ACS OMEGA

http://pubs.acs.org/journal/acsodf

Article

Dynamic Batch Process Monitoring Based on Time-Slice Latent Variable Correlation Analysis

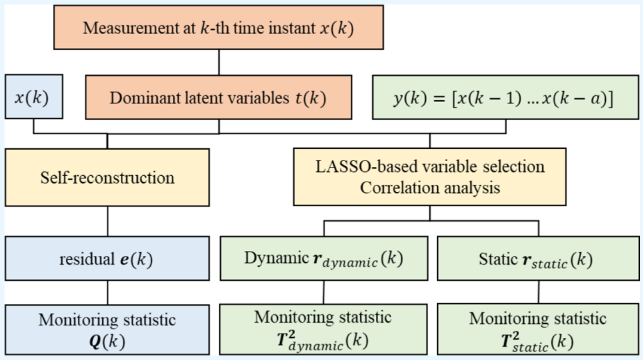
Le Du, Wenhao Jin, Yang Wang, and Qingchao Jiang*

Cite This: *ACS Omega* 2022, 7, 41069–41081

Read Online

ACCESS | Metrics & More | Article Recommendations

ABSTRACT: Batch processes are generally characterized by complex dynamics and remarkable data collinearity, thereby rendering the monitoring of such processes necessary but challenging. This paper proposes a data-driven time-slice latent variable correlation analysis-based model predictive fault detection framework to ensure accurate fault detection in dynamic batch processes. The three-way batch process data are first unfolded into the two-way time slice. For each single time slice, process data are mapped to both major latent variables and residual subspaces to deal with the variable-wise data collinearity and extract dominant data information. A measurement status is then determined with a canonical correlation analysis of the major latent variables and correlated variables, using both the time and batch perspectives. Prediction-based residuals are generated, which provide the basis for identifying the property of faults detected, namely, static or dynamic. Based on experiments using a simulated penicillin production and an industrial inject molding process, the proposed monitoring scheme has been proven feasible and effective.



1. INTRODUCTION

Batch processes take a significant part in producing high value-added products, and batch process monitoring is important in keeping favorable operation conditions.[1−3] For one thing, the complex reaction or process characteristic makes the establishment of a mathematical model difficult, and this problem limits the usage of the model-based monitoring approach.[4] For another, with the further development of data acquisition technology, mass of process data can be obtained. Data-driven process monitoring, especially the multivariate statistical process monitoring (MSPM) methods, becomes popular.[5−9]

Principal component analysis (PCA), partial least squares (PLS), and canonical correlation analysis (CCA) are three MSPM approaches that have been widely used recently.[10−14] Batch processes can be analyzed using multiway PCA (MPCA) and multiway PLS (MPLS), and time-slice CCA methods had been developed. The MPCA method unfolds three-way batch process data into two-way, on which PCA is then performed.[15] The variable-wise correlation is considered by projecting the process data into both dominant and residual subspaces. MPLS also requires the conversion of three-way data to two-way and then carries out the PLS between the latter and the quality variables.[16] Process data are then projected into a quality relevant subspace for process monitoring. Time-slice CCA characterizes the relationship between different operation units and is used for monitoring the key operation unit.[17] The effectiveness of these methods had been demonstrated. However, the complex dynamics in batch processes is not thoroughly explored and characterized by these methods.

To deal with process dynamics, various dynamic process monitoring methods were proposed.[18−20] For dynamic batch processes, multiway dynamic monitoring methods were proposed,[21,22] among which dynamic MPCA, dynamic MPLS, and dynamic CCA methods are the most extensively used.[23,24] In order to mine dynamic characteristic of the batch process, a two-dimensional localized dynamic support vector data description method is proposed, and this method also mines the local behavior of process data well.[25] In dynamic monitoring methods, the correlation in the time series is explored. To characterize the correlation in both the time and batch directions, two-dimensional monitoring models such as two-dimensional dynamic PCA and PLS were developed.[26,27] A two-dimensional deep correlated representation learning method was also proposed to solve the problem of dynamics and nonlinearity; on the basis of data slicing, a stacked autoencoder-based deep neural network is constructed to

Received: July 14, 2022
Accepted: September 19, 2022
Published: October 31, 2022

characterize the correlation among the process variables, effectively improving the monitoring performance.[28] Recently, a multiobjective two-dimensional CCA monitoring method was proposed.[24] By comparing the correlation information from the previous samples and previous batches, the status of a measurement can be examined. In addition, the related methods of neural networks have also been applied to deal with data with nonlinear and dynamic properties; in a deep autoencoder thermography method, the layer-by-layer feature visualization reveals how the model extracts defect features.[29] However, the following deflects require further discussion. First, high collinearity may exist in the variable-wise data, which may cause inefficiency of conventional CCA methods.[30] Second, the stochastic optimization method is used to select the most correlated variables and is considerably computationally expensive, which makes establishing the time-slice monitoring model inappropriate. Third, the property of a detected fault is not identified (a dynamic-related fault or a static fault).

This study proposes a data-driven time-slice latent variable correlation analysis-based model predictive fault detection approach for efficient dynamic batch process monitoring. Compared to the existing methods, this study solved the problem of time-slice data collinearity. Variable selection using the least absolute shrinkage and selection operator (LASSO) method reduces the computational cost, and the property of detecting faults is distinguished. The novelty and contributions are summarized as follows:

(1) The three-way data are unfolded into the two-way time slice, and the measurements are mapped to both major latent variables and residual subspaces, addressing variable-wise collinearity. Then, the correlation between a measurement and previous samples is analyzed in the dominant subspace, through which the process dynamics is characterized. The correlation between the current and prior time slices is used to evaluate the status of a sample.

(2) LASSO is employed to efficiently select variables that are suitable for prediction from the time perspective and batch perspective. The computational cost of this method is significantly lower than the existing selection methods based on random optimization.

(3) Prediction-based fault detection residual is generated. It is further divided into two categories: dynamic and static. Following that, the properties of a detected fault are determined.

(4) Theoretical analysis and experiments demonstrate the feasibility and superiority of the proposed monitoring scheme.

The rest of this article is presented in the following structure. Section 2 reviews the basic CCA process monitoring for batch processes. Section 3 details the proposed model predictive batch process monitoring method. Then, Section 4 conducts the two experimental studies. Finally, Section 5 presents the conclusions and discussions.

2. PRELIMINARIES AND PROBLEM FORMULATION

2.1. CCA-Based Batch Process Monitoring. CCA is a classical multivariate statistical analysis method for exploring and characterizing the correlation between two parts of random variables. Given random variables $\boldsymbol{x} \in \mathfrak{R}^p$ and $\boldsymbol{y} \in \mathfrak{R}^q$, p and q determine the numbers of variables, CCA attempts to calculate the canonical correlation vectors $\boldsymbol{J}_i \in \mathfrak{R}^{p\times 1}$ and $\boldsymbol{L}_i \in \mathfrak{R}^{q\times 1}$ such that the correlation between $\boldsymbol{J}_i^T\boldsymbol{x}$ and $\boldsymbol{L}_i^T\boldsymbol{y}$ is maximized. The optimization problem is formulated as[31,32]

$$(\boldsymbol{J}_i, \boldsymbol{L}_i) = \underset{(\boldsymbol{J}_i,\boldsymbol{L}_i)}{\operatorname{argmax}} \frac{\boldsymbol{J}_i^T \sum_{xy} \boldsymbol{L}_i}{(\boldsymbol{J}_i^T \sum_x \boldsymbol{J}_i)^{1/2} \left(\boldsymbol{L}_i^T \sum_y \boldsymbol{L}_i\right)^{1/2}} \quad (1)$$

where $\boldsymbol{\Sigma}_x$, $\boldsymbol{\Sigma}_y$, and $\boldsymbol{\Sigma}_{xy}$ are covariance matrices. Solution to eq 1 can be acquired through singular value decomposition (SVD) on a matrix K as

$$\boldsymbol{K} = \sum\nolimits_x^{-1/2} \sum\nolimits_{xy} \sum\nolimits_y^{-1/2} = \boldsymbol{R\Xi V}^T \quad (2)$$

where $\boldsymbol{\Xi} = \begin{bmatrix} \operatorname{diag}(\sigma_1, \cdots, \sigma_l) & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \in \mathfrak{R}^{p\times q}$ is a correlation matrix and $l = \operatorname{rank}(\boldsymbol{\Sigma}_{xy})$. Then, we derive canonical correlation matrices as[31,32]

$$\boldsymbol{J} = [\boldsymbol{J}_1 \cdots \boldsymbol{J}_p] = \sum\nolimits_x^{-1/2} \boldsymbol{R},$$
$$\boldsymbol{L} = [\boldsymbol{L}_1 \cdots \boldsymbol{L}_q] = \sum\nolimits_y^{-1/2} \boldsymbol{V} \quad (3)$$

Batch process data can be thought of having three dimensions, that is, variable, time, and batch. To deal with batch process data, first, is to unfold the three-way data into two-way data. After data normalization, a current sample data matrix $\boldsymbol{X}(k)$ containing the current samples and a previous sample data matrix $\boldsymbol{Y}(k)$ containing previous samples are constructed. Then, CCA is performed between $\boldsymbol{X}(k)$ and $\boldsymbol{Y}(k)$, and canonical correlation matrices $\boldsymbol{J}(k)$ and $\boldsymbol{L}(k)$ and correlation matrix $\boldsymbol{\Xi}(k)$ are obtained. For a measurement at the k-th instant, $\boldsymbol{x}(k) \in \mathfrak{R}^{p\times 1}$ and $\boldsymbol{y}(k) = [\boldsymbol{x}(k-1)^T \cdots \boldsymbol{x}(k-a)^T]^T \in \mathfrak{R}^{q\times 1}$, where a is the number of lagged variables, and a fault detection residual vector is generated as[24]

$$\boldsymbol{r}(k) = \boldsymbol{J}^T(k)\boldsymbol{x}(k) - \boldsymbol{\Xi}(k)\boldsymbol{L}^T(k)\boldsymbol{y}(k) \quad (4)$$

Then, the T^2 statistic for the residual is established as[24]

$$T^2(k) = \boldsymbol{r}(k)^T \sum\nolimits_r^{-1}(k)\boldsymbol{r}(k) \quad (5)$$

where $\boldsymbol{\Sigma}_r(k)$ is the covariance matrix of the residual $\boldsymbol{r}(k)$. Notably, when the time series correlation does not exist or the correlation is not considered, the second term in eq 4, $\boldsymbol{\Xi}(k)\boldsymbol{L}^T(k)\boldsymbol{y}(k)$, becomes zero; then, eq 5 becomes the classical T^2 monitoring.

2.2. Problem Formulation. The following problems exist in the abovementioned CCA-based batch process monitoring.

First, eq 2 involves the inverse operation of the covariance matrix. When the variable-wise correlation and data collinearity exist, the inverse operation is numerically unstable. A similar problem also exists in the T^2 test. The variable-wise correlation requires consideration and characterization.

Second, determining the involved variables in the extended sample $\boldsymbol{y}(k)$ is important. In ref 24, a multiobjective optimization method is introduced to select the most correlated variables. Nevertheless, the abovementioned stochastic numerical optimization-based method is computation expensive, and establishing the time-slice model is difficult. A

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

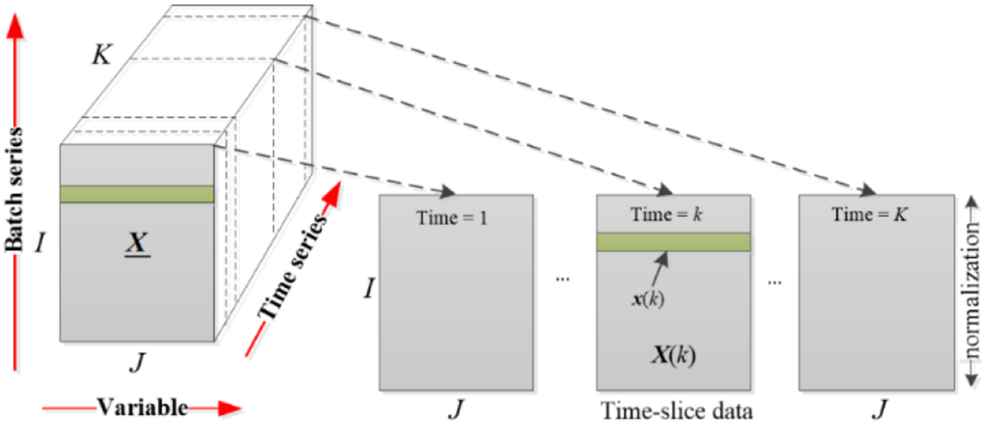


Figure 1. Time-slice data unfolding and normalization.

computationally efficient correlated variable selection method is desired.

Third, a fault may affect either the dynamic or static property of a process. However, the existing batch process monitoring methods do not discriminate the dynamic or static property of a fault. After a fault is detected, the properties of the fault need to be further determined.

3. PREDICTIVE PROCESS MONITORING FOR DYNAMIC BATCH PROCESSES

3.1. Predictive Batch Process Monitoring. A batch process is generally characterized by a complex variable

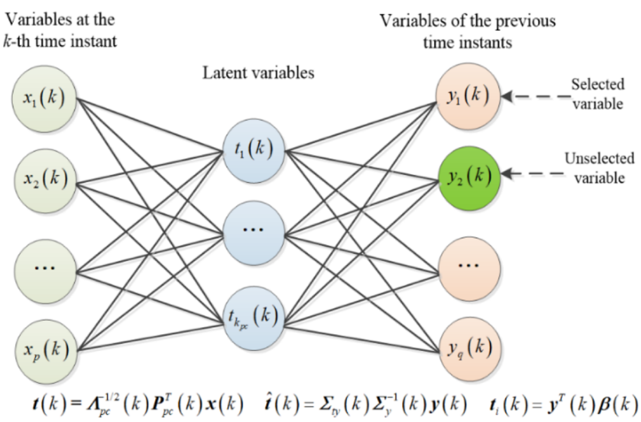


Figure 2. Illustration of the latent variable analysis and variable selection at the k-th time slice.

correlation and remarkable dynamics. To establish an efficient batch process monitoring scheme, all these complex characteristics should be addressed. Here, we individually detail the proposed predictive monitoring approach for batch processes, which is composed of the following two parts.

3.1.1. Offline Modeling. Step 1: the three-way batch process data $\underline{X}(I \times J \times K)$ are converted to two-way time-slice data $\{X(k)\}$ using the batch-wise unfolding and normalized along the batch perspective, where $\underline{X}$ denotes three-way data with I batches, $J(=p)$ denotes variable numbers, and K denotes time instants. Figure 1 presents data unfolding and normalization.

Step 2: at each time slice, a CCA monitoring model is established. Let the data at the k-th time slice be $X(k)$. To deal with the inefficiency of conventional CCA methods caused by the variable-wise high collinearity, the core characteristics of the time-slice data are better reflected and the data are projected into both dominant latent variable and residual subspaces. First, SVD is performed on the covariance matrix of $X(k)$ as

$$\begin{aligned}\sum\nolimits_x(k) &= \frac{X^T(k)X(k)}{I-1} \\ &= [P_{pc}(k)P_{\text{res}}(k)]\begin{bmatrix}\Lambda_{pc}(k) & 0 \\ 0 & \Lambda_{\text{res}}(k)\end{bmatrix}[P_{pc}^T(k)P_{\text{res}}^T(k)]\end{aligned} \tag{6}$$

then, for a sample $x(k)$ in $X(k)$, the sample is mapped to the major latent variables by $P_{pc}(k)$ as

$$t(k) = \Lambda_{pc}^{-1/2}(k)P_{pc}^T(k)x(k) \in \Re^{k_{pc}(k)\times 1} \tag{7}$$

where $k_{pc}(k)$ denotes the number of retained latent variables that occupy 85 to 95% of the original data variance at time instant k. The historical data of the k-th time slice in the latent variable subspace are denoted as $T(k)$. A residual vector that represents the data reconstruction error is constructed as

$$e(k) = x(k) - P_{pc}(k)P_{pc}^T(k)x(k) \tag{8}$$

Step 3: an extended sample $y(k)$ is constructed to include samples from the previous time slices as $y(k) = [x(k-1)^T x(k-2)^T \cdots x(k-a)^T]^T$. Let the corresponding data matrix be $Y(k)$ to include data from previous time slices. To characterize the process dynamics, CCA is carried out between $T(k)$ and previous time-slice data $Y(k)$. SVD is performed on a matrix $G_T(k)$ as

$$\begin{aligned}G_T(k) &= \sum\nolimits_t^{-1/2}(k)\sum\nolimits_{ty}(k)\sum\nolimits_y^{-1/2}(k) \\ &= R_T(k)\Xi_T(k)V_T(k)\end{aligned} \tag{9}$$

where $\sum_t(k) = \frac{T^T(k)T(k)}{I-1}$, $\sum_y(k) = \frac{Y^T(k)Y(k)}{I-1}$, and $\sum_{ty}(k) = \frac{T^T(k)Y(k)}{I-1}$. $\Xi_T(k)$ represents the correlation matrix at the k-th time instant. Canonical correlation vectors are obtained as

$$J_T(k) = [J_{T1}(k)\cdots J_{Tk_{pc}}(k)] = \sum\nolimits_t^{-1/2}(k)R_T(k) \tag{10}$$

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

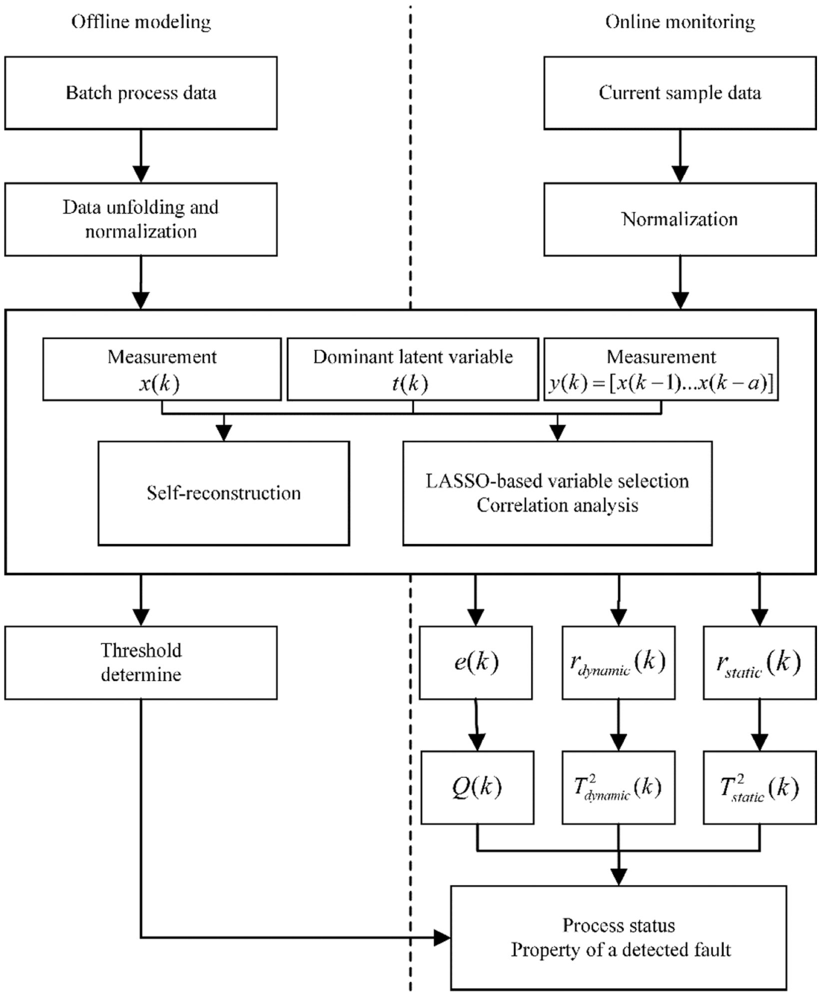


Figure 3. Schematic of the proposed predictive monitoring scheme.

Table 1. Measured Variables in the FBPCP

no.	description	no.	description
1	aeration rate	7	carbon dioxide concentration
2	agitator power	8	pH
3	substrate feed rate	9	bioreactor temperature
4	substrate feed temperature	10	generated heat
5	dissolved oxygen concentration.	11	cooling/heating water flow rate
6	culture volume		

$$\boldsymbol{L}_T(k) = [\boldsymbol{L}_{T1}(k)\cdots\boldsymbol{L}_{Tq}(k)] = \sum\nolimits_y^{-1/2}(k)\boldsymbol{V}_T(k) \tag{11}$$

To apply CCA to monitoring processes, the residuals are constructed as

$$\boldsymbol{r}_T(k) = \boldsymbol{J}_T^T(k)\boldsymbol{t}(k) - \Xi_T(k)\boldsymbol{L}_T^T(k)\boldsymbol{y}(k) \tag{12}$$

Remarkably, the extended data matrix $\boldsymbol{Y}(k)$ can have high dimension and complex correlation. Then, determining appropriate variables in $\boldsymbol{Y}(k)$ is important. Looking at the residual in eq 12, we can obtain that

$$\boldsymbol{r}_T(k) = \boldsymbol{R}_T^T(k)\Xi_T^{-1/2}(k)\left[\boldsymbol{t}(k) - \sum\nolimits_{ty}(k)\sum\nolimits_y^{-1}(k)\boldsymbol{y}(k)\right] \tag{13}$$

where $\hat{\boldsymbol{t}}(k) = \Sigma_{ty}(k)\Sigma_y^{-1}(k)\boldsymbol{y}(k)$ is the LS estimation of $\boldsymbol{t}(k)$ using $\boldsymbol{y}(k)$. The residual depends on the LS regression between $\boldsymbol{t}(k)$ and $\boldsymbol{y}(k)$. First, not all variables in $\boldsymbol{y}(k)$ contribute to the regression of $\boldsymbol{t}(k)$. Including nonbeneficial variables may induce disturbance. Second, the LS regression involves the calculation of the inverse of $\boldsymbol{y}(k)$. However, when the collinearity exists in $\boldsymbol{y}(k)$, LS also performs poorly.

To solve the problems mentioned above, this paper introduced the LASSO method. In the field of statistics, the LASSO becomes popular in solving the penalized regression problem, which imposes a bound on the L_1-norm of the regression coefficients, resulting in coefficient shrinkage. Many coefficients may become zero. As a result, the LASSO achieves variable selection and regression modeling simultaneously. When the LASSO is used for regression analysis, L_1-regularization is introduced to eliminate independent variables with little effect on dependent variables so that variables favorable for prediction could be selected from numerous independent variables.[33] It also automatically handles the high data collinearity by removing redundant variables. Thus, the LASSO increases model interpretability compared to least squares regression. Here, the LASSO is used to identify correlated variables in $\boldsymbol{y}(k)$.

Given the time-slice sample $\boldsymbol{t}_i(k) = [t_i^1(k), \cdots, t_i^I(k)]^T$ of the i-th latent variable at the time instant k and the variables $\boldsymbol{Y}(k)$

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

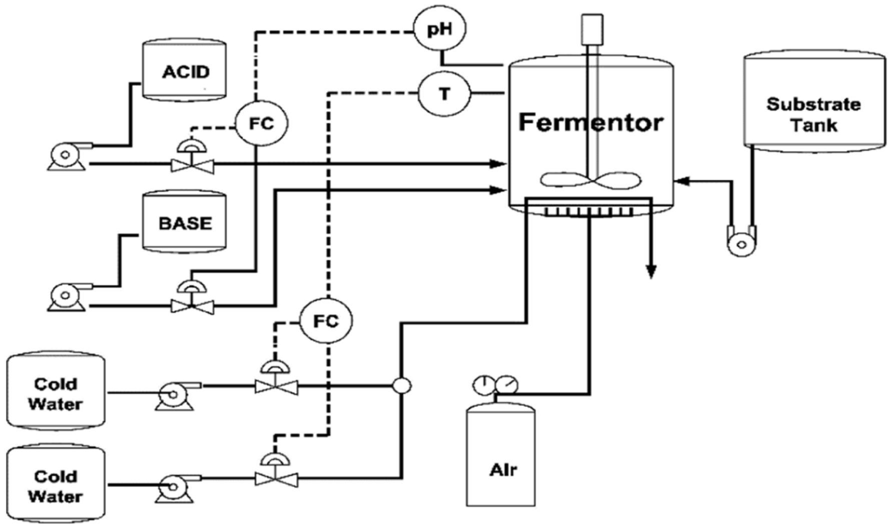


Figure 4. Simplified flowchart of the FBPCP.

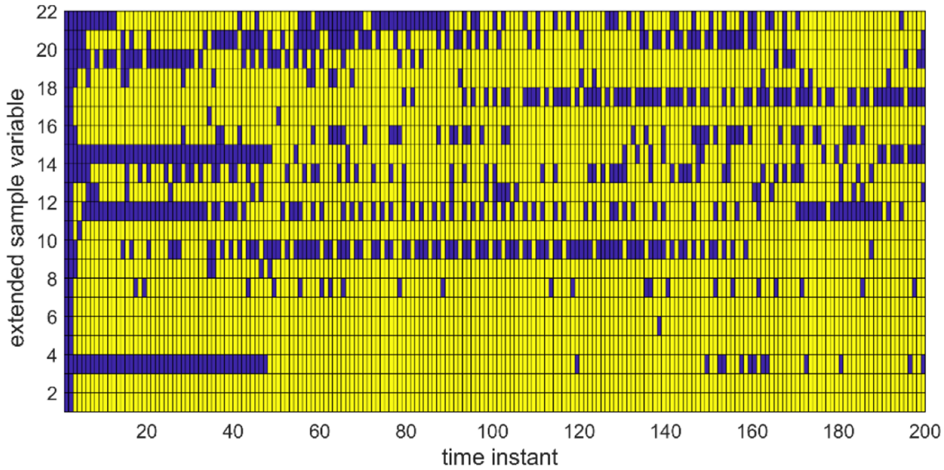


Figure 5. Variable selection results for the FBPCP (the yellow grid represents the selected variable, and the blue grid represents the unselected variable).

from the previous time slices, the LASSO-based maximum relevant independent variable selection is expressed as the following optimization problem

$$\min_{\beta(k)}\left\{\frac{1}{I}\|\boldsymbol{t}_i(k)-\boldsymbol{Y}(k)\boldsymbol{\beta}(k)\|_2^2\right\}$$
$$\text{s. t. } \|\boldsymbol{\beta}(k)\|_1 \le \delta \tag{14}$$

where $\boldsymbol{\beta}(k)$ is the correlation coefficient between $\boldsymbol{Y}(k)$ and $\boldsymbol{t}_i(k)$ and $\delta \ge 0$ is a L_1-penalty term used to control the number of independent variables which are selected. By the Lagrange multiplier method, the problem shown in eq 14 can be transformed into the following form

$$\boldsymbol{\beta}(k)=\underset{\beta(k)}{\operatorname{argmin}}\left\{\frac{1}{I}\|\boldsymbol{t}_i(k)-\boldsymbol{Y}(k)\boldsymbol{\beta}(k)\|_2^2+\lambda\|\boldsymbol{\beta}(k)\|_1\right\} \tag{15}$$

where λ is associated with δ and is used to adjust penalty weights. Generally, the value of λ is a sequence and the optimal value of λ is selected by cross-validation in the LASSO function to prevent the model from overfitting. After λ is set, the partial independent variables, which are most important for predicting $\boldsymbol{t}_i(k)$, are selected from the extended sample $\boldsymbol{Y}(k)$. The details of the LASSO-based communication variable selection algorithm are shown in Algorithm I.

3.1.1.1. Algorithm I LASSO-Based Lagged Variable Selection. Step (1): for the k-th time slice, obtain the PCs $\boldsymbol{t}(k)$.

Step (2): for the i-th PC $\boldsymbol{t}_i(k)$, establish the LS regression model between $\boldsymbol{t}_i(k)$ and extended sample $\boldsymbol{y}(k)$. Select the most important lagged variables through the LASSO denoted as $\{\boldsymbol{y}_{k,i}\}$.

Step (3): repeat step 2 for all the $k_{pc}(k)$ PCs; obtain the selected lagged variables as $\boldsymbol{y}(k)=\{\boldsymbol{y}_{k,1}\}\cup\cdots\cup\{\boldsymbol{y}_{k,k_{pc}(k)}\}$.

Step (4): repeat steps 1 to 3 for all the K time slices.

Figure 2 presents an illustration of the latent variable correlation analysis and variable selection for batch processes.

Step 4: using the data of selected variables, the CCA-based residual is generated. The residual is further decomposed as the dynamic and static parts, namely,

$$\boldsymbol{r}_T(k)=[\boldsymbol{r}_{\text{dynamic}}^T(k)\boldsymbol{r}_{\text{static}}^T(k)]^T \tag{16}$$

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

where $\boldsymbol{r}_{\text{dynamic}}(k) \in \Re^{k_{\text{dynamic}}(k)}$ and $\boldsymbol{r}_{\text{static}}(k) \in \Re^{k_{pc}(k)-k_{\text{dynamic}}(k)}$. Through the accumulated correlation method, the number of dynamic features $k_{\text{dynamic}}(k)$ can be expressed as,[17]

$$\text{Cum}(k_{\text{dynamic}}(k)) = \frac{\sum_{i=1}^{k_{\text{dynamic}}(k)} \sigma_i(k)}{\sum_{i=1}^{l(k)} \sigma_i(k)} \geq \eta \tag{17}$$

in order to preserve the most correlation information, η is generally determined as 80−95%. Correspondingly, the covariance matrix $\Sigma_{rT}(k)$ is divided as

$$\sum_{rT}(k) = \begin{bmatrix} \sum_{\text{dynamic}}(k) & \mathbf{0} \\ \mathbf{0} & \sum_{\text{static}}(k) \end{bmatrix} \tag{18}$$

where

$$\begin{aligned} \sum_{\text{dynamic}}(k) &= \boldsymbol{I}_{k_{\text{dynamic}}(k)} - \Xi_{\text{dynamic}}(k)\Xi_{\text{dynamic}}^T(k) \\ &= \text{diag}((1-\rho_1^2(k)), \cdots, (1-\rho_{k_{\text{dynamic}}}^2(k))) \end{aligned} \tag{19}$$

$$\begin{aligned} \sum_{\text{static}}(k) &= \boldsymbol{I}_{k_{pc}(k)-k_{\text{dynamic}}(k)} - \Xi_{\text{static}}(k)\Xi_{\text{static}}^T(k) \\ &= \text{diag}((1-\rho_{k,\text{dynamic}+1}^2(k), \cdots, 1) \end{aligned} \tag{20}$$

Step 5: establish the monitoring statistics and confirm the thresholds. On the basis of the residuals $\boldsymbol{r}_{\text{dynamic}}(k)$ and $\boldsymbol{r}_{\text{static}}(k)$, the status of the process can easily be identified by the following three statistics

$$\begin{aligned} T_{\text{dynamic}}^2(k) &= \boldsymbol{r}_{\text{dynamic}}^T(k)\sum_{\text{dynamic}}^{-1}(k)\boldsymbol{r}_{\text{dynamic}}(k) \\ &\sim \chi^2(k_{\text{dynamic}}(k)) \end{aligned} \tag{21}$$

$$T_{\text{static}}^2(k) = \boldsymbol{r}_{\text{static}}^T(k)\sum_{\text{static}}^{-1}(k)\boldsymbol{r}_{\text{static}}(k) \sim \chi^2(k_{\text{static}}(k)) \tag{22}$$

$$\begin{aligned} Q(k) &= \boldsymbol{e}^T(k)\boldsymbol{e}(k) \\ &= \boldsymbol{x}^T(k)(\boldsymbol{I}_{p\times p} - \boldsymbol{P}_{pc}(k)\boldsymbol{P}_{pc}^T(k))\boldsymbol{x}(k) \sim g\chi^2(h) \end{aligned} \tag{23}$$

where g and h can be calculated from the normal operating data. Notably, the Q statistic is the same with the MPCA Q statistic, and other details on the threshold determination can be found in ref 34.

3.1.2. Online Monitoring. Step 1: normalize the current sample using the statistics of the normal historical sample at time slice k.

Step 2: project the normalized online sample into the latent variables and residual subspaces.

Step 3: calculate the dynamic and static residuals; calculate the corresponding monitoring statistics.

Step 4: determine whether the process status is faulty and identify whether the fault is dynamic or static.

Figure 3 illustrates the proposed time-slice latent variable correlation analysis-based predictive monitoring scheme.

3.2. Characteristic Analysis. The proposed predictive monitoring method provides the optimal fault detection results when the relationship between the samples of the k-th instant and previous instants can be described as

$$\boldsymbol{A}(k)(\boldsymbol{t}(k) + \boldsymbol{\varepsilon}(k)) = \boldsymbol{B}(k)\boldsymbol{y}(k) \tag{24}$$

where $\boldsymbol{A}(k)$ and $\boldsymbol{B}(k)$ denote parameter matrices and $\boldsymbol{\varepsilon}(k)$ denotes noise.

3.2.1. Comparison with the Classical MPCA Method. MPCA establishes the T^2 on the extracted latent variables t and established the Q statistic on the residual $\boldsymbol{e}$. The key difference between MPCA and the proposed predictive monitoring method is that the predictive monitoring method considers the correlation between the current and previous samples, which is efficient for fault detection when process dynamics exists. The superiority of the proposed predictive monitoring method over MPCA is theoretically analyzed in Remark 1.

Remark 1: the nondetection rate (NDR) of T^2 statistic can be expressed as $\text{NDR}(T^2, f) = F_{\chi^2}(\chi_\alpha^2(k_{pc}); k_{pc}, \nu)$, where $F_{\chi^2}(T_{cl}^2; k_{pc}, \nu)$ is the cumulative distribution function of the noncentral χ^2 distribution with noncentral parameter $\nu = (\Theta f)^T \boldsymbol{\Sigma}_{\boldsymbol{x}}^{-1}(\Theta f)$ and the degree of freedom k_{pc}.[32] The degree of freedoms k_{pc} in the MPCA T^2 and the predictive monitoring method T_r^2 are the same. Let the fault sample be described as $\boldsymbol{x}_f(k) = \boldsymbol{x}_N(k) + \Theta f$, where $\boldsymbol{x}_N(k)$ denotes the normal data and Θf denotes the data with a possible fault. $\nu_{\text{PCA}} = (\Theta f)^T \boldsymbol{\Sigma}_{\boldsymbol{x}(k)}^{-1}(\Theta f)$ and $\nu_{\text{MPM}} = (\Theta f)^T \boldsymbol{\Sigma}_{r(k)}^{-1}(\Theta f)$. Then, by proving that $\nu_{\text{MPM}} \geq \nu_{\text{PCA}}$, we can obtain that the $\text{NDR}_{\text{MPM}}(T^2, f) \leq \text{NDR}_{\text{PCA}}(T^2, f)$. Here, we no longer proceed to the proof details.

3.2.2. Comparison with the Existing CCA Monitoring Methods. The proposed predictive monitoring method projects data into a latent variable subspace and deals with the variable-wise correlation. The property of a detected fault is identified, either a dynamic- or static-related fault.

3.2.3. Comparison with the Existing Multiobjective CCA Monitoring Method.[24] Compared with the stochastic optimization-based variable selection method, the computation of LASSO-based variable selection is more efficient. The possible collinearity in the candidate variables is also addressed by the LASSO.

3.3. Extension to the Two-Dimensional Dynamic Version. The abovementioned model is a one-dimensional dynamic monitoring model in which the correlation only needed to be considered in the time series. However, the dynamics may exist in both the time and batch directions when dealing with batch processes, that is, the status of a current sample is affected by both the previous samples and batches. Under this condition, the extended sample is appropriately expressed as follows,[24] where a and b represent the number of lagged variables in time and batch dimension,

$$\begin{aligned} \boldsymbol{y}(k) = [&\boldsymbol{x}(k-1, j)^T \boldsymbol{x}(k-2, j)^T \cdots \boldsymbol{x}(k-a, j)^T \cdots \\ &\boldsymbol{x}(k, j-1)^T \cdots \boldsymbol{x}(k-a, j-b)^T] \end{aligned} \tag{25}$$

Two existing problems must be addressed in extending the proposed predictive monitoring method to the two-dimensional model: first, the number of included variables in eq 25 can be considerably large, while not all variables are beneficial for the modeling. Second, considerable nonlinearity may exist in the large number of variables. However, the LASSO-based variable selection automatically selects the beneficial variables and simultaneously deals with the considerable data collinearity in $\boldsymbol{y}(k)$.

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

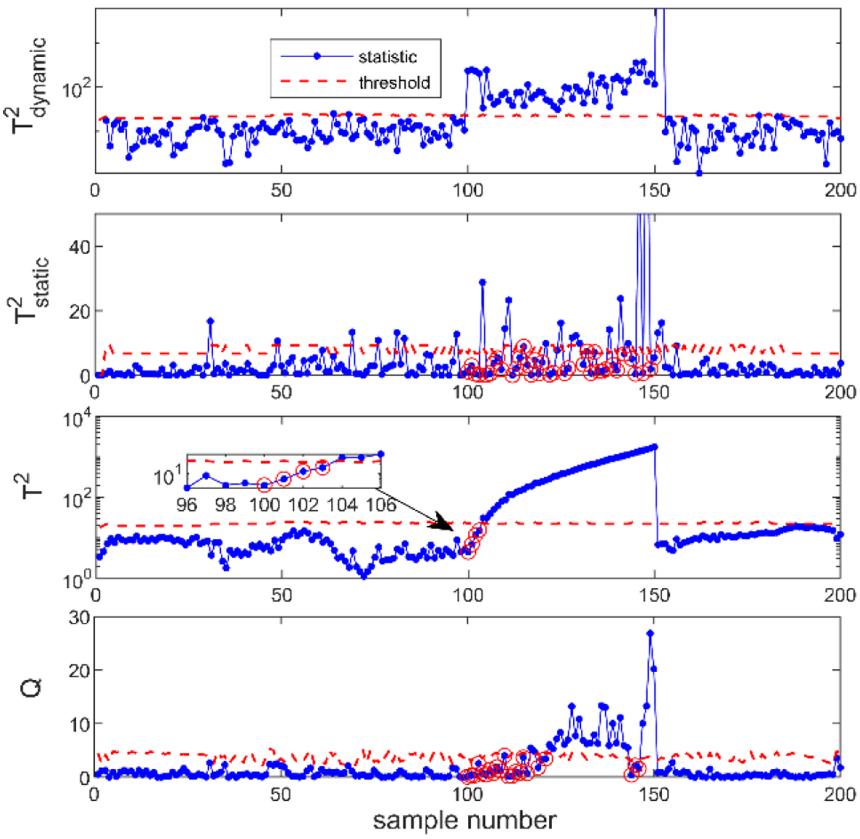


Figure 6. Monitoring results using predictive monitoring and MPCA for the FBPCP fault 1.

4. EXPERIMENTAL STUDIES

The functionality and superiority of the proposed predictive monitoring method are demonstrated through two examples.

4.1. Case Study on a Fed-Batch Penicillin Cultivation Process. The fed-batch penicillin cultivation process (FBPCP), which has been extensively studied during recent years, is characterized by complex correlation and remarkable dynamics.[35,36] Most of the important cell masses are produced at the beginning of the culture, and penicillin is produced during the exponential growth phase. After a period, the process reaches the stationary phase. A simulator was developed by the monitoring and control group of the Illinois Institute of Technology and is used to verify the validity of the proposed monitoring scheme.[35] Eleven variables are considered here, which is the same as the ref 36 and listed in Table 1. Figure 4 presents a simplified flowchart of the process. We no longer go into the detail of the simulation process, given its popularity.

Under normal operating conditions, 150 batches are generated through simulation to establish the monitoring model. Each batch running is simulated to be with 200 h, and samples are taken every hour. First, the process measurements are unfolded into the two-way time slice and normalized along the batch perspective in each time slice. Then, the measurements are mapped into major latent variables which preserve 90% variance information and a residual subspace. The previous two samples of each time instant are used to construct the $\boldsymbol{y}(k)$. Then, the LASSO-based variable selection is performed. Figure 5 presents the variable selection results at each time instant. Then, fault detection prediction residual is generated, which is further divided into the static (unpredictable) and dynamic-related (predictable) subspaces. On the basis of the residuals, monitoring statistics are established. The computation time for the proposed predictive monitoring method is 583 s, which is much faster than that of the stochastic optimization-based monitoring model which takes more than 10,000 s.[24]

As a test to verify whether the proposed predictive monitoring method can detect faults better, three different types of fault data are simulated as follows:

Case 1: a ramp change is introduced to variable 1 from the 100th to the 150th points; case 2: a step change is introduced to variable 2 from the 100th to the 150th points; and case 3: a ramp change is introduced to variable 3 from the 100th to the 150th points.

Figure 6 presents the monitoring results using MPCA and the predictive monitoring method for case 1. At the beginning of the fault, the process dynamics is changed by the fault, and the T^2_{dynamic} first detects the fault. After the fault magnitude enlarges, the MPCA also detects the fault in the T^2 statistic. The predictive monitoring method has an earlier alarm time of 4 h than the conventional MPCA method, which is important in practical applications.

Figure 7 presents the monitoring results for case 2 using the predictive monitoring and the conventional MPCA. Apparently, the fault is only detected by the T^2_{dynamic} of the predictive monitoring. Conventional MPCA cannot alarm the fault. Given that the fault magnitude is small, the fault is detected only at the beginning and the end of the fault. Figure 8 shows the monitoring results for case 3 using the predictive monitoring and the MPCA. Evidently, the T^2_{dynamic} first detects

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

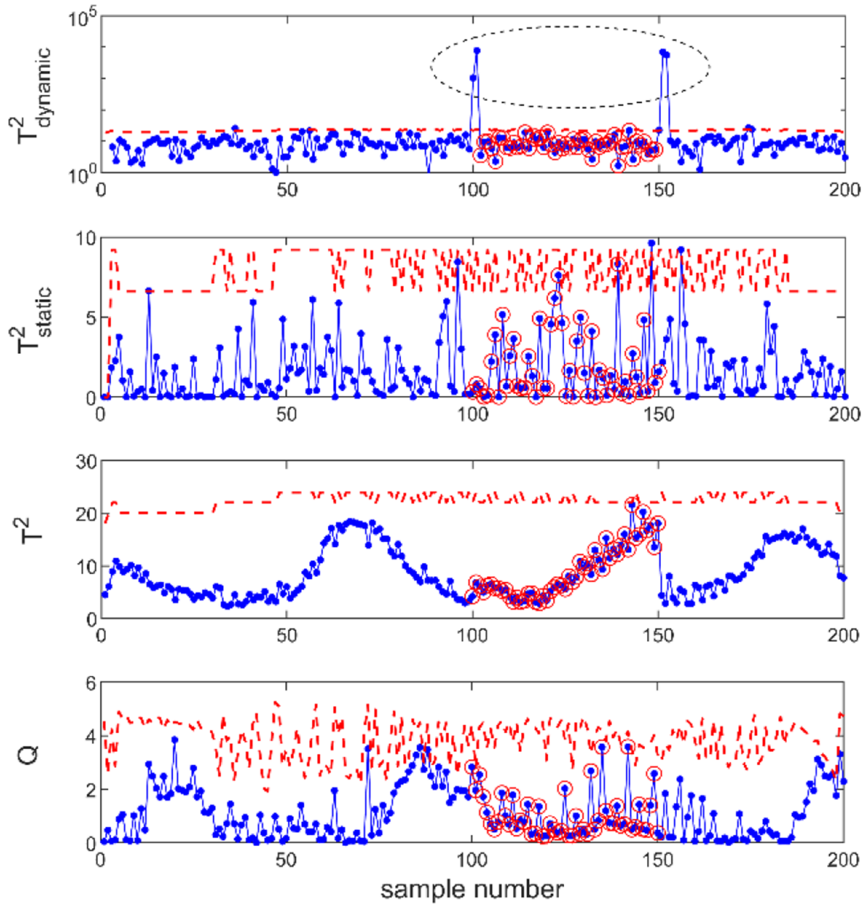


Figure 7. Monitoring results using predictive monitoring and MPCA for the FBPCP fault 2.

the fault. The abovementioned results indicate that considering the process dynamic is important in batch process monitoring because a fault can affect the process dynamics at the early fault stage. The effectiveness and superiority of the scheme are verified.

4.2. Application on an Industrial Injection Molding Process. The injection molding process (IMP) is a typical batch process that plays an important role in injection production industry. Figure 9 shows a simplified flowchart of a reciprocating-screw IMP. We no longer go into the detail, but further knowledge can be found in refs 24 and 37. Here, 17 measured variables are included, which are presented in Table 2.

Under normal operating conditions, a batch is composed of 100 samples, while a data set is mainly composed of 150 batches which are used as the training data. The batch process data are unfolded into time-slice data, and then, in each time slice, the process data are projected into a dominant subspace which contains 90% of data variance. Two previous samples are included to construct the $\boldsymbol{y}(k)$. Figure 10 presents the variable selection results. Then, prediction-based residual is generated, and the residual is further divided as the predictable and unpredictable subspaces. In order to distinguish the property and the status of a detected fault, the monitoring statistics are established. The entire modeling procedures take approximately 610 s, a rate much faster than the stochastic optimization model which takes more than 10,000 s. As a test to verify the monitoring performance, three cases with different faults are considered:

Fault 1: a ramp drift is introduced into the injection position sensor from the 31st to the 70th points.

Fault 2: a step change is introduced into the 10th variable sensor.

Fault 3: an unknown insufficient injection fault.

Monitoring results for case 1 use the proposed predictive monitoring. Figure 11 presents the conventional MPCA. Apparently, the Q statistic, shared by both, first detects the fault. Therefore, the fault affects the variable-wise correlation at the beginning of the fault. The process dynamics is not destroyed, and the fault is a dynamic-unrelated fault. Figure 12 presents the monitoring results for case 2 using the proposed predictive monitoring and conventional MPCA. Most of the faulty points are detected by the T^2_{static} of the predictive monitoring method, while the NDRs in the other statistics are considerably high. Thus, the fault is a static fault that does not cause significant effects on the process dynamic. The PCA T^2 can also detect the fault, but the NDR is much higher than the T^2_{static} because the conventional PCA does not discriminate the property of a fault, which introduces monitoring redundancy. Figure 13 presents the monitoring results for case 3 using the proposed predictive monitoring and conventional MPCA. The T^2_{dynamic} first detects the fault, indicating that the process dynamics is affected at the onset of the fault.

The abovementioned experimental results and analysis verified that the proposed predictive monitoring method involves the process dynamic information and is more computationally efficient than the multiobjective CCA

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

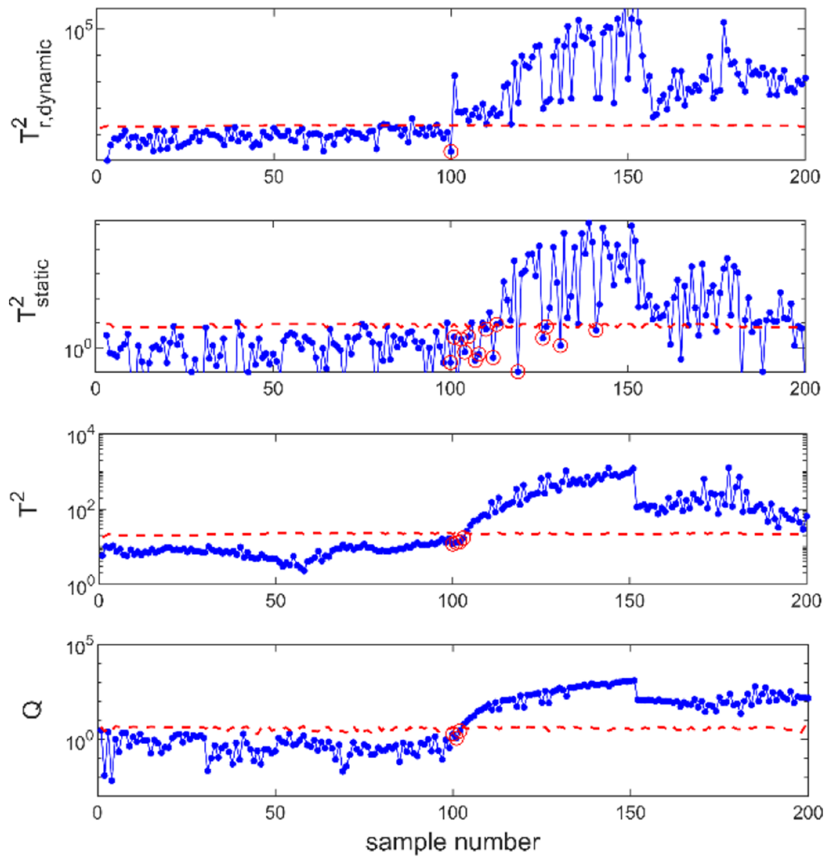


Figure 8. Monitoring results using predictive monitoring and MPCA for the FBPCP fault 3.

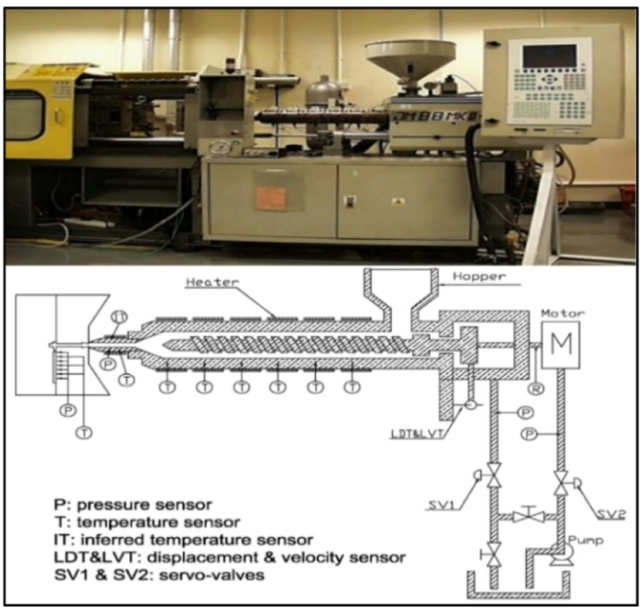


Figure 9. Industrial IMP[28] (reprinted with permission from [Data-Driven Two-Dimensional Deep Correlated Representation Learning for Nonlinear Batch Process Monitoring]. Copyright [2020] [IEEE]).

method. Moreover, the predictive monitoring method effectively divides the monitoring subspace into the dynamic- and static-related parts, which identified whether the process is faulty and whether the fault is dynamic or static.

Table 2. Measured Variables in the IMP

no.	name	no.	name
1	mold position	10	mold velocity
2	ejector pin position	11	ejector pin velocity
3	injection position	12	screw velocity
4	system pressure	13	nozzle temperature
5	mold adjustment	14	zone 1 temperature
6	plasticization	15	zone 2 temperature
7	nozzle pressure	16	zone 3 temperature
8	injection speed	17	zone 4 temperature
9	back pressure		

5. CONCLUSIONS

This study proposes a data-driven predictive fault detection scheme for dynamic batch process monitoring. By first projecting the batch process data into both major latent variables and residual subspaces, the variable-wise correlation is addressed. Then, the prediction-based monitoring method is established by performing CCA between the latent variable subspace and previous samples. LASSO-based variable selection is performed to select the most correlated variables in the model. According to the generated prediction-based residuals, dynamic residuals and static residuals are further discriminated. Then, dynamic and static monitoring statistics are established to identify the process status and fault property. The functionality and effectiveness of the suggested monitoring method are verified through experiments on a simulated FBPCP and an industrial IMP. Since the fault property is identified, the problem of fault location and classification can

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

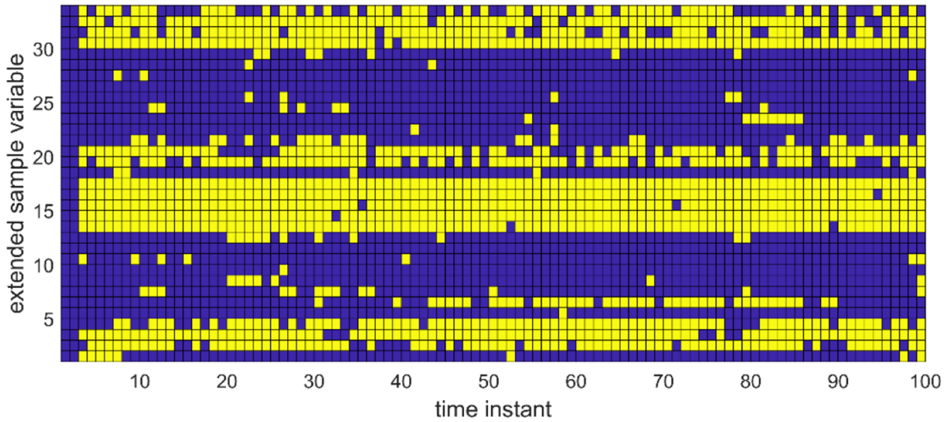


Figure 10. Variable selection results for the IMP (the yellow grid represents the selected variable, and the blue grid represents the unselected variable).

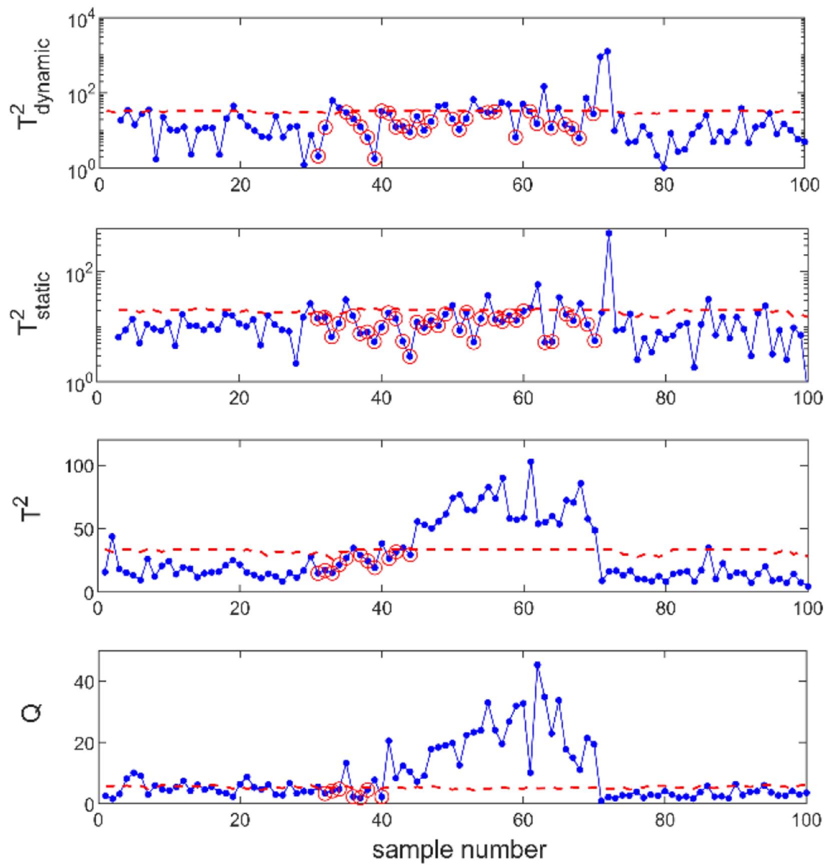


Figure 11. Monitoring results for the IMP fault 1.

be further studied in the future work. Besides, the current work uses only process data to establish the monitoring model for dynamic processes. Given that a part of process knowledge is usually available and the wide application of data-knowledge-based hybrid modeling,[38] how to incorporate process knowledge to improve the modeling and monitoring performance for dynamic processes also needs further exploration.

■ AUTHOR INFORMATION

Corresponding Author

Qingchao Jiang – *Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China University of Science and Technology, Shanghai 200237, P. R. China; Key Laboratory of Complex System Safety and Control, Ministry of Education, Chongqing University, Chongqing 400044, P. R. China;* orcid.org/0000-0002-3402-9018; Email: qchjiang@ecust.edu.cn

Authors

Le Du – *Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China University of Science and Technology, Shanghai 200237, P. R. China; Key Laboratory of Complex System Safety and Control, Ministry of Education, Chongqing University, Chongqing 400044, P. R. China*

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

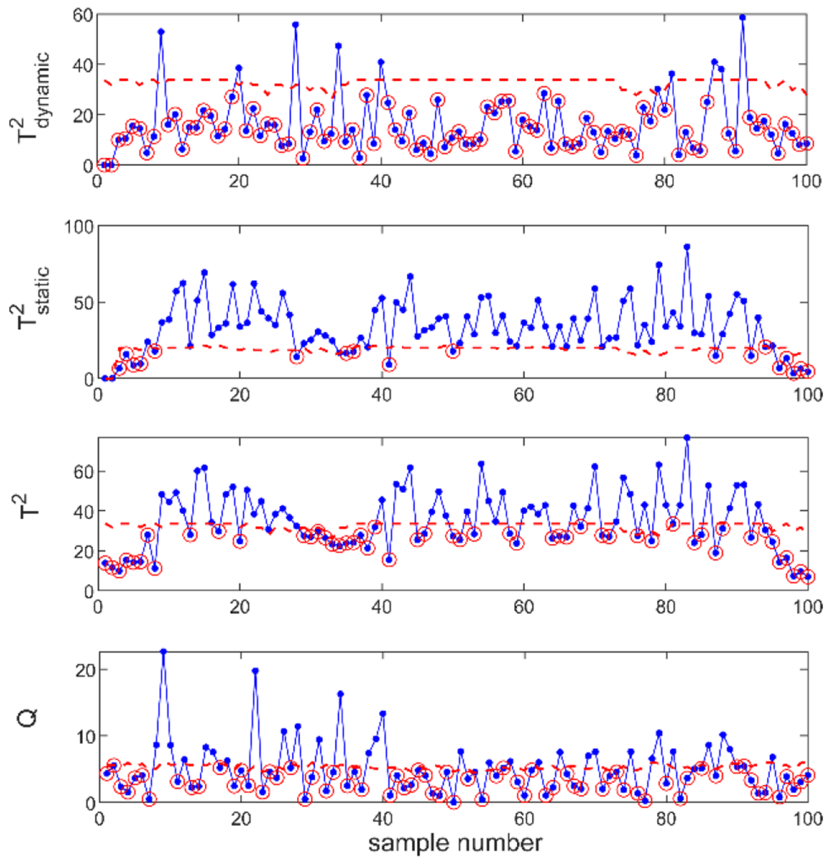


Figure 12. Monitoring results for the IMP fault 2.

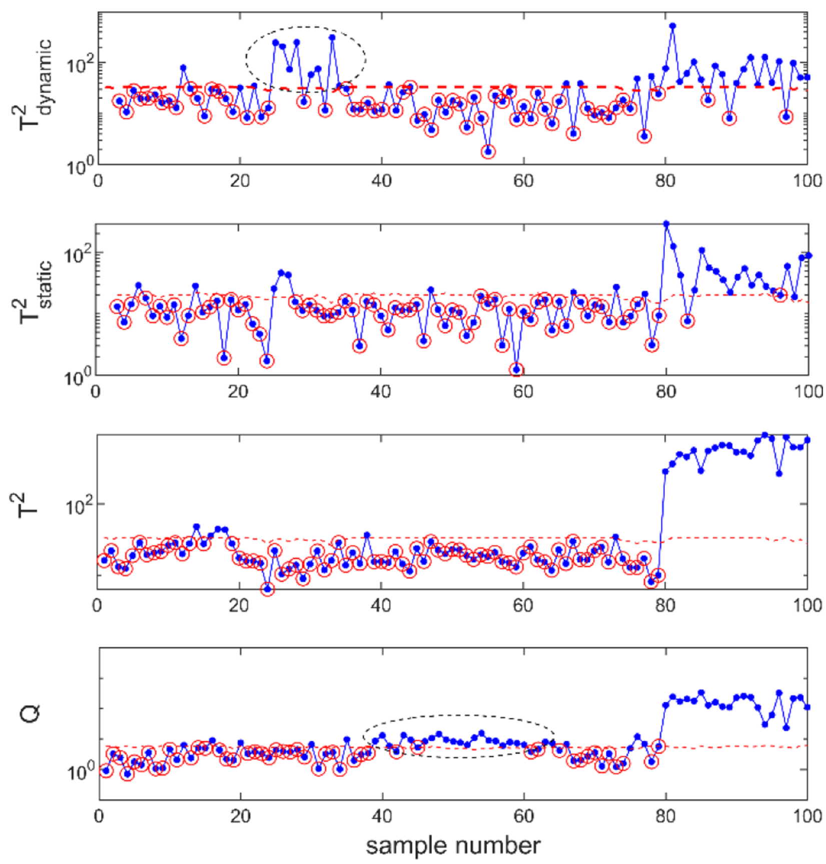


Figure 13. Monitoring results for the IMP fault 3.

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081

Wenhao Jin − *Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, East China University of Science and Technology, Shanghai 200237, P. R. China*

Yang Wang − *School of Electric Engineering, Shanghai Dianji University, Shanghai 200240, P. R. China*

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.2c04445

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

The authors gratefully acknowledge the support from the following foundations: National Key R&D Program of China under grant no. 2021YFC2101100, National Natural Science Foundation of China under grants 61973119 and 62003206, and Shanghai Rising-Star Program under grant 20QA1402600.

■ REFERENCES

(1) Rendall, R.; Chiang, L. H.; Reis, M. S. Data-driven methods for batch data analysis−A critical overview and mapping on the complexity scale. *Comput. Chem. Eng.* **2019**, *124*, 1−13.

(2) Rato, T. J.; Reis, M. S. Optimal selection of time resolution for batch data analysis. Part I: Predictive modeling. *AIChE J.* **2018**, *64*, 3923−3933.

(3) Zhu, J.; Wang, Y.; Zhou, D.; Gao, F. Batch process modeling and monitoring with local outlier factor. *IEEE Trans. Control Syst. Technol.* **2018**, *27*, 1552−1565.

(4) Gao, Z.; Cecati, C.; Ding, S. X. A survey of fault diagnosis and fault-tolerant techniques—Part I: Fault diagnosis with model-based and signal-based approaches. *IEEE Trans. Ind. Electron.* **2015**, *62*, 3757−3767.

(5) Yin, S.; Ding, S. X.; Xie, X.; Luo, H. A Review on Basic Data-Driven Approaches for Industrial Process Monitoring. *IEEE Trans. Ind. Electron.* **2014**, *61*, 6418−6428.

(6) Qin, Y.; Zhao, C.; Gao, F. An iterative two-step sequential phase partition (ITSPP) method for batch process modeling and online monitoring. *AIChE J.* **2016**, *62*, 2358−2373.

(7) Tulsyan, A.; Garvin, C.; Undey, C. Industrial batch process monitoring with limited data. *J. Process Control* **2019**, *77*, 114−133.

(8) Jiang, Q.; Yan, X.; Huang, B. Review and perspectives of data-driven distributed monitoring for industrial plant-wide processes. *Ind. Eng. Chem. Res.* **2019**, *58*, 12899−12912.

(9) Jiang, Q.; Yan, S.; Cheng, H.; Yan, X. Local-Global Modeling and Distributed Computing Framework for Nonlinear Plant-Wide Process Monitoring With Industrial Big Data. *IEEE Trans. Neural Netw. Learn. Syst.* **2021**, *32*, 3355−3365.

(10) Jiang, Q.; Yan, X.; Huang, B. Performance-Driven Distributed PCA Process Monitoring Based on Fault-Relevant Variable Selection and Bayesian Inference. *IEEE Trans. Ind. Electron.* **2016**, *63*, 377−386.

(11) Zhu, J.; Ge, Z.; Song, Z.; Gao, F. Review and big data perspectives on robust data mining approaches for industrial process modeling with outliers and missing data. *Annu. Rev. Control* **2018**, *46*, 107−133.

(12) Wang, Y.; Si, Y.; Huang, B.; Lou, Z. Survey on the theoretical research and engineering applications of multivariate statistics process monitoring algorithms: 2008−2017. *Can. J. Chem. Eng.* **2018**, *96*, 2073−2085.

(13) Cao, Y.; Yuan, X.; Wang, Y.; Gui, W. Hierarchical hybrid distributed PCA for plant-wide monitoring of chemical processes. *Control. Eng. Pract.* **2021**, *111*, 104784.

(14) Jiang, Q.; Yan, X.; Yi, H.; Gao, F. Data-Driven Batch-End Quality Modeling and Monitoring Based on Optimized Sparse Partial Least Squares. *IEEE Trans. Ind. Electron.* **2020**, *67*, 4098−4107.

(15) Nomikos, P.; MacGregor, J. F. Monitoring batch processes using multiway principal component analysis. *AIChE J.* **1994**, *40*, 1361−1375.

(16) Nomikos, P.; MacGregor, J. F. Multi-way partial least squares in monitoring batch processes. *Chemom. Intell. Lab. Syst.* **1995**, *30*, 97−108.

(17) Jiang, Q.; Gao, F.; Yi, H.; Yan, X. Multivariate statistical monitoring of key operation units of batch processes based on time-slice CCA. *IEEE Trans. Control Syst. Technol.* **2019**, *27*, 1368−1375.

(18) Dong, Y.; Qin, S. J. New Dynamic Predictive Monitoring Schemes based on Dynamic Latent Variable Models. *Ind. Eng. Chem. Res.* **2020**, *59*, 2353−2365.

(19) Tong, C.; Shi, X. Decentralized monitoring of dynamic processes based on dynamic feature selection and informative fault pattern dissimilarity. *IEEE Trans. Ind. Electron.* **2016**, *63*, 3804−3814.

(20) Shang, C.; Yang, F.; Gao, X.; Huang, X.; Suykens, J. A.; Huang, D. Concurrent monitoring of operating condition deviations and process dynamics anomalies with slow feature analysis. *AIChE J.* **2015**, *61*, 3666−3682.

(21) Zhang, S.; Zhao, C. Slow-feature-analysis-based batch process monitoring with comprehensive interpretation of operation condition deviation and dynamic anomaly. *IEEE Trans. Ind. Electron.* **2018**, *66*, 3773−3783.

(22) Hu, K.; Yuan, J. Statistical monitoring of fed-batch process using dynamic multiway neighborhood preserving embedding. *Chemom. Intell. Lab. Syst.* **2008**, *90*, 195−203.

(23) Chen, J.; Liu, K. C. On-line batch process monitoring using dynamic PCA and dynamic PLS models. *Chem. Eng. Sci.* **2002**, *57*, 63−75.

(24) Jiang, Q.; Gao, F.; Yan, X.; Yi, H. Multiobjective two-dimensional CCA-based monitoring for successive batch processes with industrial injection molding application. *IEEE Trans. Ind. Electron.* **2018**, *66*, 3825−3834.

(25) Wang, X.; Wang, Y.; Deng, X.; Cao, Y. A Batch Process Monitoring Method Using Two-Dimensional Localized Dynamic Support Vector Data Description. *IEEE Access* **2020**, *8*, 181192−181204.

(26) Yao, Y.; Gao, F. Statistical monitoring and fault diagnosis of batch processes using two-dimensional dynamic information. *Ind. Eng. Chem. Res.* **2010**, *49*, 9961−9969.

(27) Lu, N.; Yao, Y.; Gao, F.; Wang, F. Two-dimensional dynamic PCA for batch process monitoring. *AIChE J.* **2005**, *51*, 3300−3304.

(28) Jiang, Q.; Yan, S.; Yan, X.; Yi, H.; Gao, F. Data-Driven Two-Dimensional Deep Correlated Representation Learning for Nonlinear Batch Process Monitoring. *IEEE Trans. Ind. Inform.* **2020**, *16*, 2839−2848.

(29) Liu, K.; Zheng, M.; Liu, Y.; Yang, J.; Yao, Y. Deep Autoencoder Thermography for Defect Detection of Carbon Fiber Composites. *IEEE Trans. Ind. Inform.* **2022**, DOI: 10.1109/TII.2022.3172902.

(30) Jiang, Q.; Chen, S.; Yan, X.; Kano, M.; Huang, B. Data-Driven Communication Efficient Distributed Monitoring for Multiunit Industrial Plant-Wide Process. *IEEE Trans. Autom. Sci. Eng.* **2022**, *19*, 1913−1923.

(31) Chen, Z.; Ding, S. X.; Peng, T.; Yang, C.; Gui, W. Fault detection for non-Gaussian processes using generalized canonical correlation analysis and randomized algorithms. *IEEE Trans. Ind. Electron.* **2017**, *65*, 1559−1567.

(32) Jiang, Q.; Ding, S. X.; Wang, Y.; Yan, X. Data-driven distributed local fault detection for large-scale processes based on the GA-regularized canonical correlation analysis. *IEEE Trans. Ind. Electron.* **2017**, *64*, 8148−8157.

(33) Tibshirani, R. Regression shrinkage and selection via the lasso. *J. R. Stat. Soc. Ser. B: Methodol.* **1996**, *58*, 267−288.

(34) Ding, S. X. *Data-driven design of fault diagnosis and fault-tolerant control systems*; Springer: London, 2014.

(35) Birol, G.; Ündey, C.; Çinar, A. A modular simulation package for fed-batch fermentation: penicillin production. *Comput. Chem. Eng.* **2002**, *26*, 1553−1565.

(36) Lee, J.-M.; Yoo, C. K.; Lee, I.-B. Enhanced process monitoring of fed-batch penicillin cultivation using time-varying and multivariate statistical analysis. *J. Biotechnol.* **2004**, *110*, 119−136.
(37) Ge, Z.; Song, Z.; Zhao, L.; Gao, F. Two-level PLS model for quality prediction of multiphase batch processes. *Chemom. Intell. Lab. Syst.* **2014**, *130*, 29−36.
(38) Jiang, Q.; Fu, X.; Yan, S.; Li, R.; Du, W.; Cao, Z.; Qian, F.; Grima, R. Neural network aided approximation and parameter inference of non-Markovian models of gene expression. *Nat. Commun.* **2021**, *12*, 2618.

https://doi.org/10.1021/acsomega.2c04445
ACS Omega 2022, 7, 41069−41081