difference between single-mode model and between-mode model is the modes involved in modeling, a single mode or multiple modes.

The novel modeling algorithm proposed here for the latter model is a trial procedure since there is uncertainty whether the information in the historical modes is significant to the new mode or not. However, this method inspires a new way to dig information from multimode process data, and it is sure that if the information in the historical mode is significant to the new mode, it will be well extracted by the regression model and the more valuable the information is, the more it will enhance the model precision for quality regression. The model precision of the between-mode model will be compared with the precision of the single-mode model to select the model for quality prediction in the next step.

3.3. Model Comparison and Selection. After building two models for the new mode, in this section, these two models are compared and one is selected as the regression model for quality prediction. The flow diagram is shown in Figure 4. The basic idea is first to compare the prediction performances of the two models and then select the one with better predictions as the quality prediction model. The mode library updating depends on the model comparison result. If the two models have similar performances, which means the historical modes have as much information for the new mode as the new mode itself, then the between-mode regression model based on the historical modes should be applied and the mode library does not need to be updated. If the two models have different performances, the one with better performance should be selected as the prediction model considering the accuracy of quality prediction. That is, when it is the single-mode model that provides better predictions, the mode library needs to be updated to include the new mode in it. If it is the between-mode model that provides better predictions, the mode library does not need to be updated. The detailed model comparison and selection procedures are introduced as follows.

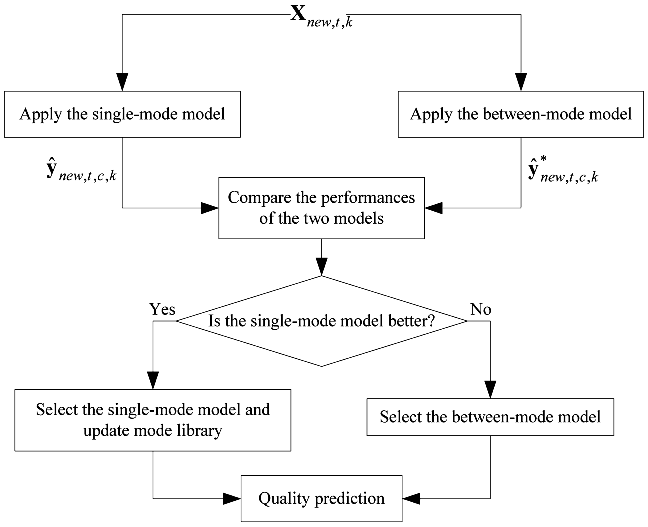

Figure 4. Flow diagram of model comparison and selection for quality prediction.

First, for new coming batches of the new mode with normalized process variables $\mathbf{X}_{\mathrm{new},t,k}(I_{\mathrm{new}} \times J_x)$, $k = 1, 2, ..., K_c$, and quality $\mathbf{y}_{\mathrm{new},t}(I_{\mathrm{new}} \times 1)$, two quality predictions, $\hat{\mathbf{y}}_{\mathrm{new},t,c,k}$ and $\hat{\mathbf{y}}^*_{\mathrm{new},t,c,k}$, are obtained for the kth time interval by applying the single-mode model and the between-mode model using eq 10 and eq 11 through eq 14, respectively,

$$\hat{\mathbf{y}}_{\mathrm{new},t,c,k} = \mathbf{X}_{\mathrm{new},t,k}\boldsymbol{\beta}_{t,c} \tag{15}$$

$$\begin{aligned} \hat{\mathbf{y}}_{\mathrm{new},t,m,k} &= \mathbf{X}_{\mathrm{new},t,k}\boldsymbol{\beta}_{m,k} \\ \mathbf{Z}_{\mathrm{new},t,k} &= [\hat{\mathbf{y}}_{new,t,1,k}, ..., \hat{\mathbf{y}}_{\mathrm{new},t,m,k}, ..., \hat{\mathbf{y}}_{\mathrm{new},t,M,k}] \\ \hat{\mathbf{y}}^*_{\mathrm{new},t,c,k} &= \mathbf{Z}_{\mathrm{new},t,k}\boldsymbol{\alpha}_{t,c} \end{aligned} \tag{16}$$

where $\hat{\mathbf{y}}_{\mathrm{new},t,c,k}$ is obtained based on the regression parameter of the new mode, $\boldsymbol{\beta}_{t,c}$, the assumed quality predictions of the historical modes, $\hat{\mathbf{y}}_{\mathrm{new},t,m,k}$, $m = 1, 2, ..., M$, comprise a matrix, $\mathbf{Z}_{new,t,k}$, and the final prediction based on the historical modes, $\hat{\mathbf{y}}^*_{\mathrm{new},t,c,k}$, is obtained by the phase-average regression parameter $\boldsymbol{\alpha}_{t,c}$ between the assumed quality predictions of the historical modes and the quality.

Then, the root-mean-square error (RMSE) values are calculated for the kth time interval within the ch phase between the predictions, $\hat{\mathbf{y}}_{\mathrm{new},t,c,k}$ and $\hat{\mathbf{y}}^*_{\mathrm{new},t,c,k}$, and the real quality, $\mathbf{y}_{\mathrm{new},t}$,

$$\mathrm{RMSE}_{c,k} = \sqrt{\frac{1}{I_{\mathrm{new}}}\sum_{i=1}^{I_{\mathrm{new}}}(y_{\mathrm{new},t,i} - \hat{y}_{\mathrm{new},t,i,c,k})^2} \tag{17}$$

$$\mathrm{RMSE}^*_{c,k} = \sqrt{\frac{1}{I_{\mathrm{new}}}\sum_{i=1}^{I_{\mathrm{new}}}(y_{\mathrm{new},t,i} - \hat{y}^*_{\mathrm{new},t,i,c,k})^2} \tag{18}$$

where i is the index for the batch, $i = 1, 2, ..., I_{\mathrm{new}}$, $y_{\mathrm{new},t,i}$, $\hat{y}_{\mathrm{new},t,i,c,k}$, and $\hat{y}^*_{\mathrm{new},t,i,c,k}$ are the ith elements of $\mathbf{y}_{\mathrm{new},t}$, $\hat{\mathbf{y}}_{\mathrm{new},t,c,k}$, and $\hat{y}^*_{\mathrm{new},t,c,k}$, $k = 1, 2, ..., K_c$.

Then, these two series, $\mathrm{RMSE}_{c,k}$ and $\mathrm{RMSE}^*_{c,k}$, $k = 1, 2, ..., K_c$, are compared by the paired t test of the hypothesis that two matched samples come from distributions with equal means. $H = 0$ indicates that the null hypothesis cannot be rejected, which means the predictions of these two models have similar accuracies. $H = 1$ indicates that the null hypothesis can be rejected, which means the predictions of these two models have different accuracies; that is, one model is better than the other. Different H values lead to different model selection strategies:

3.3.1. H = 0. The two models have similar performances for quality prediction; that is, the between-mode regression model could provide predictions which are as good as those the single-mode model provides, which means the historical modes have enough information for the new mode. Although sharing similar performances means either of the two models is applicable, considering the saving space burden of the mode library and the efficiency of mode library updating, it is suggested to select the between-mode model rather than the single-mode model. Therefore, the mode library does not need to be updated. Moreover, the new mode should be classified as the interpolation of the historical modes.

3.3.2. H = 1. The two models have different performances: thus, the one with better performance should be selected as the prediction model considering the accuracy of quality prediction.

To compare the performances and determine which model is better, the mean of RMSE values are calculated along the time direction for phase c,

$$\mathrm{RMSE}_{c,\mathrm{mean}} = \frac{1}{K_c}\sum_{i=1}^{K_c}\mathrm{RMSE}_{c,k} \tag{19}$$

$$\mathrm{RMSE}^*_{c,\mathrm{mean}} = \frac{1}{K_c}\sum_{i=1}^{K_c}\mathrm{RMSE}^*_{c,k} \tag{20}$$

where K_c is the number of the time intervals of phase c.

Compare $\mathrm{RMSE}_{c,\mathrm{mean}}$ and $\mathrm{RMSE}^*_{c,\mathrm{mean}}$, and then select the model with lower value as the regression model for quality prediction.

3.3.2.1. $RMSE_{c,mean} > RMSE^*_{c,mean}$. When the between-mode model provides better predictions, it means that the historical modes have valuable quality-relative information for the new mode, but the single-mode model does not have that information. This is possible because the single-mode model may be limited to the available batches of the new mode and does not cover all valuable quality-related information for the new mode, which the historical modes have. Therefore, the new mode should be classified as the interpolation of the historical modes. To use the valuable quality-related information, the between-mode model should be applied and the mode library does not need to be updated.

3.3.2.2. $RMSE_{c,mean} < RMSE^{*}_{c,mean}$. When the single-mode model provides better predictions, it means that the historical modes do not have valuable quality-relative information for the new mode, but the single-mode model can extract this information from the available batches of the new mode. Thus, the new mode should be classified as the extrapolation of the historical modes and the single-mode model should be applied and the mode library needs to be updated to include the new mode.

As shown in Figure 4, after the comparison, the selected model with better performance will be utilized as the regression model for quality prediction. To be clear, no matter which model performs better, no more batches are needed to retrain the model since generally the models have been trained by enough batches and are deemed to be able to capture the quality information within the single mode or the multiple modes.

3.4. Online Quality Prediction. After the selection of the quality regression model from the single-mode model and the between-mode model, the selected model will be applied online to new observations of the new mode for quality prediction. For the two possible situations, the online quality prediction for the new observation at the kth time interval, $\mathbf{x}_{\mathrm{new},k}(1 \times J_x)$, which is normalized by the mean and standard deviation calculated from training data of the new mode, is conducted as follows, and the current phase c can be determined by the time index.

If the single-mode model is selected, the prediction for the new sample $\mathbf{x}_{\mathrm{new},k}$ is calculated based on the average regression parameter of the current phase c, $\boldsymbol{\beta}_{t,c}$,

$$\hat{y}_{\mathrm{new},c,k} = \mathbf{x}_{\mathrm{new},k}\boldsymbol{\beta}_{t,c} \tag{21}$$

If the between-mode model is selected, the prediction for the new sample $\mathbf{x}_{\mathrm{new},k}$ is calculated through the regression models for the historical modes,

$$\begin{aligned} \hat{y}_{\mathrm{new},m,c,k} &= \mathbf{x}_{\mathrm{new},k}\boldsymbol{\beta}_{m,c} \\ \mathbf{z}_{\mathrm{new},k} &= [\hat{y}_{\mathrm{new},1,c,k}, ..., \hat{y}_{\mathrm{new},m,c,k}, ..., \hat{y}_{\mathrm{new},M,c,k}] \\ \hat{y}_{\mathrm{new},c,k} &= \mathbf{z}_{\mathrm{new},c,k}\boldsymbol{\alpha}_{t,c} \end{aligned} \tag{22}$$

where the assumed quality predictions of the historical modes, $\hat{y}_{\mathrm{new},m,c,k}$, $m = 1, 2, ..., M$, comprise a vector $\mathbf{z}_{\mathrm{new},k}$ and the final prediction, $\hat{y}_{\mathrm{new},c,k}$, is obtained by the phase-average regression parameter $\boldsymbol{\alpha}_{t,c}$ of the between-mode model.

4. ILLUSTRATION AND DISCUSSION

4.1. Process Description. The proposed algorithm is illustrated by a typical multiphase batch process, injection molding, which is an important manufacturing process. Figure 5 shows a simplified schematic diagram of an injection molding machine. 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 until the part becomes sufficiently rigid for ejection. Besides, plasticization takes place in the barrel in the early cooling phase, where polymer is melted and conveyed to the barrel front by screw rotation, preparing for the next cycle. It can be readily implemented for experiments, in which, all key process conditions such as the

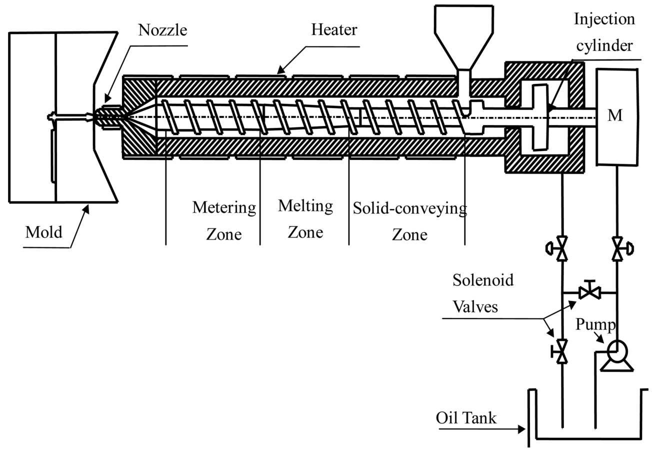

Figure 5. Simplified schematic diagram of injection molding machine.

temperatures, pressures, displacement, and velocity can be online measured by their corresponding transducers, providing abundant process information.[29,30] A one-dimension index, mass (g), is chosen to evaluate the product quality, whose real values can be directly measured by instruments.

The material used in this work is high-density polyethylene (HDPE). Ten process variables and one quality variable as shown in Table 1 are selected for modeling. In this work, the

Table 1. Process Variables for Injection Molding Start-up Process

	description	unit
process variable no.		
1	SV1 opening	%
2	SV2 opening	%
3	screw velocity	mm/s
4	ejector stroke	mm
5	mold stroke	mm
6	mold velocity	mm/s
7	injection pressure	bar
8	barrel temperature 1	°C
9	barrel temperature 2	°C
10	barrel temperature 3	°C
quality variable no.		
1	mass	g

injection velocity is set at 25 mm/s, and different operation modes are obtained by setting the packing pressure (PP) and barrel temperature (BT) at different values. Detailed experiment settings of operation modes are listed in Table 2. Thirty batches are obtained for each mode. All batches have been synchronized so the time index k can indicate the location of each time interval along the time direction.

4.2. Phase-Based Quality Regression Modeling. Phase division is implemented to divide a batch cycle into phases. Using indicator variables, each batch cycle can be divided into four phases. Two process variables, screw velocity and the SV1 (servo-valve 1) opening, which are respectively the third and the first process variables listed in Table 1, are chosen to be indicator variables based on process knowledge. When the value of screw velocity is not zero, it means the screw moves forward, revealing the starting of one batch cycle. Meanwhile, the SV1 opening can be used to indicate the end of a batch cycle. Screw velocity can indicate the switch points of phases. In

Table 2. Different Operation Modes Caused by Different Settings of Packing Pressure (PP) and Barrel Temperature (BT)

	for given settings	
mode	PP (bar)	BT (°C)
mode 1	25	180
mode 2	30	180
mode 3	35	180
mode 4	25	200
mode 5	30	200
mode 6	35	200

Figure 6, the phase division results are illustrated by one random batch in the training group and the four phases (I–IV)

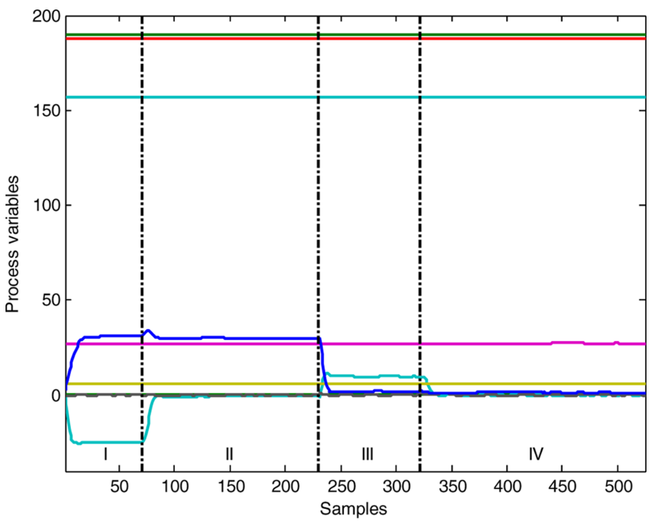

Figure 6. Process trajectories and phase division results (solid lines refer to the process trajectories; dashed–dotted lines refer to the phase boundaries of (I) injection phase, (II) packing–holding phase, (III) plasticization phase, and (IV) cooling phase).

are separated from each batch process, injection, packing–holding, plasticization, and cooling.

After phase division, for each phase, single-mode regression models for each historical mode as well as the new mode are established based on each mode alone. Moreover, between-mode regression model for the new mode is established based on the new mode together with the historical modes. The prediction performances of these two models for the new mode are compared in the next section.

4.3. Model Comparison and Selection. To illustrate the proposed algorithm, three typical cases are discussed in this part. Considering the possible situations, mode 1, mode 2, and mode 3 listed in Table 2 are investigated in both case 1 and case 2, whereas the arrangements of the new mode and the historical modes are different. In case 3, mode 4, mode 5, and mode 6 are utilized and the situation in which only limited batches are obtained for the new mode is investigated. The details are as follows.

In case 1, mode 1 and mode 3 are considered as the historical modes in the mode library and mode 2 is considered as the new mode. This case is used to find out whether mode 2, which has a PP value set in the middle of the PP values of mode 1 and mode 3, as shown in Table 2, can be represented by the information extracted from mode 1 and mode 3. The analysis results evaluated of two RMSE values along the time direction are shown in Figure 7, for which the paired t test shows $H = 1$

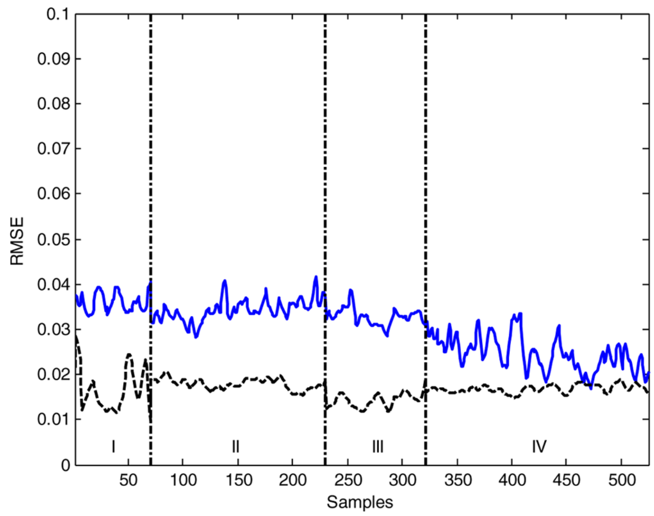

Figure 7. RMSE values along the time direction for case 1 (solid line refers to the results of the between-mode model; dashed line refers to the results of single-mode model; dotted–dashed lines refer to the phase boundaries of phases I–IV).

for all four phases. It means that the predictions of the two models have different performances within the four phases, and the one with better performance should be selected as the prediction model considering the accuracy of quality prediction. From Figure 7, the RMSE values of the between-mode model are higher than those of the single-mode model, which is confirmed by the mean of RMSE values along the time direction calculated for each phase listed in Table 3, where all

Table 3. Mean RMSE Values along Time Direction within Four Phases (I–IV) of Between-Mode Model and Single-Mode Model for Case 1

	mean RMSE along time direction			
model	I	II	III	IV
between-mode model	0.0360	0.0343	0.0328	0.0247
single-mode model	0.0168	0.0179	0.0143	0.0168

mean RMSE values for the four phases of the between-mode model are higher than those of the single-mode model. Consequently, it can be concluded that the single-mode model provides better predictions than the between-mode model, and this single-mode model should be used as the quality prediction model for online quality prediction for the new mode. This analysis result shows that although mode 2 has the PP value set in the middle of the PP values of mode 1 and mode 3, it cannot be represented by the quality-related information extracted from mode 1 or mode 3 for quality regression. Therefore, mode 2 is classified as the extrapolation of mode 1 and mode 3, and to include the information on mode 2, the mode library needs to be updated.

In case 2, modes 1 and 2 are considered as the historical modes and mode 3 is considered as the new mode. This case is similar to case 1 and used to find out whether an analysis result similar to the result of case 1 can be obtained, that is, whether mode 3 cannot be represented by the information extracted from mode 1 or mode 2. The analysis results evaluated by two

RMSE values along the time direction are shown in Figure 8, for which the paired t test shows $H = 1$ for the first three phases, but for the fourth phase, $H = 0$. For the first three phases, from Figure 8, the RMSE values of the between-mode model are lower than those of the new-mode model, and for the fourth phase, these two RMSE values are very near to each other. This is confirmed by the mean of RMSE values calculated for each phase listed in Table 4, where for the first three phases, the two mean RMSE values have big differences, whereas for the fourth phase the two mean RMSE values are very near. It can be concluded that in general the between-mode model provides better predictions than the single-mode model, so the between-mode model should be used as the quality prediction model for online quality prediction for the new mode. Therefore, in this case, it can be concluded that mode 1 and mode 2 have valuable quality-related information for mode 3, and mode 3 is the interpolation of mode 1 and mode 2.

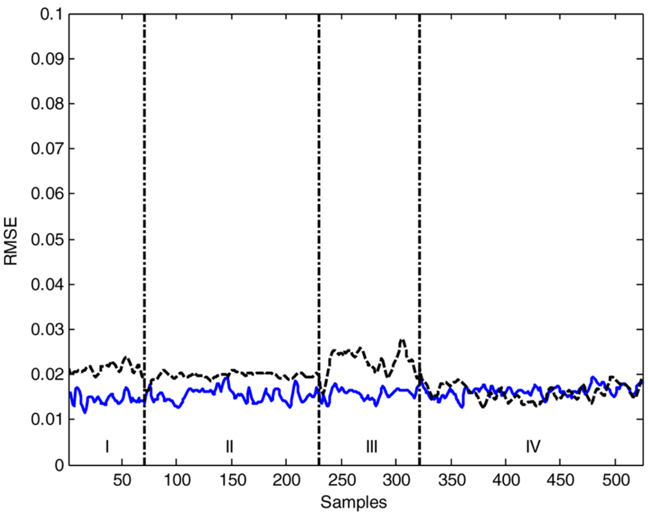

Figure 8. RMSE values along the time direction for case 2 (solid line refers to the results of the between-mode model; dashed line refers to the results of the single-mode model; dotted−dashed lines refer to the phase boundaries of phases I−IV).

Table 4. Mean RMSE Values along Time Direction within Four Phases (I−IV) of Between-Mode Model and Single-Mode Model for Case 2

model	mean RMSE along time direction I	II	III	IV
between-mode model	0.0145	0.0154	0.0157	0.0163
single-mode model	0.0213	0.0197	0.0228	0.0160

It should be noted that although this case is similar to case 1, the conclusion is opposite to case 1. Comparing the conclusion of case 2, which is that mode 1 and mode 2 have valuable quality-related information for mode 3, with the conclusion of case 1, which is that mode 1 and mode 3 do not have valuable quality-related information for mode 2, it shows that mode 2 is more informative and representative than mode 3 in quality prediction. Therefore, the quality-related information from mode 2 is more important than mode 3 and more attention should be paid to mode 2 than mode 3 in quality analysis. Besides, attention should be paid to the difference of the fourth phase from the other phases in case 2. The similar RMSE values along the time direction within the fourth phase of these two models reveal that the quality-related information extracted from the new mode and the historical multiple modes are similar and have similar impacts on quality prediction. Since the only difference between the new mode and the historical modes is the PP settings, it can be inferred that the setting difference between different modes does not impact quality prediction performances for the fourth phase so much as the other phases. This is actually consistent with the process knowledge that the fourth phase, the cooling phase, during which the plastic in the mold cools and turns solid until being ejected out from the mold, indeed has no manipulated variables which can directly impact the considered quality, mass, after the mold gate freezing.[16] Therefore, the similarity of the RMSE values along the time direction within the fourth phase of these two models is possible and reasonable.

In case 3, mode 4, mode 5, and mode 6 are considered as the historical modes and a few new batches of mode 6 are obtained and considered as the new mode. However, the number of new batches is limited, which means generally the single-mode regression model could not represent the quality-related relationship of mode 6 well. This case is used to test whether the information on mode 6 existing in the mode library can be found out by the between-mode model and can help provide better quality prediction performance than the single-mode model. The analysis results evaluated by two RMSE values along the time direction are shown in Figure 9, for which the paired t test shows $H = 1$ for all four phases. It can be seen in Figure 9 that the two models have different performances, and the one with better performance should be selected as the prediction model. The means of RMSE values calculated for each phase are listed in Table 5. Clearly, all the mean RMSE values of the between-mode model are lower than those of the single-mode model, which means that the between-mode model provides better predictions than the single-mode model, so the new batches of mode 6 are identified belonging to a mode which is the interpolation of mode 4, mode 5 and mode 6, and the mode library does not need to be updated. This

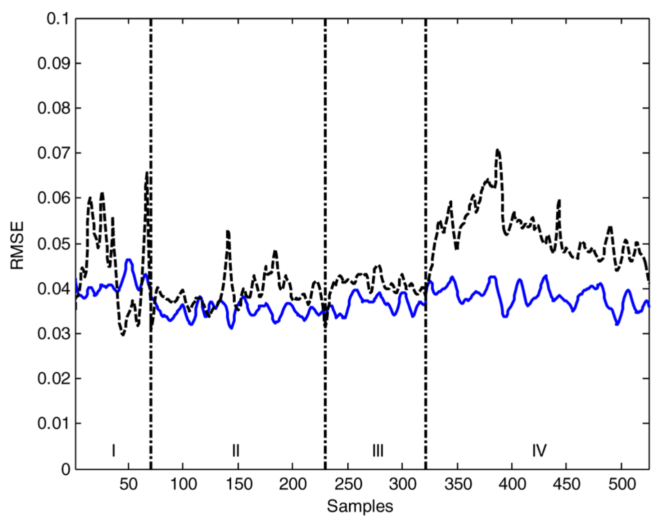

Figure 9. RMSE values along the time direction for case 3 (solid line refers to the results of the between-mode model; dashed line refers to the results of single-mode model; dotted−dashed lines refer to the phase boundaries of phases I−IV).

Table 5. Mean RMSE Values along Time Direction within Four Phases (I−IV) of Between-Mode Model and Single-Mode Model for Case 3

model	mean RMSE along time direction			
	I	II	III	IV
between-mode model	0.0409	0.0350	0.0365	0.0383
single-mode model	0.0444	0.0389	0.0410	0.0523

analysis result is consistent with the common thought that the model based on limited batches in general cannot represent a quality regression relationship well, but the model based on mode library with enough batches can. Through the analysis, the new mode with limited batches is matched with the information which already exists in the mode library, and consequently, the prediction accuracy is improved compared with using the single-mode model with the quality-related information only from the limited batches.

4.4. Online Quality Prediction. After model comparison and selection, the selected model is used as the quality prediction model and online quality predictions can be obtained. To illustrate the effectiveness of the model comparison and selection in this work, quality prediction is conduced online for some new batches of the new modes in the three cases mentioned in last section, and the results of the selected method compared with the other one are evaluated by RMSE of all time intervals $(\sum_{i=1}^{I_{ts}} K_{i,c})$ within the cth phase of these I_{ts} testing batches. The results are listed in Table 6a−c for case 1 to case 3, respectively. To be clear, the selected methods for the three cases are emphasized in bold type in Table 6. Take case 1, for example; based on the analysis about Figure 7 and Table 3 in the last section, it has been concluded that the single-mode model provides better prediction performance than the between-mode model, so the single-mode model is selected as the prediction model and it is in bold type in Table 6a. It can be seen that all RMSE values of the single-mode model for the four phases are lower than those of the between-mode model. So, from the comparison of the quality performance between these two models, the better performance of the single-mode model is confirmed; that is, the selected model after model comparison and selection illustrates the better performance for new coming batches of the new mode. For case 2 and case 3, similar conclusions can be obtained from Table 6b,c. Therefore, it can be concluded the algorithm proposed in this work can provide satisfactory online quality prediction results.

Table 6. RMSE of online quality predictions within four phases (I−IV) of between-mode model and single-mode model for (a) case 1, (b) case 2, and (c) case 3

model	RMSE			
	I	II	III	IV
(a) Case 1				
between-mode model	0.0445	0.0409	0.0394	0.0309
single-mode model	**0.0213**	**0.0237**	**0.0176**	**0.0227**
(b) Case 2				
between-mode model	**0.0216**	**0.0222**	**0.0199**	**0.0202**
single-mode model	0.0303	0.0264	0.0276	0.0239
(c) case 3				
between-mode model	**0.0196**	**0.0168**	**0.0168**	**0.0152**
single-mode model	0.0370	0.0225	0.0185	0.0317

In conclusion, the proposed novel between-mode regression modeling provides a new way to extract quality-related information from a mode library. And after the comparison and selection between the between-mode model and the new-mode model, the selected model can guarantee satisfactory prediction performance. Meanwhile, valuable information for mode library update can be provided.

It should be noted only normal batches in different modes are utilized in this work while a faulty batch problem is not discussed. Fault detection is another important research direction for batch processes, and it is achievable to detect a faulty batch from normal batches.[9,10,25] However, a faulty batch often happens accidentally due to some unexpected factor, which means in general the situation of a faulty batch does not repeat itself stably for several batches to comprise a normal mode. Thus, to focus on the between-mode quality analysis originally proposed in this work, it is assumed that each mode comprised of a number of stable batches is normal. And the main contribution of this work is to analyze the quality-related relationship between a new normal mode and the historical normal modes in a mode library for quality prediction. Considering the space limitations, the faulty batch problem is not discussed in this work. But it is still interesting to deal with this problem in the future as an extension of this work.

5. CONCLUSION

In the present work, a multimode quality analysis based on between-mode analysis is proposed for multiphase batch processes. For each phase, a between-mode quality regression model is established based on the new mode and the historical modes in the mode library, which is compared with the regression model purely based on the new mode. After comparison, the model with better prediction performance is selected as the quality prediction model. Consequently, online quality prediction is performed based on the selected model. Meanwhile, the mode library is updated when necessary according to between-mode quality analysis. In the application to the injection molding process with multiple operation modes, the proposed strategy works well for between-mode quality analysis and quality prediction.

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Notes

The authors declare no competing financial interest.

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