

## Data-Driven Model Predictive Monitoring for Dynamic Processes

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**Abstract:** Process monitoring plays an important role in maintaining favorable process operation conditions and is gaining increasing attention in both academic community and industrial applications. This paper proposes a data-driven model predictive fault detection method to achieve efficient monitoring of dynamic processes. First, a measurement sample is projected into a dominant latent variable subspace that captures main variance of the process data and a residual subspace. Then the dominant latent variable subspace is further decomposed as a dynamic feature subspace and a static feature subspace. A fault detection residual is generated in each subspace, and corresponding monitoring statistic is established. By using the model predictive monitoring scheme, not only the status of a process but also the type of a detected fault, namely a dynamic feature fault or a static feature fault, can be identified. Effectiveness of the proposed data-driven model predictive monitoring scheme is tested on a lab-scale distillation process.

**Keywords:** Model predictive process monitoring, data-driven process monitoring, dynamic processes, canonical correlation analysis, fault detection.

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### 1. INTRODUCTION

Process monitoring plays an important role in guaranteeing process safety and product quality [1-3]. Currently, an industrial process is generally characterized by large scale and considerable complexity. Establishing a first principle model is generally difficult, which limits the applicability of a model-based method [4, 5]. On the other hand, because of the rapid advancement of sensing techniques, a lot of process data are generally available. Data-driven monitoring methods that extract meaningful features are of increasing attention, among which the multivariate statistical process monitoring (MSPM) methods are the most widely used [6, 7].

Among MSPM methods, principal component analysis (PCA) and canonical correlation analysis (CCA) are the most widely used ones. PCA projects process data into a dominant subspace that captures main variance and a residual subspace that reflects the modelling uncertainty [8, 9]. CCA characterizes the correlation relationship between two sets of random variables, and projects process data into the most correlated subspaces. For process monitoring, both PCA and CCA have been widely used [5]. Key advantage of the PCA monitoring lays in the capability of dealing with large-scale processes with considerable data collinearity, while key advantage of the CCA lays in the capability of generating optimal fault detection residuals. However, the basic PCA and CCA methods do not focus on the process dynamics [10, 11].

To handle process dynamics, the time-lagged-shift methods were developed [12]. Dynamic PCA has been proposed which projects the time-lagged measurements into a dominant subspace and a residual subspace [12, 13]. Dynamic CCA has also been proposed which characterizes the correlation between time-lagged measurements [10, 14]. However, when the high data collinearity exists, the CCA methods generally cannot function well. More recently, dynamic latent variable (DLV) methods have been proposed and intensively studied [15, 16]. However, these DLV models generally use the one-step prediction for monitoring, which may not be appropriate in complex dynamic conditions. Also, the determination of the order of a dynamic model remains challenging.

This paper proposes a data-driven model predictive fault detection method for efficient monitoring of dynamic processes. First, high-dimension process data are projected into a dominant latent variable subspace and a residual subspace, through which the data collinearity are removed. Second, CCA is performed between the current latent variables and the time-lagged latent variables, during which the model order is automatically determined by preserving the maximum correlation coefficients. Then the process dominant latent variable subspace is further decomposed as the dynamic feature subspace and the static feature subspace. Fault detection residual is generated in each subspace and corresponding monitoring statistic is constructed, through which both the process status and the type of a detected fault can be identified.

The remainder of this article is organized as follows. In section 2, the CCA basics are briefly reviewed and the dynamic process monitoring problem is formulated. In section 3, the proposed model predictive process monitoring scheme is detailed. Then case studies are provided in Section 4. Finally, conclusions are presented in Section 5.

## 2. PRELIMINARIES AND MOTIVATION

### 2.1 Canonical Correlation Analysis

CCA is a classical multivariate analysis method that explores correlation between two sets of random variables. Given  $\mathbf{u} \in \mathcal{R}^{p \times 1}$  and  $\mathbf{y} \in \mathcal{R}^{q \times 1}$ , where  $p$  and  $q$  are the numbers of variables, CCA tries to find canonical vectors  $\mathbf{J}$  and  $\mathbf{L}$  such that the correlation between  $\mathbf{J}^T \mathbf{u}$  and  $\mathbf{L}^T \mathbf{y}$  are maximized, namely [17, 18]

$$(\mathbf{J}, \mathbf{L}) = \arg \max_{(\mathbf{J}, \mathbf{L})} \frac{\mathbf{J}^T \boldsymbol{\Sigma}_{uy} \mathbf{L}}{(\mathbf{J}^T \boldsymbol{\Sigma}_u \mathbf{J})^{1/2} (\mathbf{L}^T \boldsymbol{\Sigma}_y \mathbf{L})^{1/2}}, \quad (1)$$

where  $\boldsymbol{\Sigma}_u$ ,  $\boldsymbol{\Sigma}_y$  and  $\boldsymbol{\Sigma}_{uy}$  are covariance matrices. Solution to the optimization problem in (1) can be obtained through singular value decomposition (SVD) on a matrix  $\mathbf{K}$  as

$$\mathbf{K} = \boldsymbol{\Sigma}_u^{-1/2} \boldsymbol{\Sigma}_{uy} \boldsymbol{\Sigma}_y^{-1/2} = \mathbf{R} \boldsymbol{\Sigma} \mathbf{V}^T, \quad (2)$$

where  $\boldsymbol{\Sigma} = \begin{bmatrix} \text{diag}(\sigma_1, \dots, \sigma_l) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \in \mathcal{R}^{p \times q}$  is a correlation matrix and  $l = \text{rank}(\boldsymbol{\Sigma})$ . Then, we derive [17, 18]

$$\mathbf{J} = \boldsymbol{\Sigma}_u^{-1/2} \mathbf{R}, \mathbf{L} = \boldsymbol{\Sigma}_y^{-1/2} \mathbf{V}. \quad (3)$$

For a sample  $\mathbf{u} \in \mathcal{R}^{p \times 1}$  and  $\mathbf{y} \in \mathcal{R}^{q \times 1}$ , the residual vector is generated as [11, 19]

$$\mathbf{r} = \mathbf{J}^T \mathbf{u} - \boldsymbol{\Sigma} \mathbf{L}^T \mathbf{y}. \quad (4)$$

Then, the  $T^2$  statistic for the residual is established as [11, 19]

$$T^2 = \mathbf{r}^T \boldsymbol{\Sigma}_r^{-1} \mathbf{r}, \quad (5)$$

where  $\boldsymbol{\Sigma}_r$  is the covariance matrix of the residual  $\mathbf{r}$ . Under the Gaussian assumption, the  $T^2$  statistic is optimal for detecting a fault that affects only  $\mathbf{u}$  [11, 19]. Similarly, the  $T^2$  test for detecting a fault that affects  $\mathbf{y}$  can be established.

### 2.2 Problem Formulation and Motivation

The above static CCA is usually used to characterize the relationship between process input and output variables. It works well once the relationship between  $\mathbf{u}$  and  $\mathbf{y}$  can be expressed as [10, 11]

$$\mathbf{A}(\mathbf{u} + \boldsymbol{\varepsilon}) = \mathbf{B}\mathbf{y}, \quad (6)$$

where  $\boldsymbol{\varepsilon}$  denotes the noise. However, a process is generally characterized by dynamics, and the correlation in time series should be considered for process monitoring. In the current work, a data-driven model predictive monitoring method is proposed which considers the correlation in both the variable direction and the time series. First, to characterize the correlation in the variable direction, the measurement subspace is decomposed into a dominant latent variable subspace and a residual subspace. Second, time series correlation is assumed to exist within the dominant latent variable subspace, and the dominant subspace is further decomposed as the dynamic feature subspace and the static feature subspace. Then fault detection residual is generated and monitoring statistic is established in each subspace, through which both the process status and the type of a detected fault can be identified.

## 3. MODEL PREDICTIVE PROCESS MONITORING

Given the process data  $\mathbf{X} \in \mathcal{R}^{N \times m}$ , where  $N$  denotes the number of samples and  $m$  denotes the number of measured variables, the first step is to decompose the data into a dominant latent variable subspace that captures main variance information of the data and a residual subspace. The decomposition can be achieved by SVD on the covariance matrix as

$$\boldsymbol{\Sigma}_X = \frac{\mathbf{X}^T \mathbf{X}}{N-1} = \begin{bmatrix} \mathbf{P}_{pc} & \mathbf{P}_{res} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Lambda}_{pc} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Lambda}_{res} \end{bmatrix} \begin{bmatrix} \mathbf{P}_{pc}^T \\ \mathbf{P}_{res}^T \end{bmatrix}, \quad (7)$$

where  $\mathbf{P}_{pc}$  projects the data into the dominant subspace that removes the data collinearity as

$$\mathbf{t} = \boldsymbol{\Lambda}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{x} \in \mathcal{R}^{k_{pc} \times 1}. \quad (8)$$

The number of retained latent variables  $k_{pc}$  is generally determined to preserve 80%~95% of all data variance. Correspondingly, the residual can be obtained as

$$\mathbf{e} = \mathbf{x} - \mathbf{P}_{pc} \mathbf{P}_{pc}^T \mathbf{x}. \quad (9)$$

The current work considers that process dynamics exist in the dominant latent variable subspace. Then a process sample at time instant  $k$  is projected into the latent variable subspace as  $\mathbf{t}_u(k)$ . Latent variables that contain information from time-lagged samples are denoted as  $\mathbf{t}_y(k) = [\mathbf{t}_u(k-1)^T, \mathbf{t}_u(k-2)^T, \dots, \mathbf{t}_u(k-\tau)^T]^T$ , where  $\tau$  is the order of a dynamic model. Then historical process data in the latent variable subspace can be obtained as  $\mathbf{T}_u$  and  $\mathbf{T}_y$ . By performing CCA between the  $\mathbf{T}_u$  and  $\mathbf{T}_y$ , we can obtain the canonical correlation vectors  $\mathbf{J}_T$  and  $\mathbf{L}_T$ , as well as the correlation matrix  $\boldsymbol{\Sigma}_T$ . For monitoring the latent variables at the sample  $k$ , the following residual can be generated

$$\begin{aligned} \mathbf{r}_u &= \mathbf{J}_T^T \mathbf{t}_u - \boldsymbol{\Sigma}_T \mathbf{L}_T^T \mathbf{t}_y \\ &= \mathbf{J}_T^T \boldsymbol{\Lambda}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{x}(k) - \boldsymbol{\Sigma}_T \mathbf{L}_T^T \boldsymbol{\Lambda}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{y}(k), \end{aligned} \quad (10)$$

where  $\mathbf{y}(k) = [\mathbf{x}(k-1)^T, \mathbf{x}(k-2)^T, \dots, \mathbf{x}(k-\tau)^T]^T$ . The CCA detects a fault relying on the correlation between variables, and therefore only the correlated samples should be selected to establish the model. Then, the order  $\tau$  is determined by preserving the maximum correlation and eliminating the irrelevant time-lagged variables. The genetic algorithm-based regularization method in reference [11] can be employed. After some derivation, we can obtain that

$$\mathbf{r}_u = \mathbf{J}_T^T (\mathbf{t}_u - \boldsymbol{\Sigma}_{T_{uy}} \boldsymbol{\Sigma}_{T_y}^{-1/2} \mathbf{t}_y), \quad (11)$$

where  $\hat{\mathbf{t}}_u = \boldsymbol{\Sigma}_{T_{uy}} \boldsymbol{\Sigma}_{T_y}^{-1/2} \mathbf{t}_y$  is the least square estimation of  $\mathbf{t}_u$  using the  $\mathbf{t}_y$ . Therefore, once the relation in process data can be expressed as

$$\mathbf{A}[\mathbf{t}(k) + \boldsymbol{\varepsilon}] = \mathbf{B}[\mathbf{t}(k-1)^T, \mathbf{t}(k-2)^T, \dots, \mathbf{t}(k-\tau)^T]^T, \quad (12)$$

the generated residual  $\mathbf{r}_u$  is optimal for detecting a fault that affects the sample at time instant  $k$ . Considering that the

process dynamic generally exists in a low-dimension subspace but not the entire latent variable space, we further divide the canonical correlation vectors as  $\mathbf{J}_T = [\mathbf{J}_{T,dynamic}, \mathbf{J}_{T,static}]$ . Correspondingly, the residual vector can be written as

$$\mathbf{r}_u = \begin{bmatrix} \mathbf{J}_{T,dynamic}^T \\ \mathbf{J}_{T,static}^T \end{bmatrix} \mathbf{t}_u - \begin{bmatrix} \boldsymbol{\varepsilon}_{T,dynamic} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\varepsilon}_{T,static} \end{bmatrix} \mathbf{L}_T^T \mathbf{t}_y. \quad (13)$$

Then the dynamic feature residual can be constructed as

$$\begin{aligned} \mathbf{r}_{dynamic} &= \mathbf{J}_{T,dynamic}^T \mathbf{t}_u - [\boldsymbol{\varepsilon}_{T,dynamic} \quad \mathbf{0}] \mathbf{L}_T^T \mathbf{t}_y \\ &= \mathbf{J}_{T,dynamic}^T \mathbf{A}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{x}(k) - [\boldsymbol{\varepsilon}_{T,dynamic} \quad \mathbf{0}] \mathbf{L}_T^T \mathbf{A}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{y}(k) \end{aligned} \quad (14)$$

The static feature residual can be constructed as

$$\begin{aligned} \mathbf{r}_{static} &= \mathbf{J}_{T,static}^T \mathbf{t}_u - [\mathbf{0} \quad \boldsymbol{\varepsilon}_{T,in}] \mathbf{L}_T^T \mathbf{t}_y \\ &= \mathbf{J}_{T,static}^T \mathbf{A}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{x}(k) - [\mathbf{0} \quad \boldsymbol{\varepsilon}_{T,in}] \mathbf{L}_T^T \mathbf{A}_{pc}^{-1/2} \mathbf{P}_{pc}^T \mathbf{y}(k) \end{aligned} \quad (15)$$

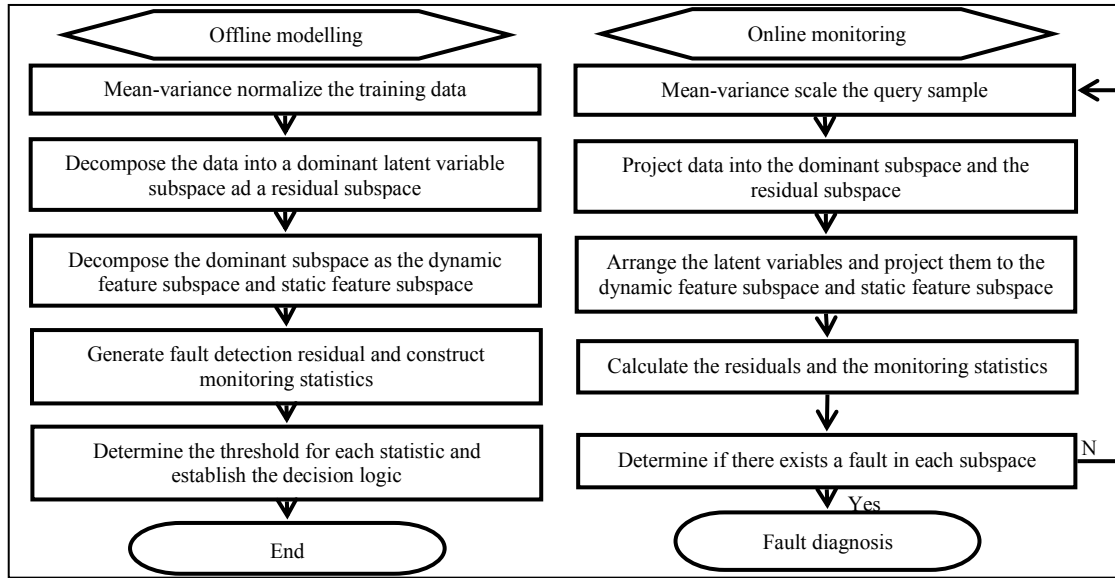


Figure 1 Schematic of the proposed model predictive monitoring

Then based on the residuals  $\mathbf{e}$ ,  $\mathbf{r}_{dynamic}$  and  $\mathbf{r}_{static}$  the following three statistics are established to identify the process status:

$$T_{dynamic}^2 = \mathbf{r}_{dynamic}^T \boldsymbol{\Sigma}_{dynamic}^{-1} \mathbf{r}_{dynamic} \sim \chi^2(k_{dynamic}), \quad (16)$$

$$T_{static}^2 = \mathbf{r}_{static}^T \boldsymbol{\Sigma}_{static}^{-1} \mathbf{r}_{static} \sim \chi^2(k_{static}), \quad (17)$$

$$Q = \mathbf{e}^T \mathbf{e} = \mathbf{x}^T (\mathbf{I}_{k \times k} - \mathbf{P}_{pc} \mathbf{P}_{pc}^T) \mathbf{x} \sim g \chi^2(h), \quad (18)$$

where  $\boldsymbol{\Sigma}_{dynamic} = \mathbf{I}_{k_{dynamic}} - \boldsymbol{\varepsilon}_{dynamic} \boldsymbol{\varepsilon}_{dynamic}^T = \text{diag}((1 - \rho_1^2), \dots, (1 - \rho_{k_{dynamic}}^2))$ ,  $\boldsymbol{\Sigma}_{in} = \mathbf{I}_{m - k_{dynamic}} - \boldsymbol{\varepsilon}_{in} \boldsymbol{\varepsilon}_{in}^T = \text{diag}((1 - \rho_{k_{dynamic}+1}^2), \dots, 1)$ ; Parameters  $g$  and  $h$  are calculated from historical data [20]. The number of selected dynamic features  $k_{dynamic}$  can be obtained by the accumulated correlation method, namely [21]

$$Cum(k_{dynamic}) = \frac{\sum_{i=1}^{k_{dynamic}} \rho_i}{\sum_{i=1}^l \rho_i} \geq \delta, \quad (19)$$

where  $\delta$  is generally determined as 80%~95% to preserve the most correlation information. Thresholds of the statistics can be determined by assume that process data follow Gaussian assumption or using the kernel density estimation. Then following decision logic can be employed to identify the process status:

$$\begin{cases} T_{dynamic}^2 \leq T_{dynamic,cl}^2 \text{ and } T_{static}^2 \leq T_{static,cl}^2 \text{ and } Q \leq Q_{cl} \Rightarrow \text{fault-free}; \\ T_{dynamic}^2 > T_{dynamic,cl}^2 \Rightarrow \text{a fault in the dynamic feature subspace}; \\ T_{dynamic}^2 \leq T_{dynamic,cl}^2 \text{ and } T_{static}^2 > T_{static,cl}^2 \Rightarrow \text{a fault in the static feature subspace}; \\ Q > Q_{cl} \Rightarrow \text{a fault affects the variable-wise correlation.} \end{cases} \quad (20)$$

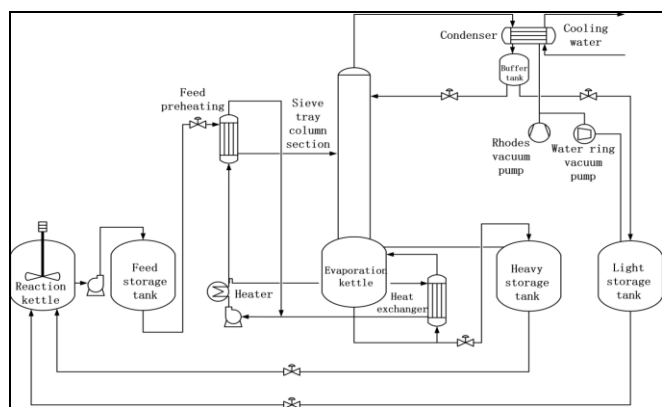
Procedures of the model predictive dynamic process monitoring scheme consists of the offline modeling and online monitoring steps, which are summarized as Figure 1.

#### 4. CASE STUDY

Glycerin is an important raw industrial material for producing high value-added products. To obtain high purity glycerin, efficient distillation process that separates glycerin from others is necessary. A lab-scale glycerin process that distillates glycerin from glycerin-water mixtures is available in the process control laboratory of the East China University of Science and Technology, which is the 1/8 scale of a real industrial process in a chemical production company. An illustration of the lab-scale distillation process is presented in Figure 2. The process consists of four typical operation units, namely the feeding unit, the heating and evaporation unit, the condensing and refluxing unit, and the production collecting unit. Twenty-one variables are measured and recorded as listed in Table 1.



(a)



(b)

Figure 2 Schematic of the experimental glycerol distillation process: (a) physical figure; (b) simplified scheme

Under normal operation condition, a set of data that contains 400 samples are collected. Based on the normal operating data, the model predictive monitoring model is established. The number of retained dominant latent variables is determined by preserving the 90% variance, the number of dynamic features is determined by preserving the 85% correlation, and the false alarm rate of each statistic is

controlled under 1% by determining the level of significance. To test the monitoring performance, the following four sets of process data with each consisting of 250 samples are generated: Fault 1: A step change of sensitive plate temperature sensor at approximately the 130th point; Fault 2: A step change of tower plate temperature sensor 5 at approximately the 130th point; Fault 3: A step change of condenser cooling water flow rate at approximately the 130th point; Fault 4: A step change of tower top reflux at approximately the 130th point.

Monitoring results for the four faults using the model predictive monitoring scheme are presented in Figures 3-6. Figure 3 shows the monitoring results of fault 1. It can be seen that the  $T_{dynamic}^2$  statistic is affected while the  $T_{static}^2$  and  $Q$  statistics remain normal, indicating that the fault 1 is a dynamic feature-related fault. Figure 4 shows the monitoring results of fault 2. It can be seen that only the  $T_{static}^2$  is affected, indicating that the fault is a static feature fault. Figure 5 shows the monitoring results of fault 3. It can be seen that the fault affects only the  $Q$  statistic, indicating that the fault affects the variable collinearity. Figure 6 shows the monitoring results of fault 4. It can be seen that all the three statistics are affected, indicating that the fault 4 is a serious fault and causes considerable influence on the process status. The model predictive monitoring scheme can not only detect a fault but also identify the type of a detected fault. The effectiveness of the model predictive monitoring is shown.

Table 1 Process variables of the distillation process

Variable number	Variable description
1	Feed flow rate
2	Sensitive plate temperature
3	Tower bottom liquid level
4	Tower top reflux
5	Overhead product flow
6	Feed storage tank level
7-18	Tower plate temperatures 1-12
19	Condenser cooling water flow rate
20	Heavy storage tank level
21	Light storage tank level

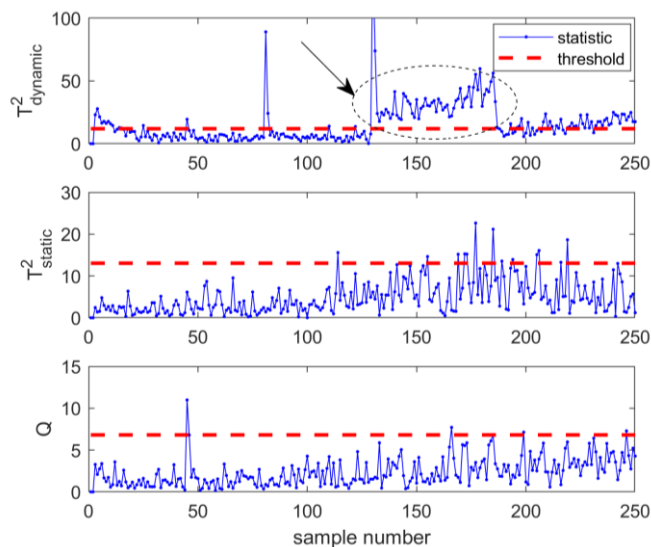


Figure 3 Monitoring results for the fault 1

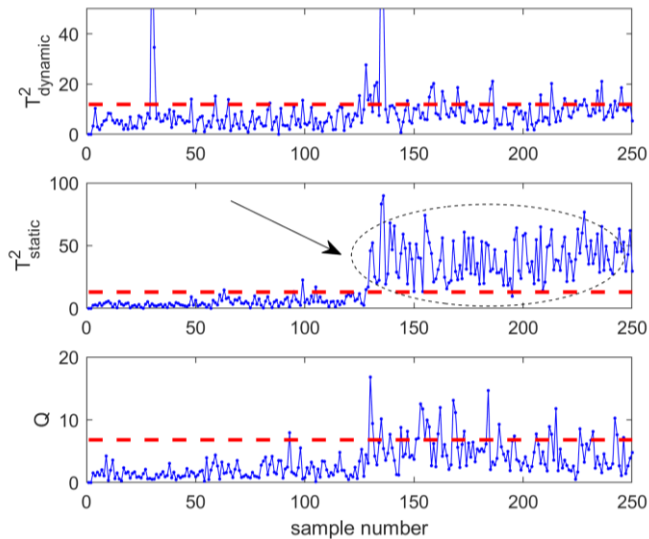


Figure 4 Monitoring results for the fault 2

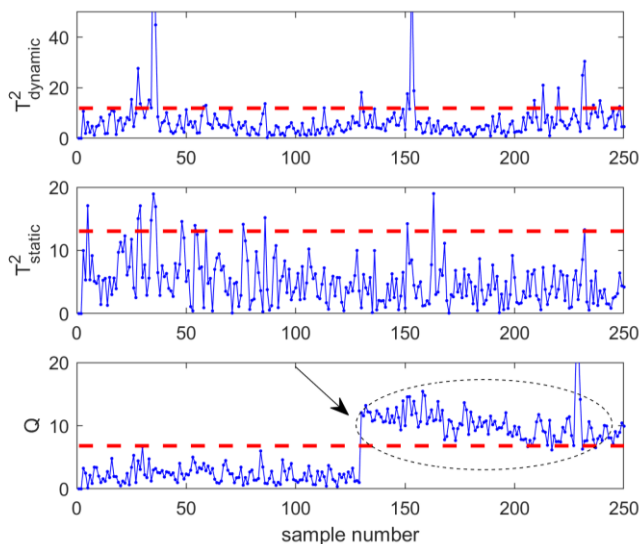


Figure 5 Monitoring results for the fault 3

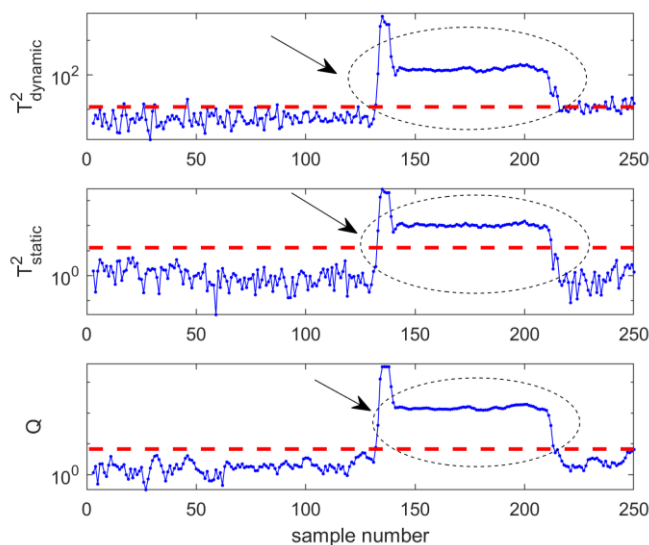


Figure 6 Monitoring results for the fault 4

## 5. CONCLUSIONS

In this work, a data-driven model predictive monitoring method was developed for efficient dynamic process monitoring. Process measurements are first projected into a dominant latent variable subspace and a residual subspace. Then the dominant latent variable subspace is further decomposed into a dynamic feature subspace and a static feature subspace, under the consideration that process dynamic exists in a low dimensional dynamic feature subspace. Fault detection residual is generated and monitoring statistic is established for each subspace, through which both the process status and the type of a detected fault can be identified. Application examples on a lab-scale distillation process verified the effectiveness of the proposed monitoring scheme.

It is noted that the current work is the preliminary study on the data-driven model predictive monitoring and only the fault detection issue is addressed. Future works can be devoted to the fault variable isolation and fault pattern diagnosis. Also, this work deals with only the linear case, while more complex process characteristics such as process nonlinearity and multimode should be discussed.

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