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Quality-Related and Process-Related Fault Monitoring With Online Monitoring Dynamic Concurrent PLS

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ABSTRACT The partial least squares (PLS) method has been widely used in quality-related industrial process monitoring because of its ability to extract quality-related information. Generally, online quality monitoring data cannot be obtained in real time, and in this case, updating the online monitoring model is a serious challenge. In this paper, an online monitoring dynamic PLS (OMD-PLS) model that uses the relation between time-delay process data and time-delay quality data is proposed. To accurately monitor the quality-related and process-related fault data, we also propose an online monitoring dynamic concurrent PLS (OMDC-PLS) model based on OMD-PLS, which has the ability to detect slight deviations. Furthermore, an alarm-parameter alarm method based on the OMDC-PLS model is proposed and effectively reduces the false alarm rate. Finally, numerical simulations and the Tennessee Eastman process are used to illustrate the effectiveness of the proposed methods.

INDEX TERMS Partial least squares, quality-related, process monitoring, dynamic.

I. INTRODUCTION

It is difficult to construct physical models of complex industrial processes. To solve this problem, a data-driven multivariate statistical model method is proposed [1]. Because of the high correlation of multiple measurements, how to capture the rela- tions between several measurements and important quality indices is a serious problem [2].

The partial least squares (PLS) method, which can effectively provide the potential relations between output (quality) varia- bles $\boldsymbol{Y}$ and input (process) variables $\boldsymbol{X}$, has become a powerful tool for quality-related fault monitoring [3]. PLS can extract latent variables with maximum covariance from $\boldsymbol{X}$ and $\boldsymbol{Y}$. Li *et al.* [2] found that the standard PLS method does not decompose $\boldsymbol{X}$ orthogonally. Moreover, PLS does not extract the latent variables in descending order of the variance in $\boldsymbol{X}$. These facts illustrate two shortcomings of the standard PLS model. First, the principal subspace of $\boldsymbol{X}$ contains variations that are orthogonal to $\boldsymbol{Y}$, which, in some cases, makes PLS unsuitable for quality-related fault monitoring. Second, the $\boldsymbol{X}$-residual of PLS usually has large variations, which makes the use of the $Q - statistic$ on the $\boldsymbol{X}$-residual inappropriate. To solve these two problems, Zhou *et al.* [4] proposed the total projection to latent structures (T-PLS) model by decomposing the $\boldsymbol{X}$-principal and $\boldsymbol{X}$-residual of the PLS. Furthermore, Yin *et al.* [5] proposed the modified partial least squares (M-PLS) model, which decomposes $\boldsymbol{X}$ orthogonally and uses singular value decomposition (SVD) to avoid iterative processes. Nevertheless, Peng *et al.* [6] found that a generalized inverse calculation process exists in the M-PLS algorithm model, which may lead to an $\boldsymbol{X}$-residual that still contains quality-related information. He proposed the efficient projection to latent structures (E-PLS) algorithm to further decompose the $\boldsymbol{X}$-residual. The T-PLS method has two disadvantages in fault monitoring. The first one is that this model monitors only the predictable $\boldsymbol{Y}$ part and ignores the unpredictable $\boldsymbol{Y}$ part. The second disadvantage is that it is unnecessary to divide $\boldsymbol{X}$ into four subspaces. To address these two deficiencies, Qin and Zheng [7] proposed the concurrent projection to latent structures (C-PLS) model based on PLS, which divided $\boldsymbol{X}$ into a prediction-related subspace and a prediction-unrelated subspace.

Recently, scholars have found that PLS and its extension algorithms focus on only global structure information and cannot suitably extract the local adjacent structure information from the data. The locality-preserving projections (LPP) method can preserve local features by projecting the global structure into an approximate linear space, but it cannot consider the overall structure and lacks detailed analysis and interpretation of the correlation between process and quality variables. By combining the advantages of LPP and PLS, Zhong *et al.* [8] proposed a quality-related global and local partial least squares (QGLPLS) model. Since QGLPLS removes the LPP constraint from the optimization objective function, the monitoring results have been seriously affected. To pay more attention to the locality-preserving characteristics, a new integration method called the locality-preserving partial least squares (LPPLS) model was proposed by Wang *et al.* [9]. To effectively retain global and local characteristics and pay more attention to the correlation of the extracted principal com- ponents, Zhou *et al.* [10] proposed the global plus local projection to latent structures (GPLPLS) model. GPLPLS, which ensures that the correlation between the data after dimension reduction is still the largest, can accurately distinguish among quality- recoverable faults, quality-unrelated faults and minor quality- related faults.

The above models consider only the static relation between $\boldsymbol{X}$ and $\boldsymbol{Y}$. However, in real industrial processes, there is a dynamic relation between $\boldsymbol{X}$ and $\boldsymbol{Y}$. A static model cannot fully describe the dynamic processes. To solve this issue, two PLS dynamic expansion methods have been proposed [11], [12]. The first one is the data preprocessing method. By constructing an augmented $\boldsymbol{X}$ consisting of large numbers of time-lagged values, the dynamic characteristics of the system are considered, and then the existing linear PLS algorithm is used to model them. In the second one, a dynamic PLS model is obtained by modifying the inner and outer PLS models.

At present, there are two data preprocessing methods. The first one [13] uses the matrix format of the finite impulse response (FIR) model, which adds a large amount of time-delay process data into $\boldsymbol{X}$. The second one [14] uses the matrix format of the autoregressive exogenous (ARX) model, which adds the time-delay process data and the time-delay quality data to $\boldsymbol{X}$ simultaneously. Ricker [11] proposed an FIR-PLS dynamic model using the FIR matrix format. Qin proposed a dynamic neural network partial least squares (D-NNPLS) model by introducing the ARX matrix format into a neural net PLS (NNPLS) [15].

The two abovementioned methods are easy to expand and have been widely used in many industrial process monitoring applications [16]–[22]. However, the data preprocessing method has some time-lagged data, which cause an increase in the computation time. In the static outer model between a filtered input and the output developed by Kaspar and Ray [12], the dynamic part of the input is removed using a dynamic filter that pro- cesses the dynamic data without augmenting the input matrix. The dynamic relation between the input and output latent varia- bles, which is considered in the inner model, is developed by designing a feedback controller. Instead of dynamically filtering the input data, Lakshminarayanan proposed a new dynamic PLS model [23] that modifies the inner PLS model to describe the relation between measured disturbances and the controlled outputs.

The above research focuses on only the inner model without modifying the outer PLS model. Li *et al.* [24] proposed an objective function to obtain a new dynamic outer model, where in a dynamic inner model was constructed using weighted input and output latent variables, and extended it to the dynamic T-PLS (D-TPLS) model. Based on a similar situation, Li *et al.* [25] improved dynamic PCA (DPCA) to the dynamic latent-variable (DLV) model. Dong and Qin [26] found that the inner model proposed by Li *et al.* [24] is not explicit and is dificult to interpret. Using the ARX model to describe the dynamic relation between process and quality latent vari- ables, Dong presented a dynamic PLS (Di-PLS) model. Inspired by Di-PLS, Dong and Qin [27] improved DPCA to the dynamic-inner PCA (DiPCA) model. Recently, Dong and Qin [28] also introduced dynamic latent variable methods for the modeling of multidimensional time series data for prediction to the essence and objectives of latent variable analytics.

In industrial processes, the process variables are more frequently sampled than the quality variables [7]. Therefore, the quality data of the current time period cannot be obtained, which means the sample numbers of new data $\boldsymbol{X}_{new}$ and $\boldsymbol{Y}_{new}$ are different. In this situation, how to update the model using the data becomes a new problem. As far as we know, little has been reported in the literature about this specific issue. In this study, we established an online monitoring dynamic PLS (OMD-PLS) model using the relation between the time-delay process data and the time-delay quality data. Based on OMD-PLS, an online monitoring dynamic C-PLS (OMDC-PLS) model, which has the ability to detect slight deviations, is proposed to monitor quality-related and process-related faults. Furthermore, we propose an alarm-parameter alarm method, which can effectively reduce the false alarm rate, in the dynamic process monitoring provided by OMDC-PLS.

The remainder of this paper is organized as follows. In Section II, the D-PLS model proposed by Li is reviewed, and the OMD-PLS and the OMDC-PLS models are proposed. In Section III, the process monitoring technology for OMDC-PLS is developed. In Section IV, the effectiveness of the proposed methods is illustrated with numerical simulations and the Tennessee Eastman process (TEP). In the last section, conclusions are presented.

II. ONLINE MONITORING DYNAMIC CONCURRENT PLS (OMDC-PLS) MODEL

The PLS was proposed by Wold *et al.* in 1983 [29]. PLS has been widely used in industrial process monitoring due to its comprehensive functions [30]. In this section, the main contents of the standard PLS and D-PLS are briefly reviewed. Then, the OMD-PLS is proposed for the online quality monitoring data that cannot be obtained in real time.

Finally, to accurately monitor the quality-related and process-related fault data, the OMDC-PLS algorithm is proposed.

A. DYNAMIC PARITIAL LEAST SQUARES (DPLS) MODEL

The standard PLS algorithm extracts the latent variables from $\boldsymbol{X}$ to interpret $\boldsymbol{Y}$ and builds a linear algebraic relation between the input scores $\boldsymbol{t} = \boldsymbol{Xw}$ and the output scores $\boldsymbol{u} = \boldsymbol{Yc}$. The selection of latent variables should satisfy two principles [31]. First, $\boldsymbol{t}$ and $\boldsymbol{u}$ should carry as much variation information as possible for $\boldsymbol{X}$ and $\boldsymbol{Y}$, respectively. Second, the degree of correlation between $\boldsymbol{t}$ and $\boldsymbol{u}$ should be maximized. The input matrix $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_n]^T \in \mathbf{R}^{\mathrm{n}\times\mathrm{m}}$ is composed of m process variables with n sample numbers. The output matrix $\boldsymbol{Y} = \left[\boldsymbol{y}_1, \boldsymbol{y}_2, \cdots, \boldsymbol{y}_n\right]^T \in \mathbf{R}^{\mathrm{n}\times\mathrm{p}}$ is composed of p quality variables with n sample numbers. On the basis of the two principles, the objective function of PLS is as follows:

$$\begin{cases} \max \boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{Yc} \\ s.t.\ \|\boldsymbol{w}\| = \|\boldsymbol{c}\| = 1. \end{cases} \tag{1}$$

The above function, which cannot extract the dynamic variations and relation between $\boldsymbol{X}$ and $\boldsymbol{Y}$, describes only the static relation between $\boldsymbol{X}$ and $\boldsymbol{Y}$. To describes a dynamic process, Li proposed the following outer model objective function [24]:

$$\begin{cases} \max\limits_{\boldsymbol{w},\boldsymbol{c},\beta_{(j)}} \left(\boldsymbol{w}^T\boldsymbol{X}_{(0)}^T\beta_{(0)} + \cdots + \boldsymbol{w}^T\boldsymbol{X}_{(d-1)}^T\beta_{(d-1)}\right)\boldsymbol{Yc} \\ s.t.\ \|\boldsymbol{w}\| = \|\boldsymbol{c}\| = 1 \\ \qquad \beta_{(0)}^2 + \beta_{(1)}^2 + \cdots + \beta_{(d-1)}^2 = 1, \end{cases} \tag{2}$$

where $\boldsymbol{X}_{(j)} = \left[\boldsymbol{x}_{d-j}, \boldsymbol{x}_{d+1-j}, \cdots, \boldsymbol{x}_{d+N-j}\right]^T \in \mathbf{R}^{(\mathrm{N}+1)\times m}$ is the input data with j time delay, $j = 0, \cdots, d-1$, $\beta_{(\mathrm{j})}$ is the weight coefficient for $\boldsymbol{X}_{(j)}\boldsymbol{w}$, $\boldsymbol{X}_{(j)}$ can be obtained by splitting $\boldsymbol{X}$ into d parts, and the number of samples in each part is $N+1$. N, n and d satisfy $N = n - d$. Function (2) maxi- mizes the dynamic linear relation of $\boldsymbol{X}$ and $\boldsymbol{Y}$ by searching for a direction vector $\boldsymbol{w}$ and a coefficient vector $\boldsymbol{\beta} = \left[\beta_{(0)}, \cdots, \beta_{(d-1)}\right]^T$. To simplify the expression, some define- tions are given as follows:

$$\boldsymbol{X}_{\mathrm{g}} = \left[\boldsymbol{X}_{(0)}, \boldsymbol{X}_{(1)}, \cdots, \boldsymbol{X}_{(d-1)}\right] \in \mathbf{R}^{(N+1)\times md}, \tag{3}$$

$$\boldsymbol{Y}_{(0)} = \left[\boldsymbol{y}_d, \boldsymbol{y}_{d+1}, \cdots, \boldsymbol{y}_{d+N}\right]^T \in \mathbf{R}^{(N+1)\times p}, \tag{4}$$

$$\boldsymbol{\beta}^T \otimes \boldsymbol{w}^T = (\boldsymbol{\beta}\otimes\boldsymbol{w})^T = \left[\beta_{(0)}\boldsymbol{w}^T, \cdots, \beta_{(d-1)}\boldsymbol{w}^T\right] \in R^{1\times md}, \tag{5}$$

where $\otimes$ represents the Kronecker product. Then, function (2) can be rephrased as follows:

$$\begin{cases} \max\limits_{\boldsymbol{w},\boldsymbol{c},\boldsymbol{\beta}}\ (\boldsymbol{\beta}\otimes\boldsymbol{w})^T\boldsymbol{X}_g^T\boldsymbol{Y}_{(0)}\boldsymbol{c} \\ s.t.\ \|\boldsymbol{w}\| = \|\boldsymbol{c}\| = \|\boldsymbol{\beta}\| = 1. \end{cases} \tag{6}$$

When $d = 1$, function (6) is the standard PLS objective function. The dynamic model contains at least one piece of time-delay data; therefore, $d \geq 2$. In this study, we are primarily concerned with the dynamic model, i.e., $d \geq 2$. Suppose that q represents the time-delay model parameter, i.e., $q = d - 1$. Then, it follows that $N + 1 = n - (d-1) = n - q$.

B. ONLINE MONITORING DYNAMIC PLS (OMD-PLS) MODEL

In actual industrial processes, the measurement frequency of the process variable is higher than that of the quality variable. Thus, we assume that the quality data of the $t \in (0, d)$ time period $\left[\boldsymbol{y}_{d+N+1-t}\cdots\boldsymbol{y}_{d+N}\right]^{\mathrm{T}}$ cannot be obtained at $\boldsymbol{Y}_{(0)}$. In addition, there is a correlation between the time-delay process data and the time-delay quality data. Therefore, $\boldsymbol{Y}_{(0)}$ in the D-PLS objective function is modified to $\boldsymbol{Y}_{\mathrm{g}} = \left[\boldsymbol{Y}_{(t)}, \boldsymbol{Y}_{(t+1)}, \cdots, \boldsymbol{Y}_{(d-1)}\right] \in \mathbf{R}^{(n-q)\times(d-\mathrm{t})p}$, where $\boldsymbol{Y}_{(j)}$ is the time-delay quality data corresponding to $\boldsymbol{X}_{(j)}$. This modification achieves two goals: (1) During online monitoring, current process data can be used to update the model, even though the quality data is not provided during the time period t, which improves the dynamic update capability of the model. (2) From the introduction of time- delay quality data, the quality-related fault detection capability of the model is improved. Herein, we denote the modified objective function as the OMD-PLS objective function,

$$\begin{cases} \max\limits_{\boldsymbol{w},\boldsymbol{c},\boldsymbol{\beta}} (\boldsymbol{\beta}\otimes\boldsymbol{w})^T\boldsymbol{X}_g^T\boldsymbol{Y}_g\boldsymbol{c} \\ s.t.\ \|\boldsymbol{w}\| = \|\boldsymbol{c}\| = \|\boldsymbol{\beta}\| = 1, \end{cases} \tag{7}$$

Lagrange multipliers are used to solve this optimization (7). We define the following:

$$\max\ J = (\boldsymbol{\beta}\otimes\boldsymbol{w})^T\boldsymbol{X}_g^T\boldsymbol{Y}_g\boldsymbol{c} + \frac{1}{2}\lambda_w\left(1 - \boldsymbol{w}^T\boldsymbol{w}\right) + \frac{1}{2}\lambda_c\left(1 - \boldsymbol{c}^T\boldsymbol{c}\right) + \frac{1}{2}\lambda_\beta\left(1 - \boldsymbol{\beta}^T\boldsymbol{\beta}\right), \tag{8}$$

Taking derivatives with respect to $\boldsymbol{w}$, $\boldsymbol{c}$ and $\boldsymbol{\beta}$ and setting the results to zero simplify the equation as follows:

$$\begin{cases} \mathbf{S}_w\boldsymbol{\beta} = \lambda_\beta\lambda_c\boldsymbol{\beta} \\ \mathbf{S}_\beta\boldsymbol{w} = \lambda_w\lambda_c\boldsymbol{w}, \end{cases} \tag{9}$$

where

$$\boldsymbol{S}_w \equiv (\boldsymbol{I}_d\otimes\boldsymbol{w})^T\boldsymbol{X}_g^T\boldsymbol{Y}_g\boldsymbol{Y}_g^T\boldsymbol{X}_g(\boldsymbol{I}_d\otimes\boldsymbol{w}) \in \mathbf{R}^{d\times d}, \tag{10}$$

$$\boldsymbol{S}_\beta \equiv (\boldsymbol{\beta}\otimes\boldsymbol{I}_m)^T\boldsymbol{X}_g^T\boldsymbol{Y}_g\boldsymbol{Y}_g^T\boldsymbol{X}_g(\boldsymbol{\beta}\otimes\boldsymbol{I}_m) \in \mathbf{R}^{m\times m}, \tag{11}$$

and $\lambda_\beta\lambda_c$ and $\lambda_w\lambda_c$ are the maximum objective function values from (8). Therefore, $\boldsymbol{\beta}$ is the maximum eigenvector of $\boldsymbol{S}_w$, and $\boldsymbol{w}$ is the maximum eigenvector of $\boldsymbol{S}_\beta$. It should be noted that $\boldsymbol{w}$ and $\boldsymbol{\beta}$ cannot be calculated directly using (9) because $\boldsymbol{S}_w$ and $\boldsymbol{S}_\beta$ depend on $\boldsymbol{w}$ and $\boldsymbol{\beta}$, respectively. We can initialize $\boldsymbol{w}$ and use (9) to calculate $\boldsymbol{w}$ and $\boldsymbol{\beta}$ iteratively, according to the method introduced in the literature [24]. The detailed OMD-PLS algorithm process is shown in TABLE 1.

In TABLE 1, $d = q + 1$. The parameters A and q are determined by two-dimensional cross-validation, as summarized in the Appendix. The OMD-PLS algorithm then has the

TABLE 1. OMD-PLS algorithm.

Algorithm 1 OMD-PLS

Normalize the raw data of the $\boldsymbol{X}$ and $\boldsymbol{Y}$ zero mean and unit variance, and determine the value of $t \in (0, d)$ according to the requirements. Calculate $\boldsymbol{X}_{g,i}$ and $\boldsymbol{Y}_{g,i}$, and set $i = 1$.

Step 1: Set $\boldsymbol{w}_i = [1, 0, \cdots, 0]^T$. $\boldsymbol{\beta}_i$ is the eigenvector corresponding to the largest eigenvalue of $\mathbf{S}_{w,i}$.

Step 2: Here, $\boldsymbol{w}_i$ is the eigenvector corresponding to the largest eigenvalue of $\boldsymbol{S}_{\beta,i}$.

Step 3: Iterate steps 1 and 2 until eigenvalues $\boldsymbol{w}_i$ and $\boldsymbol{\beta}_i$ converge.

Step 4: Update $\boldsymbol{Y}_{g,i}$:

$\boldsymbol{t}_{g,i} = \mathbf{X}_{g,i}(\boldsymbol{\beta}_i \otimes \boldsymbol{w}_i)$, $\boldsymbol{q}_i = \boldsymbol{Y}_{g,i}^T \boldsymbol{t}_{g,i} / \boldsymbol{t}_{g,i}^T \boldsymbol{t}_{g,i}$, $\boldsymbol{Y}_{g,i+1} = \boldsymbol{Y}_{g,i} - \boldsymbol{t}_{g,i} \boldsymbol{q}_i^T$,

Step 5: Update $\mathbf{X}_{g,i}$:

Set $j = 0$,

1) $\boldsymbol{t}_{(j),i} = X_{(j),i}^T \boldsymbol{w}_i$, $\boldsymbol{p}_{(j),i} = \boldsymbol{X}_{(j),i}^T \boldsymbol{t}_{(j),i} / \boldsymbol{t}_{(j),i}^T \boldsymbol{t}_{(j),i}$,

$\boldsymbol{X}_{(j),i+1} = \boldsymbol{X}_{(j),i} - \boldsymbol{t}_{(j),i} \boldsymbol{p}_{(j),i}^T$,

2) Set $j = j + 1$, return to 1) until $j > d - 1$,

3) $\boldsymbol{X}_{g,i+1} = \left[\boldsymbol{X}_{(0),i+1}, \boldsymbol{X}_{(1),i+1}, \cdots, \boldsymbol{X}_{(d-1),i+1}\right]$.

Step 6: Let $i = i + 1$; return to step 1 until $i > \mathrm{A}$.

following parameters:

$$\begin{cases} \boldsymbol{B} = [\boldsymbol{\beta}_1, \cdots, \boldsymbol{\beta}_{\mathrm{A}}] \in R^{d \times \mathrm{A}} \\ \boldsymbol{W} = [\boldsymbol{w}_1, \cdots, \boldsymbol{w}_{\mathrm{A}}] \in R^{m \times \mathrm{A}} \\ \boldsymbol{T}_g = [\boldsymbol{t}_{g,1}, \cdots, \boldsymbol{t}_{g,\mathrm{A}}] \in R^{(n-q) \times \mathrm{A}} \\ \boldsymbol{Q} = [\boldsymbol{q}_1, \cdots, \boldsymbol{q}_{\mathrm{A}}] \in R^{(d-t)p \times \mathrm{A}} \\ \boldsymbol{P}_{(j)} = [\boldsymbol{p}_{(j),1}, \cdots, \boldsymbol{p}_{(j),\mathrm{A}}] \in R^{m \times \mathrm{A}}. \end{cases} \tag{12}$$

where $i = 1, \cdots, A$ and $j = 0, \cdots, d-1$. To directly calculate the dynamic scores $\boldsymbol{T}_g$ from $\boldsymbol{X}_g$, a weight matrix $\boldsymbol{R}_g$ is defined as follows:

$$\begin{cases} \boldsymbol{R}_{(j)} = \boldsymbol{W}\left(\boldsymbol{P}_{(j)}^T \boldsymbol{W}\right)^{-1} \\ \boldsymbol{R}_{\mathrm{B}(j)} = \left[\mathrm{B}_{(j),1} \boldsymbol{R}_{(j),1}, \cdots, \mathrm{B}_{(j),\mathrm{A}} \boldsymbol{R}_{(j),\mathrm{A}}\right] \\ \boldsymbol{R}_g = \left[\boldsymbol{R}_{\mathrm{B}(1)}; \cdots; \boldsymbol{R}_{\mathrm{B}(d-1)}\right], \end{cases} \tag{13}$$

where $\mathrm{B}_{(j),i}$ is the element in the jth row and the ith column of $\boldsymbol{B}$. The formulae show that $\boldsymbol{T}_g = \boldsymbol{X}_g \boldsymbol{R}_g$.

The OMD-PLS model can be presented as follows:

$$\begin{cases} \boldsymbol{X}_{(j)} = \hat{\boldsymbol{X}}_{(j)} + \tilde{\boldsymbol{X}}_{(j)} = \boldsymbol{T}_{(j)} \boldsymbol{P}_{(j)}^T + \tilde{\boldsymbol{X}}_{(j)} \\ \boldsymbol{Y}_g = \hat{\boldsymbol{Y}}_g + \tilde{\boldsymbol{Y}}_g = \boldsymbol{T}_g \boldsymbol{Q}^T + \tilde{\boldsymbol{Y}}_g. \end{cases} \tag{14}$$

C. ONLINE MONITORING DYNAMIC CONCURRENT PLS (OMDC-PLS) MODEL

The D-PLS algorithm extracts $\boldsymbol{T}_g$ to maximize the covariance between $\boldsymbol{X}_g$ and $\boldsymbol{Y}_{(0)}$. The dynamic scores $\boldsymbol{T}_g$ relate only to the predictable portion of $\boldsymbol{Y}_{(0)}$ [7]. Based on D-PLS, D-TPLS monitors $\boldsymbol{T}_g$ only and neglects the information in $\boldsymbol{Y}_{(0)}$, which is not predicted by $\boldsymbol{X}_g$. To achieve a more reliable monitoring method of the dynamic process operation data and the dynamic quality data, we extend the static C-PLS model to the OMDC-PLS model. Three objectives are achieved: (1) The dynamic scores $\boldsymbol{U}_{gc}$, which compose the covariation subspace (CVS) and are directly related to $\hat{\boldsymbol{Y}}_g$, are extracted by OMDC-PLS; (2) The unpredictable output of $\tilde{\boldsymbol{Y}}_{gc}$ is decom- posed by PCA into the output-principal subspace (OPS) and the output-residual subspace (ORS); and (3) The direct relation between $\boldsymbol{X}_g$ and $\boldsymbol{U}_{gc}$ is $\boldsymbol{U}_{gc} = \boldsymbol{X}_g \boldsymbol{R}_{gc}$. The predict- table output-unrelated but input-related subspace $\tilde{\boldsymbol{X}}_{gc}$ is obtained by projecting $\boldsymbol{X}_g$ onto $span\{\boldsymbol{R}_{gc}\}^{\perp}$. Then, $\tilde{\boldsymbol{X}}_{gc}$ can be further decomposed by PCA into the input-principal subspace (IPS) and the input-residual subspace (IRS). The OMDC-PLS procedure is shown in TABLE 2.

TABLE 2. OMDC-PLS algorithm.

Algorithm 2 OMDC-PLS

Step 1: The predictable output $\hat{\boldsymbol{Y}}_g = \boldsymbol{T}_g \boldsymbol{Q}^T$ is calculated by **Algorithm 1**; then, perform SVD on $\hat{\boldsymbol{Y}}_g$ as follows,

$$\hat{\boldsymbol{Y}}_g = \boldsymbol{U}_{gc} \boldsymbol{D}_{gc} \boldsymbol{V}_{gc}^T \equiv \boldsymbol{U}_{gc} \boldsymbol{Q}_{gc}^T, \tag{15}$$

where $\boldsymbol{Q}_{gc} = \boldsymbol{V}_{gc} \boldsymbol{D}_{gc}$ and $\boldsymbol{U}_{gc}$ and $\boldsymbol{V}_{gc}$ are dimensionality reduction matrices obtained by selecting the first l_{gc} principal components as $l_{gc} = rank(\boldsymbol{Q})$.

$\boldsymbol{V}_{gc}$ is orthonormal, and $\boldsymbol{T}_g = \boldsymbol{X}_g \boldsymbol{R}_g$; therefore, $\boldsymbol{U}_{gc} = \boldsymbol{X}_g \boldsymbol{R}_g \boldsymbol{Q}^T \boldsymbol{V}_{gc} \boldsymbol{D}_{gc}^{-1}$.

Define $\boldsymbol{R}_{gc} = \boldsymbol{R}_g \boldsymbol{Q}^T \boldsymbol{V}_{gc} \boldsymbol{D}_{gc}^{-1}$, i.e., $\boldsymbol{U}_{gc} = \boldsymbol{X}_g \boldsymbol{R}_{gc}$.

Step 2: The unpredictable output is calculated as $\tilde{\boldsymbol{Y}}_{gc} = \hat{\boldsymbol{Y}}_g - \boldsymbol{U}_{gc} \boldsymbol{Q}_{gc}^T$. Then, PCA is performed on $\tilde{\boldsymbol{Y}}_{gc}$ with l_{gy} principal components,

$$\tilde{\boldsymbol{Y}}_{gc} = \boldsymbol{T}_{gy} \boldsymbol{P}_{gy}^T + \tilde{\boldsymbol{Y}}_{gr}, \tag{16}$$

where l_{gy} is determined by the cumulative percent variance ($\mathrm{CPV} \geq 0.85$).

Step 3: Project $\boldsymbol{X}_g$ on $span\{\boldsymbol{R}_{gc}\}^{\perp}$ to obtain the predictable output-unrelated input, i.e., $\tilde{\boldsymbol{X}}_{gc} = \boldsymbol{X}_g - \boldsymbol{U}_{gc} \boldsymbol{R}_{gc}^{\dagger}$. Then, perform PCA on $\tilde{\boldsymbol{X}}_{gc}$ with l_{gx} principal components,

$$\tilde{\boldsymbol{X}}_{gc} = \boldsymbol{T}_{gx} \boldsymbol{P}_{gx}^T + \tilde{\boldsymbol{X}}_{gr}, \tag{17}$$

where $\boldsymbol{R}_{gc}^{\dagger} = \left(\boldsymbol{R}_{gc}^T \boldsymbol{R}_{gc}\right)^{-1} \boldsymbol{R}_{gc}^T$ and l_{gx} is determined by the same method as l_{gy}.

After processing by **Algorithm 2**, the OMDC-PLS model can be presented as follows:

$$\begin{cases} \boldsymbol{X}_g = \boldsymbol{U}_{gc} \boldsymbol{R}_{gc}^{\dagger} + \boldsymbol{T}_{gx} \boldsymbol{P}_{gx}^T + \tilde{\boldsymbol{X}}_{gr} \\ \boldsymbol{Y}_g = \boldsymbol{U}_{gc} \boldsymbol{Q}_{gc}^T + \boldsymbol{T}_{gy} \boldsymbol{P}_{gy}^T + \tilde{\boldsymbol{Y}}_{gr}, \end{cases} \tag{18}$$

where $\boldsymbol{U}_{gc}$ are the dynamic scores directly related to predictable- output. $\boldsymbol{T}_{gx}$ are the principal input scores, which are unrelated to the predictable output. $\boldsymbol{T}_{gy}$ are unpredictable-output principal scores. $\boldsymbol{Q}_{gc}$, $\boldsymbol{R}_{gc}^{\dagger}$, $\boldsymbol{P}_{gx}$ and $\boldsymbol{P}_{gy}$ are the loading matrices. $\tilde{\boldsymbol{X}}_{gr}$ and $\tilde{\boldsymbol{Y}}_{gr}$ are the residuals of $\boldsymbol{X}_g$ and $\boldsymbol{Y}_g$, respectively. And $\boldsymbol{u}_{gc}^T$, $\boldsymbol{t}_{gx}^T$, $\boldsymbol{t}_{gy}^T$, $\boldsymbol{x}_g^T$, $\tilde{\boldsymbol{x}}_{gr}^T$, $\boldsymbol{y}_g^T$ and $\tilde{\boldsymbol{y}}_{gr}^T$ denote specific rows of $\boldsymbol{U}_{gc}$, $\boldsymbol{T}_{gx}$, $\boldsymbol{T}_{gy}$, $\boldsymbol{X}_g$, $\tilde{\boldsymbol{X}}_{gr}$, $\boldsymbol{Y}_g$ and $\tilde{\boldsymbol{Y}}_{gr}$, respectively. These single samples are related as follows:

$$\begin{cases} \boldsymbol{u}_{gc} = \boldsymbol{R}_{gc}^T \boldsymbol{x}_g \\ \boldsymbol{t}_{gx} = \boldsymbol{P}_{gx}^T \tilde{\boldsymbol{x}}_{gc} \\ \boldsymbol{t}_{gy} = \boldsymbol{P}_{gy}^T \tilde{\boldsymbol{y}}_{gc} \\ \tilde{\boldsymbol{x}}_{gr} = \left(\boldsymbol{I} - \boldsymbol{P}_{gx}\boldsymbol{P}_{gx}^T\right) \tilde{\boldsymbol{x}}_{gc} \\ \tilde{\boldsymbol{y}}_{gr} = \left(\boldsymbol{I} - \boldsymbol{P}_{gy}\boldsymbol{P}_{gy}^T\right) \tilde{\boldsymbol{y}}_{gc}, \end{cases} \tag{19}$$

where $\tilde{\boldsymbol{x}}_{gc} = \boldsymbol{x}_g - \boldsymbol{R}_{gc}^{\dagger T} \boldsymbol{u}_{gc}$, and $\tilde{\boldsymbol{y}}_{gc} = \boldsymbol{y}_g - \boldsymbol{Q}_{gc}\boldsymbol{u}_{gc}$.

III. DYNAMIC PROCESS MONITORING TECHNOLOGY

After modeling with OMDC-PLS, $\boldsymbol{U}_{gc}$, $\boldsymbol{T}_{gx}$, $\tilde{\boldsymbol{X}}_{gr}\tilde{\boldsymbol{X}}_{gr}$, $\boldsymbol{T}_{gy}$ and $\tilde{\boldsymbol{Y}}_{gr}$, which represent covariation in the corresponding subspaces, can be monitored with the appropriate statistical technique.

A. PROCESS MONITORING INDICATORS IN OMDC-PLS

Because $\boldsymbol{U}_{gc}$ is an orthogonal matrix, the elements of $\boldsymbol{u}_{gc}$ have a zero mean with variance $1/(n-1)$. The T^2 statistic then provides more reasonable monitoring as follows:

$$T_c^2 = (n-1)\, \boldsymbol{u}_{gc}^T \boldsymbol{u}_{gc}. \tag{20}$$

According to PCA process monitoring technology [32], $\boldsymbol{T}_{gx}$ and $\tilde{\boldsymbol{X}}_{gr}$ can be monitored using the T^2 statistic and the Q statistic as follows:

$$T_x^2 = \boldsymbol{t}_{gx}^T \boldsymbol{\Lambda}_x^{-1} \boldsymbol{t}_{gx}, \tag{21}$$

$$Q_x = \left\|\tilde{\boldsymbol{x}}_{gr}\right\|^2, \tag{22}$$

where $\boldsymbol{\Lambda}_x = \boldsymbol{T}_{gx}^T \boldsymbol{T}_{gx} \big/ (n-1)$.

Similarly, $\boldsymbol{T}_{gy}$ and $\tilde{\boldsymbol{Y}}_{gr}$ can be monitored by the T^2 statistic and the Q statistic as follows:

$$T_y^2 = \boldsymbol{t}_{gy}^T \boldsymbol{\Lambda}_y^{-1} \boldsymbol{t}_{gy}, \tag{23}$$

$$Q_y = \left\|\tilde{\boldsymbol{y}}_{gr}\right\|^2, \tag{24}$$

where $\boldsymbol{\Lambda}_y = \boldsymbol{T}_{gy}^T \boldsymbol{T}_{gy} \big/ (n-1)$.

To monitor the dynamic process based on the statistical methods described above, we calculate the control limits from the statistics of the modeling data. The C-PLS algorithm proposed by Qin and Zheng [7], the OSC-MPLS algorithm proposed by Wang and Yin [33] and the OMDC-PLS algorithm proposed herein all use SVD to orthogonalize the modeling scores. If n is sufficiently large, the T^2 and Q indices approximately follow χ^2 distributions [34]. Therefore, the control limits of the T^2 statistic and of the Q statistic are calculated as follows:

$$\begin{cases} J_{th,T^2} = \chi_{l,\alpha}^2 \\ J_{th,Q} = g\chi_{h,\alpha}^2, \end{cases} \tag{25}$$

where l is the number of the principal component; $1-\alpha$ represents the confidence; and $g = b/2a$ and $h = 2a^2/b$, where a and b are the mean and the variance, respectively, of the Q statistic.

There are always some differences caused by noise and minor faults that do not affect normal operating conditions between the variations in the model data and the online detection data under normal conditions. Noise and minor faults usually exist in the process data as subcomponents. In OMDC-PLS model process monitoring, these subcomponents are introduced in $\tilde{\boldsymbol{X}}_{gr} d$ times, resulting in control limits of the online normal data ($\hat{J}_{th,Q_x}$) that are Ti times the control limits of the modeling data (J_{th,Q_x}). That is, $\hat{J}_{th,Q_x} = Ti\, J_{th,Q_x} = Ti\, g_x\chi_{h_x,\alpha}^2$. We have thus found the following relation between the multiple Ti and parameter d through the experiments described in section 4.2.3:

$$Ti = 1.281 + 0.1358d - 0.0018d^2, \quad 2 \le d \le 40; \tag{26}$$

therefore, the Q_x statistic has two control limits, J_{th,Q_x} and $\hat{J}_{th,Q_x}$. While J_{th,Q_x} can detect noise and minor faults, $\hat{J}_{th,Q_x}$ can detect more serious faults.

When using online monitoring, we need a process data matrix $\boldsymbol{X}_{new} = \left[\boldsymbol{x}_{\mathrm{new},1}, \boldsymbol{x}_{\mathrm{new},2}, \cdots, \boldsymbol{x}_{\mathrm{new,d}}\right]^T \in \mathbf{R}^{d\times m}$ to build the dynamic process data $\boldsymbol{x}_{gnew} = \left[\boldsymbol{x}_{\mathrm{new,d}}^T, \cdots, \boldsymbol{x}_{\mathrm{new},1}^T\right]$, where $\boldsymbol{x}_{\mathrm{new,d}}$ is the current process data and $\boldsymbol{x}_{\mathrm{new},1}$, $\boldsymbol{x}_{\mathrm{new},2}, \cdots,$ $\boldsymbol{x}_{\mathrm{new},(d-1)}$ is the time-delay process data. Similarly, a quality data matrix $\boldsymbol{Y}_{\mathrm{new}} = \left[\boldsymbol{y}_{\mathrm{new},1}, \boldsymbol{y}_{\mathrm{new},2}, \cdots, \boldsymbol{y}_{\mathrm{new,(d-t)}}\right]^T \in \mathbf{R}^{(d-t)\times p}$ is needed to build the dynamic quality data $\boldsymbol{y}_{gnew} = \left[\boldsymbol{y}_{\mathrm{new},(d-t)}^T, \cdots, \boldsymbol{y}_{\mathrm{new},1}^T\right]$, where $\boldsymbol{y}_{\mathrm{new},(d-t)}$ is the current measurable quality data and $\boldsymbol{y}_{\mathrm{new},1}$, $\boldsymbol{y}_{\mathrm{new},2}, \cdots,$ $\boldsymbol{y}_{\mathrm{new,(d-t-1)}}$ is the time-delay quality data. New scores and residuals are then constructed as follows:

$$\begin{cases} \boldsymbol{u}_{gcnew} = \boldsymbol{R}_{gc}^T \boldsymbol{x}_{gnew} \\ \boldsymbol{t}_{gxnew} = \boldsymbol{P}_{gx}^T \tilde{\boldsymbol{x}}_{gcnew} \\ \boldsymbol{t}_{gynew} = \boldsymbol{P}_{gy}^T \tilde{\boldsymbol{y}}_{gcnew} \\ \tilde{\boldsymbol{x}}_{grnew} = \left(\boldsymbol{I} - \boldsymbol{P}_{gx}\boldsymbol{P}_{gx}^T\right) \tilde{\boldsymbol{x}}_{gcnew} \\ \tilde{\boldsymbol{y}}_{grnew} = \left(\boldsymbol{I} - \boldsymbol{P}_{gy}\boldsymbol{P}_{gy}^T\right) \tilde{\boldsymbol{y}}_{gcnew}, \end{cases} \tag{27}$$

where $\tilde{\boldsymbol{x}}_{gcnew} = \boldsymbol{x}_{gnew} - \boldsymbol{R}_{gc}^{\dagger T} \boldsymbol{u}_{gcnew}$ and $\tilde{\boldsymbol{y}}_{gcnew} = \boldsymbol{y}_{gnew} - \boldsymbol{Q}_{gc}\boldsymbol{u}_{gcnew}$. We then calculate the new statistics T_{cnew}^2, T_{xnew}^2, Q_{xnew}, T_{ynew}^2 and Q_{ynew}, which are compared with the corresponding control limits to monitor the process as follows:

1. If $T_{cnew}^2 > J_{th,T_c^2} = \chi_{l_{gc},\alpha}^2$, a predictable-quality-related fault is detected in $\boldsymbol{x}_{gnew}$,

2. If $T_{xnew}^2 > J_{th,T_x^2} = \chi_{l_{gx},\alpha}^2$ or $Q_{xnew} > \hat{J}_{th,Q_x} = Ti\, g_x\chi_{h_x,\alpha}^2$, a predict- table quality-unrelated but process-related fault is detected in $\boldsymbol{x}_{gnew}$,

3. If only $Q_{xnew} > J_{th,Q_x} = g_x\chi_{h_x,\alpha}^2$, noise or minor faults are detected in $\tilde{\boldsymbol{x}}_{grnew}$,

4. If $Q_{xnew} > \hat{J}_{th,Q_x}$ and $T_{ynew}^2 > J_{th,T_y^2} = \chi_{l_{gy},\alpha}^2$ or else if $Q_{xnew} > \hat{J}_{th,Q_x}$ and $Q_{ynew} > J_{th,Q_y} = g_y\chi_{h_y,\alpha}^2$, a potentially unpredictable quality- related fault is detected in $\tilde{\boldsymbol{x}}_{grnew}$,

5. If $T_{ynew}^2 > J_{th,T_y^2} = \chi_{l_{gy},\alpha}^2$ or $Q_{ynew} > J_{th,Q_y} = g_y\chi_{h_y,\alpha}^2$, an unpredic- table quality-related fault is detected.

B. DYNAMIC PROCESS MONITORING TECHNOLOGY FOR OMDC-PLS

In this section, the proposed set of dynamic process monitoring technologies are described for OMDC-PLS that aim to achieve two objectives: (1) $N\mathrm{um}_{T_c^2}$, $N\mathrm{um}_{T_x^2}$, $N\mathrm{um}_{T_y^2}$ and $N\mathrm{um}_{Q_y}$ are defined as the alarm parameters of T^2_{cnew}, T^2_{xnew}, T^2_{ynew} and Q_{ynew}, respectively, and $N\mathrm{um}_{Q_x,J}$ and $N\mathrm{um}_{Q_x,\hat{J}}$ are defined as the alarm parameters of Q_{xnew}. If the statistics exceed the corresponding control limits, the corresponding alarm parameters will advance by one. If not, the corresponding alarm parameters will be set to zero. The fault alarm will not be triggered until the alarm parameters exceed the parameter limit (PL). The PL should initialize the appropriate values, and the appropriate values can effectively reduce the FAR. Excessive value of PL will affect the process monitoring results. (2) MU is defined as the model update parameter to implement the model update function. The number of stored data samples exceeds MU will trigger the model update function. The dynamic process monitoring technology is presented in TABLE 3. To describe in more detail the implementation procedure in TABLE 3, Fig. 1 is given.

IV. DYNAMIC PROCESS MONITORING TECHNOLOGY

In this section, three experiments are performed. First, we use synthetic simulations to emulate some representative faults to illustrate the effectiveness of OMDC-PLS in detecting quality-related and process-related faults. Second, the TEP is used to verify the quality-related dynamic process modeling and monitoring. Third, the relations between multiple Ti and the parameter d are obtained through experiments based on the TEP.

A. SIMULATIONS OF QUALITY-RELATED AND PROCESS-RELATED FAULT MONITORING

1) NUMERICAL SIMULATION MODEL AND FAULT-ADDING METHOD

The initial input and output data are generated as follows:

$$\begin{cases} \boldsymbol{t}_{k-2} = \boldsymbol{t0}_{k-2} + [10;\,10;\,10] \\ \boldsymbol{x}_{k-2} = \boldsymbol{P}\boldsymbol{t}_{k-2} + \boldsymbol{e}_{k-2} \\ \boldsymbol{y}_{k-2} = \boldsymbol{C}\boldsymbol{x}_{k-2} + \boldsymbol{v}_{k-2} \\ \boldsymbol{t}_{k-1} = \alpha_1\boldsymbol{t}_{k-2} + \boldsymbol{t0}_{k-1} + [10;\,10;\,10] \\ \boldsymbol{x}_{k-1} = \boldsymbol{P}\boldsymbol{t}_{k-1} + \boldsymbol{e}_{k-1} \\ \boldsymbol{y}_{k-1} = \boldsymbol{C}\boldsymbol{x}_{k-1} + \boldsymbol{C}_2\boldsymbol{x}_{k-2} + \beta_1\boldsymbol{y}_{k-2} + \boldsymbol{v}_{k-1}, \end{cases} \tag{28}$$

The inputs and outputs are generated by the following dynamic model [24]:

$$\begin{cases} \boldsymbol{t}_k = \alpha_1\boldsymbol{t}_{k-1} + \alpha_2\boldsymbol{t}_{k-2} + \boldsymbol{t}_k^* \\ \boldsymbol{x}_k = \boldsymbol{P}\boldsymbol{t}_k + \boldsymbol{e}_k \\ \boldsymbol{y}_k = \boldsymbol{C}\boldsymbol{x}_k + \boldsymbol{C}_2\boldsymbol{x}_{k-1} + \beta_1\boldsymbol{y}_{k-1} + \beta_2\boldsymbol{y}_{k-2} + \boldsymbol{v}_k, \end{cases} \tag{29}$$

where

$$\beta_1 = \begin{bmatrix} 0.2485 & 0.1552 \\ -0.4856 & -0.3011 \end{bmatrix}, \quad \beta_2 = \begin{bmatrix} -0.3042 & -0.3009 \\ 0.3265 & 0.4914 \end{bmatrix},$$

TABLE 3. OMDC-PLS dynamic process monitoring technology.

Dynamic process monitoring technology
Offline modeling and initialization: The OMDC-PLS model is built from standardized modeling data matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$, and all control limits are calculated. Then, all alarm parameters are set to 0, PL=5, $MU=100$, $i=0$, and $j=0$. Here, $\boldsymbol{x}_{\mathrm{new},(1+i)}, \boldsymbol{x}_{\mathrm{new},(2+i)}, \cdots, \boldsymbol{x}_{\mathrm{new},(d\text{-}1+i)}$ and $\boldsymbol{y}_{\mathrm{new},(1+i)}, \boldsymbol{y}_{\mathrm{new},(2+i)}, \cdots, \boldsymbol{y}_{\mathrm{new},(d\text{-}t\text{-}1+i)}$ are provided to initialize the dynamic data for online monitoring.
Online monitoring:
Step 1: Currently measurable sample data ($\boldsymbol{x}_{\mathrm{new},(d+i)}$, $\boldsymbol{y}_{\mathrm{new},(d\text{-}t+i)}$) are obtained to compose process data $\boldsymbol{X}_{new} = [\boldsymbol{x}_{\mathrm{new},(1+i)}, \boldsymbol{x}_{\mathrm{new},(2+i)}, \cdots, \boldsymbol{x}_{\mathrm{new},(d+i)}]^{\mathrm{T}}$ and quality data $\boldsymbol{Y}_{new} = [\boldsymbol{y}_{\mathrm{new},(1+i)}, \boldsymbol{y}_{\mathrm{new},(2+i)}, \cdots, \boldsymbol{y}_{\mathrm{new},(d\text{-}t+i)}]^{\mathrm{T}}$, which are converted to the dynamic data $\boldsymbol{x}_{gnew} = [\boldsymbol{x}^T_{\mathrm{new},(d+i)}, \cdots, \boldsymbol{x}^T_{\mathrm{new},(1+i)}]$ and $\boldsymbol{y}_{gnew} = [\boldsymbol{y}^T_{\mathrm{new},(d\text{-}t+i)}, \cdots, \boldsymbol{y}^T_{\mathrm{new},(1+i)}]$, respectively.
Step 2: Calculate new statistical parameters T^2_{cnew} , T^2_{xnew} , T^2_{ynew} , Q_{ynew} and Q_{xnew} and then compare these statistical results with the corresponding control limits. 1) If none of the new statistical results exceed the control limit, zero all the alarm parameters and go to Step 4; 2) If any one of T^2_{cnew} , T^2_{xnew} , T^2_{ynew} , Q_{ynew} or Q_{xnew} exceeds the corresponding control limit, increase the corresponding alarm parameter by one. Parameters with statistical results that do not exceed the control limit are set to zero. Then, go to Step 3.
Step 3: Compare $Num_{T_c^2}$, $Num_{T_x^2}$, $Num_{T_y^2}$, Num_{Q_y} , $Num_{Q_x,J}$ and $Num_{Q_x,\hat{j}}$ with PL , 1) If $Num_{Q_x,J} > PL$, then noise or minor faults are detected. 2) If $Num_{T_c^2} > PL$, a predictable quality-related fault is detected. 3) If $Num_{T_x^2} > PL$ or $Num_{\hat{Q}_x} > PL$, a predictable quality-unrelated fault is detected. 4) If $Num_{T_y^2} > PL$ or $Num_{Q_y} > PL$, an unpredictable quality-related fault is detected. 5) If $Num_{Q_x,\hat{j}} > PL$ and $Num_{T_y^2} > PL$ or $Num_{Q_y} > PL$, a potentially unpredictable quality-related fault is detected. If only 1) is satisfied, raise the alarm to indicate a slight deviation. If any one of 2)-5) is satisfied, a serious fault alarm will occur, indicating that the fault starting point is $i-FA+1$. If none of 1)-5) are satisfied, the alarm does not trigger. Let $i=i+1$, and then go to Step 1.
Step 4: Substitute $\boldsymbol{x}_{\mathrm{new},(d+i)}$ and $\boldsymbol{y}_{\mathrm{new},(d\text{-}t+i)}$ into $\boldsymbol{X}_j = [\boldsymbol{X}_j; \boldsymbol{x}^T_{\mathrm{new},(d+i)}]$ and $\boldsymbol{Y}_j = [\boldsymbol{Y}_j; \boldsymbol{y}^T_{\mathrm{new},(d\text{-}t+i)}]$, respectively. Let $j=j+1$ and $i=i+1$.
Step 5: If $j=MU$, j old sample data are removed from $\boldsymbol{X}$ and $\boldsymbol{Y}$. Then, substitute $\boldsymbol{X}_j$ and $\boldsymbol{Y}_j$ into $\boldsymbol{X}$ and $\boldsymbol{Y}$, respectively. Update the OMDC-PLS model. Set $j=0$, and go to Step 1. Otherwise, go to Step 1.

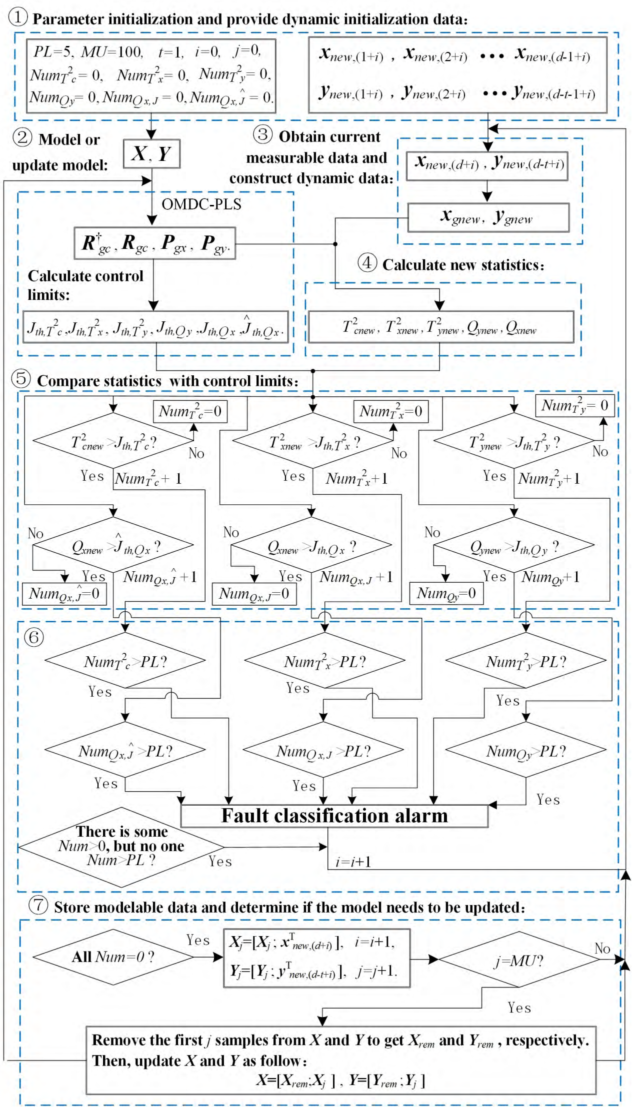

FIGURE 1. The dynamic process monitoring technology flow chart.

$$
P = \begin{bmatrix} 0.5586 & 0.2042 & 0.2042 \\ 0.2007 & 0.0492 & 0.4429 \\ 0.0874 & 0.6062 & 0.0664 \\ 0.9332 & 0.5463 & 0.3743 \\ 0.2594 & 0.0958 & 0.2491 \end{bmatrix},
$$

$$
C = \begin{bmatrix} 0.9249 & 0.4350 \\ 0.6295 & 0.9811 \\ 0.8783 & 0.0960 \\ 0.6417 & 0.5275 \\ 0.7984 & 0.5456 \end{bmatrix}^T,
$$

$$
C_2 = \begin{bmatrix} 1.7198 & -0.3715 \\ 0.5835 & 1.5011 \\ 1.4236 & 1.3226 \\ 0.4963 & -1.4145 \\ -2.5717 & 1.0696 \end{bmatrix}^T,
$$

$$
\alpha_1 = \begin{bmatrix} 0.4389 & 0.1210 & -0.0862 \\ -0.2966 & -0.0550 & 0.2274 \\ 0.4538 & -0.6573 & 0.4239 \end{bmatrix},
$$

$$
\alpha_2 = \begin{bmatrix} -0.2998 & -0.1905 & -0.2669 \\ -0.0204 & -0.1585 & -0.2950 \\ 0.1461 & -0.0755 & 0.3749 \end{bmatrix},
$$

$$
t_k = \begin{cases} \boldsymbol{t0}_k + [10; 10; 10], & 250 > k \geq 1 \\ \boldsymbol{t0}_k - [5; 5; 5], & 500 > k \geq 250 \\ \boldsymbol{t0}_k + [1; 1; 1]\sin(0.1k), & 750 > k \geq 500 \\ \boldsymbol{t0}_k & 1000 > k \geq 750, \end{cases}
$$

where $\boldsymbol{e}_k \sim \boldsymbol{N}(0, 0.1^2\boldsymbol{I}_3)$, $\boldsymbol{v}_k \sim \boldsymbol{N}(0, 0.1^2\boldsymbol{I}_3)$, and $\boldsymbol{t0}_k \sim \boldsymbol{N}(0, 2^2\boldsymbol{I}_3)$. Based on the dynamic model, 1000 samples $(\boldsymbol{X}, \boldsymbol{Y})$ are generated under normal operating conditions. To search for the optimal A and q using the two-dimensional cross-validation- based approach (see Appendix), $A_{\max} = 5$ and $q_{\max} = 10$ are selected. The data in Fig. 2 show that $A = 3$, $q = 3$ are obtained for 1000 samples $(\boldsymbol{X}, \boldsymbol{Y})$.

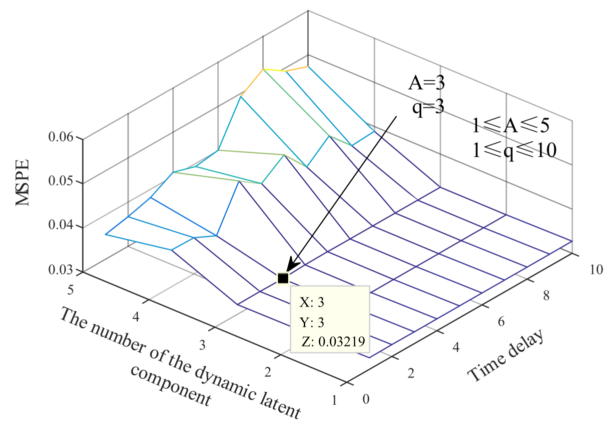

FIGURE 2. Two-dimensional cross-validation results for (X, Y).

Faults are added to the input space and the output space as follows:

$$
x_k = x_k^* + \Xi_x f_x, \tag{30}
$$

$$
y_k = y_k^* + \Xi_y f_y, \tag{31}
$$

where Ξ_x and Ξ_y are the fault-free values and f_x and f_y are the corresponding fault magnitudes. Using formulae (30) and (31), we generate 1000 online samples $(\boldsymbol{X}, \boldsymbol{Y})^{Online}$, which consist of 249 normal samples and 751 fault samples. In this study, we set $t = 1$ and build the C-PLS model from $(\boldsymbol{X}, \boldsymbol{Y})$ to obtain the load matrices $\boldsymbol{R}_c$, $\boldsymbol{P}_y$ and $\boldsymbol{P}_x$; thus, we obtain Ξ_x and Ξ_y [7].

2) PREDICTABLE QUALITY-RELATED FAULTS

In CVS, we set $f_x = 1$ and choose Ξ_x to be the first column of $\boldsymbol{R}_c$ to obtain $(\boldsymbol{X}, \boldsymbol{Y})^{T^2_{cnew}}$. Fault detection of $(\boldsymbol{X}, \boldsymbol{Y})^{T^2_{cnew}}$ is performed using OMDC-PLS. The fault detection result in Fig. 3 shows that only T^2_{cnew} detects the fault, whereas the other statistics are not affected. This result means that the fault detected by T^2_{cnew} is a predictable quality-related fault.

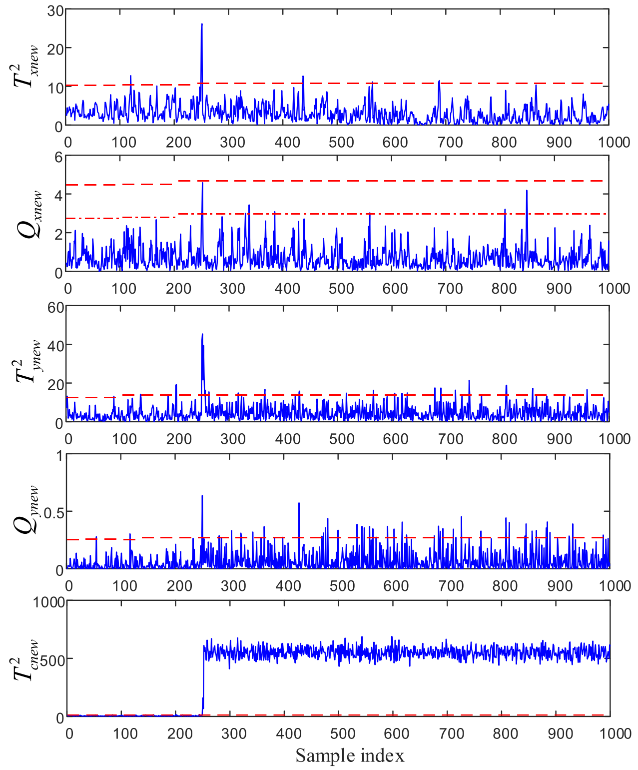

FIGURE 3. Fault occurs in CVS.

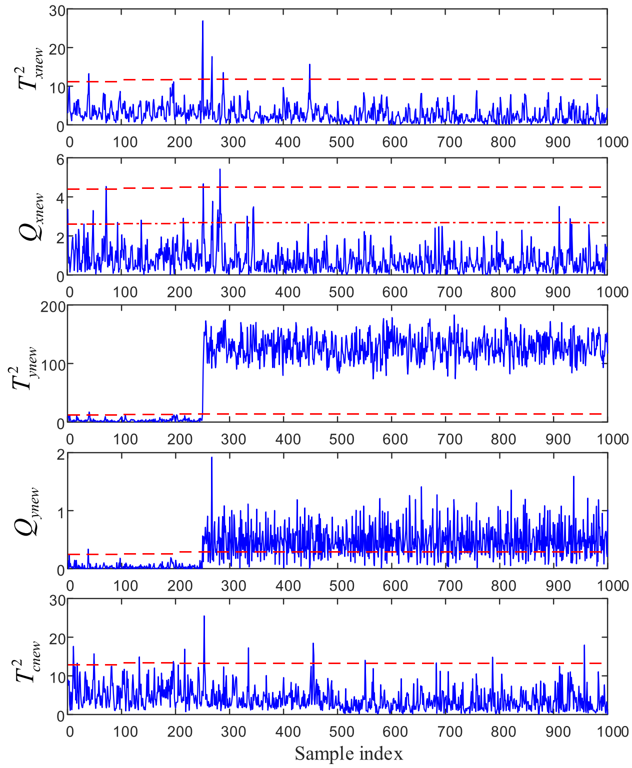

FIGURE 4. Fault occurs in OPS.

3) UNPREDICTABLE QUALITY-RELATED FAULT

To generate a fault in OPS, we set $f_y = 50$, and we choose Ξ_y to be the first column of $\boldsymbol{P}_y$ to obtain $(\boldsymbol{X}, \boldsymbol{Y})^{T^2_{ynew}}$. Fault detection of $(\boldsymbol{X}, \boldsymbol{Y})^{T^2_{ynew}}$ is performed using the OMDC-PLS dynamic process monitoring technology. The fault detection results in Fig. 4 show that both T^2_{ynew} and Q_{ynew} detect the fault. The results imply that the fault detected by both T^2_{ynew} and Q_{ynew} is an unpredictable quality-related fault.

4) POTENTIALLY UNPREDICTABLE QUALITY-RELATED FAULT

In IRS, we set $f_x = 16$ and choose Ξ_x to be the first column of $\left(\boldsymbol{I} - \boldsymbol{P}_x \boldsymbol{P}_x^T\right) \left[\boldsymbol{I} - \boldsymbol{R}_c \left(\boldsymbol{R}_c^T \boldsymbol{R}_c\right)^{-1} \boldsymbol{R}_c^T\right]$ to obtain $(\boldsymbol{X}, \boldsymbol{Y})^{Q_{xnew}}$. Fault detection of $(\boldsymbol{X}, \boldsymbol{Y})^{Q_{xnew}}$ is performed using the OMDC-PLS dynamic process monitoring technology. The fault detection result in Fig. 5 shows that T^2_{ynew} and Q_{ynew} detect the fault; thus, the fault is identified as an unpredictable quality- related fault. Moreover, both $\hat{J}_{th,Q_x}$ and J_{th,Q_x} of Q_{xnew} also detect the fault. This result implies that Q_{xnew} can detect potentially unpredictable quality-related faults in the input space.

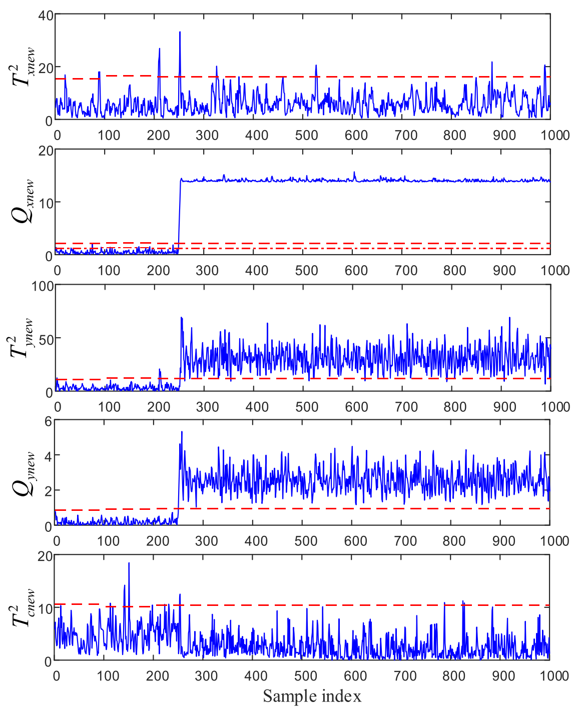

FIGURE 5. Fault occurs in IRS.

5) PREDICTABLE QUALITY-UNRELATED BUT PROCESS-RELATED FAULT

Here, we need to explain that the implementation of the minor fault detection capability of OMDC-PLS is similar to the principle of the existing dynamic PCA algorithm [35]. The data matrices $\boldsymbol{X}$ used in both OMDC-PLS and dynamic PCA introduce d-1 delay data. Suppose that there are minor faults, which exist in the form of subcomponents, in $\boldsymbol{X}$. Minor faults are repeated for a total of d times, so the magnitude of the minor fault is amplified so that it can be effectively detected. The minor fault detection capability of the OMDC-PLS algorithm proposed in this paper can further distinguish whether the minor fault is related to unpredictable quality, which is an ability that dynamic PCA does not have, and it is also the contribution of the proposed algorithm.

To demonstrate the characteristics of the algorithm, in IPS, we set $f_x = 7$ and choose Ξ_x to be the first column of $\boldsymbol{P}_x$ to obtain $(\boldsymbol{X}, \boldsymbol{Y})^{T^2_{xnew}}$. Fault detection of $(\boldsymbol{X}, \boldsymbol{Y})^{T^2_{xnew}}$ is performed using the OMDC-PLS dynamic process monitoring techno- logy. The fault detection results in Fig. 6 show that T^2_{xnew} detects the fault. This result means that the fault detected by T^2_{xnew} is a predictable quality-unrelated but process-related fault. Only J_{th,Q_x} of Q_{xnew} detects a fault, indicating that the fault is a minor fault. From the trend in the Q_{ynew} statistics, this minor fault is a minor unpredictable quality-related fault, which means that there is a minor unpredictable quality- related fault in the predictable quality-unrelated but process- related fault.

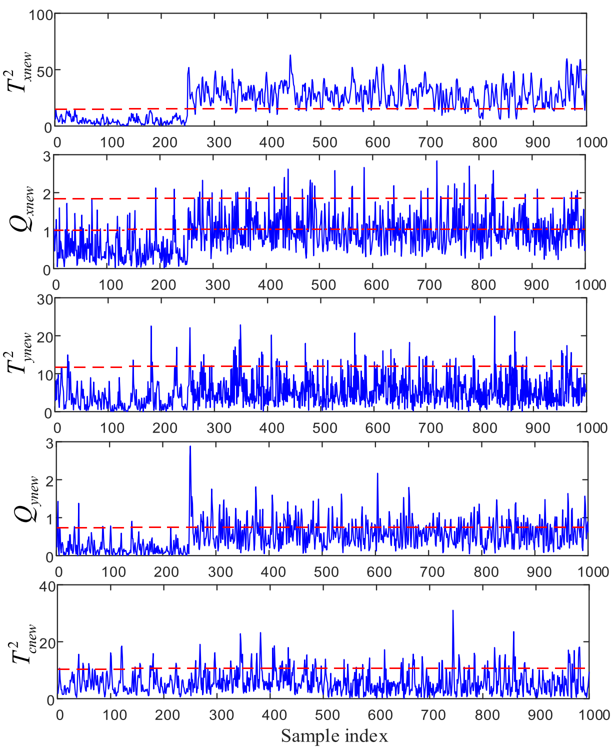

FIGURE 6. Fault occurs in IPS.

B. CASE STUDY ON THE TENNESSEE EASTMAN PROCESS (TEP)

The variables for the TEP include 12 manipulated variables and 41 measured variables. The measurement interval for the process variables is usually 3 minutes. A detailed introduce- tion to the TEP can be found in the literature [36]. The TEP simulation data are downloaded from Prof. Richard D. Braatz's website.[1] Based on the data, monitoring with OMDC-PLS, C-PLS and D-TPLS is performed.

[1] [Online]. Available: http://web.mit.edu/braatzgroup/links.html

1) EXPERIMENTAL DATA AND PARAMETER INITIALIZATION

In this experiment, the process measurements XMEAS(1-36) and the manipulated variables XMV(1-11) are selected to compose $\boldsymbol{X}$. The quality measurements XMEAS(37-41) are selected to compose $\boldsymbol{Y}$. The initial modeling data are d00 normal operating data with a sample size of 500.The number of online monitoring data samples is 980, including the first 500 normal data samples and the last 480 fault data samples.The fault data with 480 samples are derived from the 21 process faults (d01-d21), of which d01-d15 are 15 known faults. For C-PLS, A = 4 is determined by 10-fold cross-validation. Set $t = 1$. For OMDC-PLS and D-TPLS, the larger the values of A and q are, the larger the calculation amount of the algorithm. The value of q should not be too large. Compared to the A value, the q value increases the calculation by a larger amount. A_{max} and q_{max} must be specified to determine a parameter that is suitable for online model updating. Therefore, $A_{max} = 4$ and $q_{max} = 10$ are selected to search for the optimal A and q by using the two dimensional cross-validation-based approach (see Appendix). The simulation result is shown in Fig. 7, where A = 4 and q = 5.

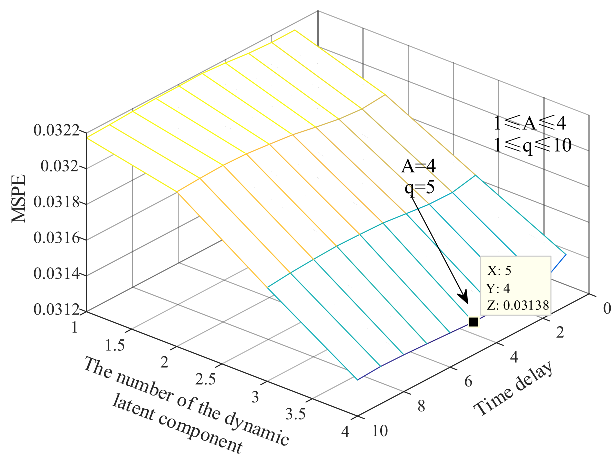

FIGURE 7. Two-dimensional cross-validation result for TEP.

2) FAULT DETECTION

Before applying a known fault, whether the fault is related to $\boldsymbol{y}$ should be determined. According to the criterion introduced in [4], nine faults [IDV(1,2,5-8,10,12,13)] are related to $\boldsymbol{y}$, and five faults [IDV(3, 4, 9, 11, 15)] are unrelated to $\boldsymbol{y}$. According to the false alarm rates (FARs) and fault detection rates (FDRs) introduced in [33], TABLE 4 and TABLE 5 list 14 fault FARs and FDRs.

In TABLE 4, the FARs of the proposed OMDC-PLS method are 0 because OMDC-PLS adopts the alarm-parameter alarm method. Therefore, the OMDC-PLS method is more suitable for quality-related fault detection. In this experiment, we set the parameter limit $PL = 5$, which means that 5 consecutive samples must all detect a fault before an alarm is raised; otherwise, no alarm will be issued.

TABLE 4. FARs of the quality-unrelated faults from the TEP (%).

Quality-unrelated faults of the TEP		Fault detection rate (%)		
Fault description		C-PLS (A=4)	OMDC-PLS (A=4, q=5)	D-TPLS (A=4, q=5)
		T^2_{cnew}	T^2_{cnew}	T^2_{ynew}
IDV(3)	D feed temperature	2.29	**0**	1.25
IDV(4)	Reactor cooling water inlet temperature	1.66	**0**	1.25
IDV(9)	D feed temperature	2.91	**0**	0.84
IDV(11)	Reactor cooling water inlet temperature	4.16	**0**	11.90
IDV(15)	Condenser cooling water valve	1.87	**0**	1.46

TABLE 5. FDRs of quality-related faults from the tep (%).

Quality-related faults of the TE process		Fault detection rate (%)						
Fault description		C-PLS (A=4)		OMDC-PLS (A=4, q=5)			D-TPLS (A=4, q=5)	
		T^2_{cnew}	Q_{xnew}	T^2_{cnew}	Q^J_{xnew}	$Q^{\hat{J}}_{xnew}$	T^2_{ynew}	Q_{snew}
IDV(1)	A/C feed ratio, B composition constant	98.54	99.38	98.54	**100**	**99.58**	98.54	99.37
IDV(2)	B composition, A/C ratio constant	96.05	98.54	**97.92**	**100**	**98.75**	54.27	97.30
IDV(5)	Condenser cooling water inlet temperature	39.29	**52.39**	**42.71**	**100**	47.5	29.23	43.66
IDV(6)	A feed loss	98.54	99.79	98.33	**100**	**100**	**99.16**	**99.79**
IDV(7)	A, B, C feed composition	67.98	99.79	**72.92**	**100**	**100**	41.76	95.63
IDV(8)	A, B, C feed composition	95.84	**97.71**	**97.08**	**99.79**	97.50	74.74	82.12
IDV(10)	C feed temperature	54.05	**67.15**	**60.21**	**100**	56.67	13.57	61.95
IDV(12)	Condenser cooling water inlet temperature	93.14	95.43	**93.96**	**100**	**96.67**	68.69	87.11
IDV(13)	Reaction kinetics	94.17	**97.92**	**94.79**	**100**	97.29	79.54	94.80

Q^J_{xnew} and $Q^{\hat{J}}_{xnew}$ represent the Q_x statistical result monitored by the two control limits, J_{th,Q_x} and $\hat{J}_{th,Q_x}$, respectively.

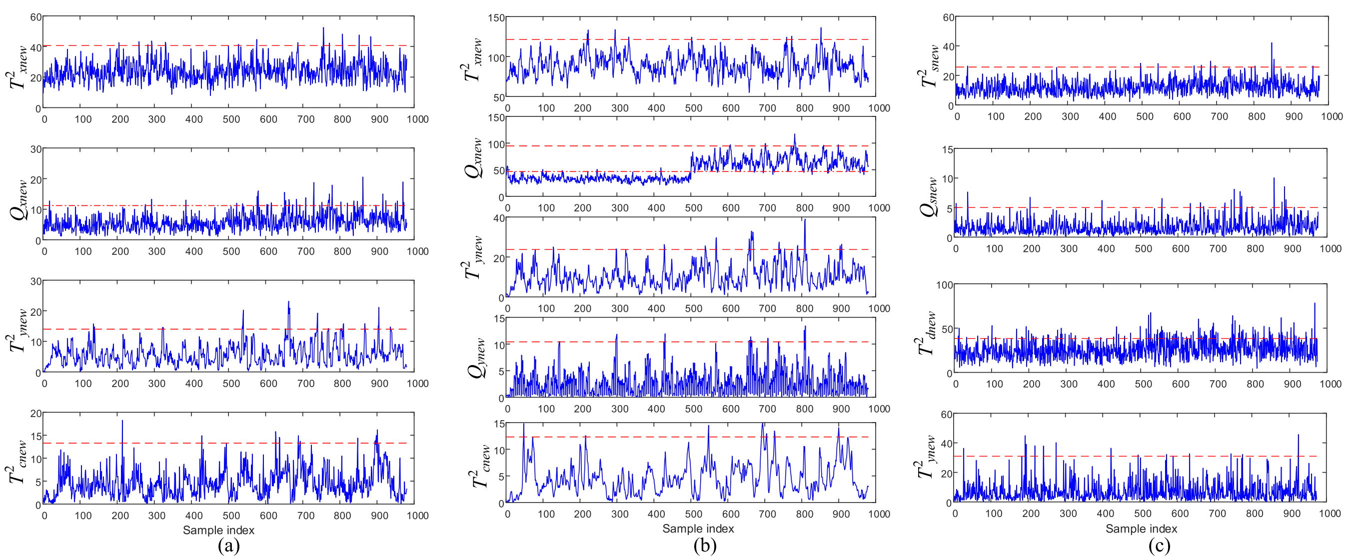

FIGURE 8. Detection results of IDV(3) by C-PLS (a),OMDC-PLS (b) and D-TPLS (c).

In a continuous industrial production process, if production is stopped from a temporary recoverable fault, large losses occur. Therefore, the dynamic process monitoring technology proposed in this study is more suitable for continuous production process monitoring.

TABLE 5 shows that the FDRs of quality-related faults are higher in the proposed OMDC-PLS method than in the C-PLS and D-TPLS method. Only in IDV(6) does the OMDC-PLS have a lower FDR than C-PLS and D-TPLS. These results show that OMDC-PLS has better quality-related fault detection capabilities than mature methods, i.e., C-PLS and D-TPLS. OMDC-PLS can successfully detect noise or minor faults in the process, as shown in the comparison in Fig. 8. As shown in Fig. 8, C-PLS and D-TPLS

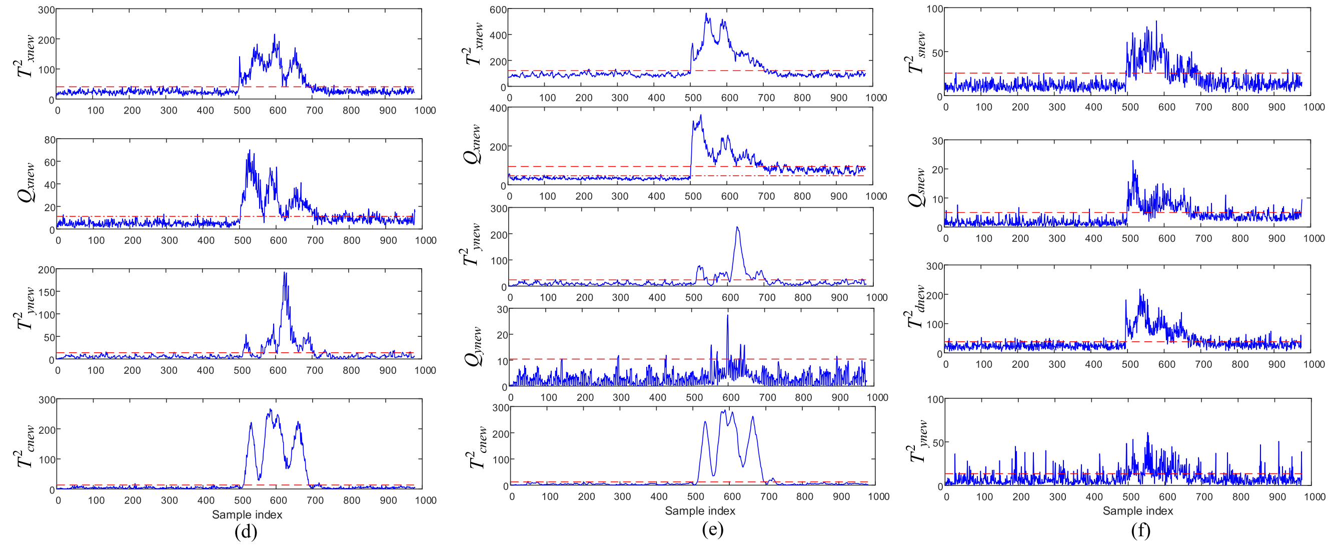

FIGURE 9. **Detection results of IDV(5) by C-PLS (d), OMDC-PLS (e) and D-TPLS (f).**

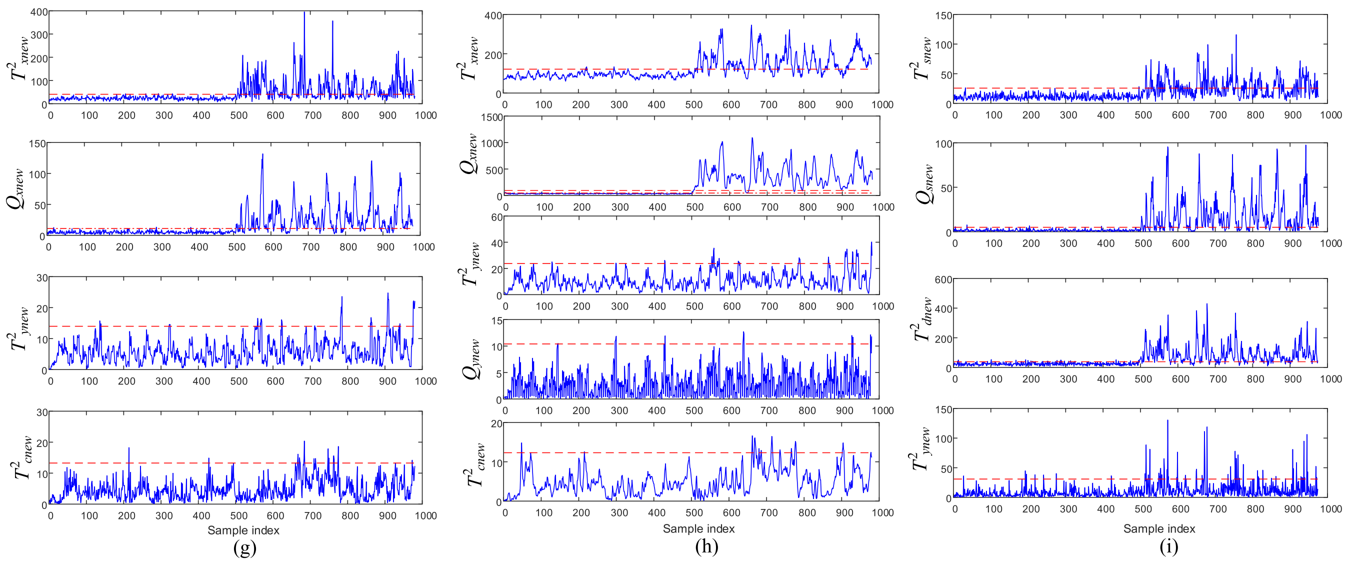

FIGURE 10. **Detection results of IDV(11) by C-PLS (g), OMDC-PLS (h) and D-TPLS (i).**

fail to detect IDV(3). In contrast, a slight deviation in the D feed temperature is fully detected by Q^J_{xnew} of OMDC-PLS, as shown in (b) of Fig. 8. This is primarily because of the introduction of time-delay process variables, which cause $\tilde{X}_{gr}$ to generate a slight deviation. The Q_x statistic can be sensitive to slight deviations. For C-PLS, Q_y is null and does not need to be monitored; therefore, we report only the monitoring results of the other four statistics.

The monitoring results of C-PLS, OMDC-PLS and D-TPLS for IDV(5) are presented in (d), (e) and (f) of Fig. 9, respectively. Fig. 9 shows that the fault is detected at the 500th point. However, the process eventually tested as normal after the 700th point. After the 700th point, a slight deviation in the condenser cooling water flow rate is fully detected by Q^J_{xnew} of OMDC-PLS. However, the C-PLS and D-TPLS methods failed to detect this slight deviation.

The monitoring results of C-PLS, OMDC-PLS and D-TPLS for IDV(11) in quality-unrelated fault detection are presented in (g), (h) and (i) of Fig. 10, respectively. As shown in the figure, the fault is detected only by T^2_{xnew} and Q_{xnew} in C-PLS and OMDC-PLS. In D-TPLS, the fault is detected by T^2_{snew}, Q_{snew} and $T^2_{\mathrm{d}new}$. Therefore, the fault is identified as a predictable quality-unrelated but process- related fault. The Q_{xnew} FDR of OMDC-PLS is higher than the Q_{xnew} FDR of C-PLS and the Q_{snew} FDR of D-TPLS. The FDRs of OMDC-PLS, C-PLS and D-TPLS are 96.7%, 77.5% and 74.1% respectively. This example shows that OMDC-PLS also performs better than C-PLS and D-TPLS in quality-unrelated fault detection.

3) RELATION BETWEEN MULTIPLE *Ti* AND PARAMETER *d*

To calculate $\hat{J}_{th,Q_x}$ directly from J_{th,Q_x}, multiple Ti are defined. There is an implicit relation between Ti and parameter d. To develop this relation, we select the d00 data set and the d00_te data set, assign $d \in [2, 40]$, and perform 39 simulations to obtain 39 sets of $\hat{J}_{th,Q_x}$ and J_{th,Q_x}. Then, 39 Ti are calculated with $d \in [2, 40]$, and the relation between Ti and d was obtained by curve fitting. The detailed process of the experiment is shown in TABLE 6.

TABLE 6. Relationship between multiple *Ti* and parameter *d*.

Step 1:	Set $\mathrm{CPV}=0.85$, $\mathrm{A}=4$, $d=2$ and $d_{\max}=40$.
Step 2:	The OMDC-PLS model was established from the d00 data set to obtain the control limit J_{th,Q_x}.
Step 3:	Based on this model, the data of d00_te are detected to obtain Q_{xnew}, and then the control limit $\hat{J}_{th,Q_x}$ of Q_{xnew} is obtained.
Step 4:	Calculate $Ti(d)=\hat{J}_{th,Q_x} / J_{th,Q_x}$, set $d=d+1$, and go to Step 2 until $d=d_{\max}$.
Step 5:	Use the MATLAB built-in polyfit function to fit the relationship between the Ti and d parameters.

V. CONCLUSIONS

In this study, we proposed the online monitoring dynamic partial least squares (OMD-PLS) model, which is suitable because the quality data of the current time period cannot be obtained in online monitoring using the relation between time-delay process data and time-delay quality data. The OMD-PLS model has a wider range of applications and stronger quality-related fault detection capabilities than DPLS. Furthermore, we propose the online monitoring dynamic concurrent PLS (OMDC-PLS) model. The OMDC- PLS model can perform quality-related and process-related fault monitoring and has stronger quality-related fault detection ability than mature methods, i.e., C-PLS and D-TPLS. We propose an alarm-parameter alarm method, which enhances the dynamic monitoring capabilities of OMDC-PLS and effect- tively reduces the magnitude of FARs. In addition, OMDC- PLS can detect slight deviations in advance and can be applied to detect minor faults, making it possible to identify whether these minor faults are related to predictable quality through trends in other statistics.

APPENDIX

METHOD FOR OBTAINING A AND q

Step 1: Initialize the parameters $\mathrm{A}_{\max}$ and $\mathrm{q}_{\max}$, and set $\mathrm{A} \in [1, \mathrm{A}_{\max}]$, $\mathrm{q} \in [1, \mathrm{q}_{\max}]$,

Step 2: Obtain quality predictions $\hat{\boldsymbol{Y}}$ using the DPLS model, and calculate the mean square error:

$$\mathrm{MSPE} = \frac{1}{n}\left\|\boldsymbol{Y} - \hat{\boldsymbol{Y}}\right\|^2$$

Step 3: A and q corresponding to the pair.

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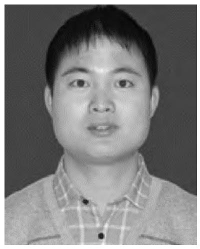

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