COMBINED MULTIVARIATE STATISTICAL PROCESS CONTROL

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Abstract: Multivariate statistical process control (MSPC) based on principal component analysis (PCA) has been widely used in chemical processes. Recently, the use of independent component analysis (ICA) was proposed to improve monitoring performance. In the present work, a new method, referred to as combined MSPC (CMSPC), is proposed by integrating PCA-based SPC and ICA-based SPC. CMSPC includes both MSPC methods as its special cases and thus provides a unified framework for MSPC. The effectiveness of CMSPC was demonstrated with its applications to a multivariable system and a CSTR process.

Keywords: Statistical Process Control, Process Monitoring, Fault Detection, Independent Component Analysis, Principal Component Analysis

1. INTRODUCTION

The successful process operation often depends on the effectiveness of fault detection. On-line process monitoring plays an important role in detecting process upsets, equipment malfunctions, or other special events as early as possible. In chemical processes, statistical process control (SPC), which is a data-based approach for process monitoring, has been used widely and successfully. Well-known SPC techniques include Shewhart control charts, cumulative sum (CUSUM) control charts, and exponentially weighted moving average (EWMA) control charts. Such SPC charts are well established for monitoring univariate processes, but univariate SPC (USPC) does not function well for multivariable processes. In order to extract useful information from multivariate process data and utilize it for process monitoring, multivariate statistical process control (MSPC) based on principal component analysis (PCA) has been developed (Jackson and Mudholkar, 1979). In the last decade or so, many successful applications have been reported and various extensions of MSPC have been proposed (Kresta et al., 1991; Kano et al., 2002a).

PCA-based SPC (PCA-SPC) and its extensions have been widely accepted in process industries. However, their achievable performance is limited due to the assumption that monitored variables are normally distributed. Recently, to further improve the monitoring performance, a new MSPC method based on independent component analysis (ICA), referred to as ICA-SPC, was proposed by Kano et al. (2002b, 2003). They demonstrated the superiority of ICA-SPC over conventional methods.

ICA-SPC, however, does not always outperform PCA-SPC. ICA-SPC should be selected when process variables do not follow normal distribution. On the other hand, ICA-SPC likely will not improve the performance in comparison with PCA-SPC if process variables are normally distributed. In a practical case, where some variables follow normal distribution and others do not, which monitoring method should be selected? In the present work, to answer this question and propose a new framework for MSPC, combined MSPC (CMSPC) is developed by integrating PCA-SPC and ICA-SPC. The performance of CMSPC is evaluated with its applications to monitoring problems of a linear multivariable system and a CSTR process.

2. PCA-BASED MSPC

PCA, which is a tool for data compression and information extraction, finds linear combinations of variables that describe major trends in a data set. For monitoring a process by using PCA-SPC, control limits are set for two kinds of statistics, T^2 and Q, after a PCA model is developed. T^2 and Q are defined as

$$T^2 = \sum_{r=1}^{R} \frac{t_r^2}{\sigma_{t_r}^2} \tag{1}$$

$$Q = \sum_{p=1}^{P} (x_p - \hat{x}_p)^2 \tag{2}$$

where t_r is the r-th principal component score and $\sigma_{t_r}^2$ is its variance. x_p and $\hat{x}_p$ are a measurement of the p-th variable and its predicted (reconstructed) value, respectively. R and P denote the number of principal components retained in the PCA model and the number of process variables, respectively. The T^2 statistic is a measure of the variation within the PCA model, and the Q statistic is a measure of the amount of variation not captured by the PCA model.

3. ICA-BASED MSPC

ICA (Jutten and Herault, 1991) is a signal processing technique for transforming measured multivariate data into statistically independent components, which are expressed as linear combinations of measured variables. In this section, an ICA algorithm and ICA-SPC are briefly described.

3.1 *Problem Definition*

It is assumed that m measured variables $x_1, x_2, \ldots, x_m$ are given as linear combinations of $n (\leq m)$ unknown independent components $s_1, s_2, \ldots, s_n$. The independent components and the measured variables are mean-centered. The relationship between them is given by

$$\boldsymbol{x} = \boldsymbol{s}\boldsymbol{A} \tag{3}$$

$$\boldsymbol{x} = \left[\, x_1 \; x_2 \; \ldots \; x_m \,\right] \tag{4}$$

$$\boldsymbol{s} = \left[\, s_1 \; s_2 \; \ldots \; s_n \,\right] \tag{5}$$

where $\boldsymbol{A}$ is a full-rank matrix, called the mixing matrix. When k samples are available, the above relationship can be rewritten as $\boldsymbol{X} = \boldsymbol{S}\boldsymbol{A}$.

The basic problem of ICA is to estimate the original components $\boldsymbol{S}$ or to estimate the mixing matrix $\boldsymbol{A}$ from the measured data matrix $\boldsymbol{X}$ without any knowledge of $\boldsymbol{S}$ or $\boldsymbol{A}$. Therefore, the practical objective of ICA is to calculate a separating matrix $\boldsymbol{W}$ so that components of the reconstructed data matrix $\boldsymbol{Y}$, given as

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{W}, \tag{6}$$

become as independent of each other as possible. The limitations of ICA are: 1) only non-Gaussian independent components can be estimated (just one of them can be Gaussian), and 2) neither signs, powers, nor orders of independent components can be estimated.

3.2 *Sphering with PCA*

Statistical independence is more restrictive than uncorrelation. Therefore, for performing ICA, measured variables $\{x_i\}$ are first transformed into uncorrelated variables $\{z_j\}$ with unit variance. This pretreatment can be accomplished by PCA and it is called sphering or prewhitening.

By defining the sphering matrix as $\boldsymbol{M}$, the relationship between $\boldsymbol{z}$ and $\boldsymbol{s}$ is given as

$$\boldsymbol{z} = \boldsymbol{x}\boldsymbol{M} = \boldsymbol{s}\boldsymbol{A}\boldsymbol{M} = \boldsymbol{s}\boldsymbol{B}^T \tag{7}$$

where $\boldsymbol{B}^T = \boldsymbol{A}\boldsymbol{M}$. Since s_i are mutually independent and z_j are mutually uncorrelated,

$$E\left[\boldsymbol{z}^T\boldsymbol{z}\right] = \boldsymbol{B}E\left[\boldsymbol{s}^T\boldsymbol{s}\right]\boldsymbol{B}^T = \boldsymbol{B}\boldsymbol{B}^T = \boldsymbol{I} \tag{8}$$

is satisfied. Here $E[\cdot]$ denotes expectation. It is assumed here that the covariance matrix of s_i, $E\left[\boldsymbol{s}^T\boldsymbol{s}\right]$, is an identity matrix, because signs and powers of s_i remain arbitrary. Equation (8) means that $\boldsymbol{B}$ is an orthogonal matrix. Therefore, the problem of estimating a full-rank matrix $\boldsymbol{A}$ is reduced to the problem of estimating an orthogonal matrix $\boldsymbol{B}$ through the sphering.

3.3 *Fixed-Point Algorithm for ICA*

The fourth-order cumulant of zero-mean random variable y is defined as

$$\kappa_4(y) = E[y^4] - 3E[y^2]^2 \tag{9}$$

By minimizing or maximizing the fourth-order cumulant $\kappa_4(\boldsymbol{z}\boldsymbol{b})$ under the constraint of $\|\boldsymbol{b}\| = 1$, columns of the orthogonal matrix $\boldsymbol{B}$ are obtained as solutions for $\boldsymbol{b}$. Finding the local extrema of the fourth-order cumulant is equivalent to estimating the non-Gaussian independent components (Delfosse and Loubaton, 1995). In the present work, a fixed-point algorithm (Hyvarinen and Oja, 1997) is used to obtain $\boldsymbol{b}$ that minimizes or maximizes the fourth-order cumulant.

For estimating n independent components that are different from each other, the following orthogonal conditions are imposed.

$$\boldsymbol{b}_i^T \boldsymbol{b}_j = 0 \qquad (i \neq j) \tag{10}$$

Thus, the current solution $\boldsymbol{b}_i$ is projected on the space orthogonal to previously calculated $\boldsymbol{b}_j (j = 1, 2, \ldots, i-1)$. By defining

$$\boldsymbol{B} = \left[\, \boldsymbol{b}_1 \ \boldsymbol{b}_2 \ \ldots \ \boldsymbol{b}_n \, \right], \tag{11}$$

independent components $\boldsymbol{Y}$ can be obtained from

$$\boldsymbol{Y} = \boldsymbol{Z}\boldsymbol{B} = \boldsymbol{X}\boldsymbol{M}\boldsymbol{B} = \boldsymbol{X}\boldsymbol{W}. \tag{12}$$

This means that the separating matrix $\boldsymbol{W}$ can be calculated from $\boldsymbol{W} = \boldsymbol{M}\boldsymbol{B}$.

The sphering matrix $\boldsymbol{M}$ uncorrelates $\boldsymbol{x}$ and scales it so that uncorrelated variables $\boldsymbol{z}$ have unit variances. Uncorrelated variables can be derived by using PCA. Therefore, the sphering matrix $\boldsymbol{M}$ can be decomposed into two parts: an uncorrelating matrix $\boldsymbol{P}$ and a scaling matrix $\boldsymbol{\Lambda}$. The uncorrelating matrix $\boldsymbol{P}$ is the same as the loading matrix of PCA. Therefore, Eq. (12) can be rewritten as

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{M}\boldsymbol{B} = \boldsymbol{X}\boldsymbol{P}\boldsymbol{\Lambda}\boldsymbol{B}. \tag{13}$$

Both $\boldsymbol{P}$ and $\boldsymbol{B}$ are orthogonal matrices.

3.4 *Monitoring of Independent Components*

The procedure of ICA-SPC is the same as USPC. The only difference lies in the variables to be monitored. That is, independent components are monitored in ICA-SPC while correlated measured variables are monitored in USPC.

A separating matrix $\boldsymbol{W}$ in Eq. (12) and control limits must be determined in order to apply ICA-SPC to monitoring problems. For this purpose, the following procedure is adopted.

(1) Acquire time-series data when a process is operated under a normal condition. Normalize each column (variable) of the data matrix, i.e., adjust it to zero mean and unit variance, if necessary.
(2) Apply ICA to the normalized data, determine a separating matrix $\boldsymbol{W}$, and calculate independent components.
(3) Determine control limits of all independent components.

For on-line monitoring, a new sample of monitored variables is scaled with the means and the variances obtained at step 1. Then, it is transformed to independent components through the separating matrix $\boldsymbol{W}$. If one or more of the independent components are outside the corresponding control limits, the process is judged to be out of control.

4. COMBINED MSPC

ICA-SPC does not necessarily outperform PCA-SPC. ICA is based on the assumption that each measured variable is given as a linear combination of non-Gaussian variables that are independent of each other. Independent components, even if they can be calculated, are meaningless and ICA-SPC does not function well when this assumption is incorrect. In the present work, a new advanced MSPC method is proposed for further improving the monitoring performance by combining ICA-SPC and PCA-SPC. The proposed method is referred to as combined MSPC (CMSPC).

4.1 *CMSPC Algorithm*

The basic and important fact of PCA-SPC is that uncorrelated variables, i.e., principal components, are monitored. On the other hand, independent components are monitored in ICA-SPC. Since statistical independence is more restrictive than uncorrelation, ICA-SPC can outperform PCA-SPC. However, if process variables are normally distributed, the monitoring performance would not necessarily be improved by using ICA-SPC. Ideally, ICA-SPC should be used for monitoring non-Gaussian independent variables, and PCA-SPC is used for monitoring uncorrelated Gaussian variables. This conclusion motivates us to integrate PCA-SPC and ICA-SPC into a new MSPC method. For realizing this integration, non-Gaussian variables and Gaussian variables have to be distinguished.

In the present work, the fourth-order cumulant is used to evaluate the non-Gaussianity of components $\{y_l\}$ derived by using ICA. The fourth-order cumulant of any Gaussian random variable is zero. In addition, the absolute value of the fourth-order cumulant increases as the non-Gaussianity increases. Therefore, non-Gaussian independent variables can be selected from $\{y_l\}$ based on their fourth-order cumulants. When the fourth-order cumulant of an independent component is larger than the threshold determined in advance, it is judged to be non-Gaussian and independent.

Consider a data matrix $\boldsymbol{X} \in \Re^{k \times m}$, where k and m are the number of samples and that of variables, respectively. All variables are mean-centered. When r of m components $\{y_1, y_2, ..., y_r\}$ are judged to be non-Gaussian, these r independent components should be monitored independently. In other words, ICA-SPC should be applied to these r independent components. However, since the other $m - r$ components $\{y_{r+1}, y_{r+2}, ..., y_m\}$ are Gaussian, these $m - r$ variables should be monitored by using PCA-SPC. In practice, the ICA algorithm might not converge if more than one component is Gaussian. Therefore, a part of $\boldsymbol{X}$, which is explained by $\{y_{r+1}, y_{r+2}, ..., y_m\}$, needs to be derived without calculating these $m-r$ components.

From Eq. (13), the first r non-Gaussian independent components are given as

$$\boldsymbol{Y}_r = \left[\, \boldsymbol{y}_1 \; \boldsymbol{y}_2 \; \cdots \; \boldsymbol{y}_r \,\right] = \boldsymbol{X}\boldsymbol{P}\boldsymbol{\Lambda}\boldsymbol{B}_r. \qquad (14)$$

A part of $\boldsymbol{X}$, which is explained by the first r non-Gaussian independent components, can be reconstructed from $\boldsymbol{Y}_r$ or $\boldsymbol{X}$.

$$\begin{aligned} \boldsymbol{X}_r &= \boldsymbol{Y}_r \boldsymbol{B}_r^T \boldsymbol{\Lambda}^{-1} \boldsymbol{P}^T \\ &= \boldsymbol{X}\boldsymbol{P}\boldsymbol{\Lambda}\boldsymbol{B}_r\boldsymbol{B}_r^T \boldsymbol{\Lambda}^{-1} \boldsymbol{P}^T \end{aligned} \qquad (15)$$

As a result, $\boldsymbol{X}_{m-r}$, which cannot be explained by $\boldsymbol{Y}_r$, is calculated as follows:

$$\begin{aligned} \boldsymbol{X}_{m-r} &= \boldsymbol{X} - \boldsymbol{X}_r \\ &= \boldsymbol{X}(\boldsymbol{I} - \boldsymbol{P}\boldsymbol{\Lambda}\boldsymbol{B}_r\boldsymbol{B}_r^T \boldsymbol{\Lambda}^{-1} \boldsymbol{P}^T). \end{aligned} \qquad (16)$$

Since $\boldsymbol{X}_{m-r}$ does not include significant non-Gaussian components, it can be monitored successfully by using PCA-SPC.

4.2 *CMSPC Procedure*

The procedure of CMSPC is summarized as follows:

(1) Acquire time-series data when a process is operated under a normal condition. Normalize each column (variable) of the data matrix, i.e., adjust it to zero mean and unit variance, if necessary.
(2) Apply ICA to the normalized data $\boldsymbol{X}$, and calculate independent components $\{y_l\}$.
(3) Calculate the fourth-order cumulant of independent components.
(4) Adopt independent components $\{y_1, y_2, \cdots, y_r\}$ with the fourth-order cumulant larger than the threshold (e.g. 0.1) as non-Gaussian independent components.
(5) The other components are regarded as Gaussian, and those variables are projected onto the original space through Eq. (16).
(6) Apply PCA to the reconstructed data $\boldsymbol{X}_{m-r}$, and calculate principal components $\{z'_1, z'_2, \cdots, z'_{m-r}\}$.
(7) Calculate T^2 and Q statistics.
(8) Determine control limits of independent components $\{y_1, y_2, \cdots, y_r\}$ and those of T^2 and Q.
(9) Monitor $\{y_1, y_2, \cdots, y_r\}$, T^2, and Q on-line.

CMSPC includes both PCA-SPC and ICA-SPC as its special cases. In fact, CMSPC is the same as PCA-SPC when no independent components are adopted in step (4), because PCA is applied to $\boldsymbol{X}_{m-r} = \boldsymbol{X}$ in such a case. On the other hand, CMSPC is the same as ICA-SPC when $r = rank(\boldsymbol{X})$. Therefore, CMSPC provides a unified framework for MSPC.

5. APPLICATION 1

In this section, USPC, PCA-SPC, ICA-SPC, and the proposed CMSPC are applied to fault detection problems of an eight-variable system:

$$\boldsymbol{x} = \boldsymbol{s}\boldsymbol{A} + \boldsymbol{v} \qquad (17)$$

$$\boldsymbol{A} = \begin{bmatrix} 0.95 & 0.82 & 0.94 & 0.14 \\ 0.23 & 0.45 & 0.92 & 0.20 \\ 0.61 & 0.62 & 0.41 & 0.20 \\ 0.49 & 0.79 & 0.89 & 0.60 \\ 0.89 & 0.92 & 0.06 & 0.27 \\ 0.76 & 0.74 & 0.35 & 0.20 \\ 0.46 & 0.18 & 0.81 & 0.02 \\ 0.02 & 0.41 & 0.01 & 0.75 \end{bmatrix}^T \qquad (18)$$

$$\boldsymbol{s} = \left[\, s_1 \; s_2 \; s_3 \; s_4 \,\right] \qquad (19)$$

where $\{s_i\}$ are uncorrelated random signals following uniform or normal distribution with unit variance ($\sigma_s = 1$). The output $\boldsymbol{x}$ is corrupted by measurement noise $\boldsymbol{v}$ following normal distribution ($\sigma_v = 0.1$). For evaluating the monitoring performance, mean shifts of $\{s_i\}$ or $\{x_j\}$ are investigated.

One data set, including 100,000 samples, obtained from a normal operating condition was used to build a PCA model, to determine a separating matrix, and also to determine control limits. To evaluate the monitoring performance, average run length (ARL) is used. ARL is the average number of points that must be plotted before a point indicates an out-of-control condition. To calculate ARL, 10,000 data sets were generated by changing seeds of the random signals $\boldsymbol{s}$ and $\boldsymbol{v}$ in each case shown in Table 1.

The control limit of each index or variable is determined so that the number of samples outside

Table 1. ARL Comparison.

Case 1				
	s_i :	uniform distribution		
	fault :	$\boldsymbol{s}_1$		
Shift size	USPC x_5	PCA-SPC T_4^2	ICA-SPC y_3	CMSPC y_3
0	98.1	99.0	101	101
0.2	82.5	84.0	59.6	59.6
0.5	42.2	43.2	18.0	18.0
1.0	16.5	12.3	5.5	5.5
Case 2a				
	s_i :	normal distribution		
	fault :	$\boldsymbol{s}_1$		
Shift size	USPC x_5	PCA-SPC T_4^2	ICA-SPC y_3	CMSPC T_4^2
0	96.0	101	97.3	101
0.2	91.9	96.0	91.7	96.0
1.0	33.5	36.6	37.6	36.6
2.0	8.9	8.1	10.8	8.1
Case 2b				
	s_i :	normal distribution		
	fault :	$\boldsymbol{s}_2$		
Shift size	USPC x_5	PCA-SPC T_4^2	ICA-SPC y_4	CMSPC T_4^2
0	103	97.5	99.8	97.5
1.0	32.3	37.4	51.6	37.4
2.0	8.3	8.5	18.5	8.5
3.0	3.2	2.7	8.0	2.7
Case 3				
	s_1, s_2 :	uniform distribution		
	s_3, s_4 :	normal distribution		
	fault :	$\boldsymbol{x}_5$		
Shift size	USPC x_5	PCA-SPC Q_4	ICA-SPC y_8	CMSPC Q_2
0	96.8	96.1	98.9	102
0.1	79.9	55.4	54.1	48.3
0.2	50.3	21.1	20.2	14.8
0.5	12.6	2.5	2.5	1.6

the control limit is 1% of the entire samples while the process is operated under a normal condition. The monitored indexes for PCA-SPC are T_4^2 and Q_4. The subscript 4 means that four principal components are retained in the PCA model. In ICA-SPC, however, each independent component is independently monitored. In CMSPC, the number of independent components and that of principal components retained in the PCA model depend on the cases. Four independent components and no principal components are retained in case 1, no independent components and four principal components in case 2, and two independent components and two principal components in case 3.

Fault detection results are summarized in Table 1. ARL decreases as the shift size increases, irrespective of the type of monitoring method. In case 1, the results have clearly shown the advantage of ICA-SPC and CMSPC over both USPC and PCA-SPC, and the ARL of ICA-SPC is the same as that of CMSPC because all original variables follow uniform distribution. On the other hand, in case 2, PCA-SPC and CMSPC are superior to ICA-SPC, and they achieve the same performance because all variables follow normal distribution. The difference between case 2a and 2b is the variable where the mean shift occurs. In case 2a, the monitoring performance of all four SPC methods is similar, and the advantage of using PCA-SPC over ICA-SPC is not clear. In case 2b, however, PCA-SPC outperforms ICA-SPC. Therefore, it is concluded that PCA-SPC functions better than or as well as ICA-SPC when all measured variables are Gaussian. Although PCA-SPC is better than ICA-SPC in case 2, these two methods do not outperform USPC. Even when measured variables are mutually correlated, USPC sometimes outperforms MSPC. In case 2b, USPC gives better performance than the others because a_{52}, which is the coefficient from s_2 to x_5 in $\boldsymbol{A}$, is larger than the others in the same row and thus the mean shift can be easily detected by monitoring x_5.

In case 3, two of four original variables follow uniform distribution and the other two variables follow normal distribution. In this case, CMSPC can detect the mean shift of x_5 earlier than the other methods. This result clearly shows the advantage of CMSPC over other SPC methods.

ICA-SPC functions well for generating and monitoring non-Gaussian independent variables, while PCA-SPC is suitable for monitoring Gaussian variables. Therefore, the answer to the question "Which MSPC method should be applied to our process?" depends on the process. However, the proposed CMSPC combines the advantages of both PCA-SPC and ICA-SPC, and thus it enables us to select the best solution automatically.

6. APPLICATION 2

In this section, four SPC methods are applied to monitoring problems of a CSTR process (Johannesmeyer and Seborg, 1999). The objective of this section is to show the usefulness of CMSPC with its application to a more realistic example.

The CSTR process used for dynamic simulations is shown in Fig. 1. The reactor is equipped with a cooling jacket. The process has two manipulated variables (valves) and five process measurements. A total of nine variables used for monitoring are listed in Table 2. Process data are generated from a normal operating condition and eight abnormal operating conditions listed in Table 3. All variables are measured every five seconds.

The control limit of each index or variable is determined in the same way as the previous section. Five principal components are retained in the PCA model for PCA-SPC. The number of non-Gaussian independent components is five,

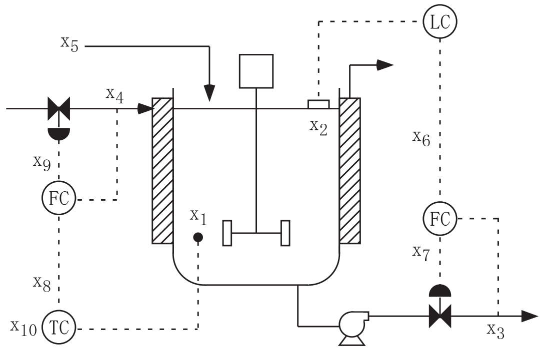

Fig. 1. CSTR with feedback control.

Table 2. Process variables.

x_1	reactor temperature
x_2	reactor level
x_3	reactor outlet flow rate
x_4	coolant flow rate
x_5	reactor feed flow rate
x_6	MV of level controller
x_7	MV of outlet flow controller
x_8	MV of temperature controller
x_9	MV of coolant flow controller

Table 3. Disturbances and faults.

Case	Operation Mode
N	normal operation
F1	dead coolant flow measurement
F2	bias in reactor temp. measurement
F3	coolant valve stiction
F4	feed flow rate - step
F5	feed concentration - ramp
F6	coolant feed temperature - ramp
F7	upstream pressure in coolant line - step
F8	downstream pressure in outlet line - step

Table 4. ARL Comparison (CSTR).

Case	USPC	PCA-SPC	ICA-SPC	CMSPC
N	94.7	115	96.6	95.4
F1	1.0	1.4	1.1	1.1
F2	7.9	8.7	8.8	8.8
F3	7.0	2.6	1.4	1.4
F4	49.5	23.1	1.0	1.0
F5	52.4	60.1	57.6	57.6
F6	60.0	61.8	55.8	55.8
F7	79.3	86.2	2.5	2.5
F8	61.7	6.6	1.0	1.0

and the other four components are monitored together by using T^2 in CMSPC. The results are summarized in Table 4. In this application, there is little or no difference of ARLs among four monitoring methods except F4, F7, and F8. In those three cases, ICA-SPC and CMSPC can detect the faults considerably earlier than USPC and PCA-SPC. In addition, ICA-SPC and CMSPC achieve the same performance in almost all cases because the faults tend to be detected at non-Gaussian independent components. The results clearly show the effectiveness of CMSPC as well as ICA-SPC.

7. CONCLUSIONS

A new advanced MSPC method, referred to as combined MSPC (CMSPC), was developed by integrating conventional PCA-SPC and recently proposed ICA-SPC. CMSPC includes both PCA-SPC and ICA-SPC as its special cases, and thus it provides a unified framework for MSPC. The application results show that CMSPC functions very well and it combines the advantages of both PCA-SPC and ICA-SPC.

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