Dynamic monitoring system for full-scale wastewater treatment plants

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Abstract This paper proposes a new process monitoring method using dynamic independent component analysis (ICA). ICA is a recently developed technique to extract the hidden factors that underlie sets of measurements, whereas principal component analysis (PCA) is a dimensionality reduction technique in terms of capturing the variance of the data. Its goal is to find a linear representation of non-Gaussian data so that the components are statistically independent. PCA aims at finding PCs that are uncorrelated and are linear combinations of the observed variables, while ICA is designed to separate the ICs that are independent and constitute the observed variables. The dynamic ICA monitoring method is applying ICA to the augmenting matrix with time-lagged variables. The dynamic monitoring method was applied to detect and monitor disturbances in a full-scale biological wastewater treatment (WWTP), which is characterized by a variety of dynamic and non-Gaussian characteristics. The dynamic ICA method showed more powerful monitoring performance on a WWTP application than the dynamic PCA method since it can extract source signals which are independent of time and cross-correlation of variables.

Keywords Biological wastewater treatment; disturbance detection and diagnosis; dynamic process; multivariate statistical process control (MSPC); independent component analysis (ICA); on-line monitoring

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Introduction

The increase in environmental restrictions in recent times has led to an increase in efforts aimed at attainment of better effluent quality of wastewater treatment plants. Achieving this goal requires advanced monitoring of plant performance. Wastewater treatment plants are slow when they have to recover from a “bad” state to a “normal” state. The early detection and isolation of faults in the biological process is therefore very effective since they allow corrective action to be taken well before the situation becomes dangerous. Some changes are not very obvious and may gradually grow until they become a serious operational problem. Process monitoring and fault detection of the biological processes are very important tasks in process system engineering since they aim to ensure the success of the planned operations and to improve the productivity of processes. In recent industrial process plants, many variables are measured in various operating units and are recorded in abundance. However, such data sets are highly correlated and are subject to considerable noise. In the absence of an appropriate processing method, only limited information can be extracted, which causes insufficient understanding of the process by the operator and may lead to unstable operation. If properly treated, this data can provide a wealth of information leading to keep the plant operators understanding the status of the process and assist them to make appropriate actions to remove abnormalities resulting from the process (Rosen and Lennox, 2001).

Traditionally, statistical process control (SPC) charts such as Shewhart, CUSUM and EWMA charts have been used to monitor processes and improve product quality. However, the weaknesses of such univariate control charts for detecting faults in multivariate processes have led to the development of many process monitoring schemes that use multivariate statistical methods based on principal component analysis (PCA) and partial least squares (PLS) (Wise *et al.*, 1996; Chiang *et al.*, 2001; Rosen and Lennox, 2001). Most multivariate statistical monitoring methods implicitly assume that the observations at one time instant are statistically independent to observations at past time instances and follow an identical multivariate Gaussian distribution. In environmental processes, variables rarely remain at steady state but are rather driven by random noise and uncontrollable disturbances. These effects result in autocorrelated data and dynamic properties of the system. This suggests that a method taking into account the serial correlations in the data is needed in order to implement a process monitoring method. Recently, several works have been proposed to tackle the autocorrelation problem and capture process dynamics. Ku *et al.* (1995) proposed dynamic PCA (DPCA) which uses an augmenting matrix with time-lagged variables. DPCA can extract the time-series model from the eigenvectors of the covariance matrix that corresponds to the zero eigenvalues. Negiz and Cinar (1997) proposed a monitoring method that utilizes a state space identification technique based on canonical variate analysis (CVA) to solve the dynamic problem. This method takes serial correlations into account during the dimension reduction step, like DPCA, and uses the state variables for computing the monitoring statistic in order to remove the serial correlation. Russell *et al.*, (2000) evaluated and compared the performance of PCA, DPCA, and CVA for detecting faults in a realistic chemical process simulation. On the other hand, there is another fundamental problem in conventional process monitoring: the non-Gaussian dilemma. While conventional monitoring methods such as PCA and PLS provide satisfactory process monitoring performance in the Gaussian distributed variables, the real measured variables and their score values of PCA and PLS do not usually follow a normal distribution. Recently, Yoo *et al.* (2004a,b) and Lee *et al.* (2003) suggested new batch and continuous monitoring methods using independent component analysis (ICA) to solve the non-Gaussian constraint problem and obtain better monitoring performance. In this paper, a dynamic ICA monitoring method which uses ICA on lagged variables is suggested to deal with the dynamic and non-Gaussian problem encountered in biological WWTP.

Methods

Independent component analysis (ICA)

What distinguishes ICA from other multivariate monitoring methods is that it looks for components that are both statistically independent and non-Gaussian. Although ICA can be considered as a useful extension of PCA, its objective differs from that of PCA. PCA is a dimensionality reduction technique in terms of capturing the variance of the data, and it is capable of extracting uncorrelated latent variables from highly correlated data. PCA can only impose independence up to second order statistics information (mean and variance) while constraining the direction vectors to be orthogonal, whereas ICA has *no orthogonality* constraint and also involves *higher-order* statistics. Second order statistics such as PCA can roughly be characterized as finding a faithful representation of a data set in the sense of the reconstruction mean-square error. In contrast, most methods that use higher-order statistics, such as ICA, endeavor to find a *meaningful* representation (Cardoso, 1998; Hyvärinen *et al.*, 2001). To illustrate the superiority of ICA over PCA, we applied the two types of analysis to a simple example system. Let’s consider two source variables that have the uniform distributions shown in Figure 1(a). The source variables are linearly independent, i.e., the values of one source variable do not convey any information about the other source variable. These

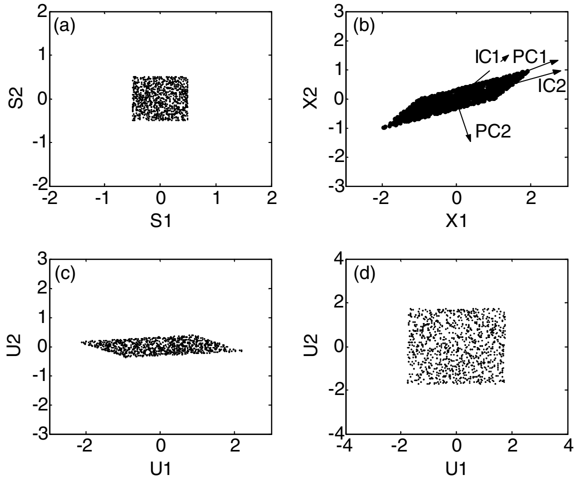

Figure 1 (a) Scatter plot of the original source data, (b) The mixtures and axes of PCA and ICA, (c) The recovered source data using PCA, (d) The recovered source data using ICA

sources are linearly mixed as follows:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \end{bmatrix}. \tag{1}$$

Figure 1(b) shows the scatter-plot of the mixtures. Note that the random variables x_1 and x_2 are not independent because it is possible to predict the value of one of them from the value of the other. When PCA is applied to these mixed variables, it gives two principal components. The axes of the first and second PCs (PC1, PC2) are shown in Figure 1(b). The first PC is the axis capturing the highest variance in the data and the second PC is the axis orthogonal to the first PC. Figure 1(c) shows the PCA solution, which differs from the original because the two principal axes are still dependent. However, the ICA solution shown in Figure 1(d) can recover the original sources since ICA not only decorrelates the data but also rotates it such that the axes of u_1 and u_2 are parallel to the axes of s_1 and s_2 [12]. The axes of the first and second independent components (IC1, IC2) are shown in Figure 1(b). The basic idea of this approach is to extract essential independent components that drive a process and to combine them with process monitoring techniques. The simple example given above clearly demonstrates that if the latent variables follow a non-Gaussian distribution, the ICA solution extracts the original source signal to a much greater extent than the PCA solution. Therefore, it is natural to infer that a monitoring system based on the ICA solution may give better results compared to PCA.

The following ICA algorithm is based on the formalism presented in the survey article of Hyvärinen *et al.* (2001). In the ICA algorithm, it is assumed 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 means. The relationship between them is given by

$$\boldsymbol{X} = \boldsymbol{AS} + \boldsymbol{E} \tag{2}$$

where $\boldsymbol{X} = [\boldsymbol{x}(1), \boldsymbol{x}(2), \ldots, \boldsymbol{x}(n)] \in R^{d \times n}$ is the data matrix (in contrast to PCA, ICA employs the transposed data matrix), $\boldsymbol{A} = [\boldsymbol{a}_1, \ldots, \boldsymbol{a}_m] \in R^{d \times m}$ is the unknown mixing matrix, $\boldsymbol{S} = [\boldsymbol{s}(1), \boldsymbol{s}(2), \ldots, \boldsymbol{s}(n)] \in R^{m \times n}$ is the independent component matrix, $\boldsymbol{E} \in R^{d \times n}$ is the residual matrix, and n is the number of samples. Here, we assume $d \geq m$ (when $d = m$, the residual matrix, $\boldsymbol{E}$, becomes the zero matrix). The basic problem of ICA is to estimate both the mixing matrix $\boldsymbol{A}$ and the independent components $\boldsymbol{S}$ from only the observed data $\boldsymbol{X}$. Alternatively, one could define the objective of ICA as follows: to find a demixing matrix $\boldsymbol{W}$ whose form is such that the rows of the reconstructed matrix $\hat{\boldsymbol{S}}$, given as

$$\hat{\boldsymbol{S}} = \boldsymbol{W}\boldsymbol{X} \tag{3}$$

become as independent of each other as possible. This formulation is not really different from the previous one, since after estimating $\boldsymbol{A}$, its inverse gives $\boldsymbol{W}$ when d equals m.

Process monitoring using ICA

On-line monitoring of measurement variables is carried out with the aim of continuously analyzing and interpreting the measurements in order to detect and isolate disturbances and faults. The implementations of the monitoring statistics of ICA are similar to those of the monitoring statistics of PCA. The ICA model is based on historical data collected during normal operation, i.e., only common cause variation is present. Future process behavior is then compared against this 'normal' or 'in-control' representation (Chiang *et al.*, 2001; Yoo *et al.*, 2002).

In the normal operating condition, designated $\boldsymbol{X}_{normal}$, $\boldsymbol{W}$ and $\boldsymbol{S}_{normal}$ are obtained using the FastICA algorithm ($\boldsymbol{S}_{normal} = \boldsymbol{W}\boldsymbol{X}_{normal}$) under the assumption that the number of variables is equal to the number of independent components. The matrices $\boldsymbol{B}$, $\boldsymbol{Q}$, and $\boldsymbol{A}$ used in ICA can be obtained by whitening ($z(k) = \boldsymbol{Q}\boldsymbol{x}(k) = \boldsymbol{Q}\boldsymbol{A}\boldsymbol{s}(k) = \boldsymbol{B}\boldsymbol{s}(k)$) and the FastICA algorithm (refer to Hyvärinen *et al.*, 2001). On the other hand, the data dimension can be reduced by selecting a few rows of $\boldsymbol{W}$ based upon the assumption that the rows with the largest sum of squares coefficient have the greatest effect on the variation of $\hat{\boldsymbol{S}}$. The selected a rows of $\boldsymbol{W}$ constitute a reduced matrix $\boldsymbol{W}_d$ (dominant part of $\boldsymbol{W}$), and the remaining rows of $\boldsymbol{W}$ constitute a reduced matrix $\boldsymbol{W}_e$ (excluded part of $\boldsymbol{W}$). We can construct a reduced matrix $\boldsymbol{B}_d$ by selecting the columns from $\boldsymbol{B}$ whose indices correspond to the indices of the rows selected from $\boldsymbol{W}$. $\boldsymbol{B}_d$ can also be computed directly using $\boldsymbol{B}_d = (\boldsymbol{W}_d\mathbf{Q}^{-1})^T$. The remaining columns of $\boldsymbol{B}$ constitute the matrix $\boldsymbol{B}_e$. Then, new independent data vectors, $\hat{\boldsymbol{s}}_{newd}(k)$ and $\hat{\boldsymbol{s}}_{newe}(k)$, can be obtained if new data for sample k, $\boldsymbol{x}_{new}(k)$, is transformed through the demixing matrices $\boldsymbol{W}_d$ and $\boldsymbol{W}_e$, i.e., $\hat{\boldsymbol{s}}_{newd}(k) = \boldsymbol{W}_d\boldsymbol{x}_{new}(k)$ and $\hat{\boldsymbol{s}}_{newe}(k) = \boldsymbol{W}_e\boldsymbol{x}_{new}(k)$, respectively.

In ICA, three types of statistics are deduced from the process model in normal operation: two D-statistics for the systematic part of the process variation and the Q-statistic for the residual part of the process variation (Yoo *et al.*, 2004a,b). The D-statistic for sample k, also known as the I^2 statistic, is the sum of the squared independent scores and is defined as follows:

$$I^2(k) = \hat{\boldsymbol{s}}_{newd}(k)^T \hat{\boldsymbol{s}}_{newd}(k) \tag{4}$$

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 confidence limits. The SPE statistic at sample k is defined as follows:

$$SPE(k) = \boldsymbol{e}(k)^T\boldsymbol{e}(k) = (\boldsymbol{x}(k) - \hat{\boldsymbol{x}}(k))^T(\boldsymbol{x}(k) - \hat{\boldsymbol{x}}(k)) \tag{5}$$

where $\hat{\boldsymbol{x}}$ can be calculated as follows:

$$\hat{\boldsymbol{x}} = \boldsymbol{Q}^{-1}\boldsymbol{B}_d\hat{\boldsymbol{s}} = \boldsymbol{Q}^{-1}\boldsymbol{B}_d\boldsymbol{W}_d\boldsymbol{x}. \tag{6}$$

A second I^2 metric (I_e^2) based on d-a excluded independent components ($\hat{\boldsymbol{s}}_{newe}(k)$) was proposed. The I_e^2 statistic has the further advantage that it can compensate for the error that results when an incorrect number of ICs is selected for the dominant part. The use of both the I^2 and I_e^2 statistics allows the entire space spanned by the original variables to be monitored through a new basis. The I_e^2 statistic is defined as follows:

$$I_e^2(k) = \hat{\boldsymbol{s}}_{newe}(k)^T \hat{\boldsymbol{s}}_{newe}(k) \tag{7}$$

The confidence limits of the I^2, I_e^2 and *SPE* statistics in ICA can be obtained by kernel density estimation (Yoo *et al.*, 2004a).

Process monitoring using dynamic ICA

Conventional monitoring methods implicitly assume that the observations at one time are statistically independent of observations at any past time. That is, they implicitly assume that the measured variable at one time instance has not only serial independence within each variable series at past time instances but also statistical inter-independence between the different measured variable series at past time instances. However, the dynamics of a typical chemical or biological process cause the measurements to be time dependent, which means that the data may have both cross-correlation and auto-correlation. PCA and ICA methods can be extended to the modeling and monitoring of a dynamic system by augmenting each observation vector with the previous l observations and stacking the data matrix in the following manner (Ku *et al.*, 1995).

$$\boldsymbol{X}(l) = \begin{bmatrix} \boldsymbol{x}_k^T & \boldsymbol{x}_{k-1}^T & \cdots & \boldsymbol{x}_{k-l}^T \\ \boldsymbol{x}_{k+1}^T & \boldsymbol{x}_k^T & \cdots & \boldsymbol{x}_{k-l+1}^T \\ \vdots & \vdots & \vdots & \vdots \\ \boldsymbol{x}_{k+p}^T & \boldsymbol{x}_{k+p-1}^T & \cdots & \boldsymbol{x}_{k+p-l}^T \end{bmatrix} \tag{8}$$

where $\boldsymbol{x}_k^T$ is the d-dimensional observation vector in the training set at time instance k, $(p+1)$ is the number of samples, and l is the number of lagged measurements. By performing ICA on the data matrix in Eq. (8), independent components where dynamic dependency is removed are extracted directly from the data, ICA on lagged variables (dynamic ICA). Here the ICA method is extended to the modeling and monitoring of dynamic system by augmenting each observation vector with the previous l observations and stacking the data matrix. Note that a statistically justified method such as Akaike's information criterion (AIC) and subspace identification method can be used for selecting the number of lags l to include in the data (Chiang *et al.*, 2001).

The dynamic ICA monitoring strategy is depicted in Figure 2. It is divided in two steps, the training procedure and the on-line monitoring procedure. First, in the training procedure, the normal operating condition (NOC) model is built using dynamic ICA and kernel density

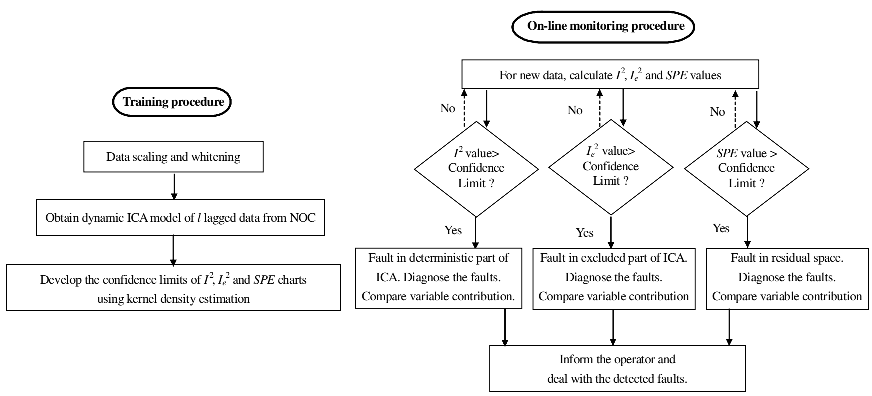

Figure 2 The proposed process monitoring scheme using the dynamic ICA method

estimation. Second, for a new on-line sample $\boldsymbol{x}_{new}$, if the I^2 statistic exceeds the limit, it indicates that a process change in the model space has occurred, if the I_e^2 statistic exceeds the limit, it indicates that a process change in the excluded model space has occurred, and if the Q-statistic of the residual space exceeds the confidence interval, it indicates the occurrence of changes that violate the ICA model. We may use the contribution plot to identify and isolate the nature of the process faults (Yoo *et al.*, 2004a).

Results and discussion

Full-scale wastewater treatment plant

The proposed monitoring method was applied to the disturbance detection at a real WWTP. In this section, the static ICA and dynamic PCA and ICA are considered to elucidate the advantages of dynamic ICA. Process data were collected from a biological WWTP which treats cokes plant wastewater from an iron and steel making plant in Korea. The data are daily average values measured between 1 Jan. 1998 and 9 Nov. 2000, with a total of 1,034 samples. This treatment plant uses a general activated sludge process that has five aeration basins (each of size 900 m^3) and a secondary clarifier (1,200 m^3). The plant layout is shown in Figure 3(a). The treatment plant has two wastewater sources: wastewater arrives either directly from a cokes making plant (called BET3) or as pretreated wastewater from an upstream WWTP at another cokes making plant (called BET2). The cokes-oven plant wastewater is produced during the conversion of coal to cokes. This type of wastewater is extremely difficult to treat because it is highly polluted and most of the chemical oxygen demand (COD) originates from large quantities of toxic, inhibitory compounds and coal-derived liquors (e.g. phenolics, thiocyanate, cyanides, poly-hydrocarbons and ammonium). In particular, the cyanide (CN) concentration of cokes wastewater is a very important variable among the influent loads (Yoo *et al.*, 2002). Sixteen variables from the WWTP were used for dynamic monitoring system: flowrate from BET2, flowrate from BET3, mixed liquor volatile suspended solid (MLVSS) at the final aeration basin, DO at the final aeration basin, cyanide from BET2, cyanide from BET3, effluent cyanide, COD influent from BET2, COD influent from BET3, effluent COD, mixed liquor suspended solid (MLSS) in the recycle, influent temperature, temperature at the final aerator, pH at the final aeration basin, and sludge volume index (SVI) in the final aerator, SVI in the settler. The values in the data set were mean centered and autoscaled to unit variance.

The data were divided into two parts. The first 720 observations were used for the development of the PCA and ICA models. In this period, the WWTP operated in an almost normal state. Several observations that were indicative of an abnormal situation confirmed

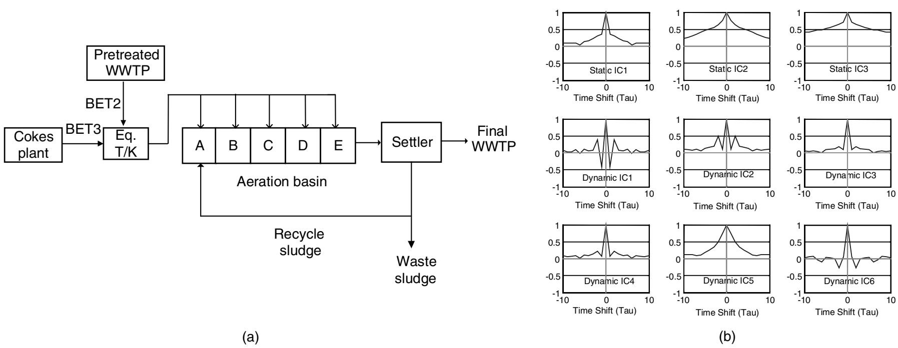

Figure 3 (a) Plant layout of a full-scale biological WWTP, (b) Auto-correlation of three ICs of the static ICA (top) and six ICs of the dynamic ICA

by the expert knowledge of two operators and a researcher were omitted in order to ensure that the training data represented the normal condition. There are several measures of a treatment management index such as the removal efficiency of COD and CN and food to microorganism (F/M) ratio, but the final judge of the normal operation was dependent on the expert knowledge. The 99% confidence limits of the monitoring charts were based on the normal operating dataset spanning two years. The remaining 314 observations were used as a test data set in order to verify the proposed dynamic monitoring method. Two lagged variables of each measurement were added to the training data matrix, where two-day lags correspond to the average hydraulic retention time (HRT) of the system (Yoo *et al.*, 2002). The method for automatically determining the number of lags described by Ku *et al.* (1995) was not used in the present work.

First, static ICA and dynamic ICA are applied to the normal operating dataset to construct each model. Using the SCREE test of the L_2 norm of the sorted demixing matrix ($\boldsymbol{W}$) against the independent component (IC) number, 3 ICs and 6 ICs are selected to be the deterministic part of the static and dynamic ICA, respectively. To investigate the merits of dynamic ICA, auto-correlation tests were applied to both cases. As shown in Figure 3(b), the static ICs have a strong auto-correlation while the dynamic ICs have a weak one. So, dynamic ICA is expected to give a better monitoring performance than static ICA since dynamic ICs encapsulate the dynamic characteristics of the process.

To compare the monitoring performance of dynamic PCA and ICA, Figure 4(a) and (b) describe the T^2 and SPE charts of the DPCA model and the I^2, I_e^2, SPE charts of the DICA model, respectively. The 99% confidence limits of each statistic chart are also shown in these figures. As shown in Figure 4, although both monitoring charts can detect a process change that has occurred between samples 103 and 120, there are too many false alarms with the SPE charts of DPCA later on, whereas DICA shows much less false alarms. To identify the most likely cause of this difference between both methods, the contributions of the dynamic ICA with two time lags from every measurement variable were plotted in Figure 5(a). In this period, the WWTP received an influent with a high temperature, high COD and high cyanide load in the aerator. It reduced the activity of the microorganisms. This results in the abnormality of the NOC, the increase of the residual parts of ICA. Because most WWTP have a high degree of non-Gaussian data (Yoo *et al.*, 2004b), ICA may give a superior monitoring performance because it extracts the key hidden (non-Gaussian) variables that influence the process.

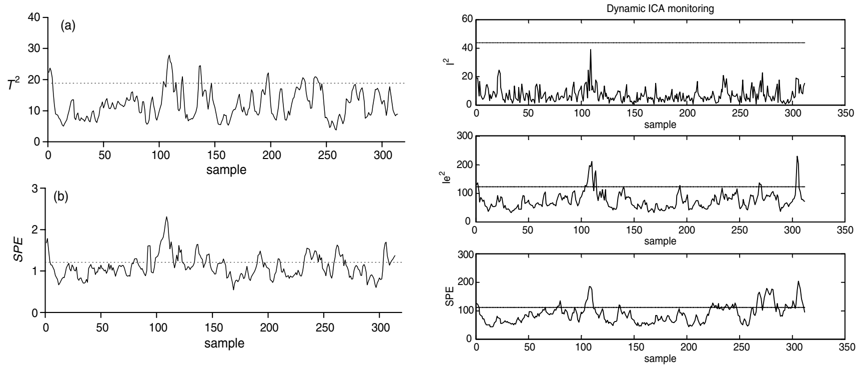

Figure 4 Dynamic PCA and ICA monitoring charts of the WWTP with the 99% confidence limits. (a) T^2 and SPE plots of the dynamic PCA (left), six PCs are used for deterministic part of the DPCA model. (b) I^2, I_e^2 and SPE plots of the dynamic ICA (right), six ICs are used for deterministic part of the DICA model

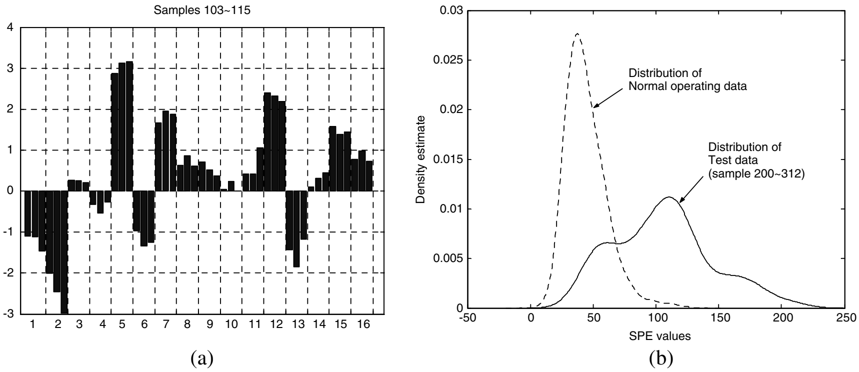

Figure 5 Contribution plot and distribution change of the *SPE* chart of the dynamic ICA. (a) contribution plot of *SPE* during samples $103 \sim 115$ (left), (b) comparison of the *SPE* distribution of normal operating data with that of the test data, sample $200 \sim 312$ (right)

After sample 200, the operating condition of the WWTP is changed a little although the new operating condition is also considered normal. This change results in a change of data structure in this period. After sample 230, the SPE chart of the dynamic ICA fluctuates above and below the confidence limit. The operators confirmed that this fluctuation of the *SPE* chart corresponds to the new operating condition, in which the microorganism had adapted to the change and the WWTP can be considered to operate normally under the new conditions. That is, because of the microorganism's adaptation ability and the control actions applied in the WWTP that bring the system to a new steady state. After the process changes or disturbances occurred, one could assume that a relation with similar variance but different mean could approximately hold. When the operating condition changes, the distribution of the normal operating data is expected to be also changed and destroyed. This can be verified by checking the change of the data distribution. Figure 5(b) shows the *SPE* distributions of the normal operating data and the test data (sample 200 to 312) in the case of dynamic ICA. Since the difference of non-Gaussian distributions is large, the *SPE* chart of the dynamic ICA can easily detect the change of the operating condition.

The difference between the PCA and ICA mainly originates from the extracted feature components; both methods extract hidden information from a multidimensional data set, but PCA looks for Gaussian components whereas ICA searches for non-Gaussian components. As is well known, a linear combination of Gaussian random variables is itself Gaussian and a linear combination of non-Gaussian random variables is itself non-Gaussian. Thus, if a data set contains any non-Gaussian component, ICA may show better feature extraction performance than PCA. Given that most process data have some degree of dynamic and non-Gaussian characteristics, ICA methods like PCA can be extended to the modeling and monitoring of dynamic systems by augmenting each observation vector with the previous l observations. ICA on lagged variables, dynamic ICA, may give more powerful monitoring performance in the case of a dynamic process since it can extract independent components from not only cross-correlated variables but also auto-correlated ones with the non-Gaussian properties.

Conclusions

The proposed monitoring method, dynamic ICA, which applies ICA to the augmenting matrix with time-lagged variables, was able to remove the major dynamics from the process and find statistically independent components from auto- and cross-correlated variables. The proposed monitoring method was applied as a dynamic monitoring system at a full-scale wastewater treatment plant. When the process variables have dynamic and non-Gaussian distributions as often found in biological processes, the dynamic ICA approach may result in better monitoring performance than the dynamic PCA since the information contained in the augmented observations has more information than a single observation and the more realistic transformation of ICA for the non-Gaussian data is considered. In the present work we have assumed that the underlying distribution of normal operating data does not change over time. However, this underlying distribution can potentially change. In fact, a small change in the distribution will have a negligible effect on the control limits of I^2 and *SPE*. When the underlying distribution changes substantially, however, the ICA model should be updated. Therefore, adaptive and dynamic ICA monitoring should be investigated in future research.

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