Fault Detection and Diagnosis Based on Modified Independent Component Analysis

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A novel multivariate statistical process monitoring (MSPM) method based on modified independent component analysis (ICA) is proposed. ICA is a multivariate statistical tool to extract statistically independent components from observed data, which has drawn considerable attention in research fields such as neural networks, signal processing, and blind source separation. In this article, some drawbacks of the original ICA algorithm are analyzed and a modified ICA algorithm is developed for the purpose of MSPM. The basic idea of the approach is to use the modified ICA to extract some dominant independent components from normal operating process data and to combine them with statistical process monitoring techniques. Variable contribution plots to the monitoring statistics (T^2 and SPE) are also developed for fault diagnosis. The proposed monitoring method is applied to fault detection and diagnosis in a wastewater treatment process, the Tennessee Eastman process, and a semiconductor etch process and is compared with conventional PCA monitoring methods. The monitoring results clearly illustrate the superiority of the proposed method. © 2006 American Institute of Chemical Engineers *AIChE J,* 52: 3501–3514, 2006
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Introduction

As chemical processes become more complex, on-line monitoring and fault diagnosis of the process are gaining importance for plant safety, maintenance, and product quality. With a large number of variables measured in chemical plants, multivariate statistical process monitoring (MSPM) approaches have been proposed to extract useful information from a large amount of process data and to detect and diagnose various faults in an abnormal operating situation. In general, MSPM is composed of the following steps:

(1) Building a data-driven model using multivariate analysis from a historical data set of normal operations.

(2) Projecting new data onto the normal model.

(3) Judging whether the new data are statistically normal or abnormal against the past in-control behavior captured by historical normal data.

(4) Identifying the variables responsible for the process to go out of control.

(5) Determining the root cause of the abnormality.

In this procedure, it is important to determine what kind of multivariate data analysis is used to build the normal operating model from historical data. The process monitoring performance depends on how well the model—based on the multivariate data analysis—fits the given data structure. The multivariate data analysis should handle high dimensional, noisy, and highly correlated data generated from chemical processes

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while extracting essential features. That is, it is required that the method can project the high-dimensional process to a low-dimensional space amenable to direct visualization and identify important features of the data.

Many monitoring schemes that use multivariate statistical methods such as principal component analysis (PCA) have been developed and widely used. PCA projects the data onto a lower-dimensional space that contains the most variance of the original data and accounts for correlations among variables.[1-10] However, PCA is a second-order method, which means it considers only mean and variance-covariance of data. PCA performs well in many cases, but lacks the ability to give high-order representations for non-Gaussian data, which is often the case for industrial data.[11] The PCA objective is only to decorrelate variables, not to make them independent. The transform defined by PCA is not useful for many purposes where optimal reduction of dimension in the mean-square sense is not needed.[12] Furthermore, in PCA-based monitoring, the control limits of Hotelling's T^2 and the *SPE* charts are developed based on the assumption that the latent variables follow a multivariate Gaussian distribution. Therefore, the use of Hotelling's T^2 and the *SPE* charts may be misleading if the latent variables tend to be non-Gaussian as a result of nonlinear characteristics of industrial processes.[13]

More recently, several MSPM methods based on ICA have been proposed.[14-20] The goal of ICA is to decompose observed data into linear combinations of statistically independent components (ICs). ICA involves higher-order statistics, that is, not only does it decorrelate the data based on second-order statistics, but it also reduces higher-order statistical dependencies.[21] Thus, ICs reveal more useful information on higher-order statistics from observed data than principal components (PCs). Li and Wang[22] introduced ICA to remove the dependencies of variables and to reduce data dimension of the monitored variables. Kano et al.[14] proposed an ICA-based statistical process control (SPC) method and showed its superiority over PCA-based methods. The basic idea is to extract essential components that drive a process using ICA and to monitor the ICs instead of the original measurements. Also, Kano et al.[16] proposed a new MSPM method based on ICA and external analysis to improve the monitoring performance and to distinguish faults from normal changes in operating conditions. However, in their method fault diagnosis is not considered, the number of monitoring charts increases as the number of ICs extracted from observed data, and false alarms may occur often given that the upper and lower control limits are devised from the assumption that the ICs follow Gaussian distributions. Lee et al.[17] proposed a method for statistical process monitoring based on ICA. They extracted independent components using ICA and separated them into dominant ICs and excluded ICs. Then they suggested three statistics: I^2 to monitor the variation within dominant ICs, I_e^2 to monitor the variation within excluded ICs, and *SPE* to monitor the variation of residuals. Kernel density estimation was used to define the control limit of each monitoring chart because each statistic was not based on Gaussianity assumptions. They also considered contribution plots for fault diagnosis, demonstrating that ICA monitoring gives more convincing results than conventional methods using PCA because the former imposes statistical independence on the individual components beyond second order and thereby can extract underlying factors that drive a process. This ICA-based monitoring method has been extended to dynamic process monitoring and batch process monitoring, respectively.[18,19] Albazzaz and Wang[20] also developed a new method for deriving SPC charts based on ICA. Their method is applied to the batch process and showed that it can detect the faults faster than a PCA-based method.

However, the ICA-based monitoring method has some drawbacks. First, it is not trivial to determine how many independent components should be extracted to establish a stable ICA model.[11] In general, all ICs up to the dimension of given data are extracted. For this reason, it incurs a high computational load. Second, unlike PCA which arranges the PCs in descending order, we cannot determine the proper order of ICs. Furthermore, random initialization of demixing matrix $\mathbf{B}$ in whitened space leads to different solutions in the ICA algorithm.

In this article, we propose a modified ICA algorithm that extracts a number of dominant ICs from multivariate data. The basic idea is to first estimate the variance of dominant ICs and the directions using PCA and then to perform conventional ICA to update the dominant ICs while maintaining the variance. A fault detection and diagnosis method based on the modified ICA is also proposed. The organization of the article is as follows. Conventional PCA monitoring is briefly reviewed in the next section, followed by a brief introduction to the ICA algorithm. Then the modified ICA algorithm and its application to process monitoring are proposed. The performance of process monitoring using the modified ICA is illustrated through three examples: a wastewater treatment process, the Tennessee Eastman Process, and a semiconductor etch process. Conclusions are given at the end of the article.

PCA Monitoring

PCA decomposes the data matrix $\mathbf{X} \in R^{n \times d}$ (where n is the number of samples and d is the number of variables) as the product of scores and loadings:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \tag{1}$$

where $\mathbf{E}$ is the residual matrix and $\mathbf{T} \in R^{n \times a}$ and $\mathbf{P} \in R^{d \times a}$ are the score and loading matrices, respectively. Here, projection into principal component space reduces the original set of variables to a latent variables. Given a new sample vector $\mathbf{x}$, the PCA score, prediction, and residual vectors are given as follows:

$$\text{Score: } \mathbf{t} = \mathbf{P}^T\mathbf{x} \tag{2}$$

$$\text{Prediction: } \hat{\mathbf{x}} = \mathbf{P}\mathbf{P}^T\mathbf{x} \tag{3}$$

$$\text{Residual: } \mathbf{e} = (\mathbf{I} - \mathbf{P}\mathbf{P}^T)\mathbf{x} \tag{4}$$

A measure of the variation within the PCA model is given by Hotelling's T^2 statistic. T^2 is the sum of the normalized squared scores, defined as

$$T^2 = \mathbf{t}^T\mathbf{D}^{-1}\mathbf{t} = \mathbf{x}^T\mathbf{P}\mathbf{D}^{-1}\mathbf{P}^T\mathbf{x} \quad (5)$$

where $\mathbf{D}$ is the diagonal matrix of the eigenvalues associated with the retained principal components. The upper control limit for T^2 can be obtained using the F-distribution.[23]

On the other hand, a measure of variation not captured by the PCA model can be monitored by using the squared prediction error (*SPE*). The *SPE* is defined as the sum of squares of $\mathbf{e}$

$$SPE = \mathbf{e}^T\mathbf{e} = \mathbf{x}^T(\mathbf{I} - \mathbf{P}\mathbf{P}^T)\mathbf{x} \quad (6)$$

The upper control limit for the *SPE* can be computed from its approximate distribution[24]

$$SPE_\alpha = \theta_1\left[\frac{c_\alpha\sqrt{2\theta_2 h_0^2}}{\theta_1} + 1 + \frac{\theta_2 h_0(h_0-1)}{\theta_1^2}\right]^{1/h_0} \quad (7)$$

where c_α is the standard normal deviate corresponding to the upper $(1-\alpha)$ percentile, $h_0 = 1 - 2\theta_1\theta_3/(3\theta_2^2)$, $\theta_i = \sum_{j=a+1}^{d}\lambda_j^i$ for $i = 1, 2, 3$, and λ_j is the eigenvalue associated with the jth loading vector of the data covariance.

Original ICA Algorithms

Several different algorithms for ICA have been proposed.[21,25] The most well known ICA algorithms are based on neural networks, higher-order statistics, and minimum mutual information. We briefly review the fast fixed-point ICA algorithm (FastICA) that was developed by Hyvärinen and Oja.[26]

Suppose that d measured variables $x_1, x_2, \ldots, x_d$ can be expressed as linear combinations of m ($\leq d$) unknown independent components $s_1, s_2, \ldots, s_m$. The independent components and the measured variables have zero mean. If we denote the random column vectors as $\mathbf{x} = [x_1, x_2, \ldots, x_d]^T$ and $\mathbf{s} = [s_1, s_2, \ldots, s_m]^T$, the relationship between them is given by

$$\mathbf{x} = \mathbf{A}\mathbf{s} \quad (8)$$

where $\mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_m] \in R^{d\times m}$ is the unknown mixing matrix. The basic problem of ICA is to estimate both the mixing matrix $\mathbf{A}$ and the independent components $\mathbf{s}$ from only the observed data $\mathbf{x}$. This solution is equivalent to finding a demixing matrix $\mathbf{W}$ whose form is such that the elements of the reconstructed vector $\hat{\mathbf{s}}$, given as

$$\hat{\mathbf{s}} = \mathbf{W}\mathbf{x} \quad (9)$$

become as independent of each other as possible.

For convenience we assume d equals m and ICs have unit variance: $E(\mathbf{s}\mathbf{s}^T) = \mathbf{I}$. The initial step in ICA is whitening, which eliminates all the cross-correlation between random variables. This transformation can be also accomplished by classical PCA. The whitening transformation is expressed as

$$\mathbf{z} = \mathbf{\Lambda}^{-1/2}\mathbf{U}^T\mathbf{x} = \mathbf{Q}\mathbf{x} \quad (10)$$

where $\mathbf{Q} = \mathbf{\Lambda}^{-1/2}\mathbf{U}^T$ is the whitening matrix, and $\mathbf{U}$ (orthogonal matrix of eigenvectors) and $\mathbf{\Lambda}$ (diagonal matrix of its eigenvalues) are generated from the eigen-decomposition of the covariance matrix $E(\mathbf{x}\mathbf{x}^T) = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$. After the transformation we have

$$\mathbf{z} = \mathbf{Q}\mathbf{x} = \mathbf{Q}\mathbf{A}\mathbf{s} = \mathbf{B}\mathbf{s} \quad (11)$$

where $\mathbf{B} = \mathbf{Q}\mathbf{A}$ is an orthogonal matrix, given that $E(\mathbf{z}\mathbf{z}^T) = \mathbf{B}E(\mathbf{s}\mathbf{s}^T)\mathbf{B}^T = \mathbf{B}\mathbf{B}^T = \mathbf{I}$.

Then we can estimate $\mathbf{s}$ from Eq. 11 as follows:

$$\hat{\mathbf{s}} = \mathbf{B}^T\mathbf{z} = \mathbf{B}^T\mathbf{Q}\mathbf{x} \quad (12)$$

From Eqs. 9 and 12, the relation between $\mathbf{W}$ and $\mathbf{B}$ can be expressed as

$$\mathbf{W} = \mathbf{B}^T\mathbf{Q} \quad (13)$$

To calculate $\mathbf{B}$, each column vector $\mathbf{b}_i$ is randomly initialized and then updated so that the ith independent component $\hat{s}_i = (\mathbf{b}_i)^T\mathbf{z}$ has maximum non-Gaussianity. The objective function that the elements of $\hat{\mathbf{s}}$ are statistically independent can be reflected by their non-Gaussianity.[26] *Negentropy*, a common measure of non-Gaussianity, is based on the information-theoretic quantity of differential entropy. Hyvärinen and Oja[26] introduced a flexible and reliable approximation of negentropy as follows:

$$J(y) \approx [E\{G(y)\} - E\{G(v)\}]^2 \quad (14)$$

where y is assumed to be of zero mean and unit variance, v is a Gaussian variable of zero mean and unit variance, and G is any nonquadratic function. These approximations are often more accurate and robust than the cumulant-based approximations. By selecting G approximately, one obtains good approximations of negentropy. Hyvärinen and Oja[26] suggested three functions for G:

$$G_1(u) = \frac{1}{a_1}\log\cosh(a_1 u) \quad (15)$$

$$G_2(u) = \exp(-a_2 u^2/2) \quad (16)$$

$$G_3(u) = u^4 \quad (17)$$

where $1 \leq a_1 \leq 2$ and $a_2 \approx 1$. Among these three functions, G_2 and G_3 are more suitable for super-Gaussian and sub-Gaussian components, respectively. G_1 is a good general-purpose contrast function and was therefore selected for use in this article. The nonquadratic function G is described in detail by Hyvärinen.[27]

Based on the approximate form for the negentropy, Hyvärinen[28] introduced a very simple and highly efficient fixed-point algorithm for ICA, calculated over sphered zero-mean vectors $\mathbf{z}$. The algorithm, known as *FastICA*, calculates one column of the matrix $\mathbf{B}$ and allows the identification of one independent component; the corresponding IC can then be found using Eq. 12. After calculating $\mathbf{B}$, we can obtain $\hat{\mathbf{s}}$ and demixing matrix $\mathbf{W}$ from Eqs. 12 and 13, respectively. More detail of the ICA

algorithm can be found in Hyvärinen and Oja,[26] Hyvärinen,[12,28] and Hyvärinen et al.[25]

Modified ICA Algorithm

ICA considers higher-order statistics, that is, it exploits information about cumulants and moments of order greater than two. When ICA is applied to chemical process data, the ICs extracted from normal operating data are able to capture the essential structure of the data and to reflect normal operation history. Thus, combining them with a statistical process monitoring technique is very useful to detect and identify various faults generated from abnormal situations.[14,17]

However, the conventional ICA-based monitoring method has some drawbacks. A fundamental treatment in the original ICA algorithm is that the number of ICs equals that of variables of given data. A high computational load is the result in the case where the number of measured variables is very large. Furthermore, unimportant ICs for detecting faults are also extracted. One approach is to reduce data dimension in advance using PCA before performing ICA, which gives a low computational load.[25] However, information needed to extract essential ICs reflecting higher-order statistics is ignored by data reduction with PCA. The second problem in the original ICA algorithm is that the extracted ICs are not ordered by their importance, whereas PCA extracts components in terms of variance captured by each PC.[11] There is no standard criterion to order the ICs. In Lee et al.[17] the order of ICs is determined by the L_2 norm of each row of $\mathbf{W}$, to apply ICA to process monitoring. It is based on the assumption that the rows of $\mathbf{W}$, $\mathbf{w}_i$, with the largest sum of squares have the greatest effect on the variation of the ICs. This method, however, has a limitation to extract and order the dominant ICs, as described later in this article with a simple illustrative example. Furthermore, in the original ICA algorithm, random initialization of the demixing matrix $\mathbf{B}$ in the whitened space can lead to different solutions. As the result of random initial conditions, the order in which the ICs are extracted may also vary when applying ICA multiple times on the same data.[11]

In this section, a modified ICA algorithm is proposed. The modified ICA algorithm can solve the above-mentioned problems of original ICA algorithm, that is, it can extract a few dominant ICs, determine the order of ICs, and give a consistent solution. The basic idea is to first use PCA to estimate initial ICs where the variance of each IC is the same as that of each PC and then to update a few dominant ICs using the FastICA algorithm. Here, it is reasonable to expect the space spanned by the major PCs is a good starting point for extracting ICs because ICA can be viewed as a modified PCA (centering and whitening) and an additional iterative process.[27,29] ICA goes one step further so that it transforms the whitened data into a set of statistically independent components.

We define the objective of modified ICA as follows: find a demixing matrix $\mathbf{W} \in R^{m\times d}$ whose form is such that the elements of the extracted vector $\mathbf{y}$, given as

$$\mathbf{y} = \mathbf{W}\mathbf{x} \tag{18}$$

become as independent of each other as possible and have been ordered by their variances that are the same as the variances of the corresponding PCs.

To solve the above problem, first of all, we extract all score components from PCA:

$$\mathbf{t} = \mathbf{U}^T\mathbf{x} \tag{19}$$

where $\mathbf{t} \in R^d$, $\mathbf{x} \in R^d$, $\mathbf{U} \in R^{d\times d}$ is the eigenvector of covariance matrix $E\{\mathbf{x}\mathbf{x}^T\} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$, and $E\{\mathbf{t}\mathbf{t}^T\} = \mathbf{\Lambda} = \mathrm{diag}\{\lambda_1, \ldots, \lambda_d\}$. In some cases, the last few eigenvalues in Λ are close to zero. In that case, we exclude them and the corresponding eigenvectors in $\mathbf{U}$. However, it is important to retain as many eigenvalues as possible because the extracted score components can give additional information to perform ICA although their variances are small. Equation 19 can be normalized as follows:

$$\mathbf{z} = \mathbf{\Lambda}^{-1/2}\mathbf{t} = \mathbf{\Lambda}^{-1/2}\mathbf{U}^T\mathbf{x} = \mathbf{Q}\mathbf{x} \tag{20}$$

where $\mathbf{Q} = \mathbf{\Lambda}^{-1/2}\mathbf{U}^T$ and $\mathbf{z}$ is the normalized score vector, given that $E(\mathbf{z}\mathbf{z}^T) = \mathbf{I}$.

In the original ICA algorithm, the variances of the extracted independent components are assumed to be all one, so that we cannot decide which ICs are more important. On the contrary, the modified ICA finds m ($\leq d$) dominant source signals or ICs satisfying $E(\mathbf{y}\mathbf{y}^T) = \mathbf{D} = \mathrm{diag}\{\lambda_1, \ldots, \lambda_m\}$ such that the elements of $\mathbf{y}$ become as independent of each other as possible, using

$$\mathbf{y} = \mathbf{C}^T\mathbf{z} \tag{21}$$

where $\mathbf{C} \in R^{d\times m}$ and $\mathbf{C}^T\mathbf{C} = \mathbf{D}$. The requirement $E(\mathbf{y}\mathbf{y}^T) = \mathbf{D}$ reflects that the variance of each element of $\mathbf{y}$ is the same as that of scores in PCA; thus we can order the ICs according to their variances.

By defining the normalized ICs as

$$\mathbf{y}_n = \mathbf{D}^{-1/2}\mathbf{y} = \mathbf{D}^{-1/2}\mathbf{C}^T\mathbf{z} = \mathbf{C}_n^T\mathbf{z} \tag{22}$$

it is clear that $\mathbf{D}^{-1/2}\mathbf{C}^T = \mathbf{C}_n^T$, $\mathbf{C}_n^T\mathbf{C}_n = \mathbf{I}$, and $E(\mathbf{y}_n\mathbf{y}_n^T) = \mathbf{I}$. We have therefore reduced the problem of finding an arbitrary demixing matrix $\mathbf{W}$ to the simpler problem of finding the matrix $\mathbf{C}_n$, which has fewer parameters to estimate as a result of the orthogonality. Thus, the objective of the proposed algorithm is changed to find source signal $\mathbf{y}_n \in R^m$ and $\mathbf{C}_n$ from $\mathbf{z} \in R^d$ such that the elements of $\mathbf{y}_n$ become as independent of each other as possible and satisfy $E(\mathbf{y}_n\mathbf{y}_n^T) = \mathbf{I}$. Note that $\mathbf{z}$ is the scaled score vector generated from PCA, which is uncorrelated and had been ordered by its original variance. Although $\mathbf{z}$ is not independent, it can be a good initial value of $\mathbf{y}_n$ because it has removed statistical dependencies of data up to the second order (mean and variance). The remaining higher-order statistical dependencies can be reduced by the following algorithm. Therefore, we can set the first m components of $\mathbf{z}$ to be the initial components of $\mathbf{y}_n$. To do this, the matrix $\mathbf{C}_n^T$ should be initialized as

$$\mathbf{C}_n^T = [\mathbf{I}_m : \mathbf{0}] \tag{23}$$

where $\mathbf{I}_m$ is the m-dimensional identity matrix and $\mathbf{0}$ is the $m \times (d - m)$ zero matrix. This initialization is based on the assump-

tion that extracted PCs are good initial estimates of ICs, and thereby give a consistent solution, unlike random initialization in the original ICA algorithm.

Denoting $\mathbf{c}_{n,i}$ as the ith column of $\mathbf{C}_n$, the modified ICA algorithm obtains the ith independent component $y_{n,i} = (\mathbf{c}_{n,i})^T\mathbf{z}$ with maximized non-Gaussianity or negentropy. The detailed procedures are given below:

(1) Choose m, the number of ICs to estimate. Set counter $i \leftarrow 1$.

(2) Take the initial vector $\mathbf{c}_{n,i}$ to be the ith row of the matrix in Eq. 23.

(3) Let $\mathbf{c}_{n,i} \leftarrow E\{\mathbf{z}g(\mathbf{c}_{n,i}^T\mathbf{z})\} - E\{g'(\mathbf{c}_{n,i}^T\mathbf{z})\}\mathbf{c}_{n,i}$, where g is the first-order derivative and g' is the second-order derivative of G, and G takes the form of Eq. 15, Eq. 16, or Eq. 17. This step is an approximate Newton iteration procedure for the optimization of the negentropy given in Eq. 14.

(4) Do the following orthogonalization: $\mathbf{c}_{n,i} \leftarrow \mathbf{c}_{n,i} - \sum_{j=1}^{i-1}(\mathbf{c}_{n,i}^T\mathbf{c}_{n,j})\mathbf{c}_{n,j}$. This orthogonalization excludes the information contained in the solutions already found.

(5) Normalize $\mathbf{c}_{n,i} \leftarrow \mathbf{c}_{n,i}/\| \mathbf{c}_{n,i} \|$.

(6) If $\mathbf{c}_{n,i}$ has not converged, go back to Step 3.

(7) If $\mathbf{c}_{n,i}$ has converged, output the vector $\mathbf{c}_{n,i}$. Then, set $i \leftarrow i + 1$ and go back to Step 2 until all m ICs are calculated.

Once $\mathbf{C}_n$ is found, then the demixing matrix $\mathbf{W}$ and mixing matrix $\mathbf{A}$ can be obtained from

$$\mathbf{W} = \mathbf{D}^{1/2}\mathbf{C}_n^T\mathbf{Q} = \mathbf{D}^{1/2}\mathbf{C}_n^T\mathbf{\Lambda}^{-1/2}\mathbf{U}^T \tag{24}$$

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}^{1/2}\mathbf{C}_n\mathbf{D}^{-1/2} \tag{25}$$

where $\mathbf{WA} = \mathbf{I}_m$. Finally, we can obtain some dominant independent components from Eq. 18. The extracted dominant components $\mathbf{y}$ reveal the majority of information and represent a meaningful representation about the observed data $\mathbf{x}$. The following equation reveals the relation between modified ICs and PCs:

$$\mathbf{y} = \mathbf{W}\mathbf{x} = \mathbf{D}^{1/2}\mathbf{C}_n^T\mathbf{\Lambda}^{-1/2}\mathbf{U}^T\mathbf{x} = \mathbf{D}^{1/2}\mathbf{C}_n^T\mathbf{\Lambda}^{-1/2}\mathbf{t} \tag{26}$$

If the original data $\mathbf{x}$ is Gaussian, no further dependency exists beyond the second-order moments of $\mathbf{x}$, and thus $\mathbf{C}_n^T$ converges to $[\mathbf{I}_m \vdots \mathbf{0}]$ and $\mathbf{y} = \mathbf{t}$. In this special case, the modified ICA converges to PCA.

One remaining issue is to determine the number of ICs. Although there is no standard criterion, we can consider some methods to determine the number of ICs.

- *Set the number of ICs to be the same as the number of PCs*

The modified ICA first uses PCA as initial estimates of ICs and the demixing matrix. This approach to determining the number of ICs assumes that the space spanned by the dominant ICs to be essentially the same as the one associated to the largest PCs. Each IC has the same variance as that of each corresponding PC. It is reasonable to set the number of ICs to be the same as that of PCs because the selected PCs is able to give a good initial value of ICs.

- *Based on negentropy of the residual part*

ICA extracts independent components following non-Gaussianity from observed data. If the number of ICs is chosen such that the majority of non-Gaussianity is included in the ICs, the residual subspace, $\mathbf{e} = \mathbf{x} - \hat{\mathbf{x}}$ given in Eq. 28, will be essentially Gaussian. Based on this, the number of ICs may be selected to give the smallest negentropy value of residuals.

- *Use cross-validation*

Cross-validation[30] is a popular statistical procedure to choose the number of factors in PCA. The basis of this method is to estimate the values of some deleted data from a model and then compare these estimates with the actual value. However, in the proposed method, multiple ICA models must be built to calculate the predicted error sum of squares (PRESS), which is more tedious than PCA case.

- *Based on the variance of the reconstruction error* (*VRE*)

Valle et al.[31] proposed VRE to determine the number of PCs in a PCA model for best reconstruction. This method can be also applied to the modified ICA algorithm. It reduces the computational load compared to that of cross-validation because only one ICA model is built and a minimum is guaranteed in the variance of the reconstruction error.

Process Monitoring Based on the Modified ICA

Based on the modified ICA algorithm, a novel statistical process monitoring method is proposed. The implementations of the monitoring statistics of ICA are similar to those of the monitoring statistics of PCA. The modified ICA model is based on historical data collected during normal operation with only common cause variation. Future process behavior is then compared against this normal operating model.

In the proposed method, two types of statistics can be obtained from the process model in normal operation: the D-statistic to monitor the systematic part change of the process variation and the Q-statistic to monitor the residual part of the process variation. The D-statistic, also known as the Hotelling's T^2 statistic, is the Mahalanobis distance defined as follows:

$$T^2 = \mathbf{y}^T\mathbf{D}^{-1}\mathbf{y} \tag{27}$$

where $\mathbf{y}$ is obtained from Eq. 18 and $\mathbf{D}$ is the diagonal matrix of the eigenvalues associated with the retained dominant ICs. The upper control limit for T^2 cannot be obtained using the F-distribution because $\mathbf{y}$ is not Gaussian. In this article, kernel density estimation is used to define the control limit.[13,17,32]

The Q-statistic for the nonsystematic part of the common cause variation of new data, also known as the *SPE* statistic, can be visualized in a chart with control limits. The *SPE* statistic is defined as follows:

$$SPE = \mathbf{e}^T\mathbf{e} = (\mathbf{x} - \hat{\mathbf{x}})^T(\mathbf{x} - \hat{\mathbf{x}}) \tag{28}$$

where $\mathbf{e} = \mathbf{x} - \hat{\mathbf{x}}$ and $\hat{\mathbf{x}}$ can be calculated as follows:

$$\hat{\mathbf{x}} = \mathbf{A}\mathbf{y} = \mathbf{A}\mathbf{W}\mathbf{x} \tag{29}$$

If the number of ICs is chosen such that the majority of non-Gaussianity is included in the ICs, the residual subspace will contain mostly random noise that can be treated as normal distribution. The upper control limit of *SPE* can then be calculated from Eq. 7. Note that the residual ICs need not to be calculated.

Once a fault is detected, fault diagnosis using the modified

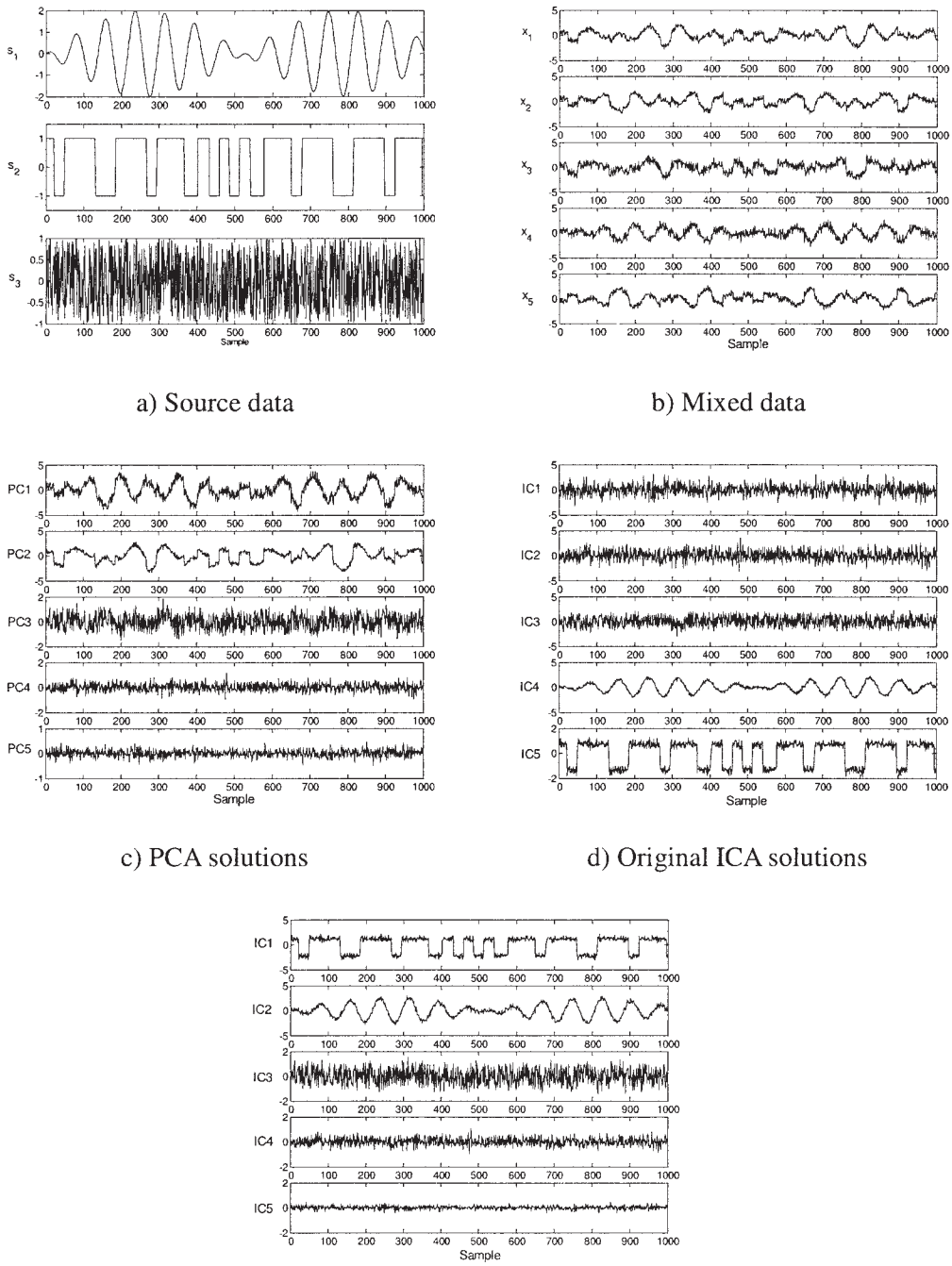


Figure 1. (a) Source data; (b) mixed data; (c) PCA solutions; (d) original ICA solutions; (e) modified ICA solutions in simple example.

ICA model can be achieved by the use of contribution plots. By interrogating the underlying process model at the point where an abnormality has been detected, contribution plots reveal the group of process variables that most influence the model or the residuals.[33] The contribution-based approach is simple to identify faults and can be generated without prior fault knowledge.[10]

In the proposed method, the T^2 statistic can be decomposed as the following equation:

$$\begin{aligned} T^2 &= \mathbf{y}^T\mathbf{D}^{-1}\mathbf{y} = \mathbf{y}^T\mathbf{D}^{-1}\mathbf{W}\mathbf{x} \\ &= \mathbf{y}^T\mathbf{D}^{-1}\sum_{j=1}^{d}\mathbf{w}_j x_j = \sum_{j=1}^{d}\mathbf{y}^T\mathbf{D}^{-1}\mathbf{w}_j x_j \\ &= \sum_{j=1}^{d} c_j \end{aligned} \tag{30}$$

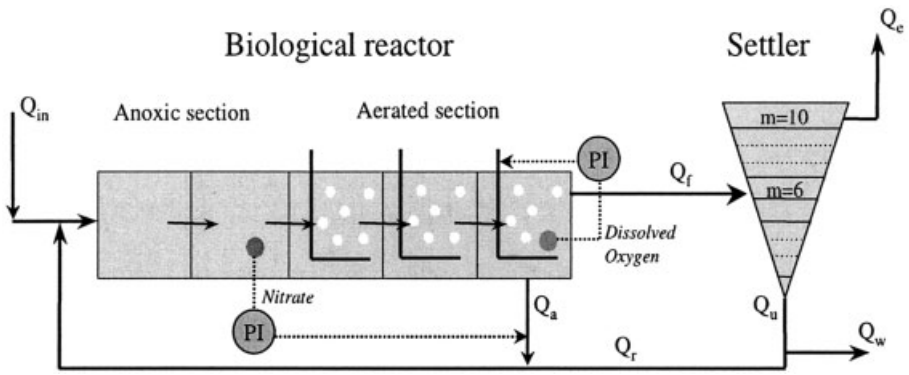


Figure 2. Flow diagram of the WWTP simulation benchmark.

Q_{in}: influent flow rate: Q_a: internal recycle flow rate: Q_e: effluent flow rate: Q_f: feed layer flow rate: Q_r: return sludge flow rate: Q_u: under flow rate: Q_w: treated water output flow rate.

Therefore, the contribution to the T^2 statistic for a new data, $\mathbf{x}$, can be represented as follows[33]:

$$c_j(T^2) = \mathbf{y}^T\mathbf{D}^{-1}\mathbf{w}_j x_j \tag{31}$$

where $c_j(T^2)$ is the contribution of the jth variable to the T^2 statistic, x_j is the jth element of $\mathbf{x}$, and $\mathbf{w}_j$ is the jth row of the demixing matrix $\mathbf{W}$.

Similarly, variable contributions can also be computed for the *SPE* statistic, that is, the variable contribution of the residuals. The contribution $c_j(SPE)$ of process variable j to the *SPE* statistic can be calculated as follows:

$$c_j(SPE) = e_j^2 \tag{32}$$

where e_j is the jth variable of $\mathbf{e} = \mathbf{x} - \hat{\mathbf{x}}$.

In this article, the upper control limit (UCL) for the T^2 contribution plot for each process variable is calculated as the mean of the contributions plus three standard deviations of the contributions for each process variable. These UCLs should not be considered to have statistical significance, but are very helpful in detecting contributions that are higher than contributions of normal operating condition data.[33] Control limits for contributions to *SPE* are calculated the same way as the Q-statistic control limits, that is, using Eq. 7.[33]

Illustrative Examples

Simple example

To illustrate the performance of the modified ICA over PCA and the original ICA, we apply these methods to a simple example system, similar to that used by Hakyin.[34] Consider three source variables that have the following distribution shown in Figure 1a:

$$s_1(k) = 2\cos(0.08k)\sin(0.006k) \tag{33}$$

$$s_2(k) = sign[\sin(0.03k) + 9\cos(0.01k)] \tag{34}$$

$$s_3(k) = \text{uniformly distributed noises in the range } [-1, 1] \tag{35}$$

These sources $\mathbf{s} = [s_1\ s_2\ s_3]^T$ are linearly mixed as $\mathbf{x} = \mathbf{As}$ with the mixing matrix

$$\mathbf{A} = \begin{bmatrix} 0.86 & 0.79 & 0.67 \\ -0.55 & 0.65 & 0.46 \\ 0.17 & 0.32 & -0.28 \\ -0.33 & 0.12 & 0.27 \\ 0.89 & -0.97 & -0.74 \end{bmatrix} \tag{36}$$

Table 1. Monitored Variables of the WWTP Benchmark

No.	Symbol	Meaning
1	$S_{NH,in}$	Influent ammonium concentration
2	Q_{in}	Influent flow rate
3	TSS_4	Total suspended solid (reactor 4)
4	$S_{O,3}$	Dissolved oxygen concentration (reactor 3)
5	$S_{O,4}$	Dissolved oxygen concentration (reactor 4)
6	K_La_5	Oxygen transfer coefficient (reactor 5)
7	$S_{NO,2}$	Nitrate concentration (reactor 2)

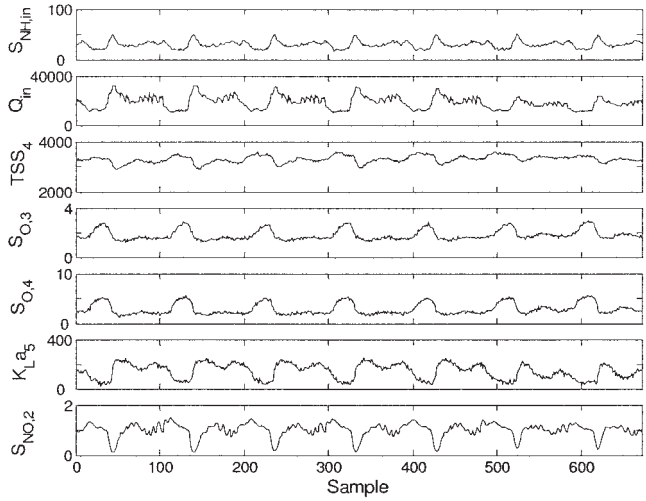
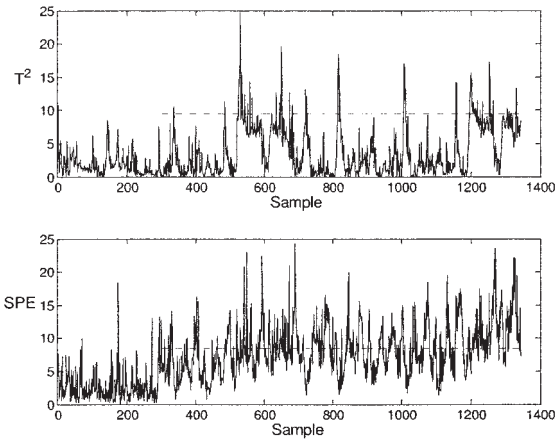
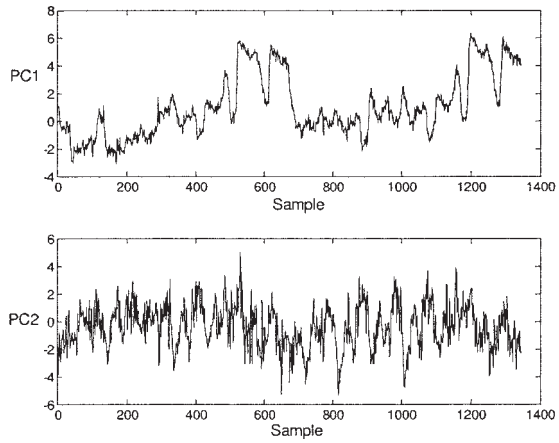


Figure 3. Variable patterns of normal operating condition data.



a) PCA monitoring



b) Pattern change in two PCs

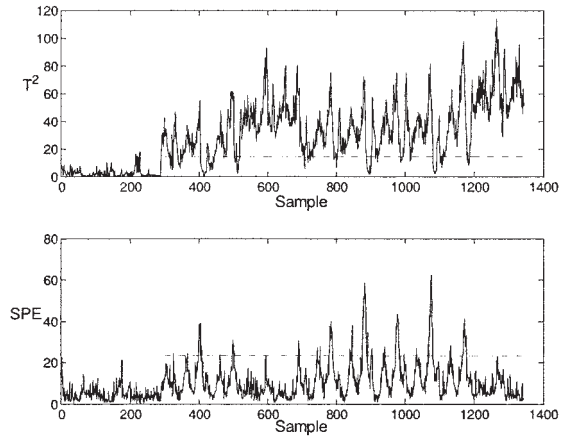
Figure 4. (a) PCA monitoring results and (b) pattern change in two PCs of the WWTP.

We generate 1000 mixed data samples of **x** and add random noises with variance 0.02 to the data. Before applying PCA, ICA, and modified ICA, **x** is mean centered and variance scaled. Figure 1b reflects the mixture data.

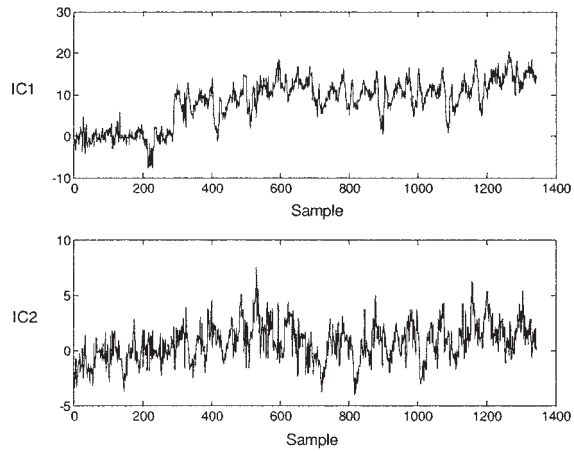
When PCA is applied to the autoscaled **x**, shown in Figure 1c, it cannot recover original signals. PCA is an optimal technique to describe the given data in the sense of mean squared error; however, it provides just a decorrelated representation of the data, not giving true independent factors of the observed data. In comparison to PCA, the ICA solution shown in Figure 1d is able to closely recover original sources. In this example, the order of ICs is determined by the L_2 norm of each $\mathbf{w}_i$, the row of **W**, which is used in the work of Lee et al.[17] However, as shown in Figure 1d, the IC1, IC2, and IC3 are random noises that have a pattern different from that of the original signals. IC4 and IC5, which are similar to the original signals, would not be chosen as dominant ICs according to the work of Lee et al.[17] This approach would select nondominant to be dominant ICs, and thereby the monitoring performance with the wrongly selected dominant signals can be poor. On the other hand, Figure 1e represents the recovered signal using the modified ICA. As shown in this figure, the modified ICA can extract dominant signals (IC1, IC2, and IC3) having the same pattern as that of the original signals. The modified IC1 resembles Variable 2 and the modified IC2 resembles Variable 1. IC4 and IC5 can be considered as just random noises. The simple example clearly demonstrates that the proposed method is very effective to extract a few dominant essential factors to a much greater extent than the PCA and original ICA solutions.

Wastewater treatment process (WWTP)

The proposed modified ICA monitoring method is tested for its ability to detect internal fault in simulated data obtained from a *benchmark simulation* of the WWTP. The activated sludge model No. 1 (ASM1) and a 10-layer settler model are used to simulate the biological reactions and the settling process, respectively. Figure 2 shows the process layout of the modeled WWTP system. The first two compartments of the



a) Modified ICA monitoring



b) Pattern change in two PCs

Figure 5. (a) Modified ICA monitoring results and (b) pattern change in two ICs of the WWTP.

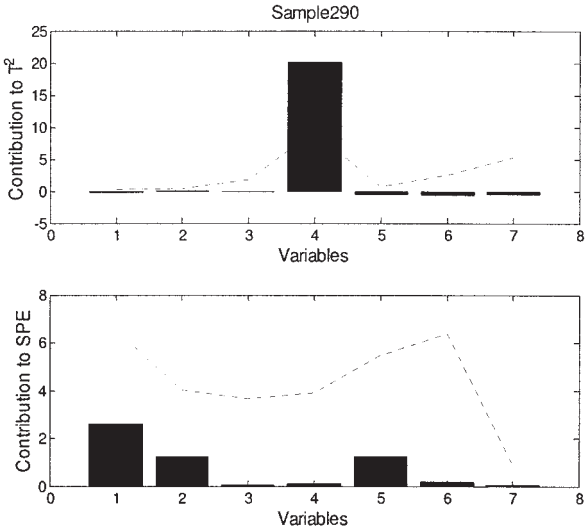


Figure 6. Variables contribution plot to T^2 and *SPE* for the WWTP at sample 290.

bioreactor are not aerated, whereas the others are. All the compartments are considered to be ideally mixed, whereas the secondary settler is modeled with a series of 10 layers with one dimension. The detailed process description is well explained in Lee et al.[17]

In Lee et al.,[17] one week's worth of normal data with the sampling time of 15 min are generated from the simulator for training data. Seven variables listed in Table 1 are selected for process monitoring because they are important and typically monitored in real WWTP systems. The simulation data exhibit periodic characteristics as shown in Figure 3 because WWTP is subject to large diurnal fluctuations in the flow rate and composition of the feed stream. Because the variables of such processes tend to fluctuate widely over a cycle, their mean and variance do not remain constant over time. Because of this, conventional multivariate statistical process monitoring (MSPM), which implicitly assumes a stationary underlying process, may lead to numerous false alarms and missed faults. In this article, we calculate the mean trajectory of diurnal fluctuations of training data and subtract it from training and test data to remove the periodicity of the data and thus improve the monitoring performance. After the periodicity has been removed, the PCA model is able to capture the variance of normal operating data up to 72% with two PCs selected by cross-validation.

To generate test data, internal faults were imposed by decreasing the nitrification rate in the biological reactor through a decrease in the specific growth rate of the autotrophs (μ_A). The autotrophic growth rate at sample 288 was a step decrease from 0.5 to 0.44 day^{-1}. In the WWTP, deterioration of the nitrification rate can strongly affect the performance of the activated sludge; thus, its early detection is important. For this small internal fault, PCA is able to detect it in *SPE* charts (Figure 4a). However, the detection rate of the *SPE* chart, defined as the percentage of the samples outside the 99% control limit, is just 43%. In contrast to the PCA result, the proposed method can detect the fault mainly in the T^2 chart (Figure 5a). The detection rate of T^2 is >83%, which demonstrates that the detection rate is greatly enhanced by the proposed method with comparable false alarm rates. Furthermore, the pattern change caused by the step decrease fault is more easily seen in the ICs plot (Figure 5b) than in the PCs plot (Figure 4b). IC1 has rapidly increased around sample 288 and retained the change up to the end, whereas PC1 does not reflect the step change, which means that fault patterns could be identified in the IC space of the proposed method more easily

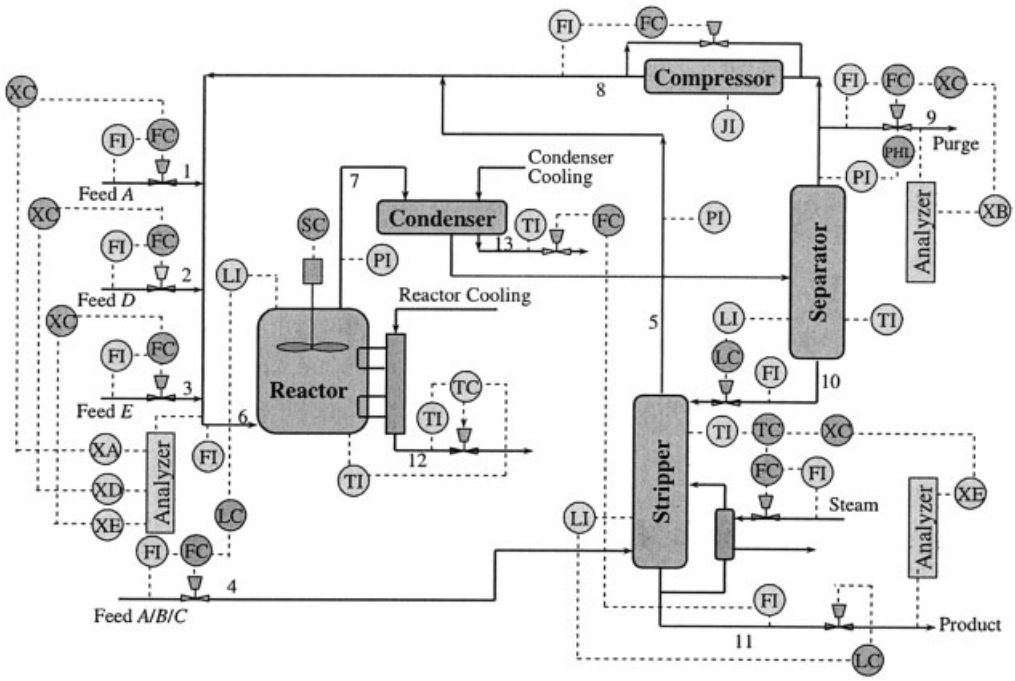


Figure 7. Process layout of the Tennessee Eastman process.

Table 2. Monitored Variables in the Tennessee Eastman Process

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

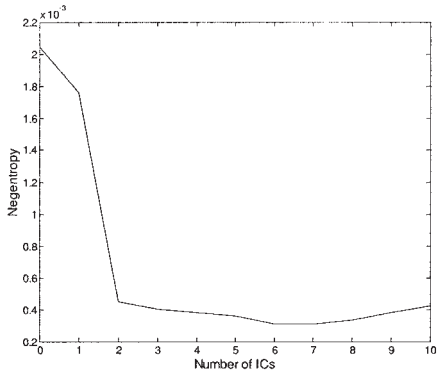
than in the PC space of conventional methods. Therefore, the proposed method is expected to be more effective than PCA for the diagnosis of fault patterns in the model space. Figure 6 shows the contribution plots of the proposed method at sample 290. From the contribution plot for the T^2 value, we can conclude that the fourth variable ($S_{O,3}$) exceeding its control limit makes the largest contribution to the T^2 statistic. The variables indicated by the contribution plots are responsible for inflating the statistic and would be related to the process fault. It should be integrated with process knowledge to determine the process fault exactly (the diagnosis activity).

Tennessee Eastman process

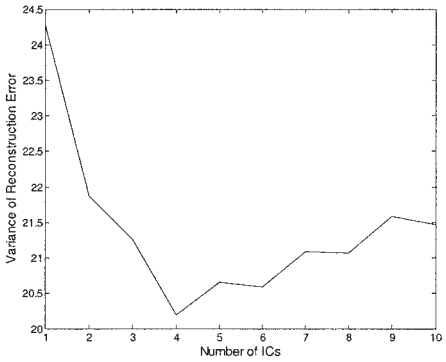
In this subsection, the proposed method is applied to the Tennessee Eastman process simulation data and is compared with PCA monitoring results. The control structure is shown schematically in Figure 7. There are five major unit operations in the process: a reactor, a condenser, a recycle compressor, a separator, and a stripper. The four reactants *A*, *C*, *D*, and *E* and the inert *B* are fed to the reactor where the products *G* and *H* are formed and a by-product *F* is also produced. The process has 22 continuous process measurements, 12 manipulated variables, and 19 composition measurements sampled less frequently. Details on the process description are well explained in Chiang et al.[9] A total of 33 variables are used for monitoring in this study. Those variables are listed in Table 2. We excluded all composition measurements because they are hard to measure on-line in practice. A sampling interval of 3 min was used to collect the simulated data for the training and testing sets. A set of programmed faults (Faults 1–21) is listed in Table 3. Both the training and testing data sets for each fault are composed of 960 observations. All faults in the test data set

Table 3. Process Faults for the Tennessee Eastman Process

No.	Description	Type
1	*A*/*C* feed ratio, *B* composition constant (stream 4)	Step
2	*B* composition, *A*/*C* ratio constant (stream 4)	Step
3	*D* feed temperature (stream 2)	Step
4	Reactor cooling water inlet temperature	Step
5	Condenser cooling water inlet temperature	Step
6	*A* feed loss (stream 1)	Step
7	*C* header pressure loss − reduced availability (stream 4)	Step
8	*A*, *B*, *C* feed composition (stream 4)	Random variation
9	*D* feed temperature (stream 2)	Random variation
10	*C* feed temperature (stream 4)	Random variation
11	Reactor cooling water inlet temperature	Random variation
12	Condenser cooling water inlet temperature	Random variation
13	Reaction kinetics	Slow drift
14	Reactor cooling water valve	Sticking
15	Condenser cooling water valve	Sticking
16	Unknown	
17	Unknown	
18	Unknown	
19	Unknown	
20	Unknown	
21	The valve for Stream 4 was fixed at the steady-state position	Constant Position



a) Negentropy change along the number of ICs



b) Variance of reconstruction error change along the number of ICs

Figure 8. Determining the number of ICs based on (a) negentropy and (b) variance of reconstruction error.

were introduced from sample 160. The data are generated by Chiang et al.[9] and can be downloaded from http://brahms.scs.uiuc.edu.

All the data were autoscaled before the application of PCA and the modified ICA. In the modified ICA, 30 score vectors are extracted from Eq. 19 to update and find ICs. Nine PCs are selected for the PCA by cross-validation and the same number of ICs is selected for fair comparison. Figure 8 shows the plot of residual negentropy and the plot of variance of reconstruction error plot along with the number of ICs. Seven ICs (based on negentropy) and four ICs (based on VRE) would be selected to be dominant components in the proposed method, respectively. To investigate the effect of the number of latent components on process monitoring performance, we plotted the overall detection rates of PCA and the proposed method for all faults against the number of components. For the data obtained after the fault occurrence, the percentage of the samples outside the 99% control limits was calculated in each simulation and termed as the *detection rate*. False alarm rates were acceptable ($<1\%$) up to 20 components in the case of the modified ICA. As opposed to the modified ICA, the false alarm rate of PCA exceeds 1% when the number of PCs is >10. Figure 9 shows that the detection rate of modified ICA-T^2 increases with the number of components, whereas that of modified ICA-*SPE* changes with smaller variation. It should be noted that the

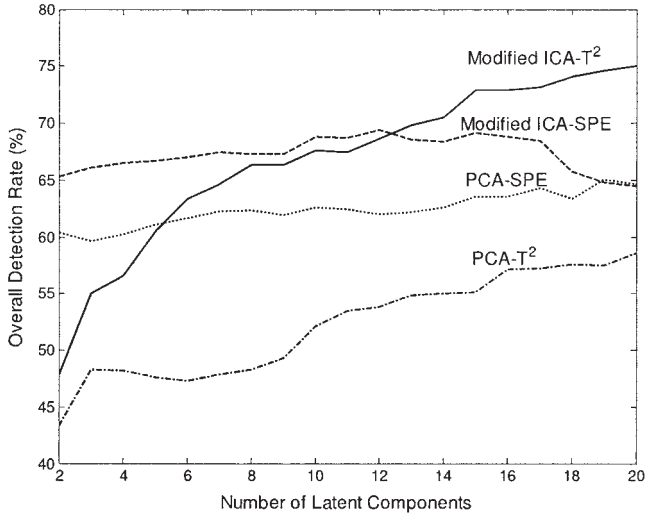


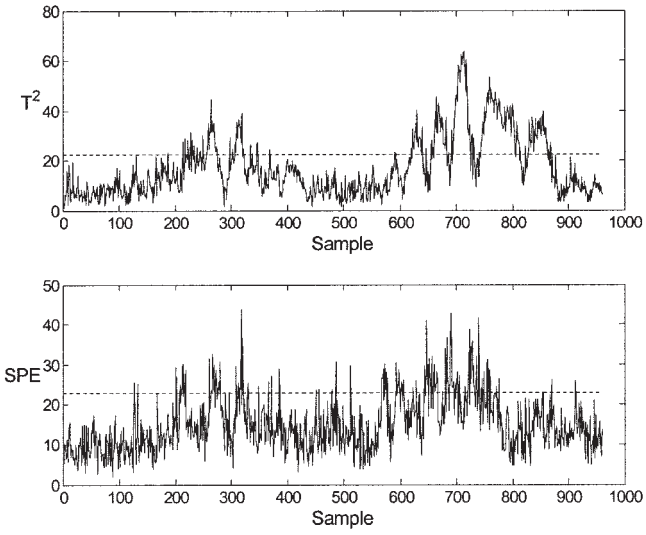
Figure 9. Overall detection rates of PCA and modified ICA against the number of latent components.

overall detection rate of the proposed method is higher than that of PCA, irrespective of the number of components.

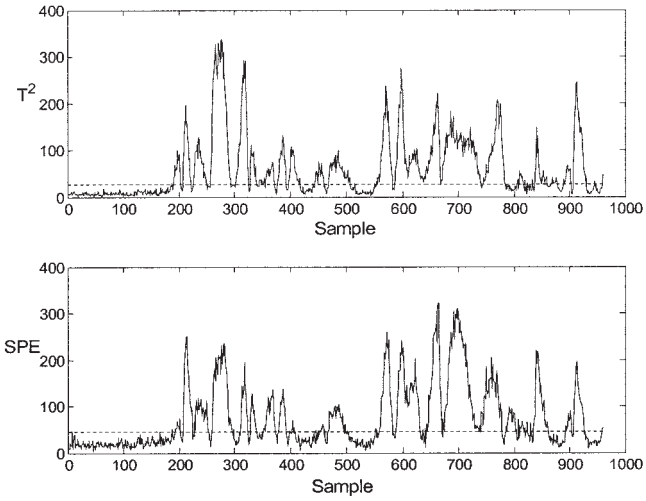
The fault detection rates of the two multivariate methods, PCA and modified ICA, for all 21 faults were computed and tabulated in Table 4. With nine PCs and nine ICs, average false alarm rates are acceptable to be 0.5% for PCA-T^2 chart, 0.8% for PCA-*SPE* chart, 0.2% for modified ICA-T^2 chart, and 0.8% for modified ICA-*SPE* chart, respectively. In Table 4, the maximum detection rate achieved for each fault except Faults 3, 9, and 15 is marked with a bold number. The detection rates for Faults 3, 9, and 15 are not considerably higher than 1% for all methods; thus, these faults are not considered in this research. As shown in Table 4, the modified ICA can detect most faults, except Fault 4 and 11, more efficiently than PCA. In particular, for Faults 10 and 16 (marked with shading), the

Table 4. Fault Detection Rates of PCA and Modified ICA in the Tennessee Eastman Process

Fault	PCA(9PCs) T^2	PCA *SPE*	Modified ICA(9ICs) T^2	Modified ICA *SPE*
1	99	**100**	**100**	**100**
2	**98**	96	**98**	**98**
3	2	1	1	1
4	6	**100**	65	96
5	**24**	18	**24**	**24**
6	99	**100**	**100**	**100**
7	42	**100**	**100**	**100**
8	97	89	97	**98**
9	1	1	1	2
10	31	17	**70**	64
11	21	**72**	43	66
12	97	90	**98**	97
13	93	**95**	**95**	94
14	81	**100**	100	**100**
15	1	2	1	2
16	14	16	**76**	73
17	74	93	87	**94**
18	89	**90**	90	**90**
19	0	**29**	25	**29**
20	32	45	**70**	66
21	33	46	**54**	19



(a) PCA monitoring



(b) Modified ICA monitoring

Figure 10. Monitoring results of the Tennessee Eastman process based on (a) PCA and (b) modified ICA in the case of Fault 10.

detection rate of the proposed method is more than twice as high as that of PCA, which shows that the modified ICA can detect small events that are difficult to detect by PCA. One thing that needs to be noted is the T^2 ability of the proposed method for detecting faults. For all cases, the detectability of T^2 is considerably enhanced by the proposed method. This result demonstrates that the proposed method is more effective than PCA to diagnose fault patterns in the feature space.

The monitoring results in the case of Fault 10 are shown in Figure 10. In the case of Fault 10, the *C* feed temperature of stream 4 is randomly changed. When the fault occurs, stripper temperature also changes, which results in a change in stripper pressure. To compensate for the changes of the stripper temperature and pressure, the stripper steam valve is manipulated by a control loop and thereby the stripper steam flow rate also changes. For this fault, PCA can detect the fault from about sample 200 (Figure 10a). However, despite the presence of the fault, there are many samples (samples 350–600 and 870–960) below the 99% control limit, giving the process operator an incorrect picture of the process status. In contrast to the PCA monitoring, the modified ICA monitoring charts show that T^2 and *SPE* statistics successfully detect the faults from sample 189 up to the end of the processing time (Figure 10b). Also, the random pattern changes caused by the fault are reflected well in the proposed method. The results of this example indicate the proposed method has a superior capability in detecting faults that are difficult to detect by conventional methods. Figure 11 shows contribution plots to T^2 and *SPE*, respectively. From this figure, we can conclude that variables 16 (Stripper pressure) and 18 (Stripper temperature) make the largest contribution to the T^2 statistic, whereas variables 19 (Stripper steam flow) and 31 (Stripper steam valve) give dominant effects on *SPE* statistic. This contribution plot correctly indicates the major variable groups affected by the fault.

Semiconductor etch process

The proposed method is applied to the fault detection of a semiconductor etch process.[35] Lam 9600 TCP metal etcher at Texas Instruments is considered in this study and the data can be obtained from http://software.eigenvector.com/Data/Etch/. The process is equipped with several sensor systems including machine state variables, optical emission spectroscopy (OES) of the plasma, and a radio-frequency monitoring (RFM) system. Wise et al.[35] tested a variety of analysis methods such as PCA, MPCA, trilinear decomposition (TLD), and parallel factor analysis (PARAFAC) for their sensitivity to specific system faults. In their results, PARAFAC is best to detect various faults, followed closely by PCA on the means, and the best combination of sensors is machine state plus RFM. This combination is more successful to detect faults than any other sensor combination when global models are considered. In this study, only machine state variables are considered for moni-

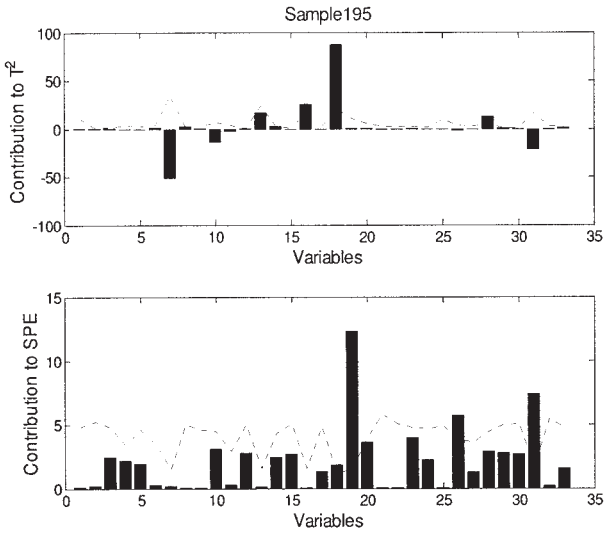


Figure 11. Variables contribution plot to T^2 and *SPE* for the Tennessee Eastman process at sample 195.

Table 5. Machine State Variables Used for Process Monitoring

1	BCL_3 flow	11	RF power
2	CL_2 flow	12	RF impedance
3	RF bottom power	13	TCP tuner
4	RFB reflected power	14	TCP phase error
5	Endpoint A detector	15	TCP impedance
6	Helium pressure	16	TCP top power
7	Chamber pressure	17	TCP reflected power
8	RF tuner	18	TCP load
9	RF load	19	Vat valve
10	Phase error		

tored variables to compare the monitoring performance of the proposed method with PCA. The variables are listed in Table 5.

The data consist of 129 wafers among which 108 normal wafers are taken during three experiments (numbers 29, 31, and 33) and 21 wafers with intentionally induced faults are taken during the same experiments by changing the TCP power, RF power, pressure, Cl_2 or BCl_3 flow rate, and He chuck pressure. The experiments were run several weeks apart and data from different experiments have a different mean and somewhat different covariance structure.

In the modeling procedure, we excluded a repeated sample from each wafer. The 56th wafer is excluded from 108 normal wafers because it has very few samples compared with other wafers. Here, the global model based on all the data and the local model based on each of the single experiments are considered in this study. Although the data are three-way batch data, multiway methods such as MPCA and PARAFAC are not considered in this article. Instead, the data were preprocessed in two ways before analysis. For one case, data from each wafer were reduced to a single vector of means of the variables over the entire wafer. Wise et al.[35] stated that PCA on the means is a reasonable choice in practice to detect various faults of the semiconductor etch process because of its simplicity and good reliability. In the other case, raw data were used for model development.

Fault detection results of PCA and the proposed method are shown in Table 6. The faults are listed in the second column of the table. In our study, all 21 faults are considered, whereas 19 faults are considered in Wise et al.[35] In the case of global and local on means, an open symbol indicates that the fault exceeded the 99% control limit, whereas a solid symbol denotes that the fault exceeded the 99% limit by a factor of five or more. In the case of global and local models on raw data, however, an open circle denotes that >15% of the time samples exceed the 95% control limit, whereas a solid circle indicates that >30% samples exceed the 95% control limit.

The number of components used to make each PCA model is selected by cross-validation and the same number of ICs is chosen for fair comparison. The number of faults caught with each method is also listed in Table 6. As shown in Table 6, fault detection performance in local models is better than that in the global model. This means that the global model will define a much larger region of the multivariate space as normal variation than would a local model, so local models are more sensitive to detect faults.[35] However, there are a few exceptional cases that faults not detected in local models are detected in the global model in the raw data case. This result may be generated from the fact that a different number of components is chosen in both cases and the numbers of samples are not sufficient to make each local model. A notable result is that the proposed method can detect more faults than PCA in all cases. In particular, the proposed method on the wafer mean can detect 15 faults, whereas PCA caught only nine faults. There are three faults (TCP-20, TCP-15, TCP+20) that exceeded the 99% confidence limit by 5 or more in the proposed method, which are never detected in the PCA case. Irrespective of the preprocessing method on data, the detection ability of proposed method is more improved over that of PCA.

Table 6. Detection Results of PCA and Modified ICA in the Semiconductor Etch Process

		Global on Means		Local on Means		Global on Raw Data		Local on Raw Data	
Exp.	Induced Fault	PCA 2PCs	Modified ICA 2ICs	PCA 2PCs	Modified ICA 2ICs	PCA 3PCs	Modified ICA 3ICs	PCA 2PCs	Modified ICA 2ICs
29	TCP+50	○	●	●	●	○	○	●	●
29	RF−12		○	○	○		○		
29	RF+10			○	○				
29	Pr+3	●	●	●	●	●	●	●	●
29	TCP+10		○	○	○				
29	BCl3+5			○	○				
29	Pr−2	●	●	●	●	●	●	●	●
29	Cl2−5		○	●	●		●		
29	He Chuck							○	○
31	TCP+30	○	●	●	●	○	●		○
31	Cl2+5			○	○				
31	RF+8	○	○	●	●		○		○
31	BCl3−5			○	○	●	●	●	●
31	Pr+2	●	●	●	●	●	●	●	●
31	TCP−20		●	●	●		○		○
33	TCP−15		●	○	●			○	○
33	Cl2−10	○	○	○	○		●		
33	RF−12			○	○				
33	BCl3+10	○	○	○	○	○	●	○	○
33	Pr+1	○	●	●	●	○	●	○	○
33	TCP+20		●	●	●				
	Total	9	15	20	20	8	13	9	12

Conclusions

This article proposes a modified ICA and a novel approach to process monitoring. Some drawbacks of original ICA are analyzed and a modified ICA algorithm is developed for MSPM. The basic idea of this approach is to use PCA to estimate initial ICs where the variance of each IC is the same as that of each PC and then to calculate dominant ICs using the FastICA algorithm. If the data are Gaussian, the space of the dominant ICs is the same as one spanned by the dominant PCs. Compared to original ICA, the proposed algorithm has the following advantages: It extracts a few dominant factors needed for process monitoring; high computational load is attenuated by extracting a few dominant ICs instead of all ICs; the ordering of ICs is considered; and it gives a consistent solution by avoiding random initializations.

The proposed method was applied to the fault detection and diagnosis of a wastewater treatment process, the Tennessee Eastman process, and a semiconductor etch process. These examples demonstrate that the proposed method detects various faults more efficiently than PCA. In particular, the extracted dominant ICs are able to reflect pattern changes better and are expected to be more useful to diagnose fault patterns in the feature space. In addition, contribution plots of the proposed method are able to reveal the group of process variables responsible for the processes to go out of control.

The present work highlights the promise of the modified ICA approach for process monitoring; however, it should be further investigated as to how to determine the number of ICs, how to extract the essential ICs more efficiently, how to improve fault identification ability, and how to extend it to other approaches such as fault reconstruction-based diagnosis.

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