Monitoring of Multimode Processes Based on Subspace Decomposition

Shuai Li,*‡‡ Xiaofeng Zhou,‡‡ Haibo Shi,‡‡ Zhi Qiao,§∥ and Zeyu Zheng†‡

*Shenyang Institute of Automation, and ‡Key Laboratory of Network Control System, Chinese Academy of Sciences, Shenyang, 110016, PR China
§NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Singapore, 117456, Republic of Singapore
∥Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, Singapore, 117542, Republic of Singapore

ABSTRACT: This paper presents a new monitoring method for multimode processes based on subspace decomposition. In the proposed method, the influence of quality variables and multimode information are considered in multimode processes modeling, which is crucially important to ensure industrial production safety and quality stabilization. Process data are decomposed into the global common subspace and the local specific subspace and monitoring is performed in each subspace to simplify the model structure. Two experiments: penicillin fermentation processes and practical foods industrial production processes, have been used to demonstrate the excellent performance of the proposed method.

1. INTRODUCTION

Process monitoring is significant and attractive for industrial production safety and quality stabilization.1–5 Multimode is one of the most significant features in the modern industrial production processes.6 Some industrial production processes frequently change because of various factors, such as alterations of raw materials and compositions, applications of different manufacturing strategies, etc.7 To ensure industrial production safety and quality stabilization of products, it is vital to develop effective monitoring methods for multimode processes.6

Multivariate statistical process monitoring (MSPM) methods, such as principal component analysis (PCA), partial least-squares (PLS) etc., may have unsatisfactory performance when directly used for multimode processes.8 To track multimode characteristics, multiple models methods,9 model library-based methods,10 localized Fisher discriminant analysis,11 and Gaussian mixture model approach6,12,13 have been proposed. Multiple models methods6 were developed by building different monitoring models for different modes that needed complete process data of each mode.14 Although it may be effective for each mode, when there are numerous modes, it is clumsy.15 Moreover, the correlations between different modes that possess useful information in modeling and monitoring are neglected. Ge et al.16 proposed an adaptive local model for multimode online monitoring, which introduced the just-in-time-learning (JITL) strategy to solve the multimode problem. Rashid et al.17 presented a hidden Markov model (HMM) for multimode processes monitoring, which utilized local ICA models to characterize various modes adaptively. The above-mentioned methods mainly consider the local characteristic in each mode, but the global characteristic is also significant. We15 considered the global characteristic and presented a subspace separation method based on manifold learning and kernel principal component analysis (KPCA), which reveals that each mode has part of the same process characteristics as in multimode processes. Then the relationships of input and output data sets were introduced, and a novel subspace separation method was presented in the context of manifold learning and kernel partial least-squares (KPLS), which reveals that each mode can be divided into two subspaces.15 It should be noted that these methods14,15 are only appropriate for multimode processes with equal mode length because each specific subspace is separated by subtracting an identical common subspace from the global space in each mode, which cannot be suitable for practical industrial production processes. Moreover, multimode information is not considered in extracting common subspace, which may lead to the loss of partial valuable information in multimode modeling.

In this paper, an effective monitoring method based on subspace decomposition is developed for multimode processes. To fulfill this purpose, each mode of the proposed method is decomposed into the global common subspace and the local specific subspace, which does not require each mode to have equal mode length. Multimode information and the influence of quality variables are considered. Moreover, global and local monitoring strategy and partial derivative contribution analysis are developed. The main contributions of this paper lie in the following aspects: (1) it provides a potential solution to the issue of nonlinear multimode processes monitoring in an efficient data-driven manner; (2) local and global characteristics are used for multimode processes modeling; (3) it is unnecessary that each mode has equal mode length for subspace decomposition; (4) the correlations between different modes, multimode information, and the influence of quality

Received: December 2, 2014
Revised: March 17, 2015
Accepted: April 1, 2015
Published: April 9, 2015

DOI: 10.1021/ie504730x
Ind. Eng. Chem. Res. 2015, 54, 3855−3864
variables are considered. Related analyses and discussions are stated to better illustrate the proposed approach.

The paper is organized as follows. In section 2, we briefly describe multimode, subspace, and the subspace separation method. In section 3, the proposed method is presented in details. Then, two experiments including penicillin fermentation processes and practical foods industrial production processes are presented in section 4. Finally, some conclusions are presented in section 5.

2. PRELIMINARIES

2.1. Multimode and Subspace. The operating conditions, such as temperature, pressure, etc., have to be adjusted to meet the production specifications, which causes various operation modes. In multimode processes, different modes have their respective specific, similar characteristics and duration time. A mode is defined as the long duration process with the same statistical characteristics, which is one part of the whole multimode processes. A simple tutorial example of multimode is stated. For data sets $X = \{X_1, X_2, \ldots, X_n\}$, $X_1 \times b_1$ denotes mode 1, where $n = (2^{m-1} \times b_1)$, $m$ is the number of variables, $n$ is the number of samples, $B$ denotes the number of modes, $b_1$ is the number of samples in each mode. However, mode is different from scale. A scale is defined as a deterministic or stochastic component of data. A simple tutorial example of scale is presented. For data sets $X^{\text{scale}} = \{X_1^{\text{scale}}, \ldots, X_L^{\text{scale}}\}$, $X_1^{\text{scale}}$ denotes scale 1, where $L$ is the number of scales. Multiscale process monitoring usually utilizes wavelet transform to decompose the original process measurements into their multiscale components according to time and frequency characteristics. It enables a separation of deterministic and stochastic features and offers a more meaningful physical interpretation of process phenomena.

In this paper, as shown in Figure 1, the main idea of subspace decomposition is decomposing the processes into multiple subspaces for monitoring. Compared with multiscale method, the proposed multimode monitoring utilizes local neighborhood relationships, multimode information and quality relations to decompose the process data into the global common subspace and the local specific subspace. In general, the structure information on data can be considered from the following sides: variable space and sample space. The global and local structures are crucial for process monitoring since the global structure defines the outer shape of the process data set and the local structure presents inner organization. It can decompose global and local characteristics and provide more meaningful interpretation for multimode processes. The global common subspace is defined as the part with global structure information on all modes, revealing neighborhood relationships of overall input data set, multimode information, and influences of output quality variables. The local specific subspace is defined as the part with local structure information on each mode. In conclusion, multiscale methods have the capabilities for noise-reduction and multiscale modeling and monitoring. However, the proposed method has the capabilities for multimode modeling and monitoring.

2.2. Subspace Separation. To overcome the disadvantages of multiple models methods, we considered the global characteristic and presented a subspace separation method. The common subspace is obtained according to the neighborhood relationships of input and output data sets. After the common subspace $\Phi(X_g)$ is obtained, the specific subspace $\Phi(X_{m})$ is calculated:

$$\Phi(X_{m}) = \Phi(X_g) - \Phi(X_{b}), \quad (m = 1, \ldots, B)$$

where $m$ denotes different modes, $\Phi(X_g)$ is the identical common subspace for each mode, $\Phi(X_{m})$ is the global space of mode $m$, and $B$ denotes the number of modes.

The problem of weight matrix stems from its inability to take similar data in each mode separately into account, as its only focus is on preserving local neighborhood relationships of all multimode data. Hence, it is necessary to construct a more efficient weight matrix by utilizing multimode information to improve the tightness of similar data in the same mode and push data in different modes far apart. Moreover, the subspace separation method is only appropriate for multimode processes with equal mode length because each specific subspace is obtained by subtracting an identical common subspace from the global space in each mode. In this paper, our subspace decomposition method considering multimode information is presented, which does not need each mode to have equal mode length and can be suitable for practical industrial production processes.

3. THE PROPOSED METHOD

The complex nonlinear multimode problem turns into a combination of a few simple subspace problems by subspace decomposition. The proposed method consists of two parts: (1) in the offline modeling phase, a subspace decomposition model is trained by normal samples, and monitoring statistics and control limits are obtained in each subspace; (2) in the online monitoring phase, the statistics of each sample are computed in each subspace, while the fault and faulty variable are recognized.

In this paper, it is considered that each mode can be decomposed into two subspaces. The influence of quality variables and multimode information are considered, which is crucial to ensure quality stabilization. The global structure information on all modes is preserved in the global common subspace and the local structure information on each mode is
Input data set \( X = \{x_1, x_2, \ldots, x_n\} \subseteq \mathbb{R}^m \) and quality variables \( Y = \{y_1, y_2, \ldots, y_n\} \subseteq \mathbb{R}^q \) are obtained, where \( n = (\sum_{i=1}^B b_i) \), \( m \) and \( q \) are the number of input and quality variables, respectively, \( n \) is the number of samples, \( B \) denotes the number of modes, \( b_i \) is the number of samples in each mode. To improve the ability to handle the nonlinear characteristic data, \( X \) is mapped to high-dimensional feature space \( \Phi(X) = \{\Phi(x_1), \Phi(x_2), \ldots, \Phi(x_n)\} \). Subsequently, \( k \) nearest neighbors of each data point in high-dimensional feature space are constructed on the basis of distance in high-dimensional feature space:

\[
||\Phi(x_i) - \Phi(x_j)|| = \sqrt{(\Phi(x_i) - \Phi(x_j))^T (\Phi(x_i) - \Phi(x_j))} = \sqrt{K(x_i, x_j) - 2K(x_i, x_j) + K(x_j, x_j)}
\]

where \( K(x_i, x_j) = \Phi^T(x_i)\Phi(x_j) \). For each sample \( \Phi(x_i) \) in high-dimensional feature space, \( j_i \) denotes the neighbors of \( \Phi(x_i) \) and the weight matrix without multimode information \( W_0 \) can be calculated by solving the optimization problem with constraints:

\[
\begin{align*}
\text{min } e(W^0) &= \sum_{i=1}^n \|\Phi(x_i) - \sum_{j=1}^n W_0^{ij}\Phi(x_j)\|^2 \\
\text{s.t. } \sum_{j=1}^n W_0^{ij} &= 1 \quad (W_0^{ij} = 0, j \notin j_i, i = 1, \ldots, n)
\end{align*}
\]

where the weight \( W_0^{ij} \) only reflects the local distance relationships of \( \Phi(x_i) \) and \( \Phi(x_j) \), which neglects multimode information. In this paper, the geometrical interpretations based on the marginal perspective\(^{25}\) are applied to solve the problem. The weights \( W_0^{ij} \) in the same mode and \( W_0^{between} \) between different modes in the proposed approach are defined as:

\[
\begin{align*}
W_0^{in} &= 1, \text{if } j \in j_i, L(x_i) = L(x_j) \\
W_0^{between} &= -1, \text{if } j \in j_i, L(x_i) \neq L(x_j) \\
W_0^{ij} &= W_0^{between} = 0, \text{else}
\end{align*}
\]

where \( L(x_i) \) denotes mode information. \( W_0^{in} \) and \( W_0^{between} \) consider the tightness of similar data in the same mode and the separability in different modes, respectively. In the proposed subspace decomposition method, local neighborhood relationships with multimode information are preserved in the global common subspace. In eq 3, when the weight \( W_0^{ij} \) increases, the distance must be reduced in order to minimize the summation. Therefore, the tightness of similar data in the same mode can be improved by increasing the weights, and data in different modes can be pushed far apart by decreasing the weights. Thus, the loss function with multimode information can be presented as follows:

\[
\begin{align*}
\text{min } e(\Phi(X_{gc})) &= \sum_{i=1}^n \|\Phi(x_{gc,i}) - \sum_{j=1}^n (\delta W_0^{ij} + (1 - \delta)(W_0^{in} + W_0^{between}))\|_2^2 \\
&\quad \times (\Phi(x_{gc,i}) - \Phi(x_{gc}))^T \\
&\text{s.t. } \Phi^T(X_{gc})M_m\Phi(X_{gc}) = I_n
\end{align*}
\]

where \( tr() \) is trace operator, \( \delta \in [0,1] \) is a trade-off parameter for balancing the two terms in the numerator of eq 5, \( I_n \) denotes an identity matrix, and \( M_m \) is symmetric and positive semidefinite:

\[
M_m = M_m^T = (I_n - (\delta W_0^{in} + (1 - \delta)(W_0^{in} + W_0^{between})))^T
\]

Quality stabilization of products in a practical industrial production process is one of the one of the greatest problems of concern, especially in multimode processes with alterations of raw materials and compositions, different manufacturing strategies, etc.\(^{7}\) Hence, to ensure the quality stabilization, the relationships of the global common subspace and output quality variables are introduced. \( Q = [q_1, \ldots, q_d] \subseteq \mathbb{R}^q \) denotes a score matrix of output quality variables \( Y \), \( Q = Y^TH \), \( H = [h_1, \ldots, h_d] \subseteq \mathbb{R}^d \) is the load matrix of \( Y \). Thus, the
Global common subspace $\Phi(\mathbf{X}_{gc}) = \{\Phi(\mathbf{x}_{gc,1}), \Phi(\mathbf{x}_{gc,2}), \ldots, \Phi(\mathbf{x}_{gc,d})\} \in \mathbb{R}^r$ can be calculated as

$$\min \beta \text{tr}(\Phi(\mathbf{x}_{gc,i})\mathbf{M}_m \Phi^T(\mathbf{x}_{gc,i})) - (1 - \beta)\Phi(\mathbf{x}_{gc,i})\mathbf{Y}^T\mathbf{h}_i$$

s.t.

$$\mathbf{h}_i^T\mathbf{h}_i = 1$$

(7)

where $\beta \in [0,1]$ is also a trade-off parameter, $j = 1, \ldots, d$. It is considered that the problem of only calculating the global common subspace is unable to learn out-of-sample in monitoring. Then a projection matrix is calculated to tackle the out-of-sample learning problem. $\mathbf{P} = [\mathbf{p}_1, \ldots, \mathbf{p}_d]$ denotes the projection matrix. Thus, each data point in high-dimensional feature space is mapped to the global common subspace, that is

$$\Phi(\mathbf{X}_{gc}) = \mathbf{P}^T\Phi(\mathbf{X})$$

(8)

The projection matrix $\mathbf{P}$ can be calculated by the following optimization problem with constraints:

$$\min \beta \text{tr}(\mathbf{p}_i^T\Phi(\mathbf{X})\mathbf{M}_m \Phi^T(\mathbf{X})\mathbf{p}_i) + (1 - \beta)\mathbf{p}_i^T\Phi(\mathbf{X})\mathbf{Y}^T\mathbf{h}_i$$

s.t.

$$\mathbf{p}_i^T\mathbf{p}_i = 1$$

(9)

However, $\Phi(\mathbf{X})$ in high-dimensional feature space is unknown on the basis of kernel function theory. To solve the out-of-sample learning problem in monitoring, it is assumed that there exists combination coefficients matrix $\mathbf{U} = [\mathbf{u}_{1,1}, \ldots , \mathbf{u}_{1,d}] \in \mathbb{R}^r$, such that

$$\mathbf{p}_i = \Phi(\mathbf{X})\mathbf{u}_i \quad (i = 1, \ldots, d)$$

(10)

The optimization problem with constraints of eq 9 can be expressed as

$$\min \beta \text{tr}(\mathbf{u}_i^T\Phi(\mathbf{X})\mathbf{M}_m \Phi^T(\mathbf{X})\Phi(\mathbf{X})\mathbf{u}_i) + (1 - \beta)\mathbf{u}_i^T\Phi(\mathbf{X})\mathbf{Y}^T\mathbf{h}_i$$

$$= \beta \text{tr}(\mathbf{u}_i^T\mathbf{K}\mathbf{M}_m \mathbf{K}_u \mathbf{u}_i) + (1 - \beta)\mathbf{u}_i^T\mathbf{K}\mathbf{Y}^T\mathbf{h}_i$$

s.t.

$$\mathbf{h}_i^T\mathbf{u}_i = 1$$

(11)

The Lagrange multiplier method is used to solve the above problem, and the following eq 12 can be obtained:

$$(\beta \mathbf{K}\mathbf{M}_m \mathbf{K} + (1 - \beta)^2/4\lambda_\mathbf{h} \mathbf{K}\mathbf{Y}^T \mathbf{Y})\mathbf{u}_i = \lambda_\mathbf{u}_i \mathbf{u}_i$$

(12)

In conclusion, the combination coefficients vectors $\mathbf{u}_i$ ($i = 1, \ldots, d$) are the eigenvectors corresponding to the smallest $d$ eigenvalues of $(\beta \mathbf{K}\mathbf{M}_m \mathbf{K} + (1 - \beta)^2/4\lambda_\mathbf{h} \mathbf{K}\mathbf{Y}^T \mathbf{Y})$. The global common subspace $\Phi(\mathbf{X}_{gc})$ and the local specific subspace $\Phi(\mathbf{X}_{ls})$ can be decomposed as below:

$$\Phi^T(\mathbf{X}) = \Phi^T(\mathbf{X}_{gc})\mathbf{P}^T + \Phi^T(\mathbf{X}_{ls})$$

$$= \Phi^T(\mathbf{X}_{gc})\mathbf{P}^T + [\Phi^T(\mathbf{X}_{ls,1}), \ldots, \Phi^T(\mathbf{X}_{ls,d})]$$

(13)

where $\Phi(\mathbf{X}_{ls}) = [\Phi(\mathbf{X}_{ls,1}), \ldots, \Phi(\mathbf{X}_{ls,d})] \in \mathbb{R}^d$ is the local specific subspace of each mode and $b_i$ is the number of samples in each mode.

In the proposed method, mode information, two statistics and $B + 1$ control limits can be calculated for monitoring in multimode processes. When a new sample $\mathbf{x}_{new}$ is obtained, its mode information should be first recognized on the basis of weight matrix $\mathbf{W} = \delta \mathbf{W}^0_d + (1 - \delta)(\mathbf{W}^m_d + \mathbf{W}^\text{between}_d)$. $\mathbf{W}$ can be denoted as

$$\mathbf{W} = \begin{bmatrix}
\mathbf{W}^1_{b_1 \times b_1} & \mathbf{W}^1_{b_1 \times b_2} & \ldots & \mathbf{W}^B_{b_1 \times b_1} \\
\mathbf{W}^1_{b_2 \times b_1} & \mathbf{W}^1_{b_2 \times b_2} & \ldots & \mathbf{W}^B_{b_2 \times b_1} \\
\vdots & \vdots & \ddots & \vdots \\
\mathbf{W}^1_{b_B \times b_1} & \mathbf{W}^1_{b_B \times b_2} & \ldots & \mathbf{W}^B_{b_B \times b_1}
\end{bmatrix}$$

(14)

The mode information $L(\mathbf{x}_{new})$ of $\mathbf{x}_{new}$ can be determined by obtaining its minimum reconstructed weight error in corresponding mode:

$$\min e(L(\mathbf{x}_{new}) = i)$$

$$= \|\|\| \Phi(\mathbf{x}_{new}) - \Phi(\mathbf{x}_b)\|\|^2$$

$$= \|\|\| \Phi(\mathbf{x}_{new}) - \Phi(\mathbf{x}_{b, +1})\|\|^2 \mathbf{W}^b_{i \times i} (i = 1, \ldots, B)$$

(15)

where $(B_i = \Sigma_{i=1}^{B-1} b_i + (1 = i, i = 2, \ldots, B))$ is the first number of each mode in weight matrix $\mathbf{W}$ and $b_i$ is the number of samples in each mode. After determining mode information on a new sample, the global common subspace $\Phi_{gc,new}$ of $\mathbf{x}_{new}$ can be computed as

$$\Phi_{gc,new} = \mathbf{P}^T \Phi(\mathbf{x}_{new})$$

$$= \mathbf{U}^T \Phi(\mathbf{x}_{new})\Phi(\mathbf{x}_{new})$$

$$= \mathbf{U}^T \Phi(\mathbf{x}_{new})$$

(16)

Then two statistic indices $T^2_{GC}$ (Hotelling’s $T^2$) of the global common subspace and SPE_{ls} (squared prediction error, SPE) of the local specific subspace are calculated as

$$T^2_{GC} = \Phi_{gc,new}^T \mathbf{A}^{-1}_{GC} \Phi_{gc,new}$$

$$= \mathbf{K}(\mathbf{x}_{new}, \mathbf{X})\mathbf{U}\mathbf{A}^{-1}_{GC}\mathbf{U}^T \mathbf{K}(\mathbf{x}_{new}, \mathbf{X})$$

(17)

$$\text{SPE}_{ls} = \|\|\| \Phi(\mathbf{x}_{new})\|^2$$

$$= \|\|\| \Phi(\mathbf{x}_{new}) - \Phi_{gc,new}^T \mathbf{P}\|^2$$

$$= \mathbf{K}(\mathbf{x}_{new}, \mathbf{x}_{new}) - 2\mathbf{K}(\mathbf{x}_{new}, \mathbf{X})\mathbf{U}\mathbf{K}(\mathbf{x}_{new}, \mathbf{X})$$

$$+ \mathbf{K}(\mathbf{x}_{new}, \mathbf{X})\mathbf{U}\mathbf{K}(\mathbf{x}_{new}, \mathbf{X})$$

(18)

where $\mathbf{A}_{GC}$ is the covariance matrix of the global common subspace and it can be expressed as

$$\mathbf{A}_{GC} = \mathbf{P}^T \Phi(\mathbf{X}_{gc}) \Phi(\mathbf{X}_{gc}) \mathbf{P}$$

$$= \frac{\mathbf{U}^T \Phi(\mathbf{X}) \Phi(\mathbf{X}) \mathbf{U}}{n - 1}$$

(19)

$$= \frac{\mathbf{U}^T \mathbf{K} \mathbf{U}}{n - 1}$$
Finally, the contributions of all variables are obtained. Each control limit of the lth variable is calculated as

$$C_l = m(\text{cont}_l) + 2.5758s(\text{cont}_l),$$

where $m(\text{cont}_l)$ and $s(\text{cont}_l)$ are the mean and standard deviation of $\text{cont}_l$, respectively. The number 2.5758 is in the contribution relation is commonly used. The fault variable is considered to be responsible for the current fault.

The flowchart of the proposed method is described in Figure 2. It is obvious that the proposed approach can decompose multimode processes in this paper can be obtained by partial derivatives. The partial derivative of the kernel function for the lth variable $\mathbf{x}_l$ is calculated as

$$\frac{\partial \mathbf{K}(\mathbf{x}_{\text{new}}, \mathbf{X})}{\partial \mathbf{x}_l} = -\frac{2}{\mathbf{x}^T} (\mathbf{x}_{\text{new},l} - \mathbf{x}_{i,l})^2 \mathbf{K}(\mathbf{x}_{\text{new},l}, \mathbf{x}_l),$$

where $\mathbf{x}_l$ is the lth variable, $\mathbf{x}_{i,l}$ denotes value of the lth variable in $\mathbf{x}_i$. For a new sample, contributions of the lth variable to the global common subspace and the local specific subspace are calculated as

$$\text{cont}_l^2 = \frac{\partial \mathbf{K}(\mathbf{x}_{\text{new}}, \mathbf{X})}{\partial \mathbf{x}_l} = \mathbf{K}(\mathbf{x}_{\text{new},l}, \mathbf{x}_l) U_{\text{GMS}}^T \mathbf{K}^T(\mathbf{x}_{\text{new},l}) \mathbf{U}^T \mathbf{U}^T \mathbf{K}^T(\mathbf{x}_{\text{new},l})$$

(24)

$$\text{cont}_{\text{SPE}}^l = \frac{\partial \text{SPE}_{\text{GMS}}}{\partial \mathbf{x}_l} = \mathbf{K}(\mathbf{x}_{\text{new},l}, \mathbf{x}_l) U_{\text{GMS}}^T \mathbf{U}^T \mathbf{K}^T(\mathbf{x}_{\text{new},l})$$

(25)

After the contributions of all variables are obtained, each control limit of the lth variable is $C_l = m(\text{cont}_l) + 2.5758s(\text{cont}_l)$, where $m(\text{cont}_l)$ and $s(\text{cont}_l)$ are the mean and standard deviation of $\text{cont}_l$, respectively. The number 2.5758 is in the contribution relation is commonly used. The fault variable is considered to be responsible for the current fault.

The flowchart of the proposed method is described in Figure 2. It is obvious that the proposed approach can decompose nonlinear multimode processes, and monitor and identify fault variables. In addition, multimode information is reflected directly in process modeling. The out-of-sample learning problem in monitoring is solved by computing a projection matrix. A simple tutorial example of the proposed method is as follows:

(1) Normal history data are used for modeling and faulty data are used for monitoring. For offline modeling, standardized input data set $\mathbf{X}$ and quality variables $\mathbf{Y}$ are obtained.

(2) $k$ nearest neighbors of each data point in high-dimensional feature space are first constructed according to eq 2.

(3) The weight matrix with multimode information is calculated according to eqs 3 and 4.

(4) The global common subspace and the local specific subspace are obtained according to eqs 7–13.

(5) Two statistics and B+1 control limits are calculated for monitoring according to eqs 16–25.

(6) For online monitoring, statistic indices of faulty data are calculated according to eqs 17–20 and 23–25.

(7) Mode information on faulty data is determined according to eqs 14 and 15.

(8) Faults and faulty variables can be obtained according to the control limits of offline modeling.”

4. EXPERIMENT RESULTS

The purpose of this section is to validate the effectiveness of the proposed method by the experiments of penicillin fermentation processes and practical foods industrial production processes.
4.1. Penicillin Fermentation Processes. The penicillin fermentation processes have the characteristics of nonlinear and multimode. Most of the necessary cell mass is generated in the initial preculture mode. Cells continue to grow to be penicillin in the fed-batch mode. Compared with the initial preculture mode, the trajectories of various variables are stable in the fed-batch mode. The multimode information can be used for multimode modeling. The data can be obtained using PenSimv2.0 simulation software, which provides a standard platform for penicillin fermentation processes monitoring and fault identification. The flowchart of the penicillin fermentation processes and the trajectories of various variables in nominal conditions are illustrated in Figures 3 and 4. The reaction time of each penicillin fermentation process is 400 h, which contains a preculture mode of about 45 h and a fed-batch mode of about 355 h. The sampling interval is 1 h. Nine process variables and one quality variable of the processes are shown in Table 2. In this paper, six runs are generated from the simulator for multimode modeling under normal operating conditions. A faulty run in which instantaneous flow at the entrance is suddenly decreased at 46 h and maintained all the time is used for monitoring and discovering the fault variable. When a fault occurs, partial derivative contribution analysis can be used to identify the fault variable.

Table 2. Input and Quality Variables in Penicillin Fermentation Processes

<table>
<thead>
<tr>
<th>input variables</th>
<th>quality variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 aeration rate (L/h)</td>
<td>1 penicillin concentration (g/h)</td>
</tr>
<tr>
<td>2 agitator power (W)</td>
<td></td>
</tr>
<tr>
<td>3 substrate feed speed (L/h)</td>
<td></td>
</tr>
<tr>
<td>4 generated heat (kcal/L)</td>
<td></td>
</tr>
<tr>
<td>5 culture volume (L/h)</td>
<td></td>
</tr>
<tr>
<td>6 carbon dioxide concentration (mmol/L)</td>
<td></td>
</tr>
<tr>
<td>7 pH</td>
<td></td>
</tr>
<tr>
<td>8 fermentor temperature (K)</td>
<td></td>
</tr>
<tr>
<td>9 dissolved oxygen saturability (%)</td>
<td></td>
</tr>
</tbody>
</table>

Figure 4. Trajectories of each variable in nominal conditions.

Figure 5. Monitoring result of fault in penicillin fermentation processes using the proposed method: (a) monitoring, (b) contribution analysis. In panel a, red lines denote control limits of different subspaces, black lines denote statistic indices. In panel b, different colors denote nine different variables. In monitoring, there is one control limit in the global common subspace according to eq 21. The control limits of different modes in the local specific subspace is different according to eq 22. In contribution analysis, the control limits of different variables are different according to eqs 24 and 25.
The standardized matrix is obtained from the original data matrix. The global common subspace and the local specific subspace of two modes are decomposed by the proposed method. The control limits are calculated. Monitoring and fault identification of each subspace are shown in Figure 5. The statistic indices of sample s which are greater than the corresponding control limits are faulty. It is shown that fault occurs from the 46th to the 400th sample. Different control limits denote corresponding identified mode information. The variable contribution which is greater than the corresponding control limit denotes a faulty variable. Different control limits in specific subspace in Figure 5 indicate that mode information is exactly recognized. Moreover, it is proved that instantaneous flow at the entrance is the fault variable, which shows that the proposed approach is suitable for multimode processes monitoring.

4.2. Foods Industrial Production Processes. The flowchart of the foods industrial production processes is illustrated in Figure 6. The products with various specifications are manufactured continuously and require monitoring to ensure production safety and quality stabilization. Multimode information for multimode modeling can be obtained according to the products with various specifications. Different modes may have unequal duration in practical foods industrial production processes. Input and quality variables are selected, as shown in Table 3. All variables are measured at practical foods production processes, providing abundant information for modeling and monitoring. The history normal data and multimode information are used for offline modeling. Each mode is decomposed and the intrinsic multimode structure can be efficiently preserved in the global common subspace. The faulty data are used to verify the accuracy of monitoring. The sampling interval is 1 min. Two products with different specifications in the same production line have similar characteristics in a common perspective and also specific characteristics and effects on multimode processes, which are decomposed based on the proposed method. It should be noted that the proposed approach is also fit for the conditions of multimode processes with more than two modes.

Three fault data sets are used to validate the effectiveness of monitoring by the proposed method. Fault 1: return air temperature is in the abnormal condition from 20th to 80th sample. Fault 2: tank temperature is deviant from 25th to 80th sample. Fault 3: there is a failure of drying machine, which

Table 3. Input and Quality Variables in Foods Production Processes

<table>
<thead>
<tr>
<th>input variables</th>
<th>quality variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 instantaneous flow at the entrance (kg/h)</td>
<td>1 moisture (%)</td>
</tr>
<tr>
<td>2 moisture at the entrance (%)</td>
<td>2 padding value (g/cm³)</td>
</tr>
<tr>
<td>3 return air temperature (°C)</td>
<td>3 entire product rate (%)</td>
</tr>
<tr>
<td>4 tank temperature (°C)</td>
<td>4 broken product rate (%)</td>
</tr>
<tr>
<td>5 actual moisture at the first exit (%)</td>
<td></td>
</tr>
<tr>
<td>6 actual temperature at the first exit (°C)</td>
<td></td>
</tr>
<tr>
<td>7 high-speed return air temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>8 high-speed loose steam flow (kg/h)</td>
<td></td>
</tr>
<tr>
<td>9 furnace temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>10 hybrid wind temperature (°C)</td>
<td></td>
</tr>
<tr>
<td>11 actual temperature at the exit (°C)</td>
<td></td>
</tr>
<tr>
<td>12 actual moisture at the exit (%)</td>
<td></td>
</tr>
</tbody>
</table>
results in disordered actual temperature at the exit from the 60th sample to the 80th sample.

In this case, all samples are obtained at equal sampling intervals. Monitoring and fault identification of each subspace by using the proposed approach for Faults 1–3 are shown in Figures 7–9. In Figure 7, it is obviously shown that Fault 1 occurs from the 20th to 80th samples and mode information can be exactly recognized. Moreover, it is evident that return air temperature is a fault variable, which shows that accurate fault identification result can be obtained by the proposed approach. Similarly, as shown in Figure 8, Fault 2 occurs from the 25th to 80th samples and mode information can be exactly recognized. In addition, tank temperature is a fault variable. Mode information and fault variable of Fault 3 are detected accurately in Figure 9. The results explain that the proposed monitoring approach for multimode processes can detect failure accurately and which mode is faulty. The proposed approach provides a strong clue to determine which variables are responsible for the output products quality. When faulty variables are recognized, quality control can be realized by adjusting faulty variables, which can improve industrial production safety and quality stabilization.

For comparing purpose, one conventional multiple model method that builds a kernel partial least-squares (KPLS) model for each mode is performed for the foods industrial production processes. The proposed method considers global and local characteristics of multimode processes. When there are various modes, the multiple model method is ineffective and needs more complete process data of each mode. Therefore, the proposed approach is more suitable for multimode processes.
monitoring, which is shown in experimental results for Fault 3 in Figures 9 and 10 based on the false negative rate and false positive rate.

5. CONCLUSIONS

A new multimode processes monitoring method based on subspace decomposition is proposed and its experiments for monitoring and fault identification are illustrated. The proposed method has attractive features, which improve the disadvantages of multiple model methods. Moreover, the multimode method has attractive features, which improve the disadvantages of multiple model methods. The proposed subspace decomposition method is building an integrated model for multimode monitoring and can be suitable for practical industrial production processes. The influence of quality variables and multimode information are used for multimode modeling to improve the accuracy of monitoring. The experimental studies on penicillin fermentation processes and practical foods industrial production processes demonstrate that the proposed approach is effective and feasible. It should be noted that the proposed approach is also fit for the conditions of multimode processes with more than two modes.

■ AUTHOR INFORMATION

Corresponding Author
E-mail: lishuai@siat.cn.

Notes
The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

This work is supported by the National High Technology Research and Development Program of China (2013AA040705-1).

REFERENCES


