Dynamic Process Monitoring Based on Integrated Statistic of Principal Component Analysis and Slow Feature Analysis

Cheng Ji, Tingting Tao, Jingde Wang*, Wei Sun*

**College of Chemical Engineering, Beijing University of Chemical Technology, North Third Ring Road 15,*

Chaoyang District, Beijing 100029, (Tel: 010-64445826; e-mail: sunwei@ mail.buct.edu.cn).

Abstract: Process monitoring has attracted extensive interest for real-time operating evaluation due to the expectation of a safe and higher-quality production in chemical industry. Principal component analysis (PCA), an effective method for data dimensionality reduction, has been widely utilized in static process monitoring. However, industrial process data generally show dynamic characteristics because certain sequences of process variables are autocorrelated due to internal mechanisms. Recently, slow feature analysis (SFA) has been proved to have a good performance in extracting the slowly changing features in dynamic processes. To monitor both static and dynamic relations, a novel dynamic process monitoring method based on integrated statistic of PCA and SFA is proposed by extracting data feature of static and dynamic variables respectively. Variables are first grouped into static and dynamic categories according to their autocorrelation. For static part, PCA is applied to extract static variable features and calculate T^2 and SPE statistics, while SFA is adopted in dynamic part for the extraction of dynamic variable features, and T^2, T_e^2, S^2 and S_e^2 statistics can be calculated accordingly. At last, these statistics can be integrated by a support vector data description (SVDD) to give a final process monitoring result. The performance of the proposed method is compared with other dynamic process monitoring methods on the benchmark Tennessee Eastman process (TEP).

Keywords: Process dynamics, Feature extraction, Mutual information, Fault detection, Support vector data description.

1. INTRODUCTION

Early detection of abnormal process deviations in chemical production plays an important role in process monitoring to guarantee product quality and production safety. With the wide application of distributed control system (DCS), massive historical operating data that contains process internal mechanism information can be obtained, which significantly accelerates the development of data-driven process monitoring methods, especially multivariate statistical methods. As a commonly used multivariate statistical method, principal component analysis (PCA) has been well adopted for process monitoring due to its extraordinary ability on dimensionality reduction. However, only static information on variable cross-correlation is considered by PCA, while the dynamic characteristics reflected in certain sequences of process variables due to process internal mechanism are neglected. The monitoring performance will be compromised if only static model is built for a dynamic process (Li and Yan, 2019).

Aiming at the time dependence of process data, numerous researches have been developed for dynamic data processing. Among them, the simplest way is to reduce sequence autocorrelation by increasing the sampling interval, but it may lead to the loss of critical process information and thus cannot achieve a desired monitoring effect. For dynamic modelling, dynamic principal component analysis (DPCA) was first introduced for process monitoring by Ku et al. (Ku et al., 1995). By introducing time lags to construct an augmented matrix, the time-varying dynamic characteristics can be further extracted by traditional PCA decomposition. This dynamic data processing idea with the application of augmented matrix has been combined with various process monitoring algorithms, such as dynamic independent component analysis (Lee et al., 2004) and dynamic canonical correlation analysis (Jiang and Yan, 2018). However, for a high dimensional process, the dimensions of data will increase significantly even though only the first-order autocorrelation is considered. On the other hand, all variables are handled with the same time lag in these dynamic methods, while the dynamic characteristics could have different effects on different variables (Li and Yan, 2019). In addition, the autocorrelation extracted by dynamic PCA is hard to interpret by just using time-lagged variables. To improve the dynamic feature extraction, dynamic latent variable models have been proposed and well developed. Li proposed a dynamic latent variable (DLV) based process monitoring method using PCA and vector autoregressive (VAR) model, by which the autoregressive PCA is first applied to extract dynamic latent variables, and then the VAR model is adopted to obtain residues of latent variables for process monitoring (Li et al., 2011). In comparison with previous techniques, DLV based methods have an advantage in extracting dynamic characteristics, but part of static information is ignored in the meantime. Recently, slow feature analysis (SFA) has begun to attract attention to dynamic process monitoring by extracting the slowly varying features in dynamic process data. Unlike traditional latent variable models, SFA enables separate descriptions of both static and dynamic variations in normal operation. According to the paper reported by Shao et al., SFA has been proved to have a better performance on dynamic process monitoring for the Tennessee Eastman process (TEP) than traditional dynamic multivariate statistical methods (Shang et al., 2015). However, few studies have been presented by separating static variables from dynamic variables and applying proper algorithms to extract static and dynamic feature respectively, which should be beneficial for monitoring both static and dynamic relations.

In this work, a dynamic process monitoring method is proposed based on integrated statistic of PCA and SFA. According to autocorrelation analysis, process variables are first grouped into static and dynamic categories. For these two categories, PCA is applied to extract data feature of static variables and calculate T^2 and SPE statistics, while SFA is adopted to extract dynamic variable features and obtain T^2, T_e^2, S^2 and S_e^2 statistics. Then the obtained statistics are integrated as an input of a support vector data description (SVDD) model for feature fusion and obtain a final process monitoring decisions. Although different statistics are used to describe a process from different perspectives, a fault usually can be detected in various statistics. The SVDD is used to comprehensively consider the changes of each statistic, by which the sensitivity to fault detection of the method can be improved. The novel dynamic process monitoring method is employed to TEP and compared with related methods, including PCA, DPCA and SFA. The results show that most faults in TEP can be earlier detected by the proposed method.

The remaining part of this paper is organized as follows. In section 2, a brief introduction to mutual information (MI), PCA, SFA and SVDD are provided. In section 3, the procedures of the proposed dynamic process monitoring model based on integrated statistic of PCA and SFA are described. In section 4, the performance of proposed method is illustrated and compared through a case study on TEP. In section 5, the paper is concluded.

2. PRELIMINARIES

In this section, the algorithms of MI, PCA, SFA and SVDD applied in the proposed process monitoring method are introduced.

2.1 Mutual information

MI is an index to measure the correlation between two random variables from the aspect of information theory. Given two random variables X and Y, the calculation of MI is given as follows (Vastano and Swinney, 1988),

$$I(X,Y)=\iint_{x,y} p(x,y)\log(\frac{p(x,y)}{p(x)p(y)}) \tag{1}$$

where $p(\cdot)$ is the marginal distribution probability density and $p(x,y)$ is the joint probability density, which can be calculated through kernel density estimation. According to Equation 1, $I(X,Y)$ is equal to zero when X and Y are completely independent, and the stronger the correlation of a pairvariables, the greater the MI value.

Similar to autocorrelation function, the MI can also be applied to measure the autocorrelation of a variable sequence by measuring the correlation between original sequence and the sequence with different time lag orders. The calculation is given by introducing a time lag parameter τ to MI,

$$I(X,X,\tau)=\iint_{x_t,x_{t+\tau}} p(x_t,x_{t+\tau})\log(\frac{p(x_t,x_{t+\tau})}{p(x_t)p(x_{t+\tau})}) \tag{2}$$

where $p(x_t,x_{t+\tau})$ is the joint distribution probability of the original sequence and the sequence with a time lag order. Considering that MI is always larger than zero, it's necessary to determine a confidence interval. In this work, massive random normally distributed sequences are generated to estimate the distribution of variable autocorrelation under static conditions using kernel density estimation. The threshold is determined under a 99% confidence level.

2.2 Principal component analysis

PCA is a classic method in data dimensionality reduction and feature extraction, which is widely utilized for static process monitoring (Kresta et al., 1991). Given a data matrix $Z_{n\times m}$ containing n sampling points of m variables after data normalization. The covariance matrix of $Z_{n\times m}$ is first calculated as follows,

$$S=\frac{1}{n-1}Z^TZ \tag{3}$$

Then the projection directions of PCA can be obtained through the singular value decomposition of the covariance matrix. On this basis, $Z_{n\times m}$ can be decomposed as follows,

$$Z=TP^T+E \tag{4}$$

where $T\in R^{n\times d}$, $P\in R^{m\times d}$ are the score matrix and the load matrix of principal components respectively. $E\in R^{n\times m}$ is the residual matrix and d is the number of selected principal components. Original data space is grouped into the principal subspace and the residual subspace, and then T^2 and SPE statistics are constructed in corresponding principal space and residual subspace for process monitoring. PCA is selected in this work to monitor the static variables for its satisfying performance in the extraction of static information.

2.3 Slow feature analysis

The core idea of SFA is to extract the slowest changing components from dynamic data as fundamental features (Wiskott and Sejnowski, 2002). Given a p-dimensional input signal $L=\{l_1,l_2,...,l_p\}$. After processed by a q-dimensional transformation function $G=\{g_1,g_2,...,g_q\}$, a q-dimensional output signal $S=\{s_1,s_2,...,s_q\}$ is obtained. where $s_j=g_j(l_j), j\in[1,2,...,q]$. The ultimate optimization goal of SFA is to determine the optimal function G and the corresponding optimization objective is given as follows,

$$\begin{aligned}
&\min\langle \dot{s}_j{}^2\rangle\\
&s.t.\\
&\langle s_j\rangle=0\\
&\langle s_j{}^2\rangle=1\\
&\langle s_i s_j\rangle=0,\forall i\neq j
\end{aligned}\tag{5}$$

where $\dot{s}_j$ is the first derivative of S. $\langle\ \rangle$ represents the variable average over a period of time. The first zero mean constraint is added to simplify the solution process, while the addition of the second constraint can prevent the numerical solution. The last constraint ensures the independence of each component in the output signal, thus avoiding redundant output. When adopting a linear transformation function, each slow feature s_j is a linear combination of input variables, which is given as follows,

$$S_j=g_j(L)=Lw_j \tag{6}$$

where w_j is the load matrix. Thus, Equation (5) can be rewritten as follows,

$$\begin{aligned}
&\min\langle \dot{s}_j{}^2\rangle=\min\langle(\dot{L}w_j)^2\rangle=\min w_j^T\langle\dot{L}^T\dot{L}\rangle w_j\\
&s.t.\\
&\langle s_j{}^2\rangle=\langle(Lw_j)^2\rangle=w_j^T\langle L^TL\rangle w_j=1
\end{aligned}\tag{7}$$

And then Equation (6) can be solved by the following generalized eigenvalue decomposition,

$$\langle\dot{L}^T\dot{L}\rangle W=\langle L^TL\rangle W\Lambda \tag{8}$$

where $\Lambda=(\lambda_1,\lambda_2,...,\lambda_q), \lambda_1<\lambda_2<\cdots<\lambda_q$ is the generalized eigenvalue matrix and $W=(w_1,w_2,...,w_q)$ is the generalized eigenvector matrix. The optimization goal of Equation (5) is exactly the main diagonal element of Λ.

2.4 Support vector data description

As a one-class grouping method, SVDD is applied in this work for a fusion of multiple monitoring statistics. The basic idea of SVDD is to build a minimal hypersphere region, which can accept target samples but reject non-targets. Given a training data set $H=\{h_1,h_2,...,h_k\}$, the optimization objective is given as follows (Tax and Duin, 2004),

$$\begin{aligned}
&\min R^2+C\sum_{h_d\in H}\zeta_d\\
&s.t.(h_d-a)^T(h_d-a)\le R^2+\zeta_d\\
&\zeta_d\ge 0,\forall d=1,2,...,k
\end{aligned}\tag{9}$$

where R and a are the radius and centre of the hypersphere. The relaxation factor ζ and the penalty weight C are introduced to improve model robustness. To solve this optimization problem, a Lagrange multiplier α_e is introduced and the duality problem of Equation (9) is given as follows,

$$\begin{aligned}
&\max\sum_{h_e\in H}\alpha_eK(h_e,h_e)-\sum_{h_e\in H}\sum_{h_f\in H}\alpha_e\alpha_fK(h_e,h_f)\\
&s.t.\sum_{h_e\in H}\alpha_e=1\\
&0\le\alpha_e\le C,\ \forall e=1,2,...,k
\end{aligned}\tag{10}$$

where $K(h_e,h_f)$ is the kernel function. In this study, Gaussian kernel is selected, which is given as follows,

$$K(h_e,h_f)=\exp(-\frac{(h_e-h_f)^2}{2\sigma^2}) \tag{11}$$

Based on the above calculations, the final radius of the hypersphere is given as follows,

$$R=\sqrt{h_k^2-2\sum_{h_e\in H}\alpha_eK(h_k,h_e)+\sum_{h_e\in H}\sum_{h_f\in H}\alpha_e\alpha_fK(h_e,h_f)} \tag{12}$$

Then the distance between a new test sample point and the hypersphere centre is given as follows,

$$D_{is}=\sqrt{z^2-2\sum_{h_e\in H}\alpha_eK(z,h_e)+\sum_{h_e\in H}\sum_{h_f\in H}\alpha_e\alpha_fK(h_e,h_f)} \tag{13}$$

If $D_{is}\le R$, it indicates the sample point is normal. Otherwise, the point will be rejected as an outlier.

3. PROCESS MONITORING METHOD BASED ON INTEGRATED STATISTIC OF PCA AND SFA

To better monitor the static and dynamic relations, a dynamic process monitoring method is proposed by separating static variables from dynamic variables. In this section, the framework of the proposed dynamic process monitoring based on integrated static of PCA and SFA and its implementation procedures are presented.

3.1 Dynamic and static variable grouping

As mentioned before, the main idea of the proposed method is to classify process variables into static part and dynamic part and employ proper algorithms to achieve better feature extraction. Therefore, the variable group according to their dynamic characteristics is implemented before establishing the process monitoring model. As shown in Figure 1, MI between each original variable sequence and the sequence with different time lag orders is introduced to measure the autocorrelation of each variable, and further represent its process dynamic characteristic. Regarding the acquisition of thresholds, a thousand Gaussian random sequences are generated to calculate the MI between independent sequences and kernel density estimation is employed to estimate its distribution. A threshold is determined under a 99% confidence level. For variable grouping, if the maximum MI value between a variable and its sequence with different time lag orders exceeds its corresponding threshold, it is grouped into the dynamic variable category, otherwise, it is grouped into the static variable category.

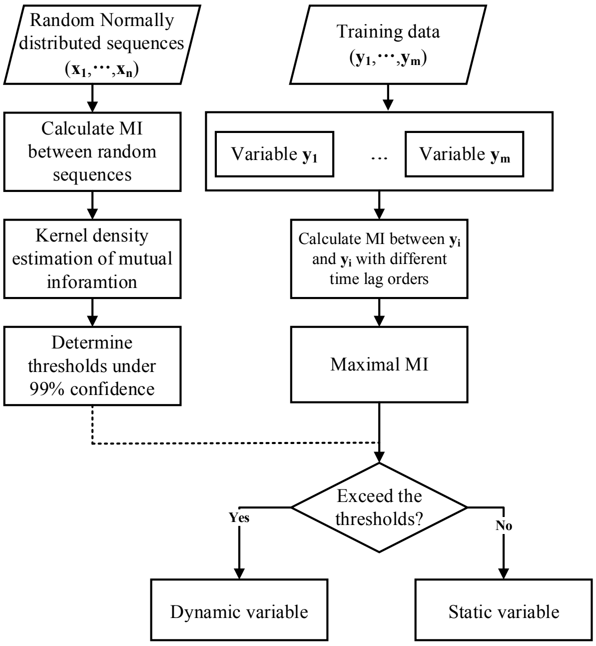

Fig. 1. Flowchart of the dynamic and static variable grouping method.

3.2 The framework of the dynamic process monitoring method based on integrated Statistic of PCA and SFA

After the variable grouping mentioned in last section, the proposed process monitoring model can be established in static part and dynamic part respectively. The flowchart of the proposed dynamic process monitoring method is shown in Figure 2, which contains offline modelling and online monitoring.

Offline modelling:

(1) Select historical data under normal conditions and normalize the selected data.

(2) Group the selected data into static and dynamic variables on the basis of the previous variable grouping method.

(3) Input the grouped static variables into a PCA model to construct T^2 and SPE statistics, while the dynamic variables are input into an SFA model to construct T^2, T_e^2, S^2 and S_e^2 statistics.

(4) Integrate the constructed statistics into a SVDD model to determine the hypersphere range under normal conditions.

Online monitoring:

(1) Normalize the real-time data with parameters obtained from historical data.

(2) Group real-time data into static and dynamic variables according to the grouping mode during offline modelling.

(3) Input static variable into the constructed PCA model and dynamic variable into the SFA model respectively to obtain real-time statistics.

(4) Input the real-time statistics into the trained SVDD fusion model to obtain a process monitoring result.

By considering static and dynamic characteristics respectively through variable grouping, PCA and SFA are employed for both static and dynamic feature extraction to achieve a better dynamic process monitoring. Finally, an integrated statistic by SVDD can be used to comprehensively measure the changes in each feature space. The performance of the proposed method will be introduced in the following section.

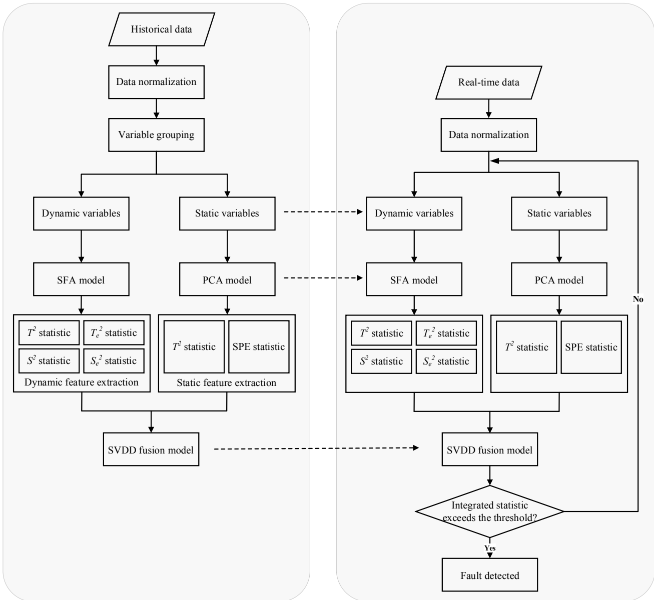

Fig. 2. Flowchart of the proposed process monitoring framework.

4. CASE STUDY

In this section, the proposed process monitoring method based on integrated statistic of PCA and SFA is applied to the TEP, and the results are compared with related methods.

4.1 Tennessee Eastman process

TEP is a widely used chemical benchmark process simulated by Eastman Chemical Company (Downs and Vogel, 1993), which has been well adopted to test newly proposed process control and monitoring methods. The data sets employed in this work are downloaded from the website provided by the Braatz research group (Braatz, 2002). The process contains 5 chemical operation units and a total of 52 variables. The variables used in this work are shown in Table 1, including 11 manipulated variables and 22 continuous process variables, and 19 composition variables are excluded for their long sampling periods. One data set obtained from normal operating conditions is applied to train the process monitoring model, and 18 fault data sets excluding fault 3, 9 and 15, which are difficult to monitor for their subtle deviations, are applied for online monitoring. The sampling frequency is 3 minutes and all the faults are introduced at the 160th sample. Detailed information about these faults can be obtained from Downs and Vogel's paper.

Table 1. Process variables in TEP

No.	Description	No.	Description
1	A feed	18	Stripper temperature
2	D feed	19	Stripper steam flow
3	E feed	20	Compressor work
4	A and C feed	21	Reactor cooling water outlet temperature
5	Recycle flow	22	Separator cooling water outlet temperature
6	Reactor feed rate	23	D feed flow
7	Reactor pressure	24	E feed flow
8	Reactor level	25	A feed flow
9	Reactor temperature	26	A and C feed flow
10	Purge rate	27	Compressor recycle valve
11	Product separator temperature	28	Purge valve
12	Product separator level	29	Separator pot liquid flow
13	Product separator pressure	30	Stripper liquid prod flow
14	Product separator underflow	31	Stripper steam valve
15	Stripper level	32	Reactor cooling water flow
16	Stripper pressure	33	Condenser cooling water flow
17	Stripper underflow		

4.2 Grouping of dynamic and static variables

As mentioned in previous section, the first step of the proposed method is to group process variables into static part and dynamic part according to autocorrelation analysis. Mutual information between original sequence and sequence with different time lag orders is applied to measure variable autocorrelation. In order to determine a confidence interval, a thousand sets of random normally distributed data are generated and applied to estimate the distribution of variable autocorrelation under static conditions using kernel density estimation with a 99% confidence level. As shown in Figure 3, the mutual information between the reactor level and its sequence with different time lag orders is small, which means the sequence of reactor level is not autocorrelated, and therefore it can be regarded as a static variable. For the stripper temperature, the mutual information is at a large value under different time lag orders, indicating a strong autocorrelation of this variable. Mutual information between each variable sequence and its sequence with different time lag orders is calculated and compared with the thresholds for variable grouping. The results are shown in Table 2. The 33 variables are grouped into 13 static variables and 20 dynamic variables.

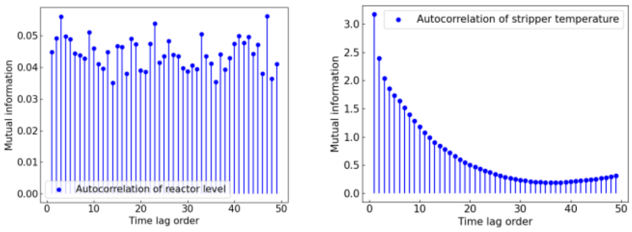

Fig. 3. (a) Fig. 3. (b)

Fig. 3. Autocorrelation analysis of variables in TEP: (a) Reactor level; (b) Stripper temperature.

Table 2. Variable groups in TEP

Static variables	4,5,6,8,10,12,14,15,17,26,29,30,33
Dynamic variables	1,2,3,7,9,11,13,16,18,19,20,21,22,23,24, 25,27,28,31,32

4.3 Process monitoring with the integrated statistic

Since the variables have been grouped into static part and dynamic part, PCA and SFA are employed to extract static and dynamic data feature respectively and calculate statistics under normal operating conditions. The T^2, SPE statistics obtained from PCA and T^2, T_e^2, S^2 and S_e^2 statistics obtained from SFA are integrated into the SVDD model for process monitoring. The fault data sets in TEP are input into the method to obtain the monitoring results. The results are compared with related methods, PCA, DPCA and SFA.

As shown in Figure 4, the proposed method is applied to monitor fault 10, which is a random variation fault that happened in the temperature of C feed. The statistic that first identifies the fault is displayed. For PCA and DPCA, this fault is difficult to detect at its early stage because the magnitude of this abnormal deviation is small. For SFA, the fault can be detected at the 182nd sample, and the fault is detected at the 180th sample by the proposed method. The results show that the proposed method has a better performance on dynamic process monitoring than traditional PCA and other dynamic process monitoring methods. Although several statistics exceed the threshold before the fault has been introduced in DPCA and the proposed method, they will not be considered as faults because they do not continuously exceed the threshold.

The fault alarm time of all 18 faults in TEP obtained by PCA, DPCA, SFA and the proposed method is shown in Table 3. The fault alarm time of a method is obtained when one of its statistics exceeds its threshold. It can be obviously obtained that almost all faults can be earlier detected by the proposed method. It can be concluded that the idea of separating static variables from dynamic variables and applying proper algorithms to extract static and dynamic feature respectively is beneficial for dynamic process monitoring.

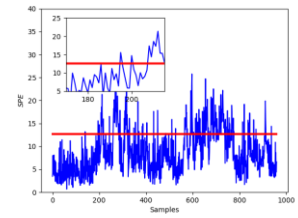

Fig. 4. (a)

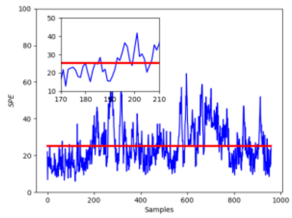

Fig. 4. (b)

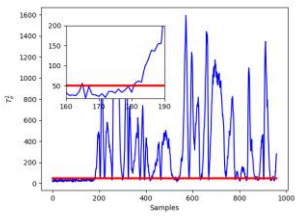

Fig. 4. (c)

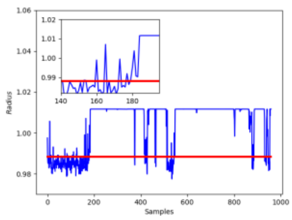

Fig. 4. (d)

Fig. 4. Process monitoring results for fault 10 in TEP: (a) PCA; (b) DPCA; (c) SFA; (d) The proposed method.

Table 3. Fault alarm time of PCA, DPCA, SFA and the proposed method for TEP

Fault No.	PCA	DPCA	SFA	Proposed method
1	163	163	161	**161**
2	175	173	174	**170**
4	161	161	161	**161**
5	161	161	161	**161**
6	161	161	161	**161**
7	161	161	161	**161**
8	180	181	180	**175**
10	209	194	182	**180**
11	166	166	166	**165**
12	163	162	162	163
13	201	198	201	**197**
14	161	162	161	**161**
16	182	177	167	**166**
17	182	180	180	**180**
18	244	240	239	**238**
19	346	171	170	**170**
20	246	241	223	**223**
21	417	420	402	**400**

5. CONCLUSIONS

In this work, a novel idea to solve dynamic process monitoring is proposed by considering the feature extraction of dynamic variables and static variables separately. Since the variables are grouped into static part and dynamic part by mutual information according to their autocorrelation, PCA is used to extract static variable feature and SFA is employed to extract dynamic variable feature. In order to comprehensively measure the changes of each feature space in the dynamic and static parts, the statistics are integrated by a SVDD model to give a final process monitoring decision. Case study on TEP shows the superiority of the proposed method compared with related methods. The proposed method provides an effective way to monitor both static and dynamic relations in dynamic processes, especially for large-scale industrial processes, as the operation of variable grouping is also helpful to reduce the calculation loads.

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