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Disturbance detection and isolation by dynamic principal component analysis

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Abstract

In this paper we extend previous work by ourselves and other researchers in the use of principal component analysis (PCA) for statistical process control in chemical processes. PCA has been used by several authors to develop techniques to monitor chemical processes and detect the presence of disturbances [1–5]. In past work, we have developed methods which not only detect disturbances, but isolate the sources of the disturbances [4]. The approach was based on static PCA models, T^2 and Q charts [6], and a model bank of possible disturbances. In this paper we use a well-known 'time lag shift' method to include dynamic behavior in the PCA model. The proposed dynamic PCA model development procedure is desirable due to its simplicity of construction, and is not meant to replace the many well-known and more elegant procedures used in model identification. While dynamic linear model identification, and time lag shift are well known methods in model building, this is the first application we are aware of in the area of statistical process monitoring. Extensive testing on the Tennessee Eastman process simulation [7] demonstrates the effectiveness of the proposed methodology.

Keywords: Dynamic multivariate statistical process control

1. Introduction

Statistical process monitoring (SPM), also often referred as statistical process control (SPC), generally defined as the use of statistical methods for process monitoring to improve process quality and productivity, has recently become of substantial interest in the chemical process industries. Conventional SPM methods originated from discrete manufacturing processes where the measured values of product quality are assumed independent and normally distributed. Such assumptions are often invalid for the measurements obtained from chemical processes due to their dynamic, multivariate, and nonlinear nature. Thus, conventional univariate SPM methods have limitations when applied to chemical processes.

Typical control charts such as Shewhart charts, cumulative sum (CUSUM) charts, and exponentially weighted moving average (EWMA) charts are used for monitoring a single variable. Applying univariate control charts to multivariate system is improper if the variables have a joint distribution with cross-correlation [8]. Multivariate control charts usually generate

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one common statistic from the values of many variables which can be plotted on a control chart. The earliest multivariate control chart uses the Hotelling's T^2 statistics which is simply the locus on the ellipse-like confidence region in the multidimensional space [8]. For n variables, T^2 can be expressed in the matrix notation

$$T^2 = \mathbf{x}^{\mathrm{T}}\mathbf{S}^{-1}\mathbf{x} \tag{1}$$

where

$$\mathbf{x} = [x_1\ x_2\ \cdots\ x_n]^{\mathrm{T}}$$

and $\mathbf{S}$ is the sample covariance matrix. T^2 can be related to the F distribution

$$T^2_{\alpha(n,m)} = \frac{n(m-1)}{m-n} F_{\alpha(n,m-n)} \tag{2}$$

where m is the sample size and $F_{\alpha(n,m-n)}$ has n and $m-n$ degrees of freedom. Several types of multivariate control charts have been proposed to take advantage of the relationships among the variables. These charts are reviewed by Alt [9] and Jackson [6]. Multivariate CUSUM charts were proposed by Healy [10] and Crosier [11]. A multivariate EWMA control chart was given by Lowry and Woodall [12]. Interestingly, these control charts utilize the T^2 in various ways.

When the number of variables is large, direct use of these multivariate control charts is not practical. Especially, as it is often the case, when the data set contains a lot of redundant information. Such redundancy results from multiple measurements of the same variables or constraining relationships between different variables. Data with such redundancy create ill-conditioning or collinearity problems. Therefore, it is suggested that such redundancy be separated from the data by selection of key variables or by data reduction methods. Principal component analysis (PCA) and partial least squares (PLS) have been widely used for this purpose. The use of PCA for quality control was first suggested in the early paper by Jackson [8]. More details on the use of PCA were later provided by Jackson [6,13]. This method has been used and extended in various applications [1–5].

An assumption of the methods mentioned above is that the variables are uncorrelated in time. In chemical processes, variables rarely remain at steady state but rather are driven by random noise and uncontrollable disturbances. The variables will move around the steady state according to the dynamic characteristics of the process and exhibit some degree of autocorrelation. It has been suggested that time series modeling approach could be used [14–17]. This approach consists of identifying a time series model, usually an autoregressive integrated moving average (ARIMA) model [18], then using this model to make one-step-ahead predictions. The prediction is then compared with the next measurement to monitor the variable. Such approaches suggested the use of univariate time series models and thus assume that the different variables are not cross-correlated. To remedy this limitation, these approaches can be extended to multivariate systems by the development of multivariate time series models [19,20], which is a quite complex task. In a previous publication [4], we have provided a detailed discussion of the PCA methods as a tool for the monitoring and isolation of process disturbances. Despite the success that the use of PCA, a multivariate technique but nevertheless a static one, had in the examples examined there, we now proceed in examining a dynamic version of the PCA approach. This is justified by the substantial amount of auto-correlation present in the variables and in the principal components of the two examples examined by Ku et al. [4].

The purpose of this paper is to show how static PCA tools could be extended to apply to dynamic multivariate systems and to examine their use for disturbance detection and isolation. We will first review the static PCA method. Next, we will show how an approximate time series model can be developed by a variation of the PCA method. We will refer to this dynamic method as 'dynamic PCA' or 'DPCA'. A design procedure will be proposed, and the method will be applied and tested on simulated processes. This method is used for detecting the existence of disturbance as well as for isolation of sources of the disturbance.

2. Principal component analysis

The principal component is defined as a linear transformation of the original variables into a new set

of variables which are uncorrelated to each other. This transformation is:

$$\mathbf{y} = \mathbf{U}^{\mathrm{T}}\mathbf{x} \tag{3}$$

The data vector $\mathbf{x}$ is centered by its mean and properly scaled. The transformation matrix $\mathbf{U}$ is composed of the eigenvectors of the covariance matrix of data, $\mathbf{S}$,

$$\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathrm{T}} \tag{4}$$

where the diagonal matrix Λ is the covariance matrix of the principal components which consists of the eigenvalues of the covariance matrix along the diagonal. The vector $\mathbf{y}$ is sometime called 'scores' or 'latent values'. The eigenvectors are called 'loading vectors' or 'latent vectors'. It is convenient to re-scale the principal components to have unit variance as suggested by Jackson [13]. This is done by dividing the eigenvectors by the squares roots of their corresponding eigenvalues. Usually, the original data can be represented by a smaller number of the principal components due to the redundancy in the data, resulting in several of the eigenvalues to be equal or close to zero. Therefore, only the first k eigenvalues, that are non-zero, and their corresponding eigenvectors are used to form a PCA model. The new scaled principal components are

$$\mathbf{y} = \mathbf{W}_k^{\mathrm{T}}\mathbf{x} = \mathbf{\Lambda}_k^{-1/2}\mathbf{U}_k^{\mathrm{T}}\mathbf{x} \tag{5}$$

The scaled principal components have zero means and unit variances. Since the covariance matrix of the scaled principal components is an identity matrix, Hotelling's T^2 can calculated as follows:

$$T^2 = \mathbf{y}^{\mathrm{T}}\mathbf{y} \tag{6}$$

which is just the sum of squares of the scores. The inverse of Eq. (5) can be used to reconstruct original variables from the reduced principal components:

$$\hat{\mathbf{x}} = \mathbf{U}_k\mathbf{\Lambda}_k^{1/2}\mathbf{y} \tag{7}$$

The sum of squares of the residuals is expressed as follows:

$$Q = (\mathbf{x} - \hat{\mathbf{x}})^{\mathrm{T}}(\mathbf{x} - \hat{\mathbf{x}}) = \mathbf{x}^{\mathrm{T}}(\mathbf{I} - \mathbf{U}_k\mathbf{U}_k^{\mathrm{T}})\mathbf{x} \tag{8}$$

It has been shown that the residuals have the properties of the noise if there are more measurements than states [1]. If the noise is random, the residuals will be random. The scalar value, Q, is a measurement of the 'goodness of fit' of the sample $\mathbf{x}$ to the model $\mathbf{W}_k$ and is directly associated with the noise which was discussed above. Therefore, the data is reduced to two variables: T^2 and Q characterizing two orthogonal subsets of the original space. T^2 represents the major variation of the data and Q represents the random noise in the data. These two variables can be used for monitoring the process. The control limit for Q was given by Jackson and Mudholkar [21]. The control limit for T^2 can be calculated by Eq. (2).

PCA can be calculated by eigenvalue decomposition of the covariance matrix $\mathbf{S}$ or by singular value decomposition of the data matrix $\mathbf{X}$, $\mathbf{S} = \mathbf{X}^{\mathrm{T}}\mathbf{X}/(m - 1)$. Note that PCA is a scale-dependent method, and thus requires a proper scaling of the data in order to obtain reasonable results. It is more common to center the data with the mean of each variable and scale them to have unit variance (auto-scaling). Many procedures have been proposed for determining the number of components to be retained in a PCA model and Jackson [22] provides a good summary of such methods. For example, a commonly used practice is to retain components with corresponding eigenvalues greater than one (auto-scaled data). The SCREE procedure is a graphical method in which one constructs a plot of the eigenvalues in descending order and looks for the 'knee' in the curve as the cut-off. Parallel analysis is a modified version of the SCREE in which the plot is augmented with a second curve showing the eigenvalues of a completely independent data set of the same size. The point where the curves cross is taken to be the cut-off. Zwick and Velicer [23] studied 5 popular methods and concluded that parallel analysis performed best. An additional popular method for selecting the number of components to retain, which was not included in the Zwick and Velicer study, is cross-validation. Cross-validation has been recommended by several authors including Wold [24] and Eastment and Krzanowski [25] and is especially attractive when the PCA model is to be used for predictive purposes. Our experience indicates that when autocorrelation and nonlinearities are present in the data as it is often the case in chemical processes, the methods just discussed can be unreliable. This seems especially true for cross-valida-

tion. Moreover, our experience [26] indicates that parallel analysis seems to work well in this application although we suggest that several approaches be applied in an effort to find some consensus.

3. Dynamic PCA method

The PCA method has been widely used in system identification and model reduction for dynamic systems [19,20,27]. However, it is not commonly used in the areas of SPM and recent studies and publications focus on this use of static PCA [1–5]. Data redundancy stems from linear relations between variables. How can we extract this information from the data? Before we apply PCA to dynamic systems, we need to address this question first. To identify the linear relations between variables is to find the null space of the data matrix $\mathbf{X}$ which is the non-trivial solution of the following equation:

$$\mathbf{Xb} = 0 \tag{9}$$

where $\mathbf{X}$ is a $m \times n$ matrix and $m \geq n$. The required condition for this solution is that the rank of $\mathbf{X}$ has to be less than n. If the rank of $\mathbf{X}$ is r, then there exist $n - r$ linear relations. The solution to the equation is the right singular vectors associated with the zero singular values:

$$\mathbf{b} = \mathbf{v}_k, \quad k = r+1, \cdots, n \text{ if } \sigma_k = 0 \tag{10}$$

The singular values and the singular vectors are defined as follows: [28]:

Definition 1 (singular value decomposition, SVD): *If* $\mathbf{X}$ *is a real* $m \times n$ *matrix then there exist orthonormal matrices*

$$\mathbf{U} = [\mathbf{u}_1, \cdots, \mathbf{u}_m] \in \mathbb{R}^{m \times m} \text{ and}$$

$$\mathbf{V} = [\mathbf{v}_1, \cdots, \mathbf{v}_n] \in \mathbb{R}^{n \times n}$$

such that

$$\mathbf{U}^{\mathrm{T}}\mathbf{X}\mathbf{V} = \mathbf{\Sigma} = diag(\sigma_1, \cdots, \sigma_p) \in \mathbb{R}^{m \times n}$$

$$p = \min\{m, n\}$$

where singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$.

The matrices $\mathbf{U}$ (left singular vectors) and $\mathbf{V}$ (right singular vectors) are orthogonal matrices, i.e. $\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{I}_m$ and $\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{V}\mathbf{V}^{\mathrm{T}} = \mathbf{I}_n$.

For example, consider the following example:

$$\mathbf{x} = [x_1 \; x_2]^{\mathrm{T}} \tag{11}$$

and let $x_2 = \alpha x_1$ and $x_1 = f(t)$. Then

$$\mathbf{X} = \begin{bmatrix} f(t_1) & \alpha f(t_1) \\ f(t_2) & \alpha f(t_2) \\ \vdots & \vdots \\ f(t_m) & \alpha f(t_m) \end{bmatrix} \tag{12}$$

and we can easily calculate that

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \text{ with } \sigma_1 = 1 + \alpha^2 \text{ and}$$

$$\mathbf{V} = \frac{1}{\sqrt{1+\alpha^2}} \begin{bmatrix} 1 & -\alpha \\ \alpha & 1 \end{bmatrix} \tag{13}$$

The zero singular value indicates that there is a linear relation between x_1 and x_2. This linear relationship is revealed by the corresponding right singular vector, $\mathbf{v}_2$:

$$-\frac{\alpha}{\sqrt{1+\alpha^2}} x_1 + \frac{1}{\sqrt{1+\alpha^2}} x_2 = 0 \Rightarrow x_2 = \alpha x_1 \tag{14}$$

The same result is obtained whether the data have been auto-scaled or not.

Consider another example:

$$\mathbf{x} = [x_1 \; x_2 \; x_3]^{\mathrm{T}} \tag{15}$$

Let $x_3 = x_1 + x_2$ represent a constraining equation such as a mass balance of a mixer or separator and let $x_1 = f_1(t)$ and $x_2 = f_2(t)$ where f_1 and f_2 are two independent functions of time then the SVD of the $m \times 3$ data matrix $\mathbf{X}$ reveals that the last singular value and singular vector are

$$\sigma_3 = 0, \; \mathbf{v}_3 = \frac{1}{\sqrt{3}} [1 \; 1 \; -1]^{\mathrm{T}} \tag{16}$$

The last singular vector reveals the exact relation among the three variables.

These examples show the results for the ideal case with no measurement or other noise. However, zero

eigenvalue or singular values are seldom found in real practice because of the presence of noise. Random noise in the data creates variation and results in converting the zero singular values to non-zero but small ones. The best solution to Eq. (9) will be the right singular vectors associated with the small singular values.

$$\mathbf{b} = \mathbf{v}_k, \quad k = r+1, \cdots, n \text{ if } \sigma_k < \sigma(E) \tag{17}$$

where $\sigma(E)$ is some threshold for small singular values. We will call the space spanned by these $\mathbf{v}_k$ vectors 'approximate null space' or 'noise subspace' which contains the linear relationships that constrain the data.

Ideally, T^2 should be constructed from the 'dominant variation subspace' which is spanned by $\mathbf{v}_k$, $k = 1,2,\cdots,r$ and represents the maximum variation of the data, and Q should be constructed from the 'noise subspace' which describes the linear constraints between variables. Obviously the 'dominant variation subspace' is orthogonal to the noise subspace and jointly they span the overall data space. However, it is difficult to determine the exact number of principal components or, equivalently, the number of constraining relationships and thus the dimensionality of their subspaces, when noise exists. An additional difficulty is introduced when the true constraining relationships are nonlinear, as it is often the case. The difficulty in selecting the correct number of the principal components will depend on the noise level of the data. The desired condition is that the noise level is not high compared to the signal level. Hence, a clear gap occurs between σ_r and σ_{r+1}. The analysis can be done theoretically by perturbation theory with some knowledge about the noise. The effect of noise on the singular values of the data matrix can be examined by perturbation theory [28]. The following theorem provides a hint to selection of number of relations:

Theorem 1 *If* $\mathbf{A}$ *and* $\mathbf{X} = \mathbf{A} + \mathbf{E}$ *are in* $\mathbb{R}^{m\times n}$ *with* $m \geq n$, *then for* $k = 1,2, \cdots, n$

$$|\sigma_k(\mathbf{A}+\mathbf{E}) - \sigma_k(\mathbf{A})| \leq \sigma_1(\mathbf{E}) = \|\mathbf{E}\|_2$$

For our problem, the matrix $\mathbf{A}$ represents the data matrix without noise and $\mathbf{E}$ represents the noise added to the data matrix. Consequently, if we assume that the noise effect is additive, we can use the following relationships:

$$\sigma_k(\mathbf{A}+\mathbf{E}) \geq \sigma_1(\mathbf{E}) \quad k = 1, \cdots, r$$

and

$$\sigma_k(\mathbf{A}+\mathbf{E}) \leq \sigma_1(\mathbf{E}) \quad k = r+1, \cdots, n$$

to determine the number, r, of principal components. The norm of $\mathbf{E}$ provides a threshold to determine which components are random noise. Unfortunately, the exact $\mathbf{E}$ is unknown and needs to be constructed. However, what is really needed is the norm of $\mathbf{E}$ which is the largest singular value of the error matrix. If the norm of $\mathbf{E}$ can be experimentally determined or estimated, one can then use this norm to determine the existing number of relations. The best estimates of $\mathbf{A}$ and $\mathbf{E}$ can then be reconstructed. Several rank-revealing decompositions require such knowledge [29–31]. An alternative way is to use the aforementioned methods for determining the number of the principal components and treating the remaining components as the noise space spanned by the linear constraints. If the actual constraining relationships are linear and static, most of the procedures for determining the number of the principal components, such as cross-validation and parallel analysis, would apply and provide reasonable answers. The major difficulty arises when the actual constraining relationships are dynamic or/and nonlinear.

Directly applying PCA on the data matrix $\mathbf{X}$ actually constructs a linear static model. When the data contains dynamic information, applying PCA on the data will not reveal the exact relations between the variables, rather a linear static approximation. It is possible to detect and isolate disturbances from a dynamic system with the use of a static PCA model as it has been demonstrated for the Tennessee Eastman simulation process [4]. However, the statistical basis of this approach is lost because the data violate the assumption of time independence. The transformed variables (scores) will be auto-correlated and possibly cross-correlated. Misleading results might be generated such as excessive false alarms especially for small size disturbances. For some dynamic systems, dynamic PCA modeling will be more useful for detecting disturbances quickly. Building a dynamic model only for the score values of the principal com-

ponents obtained from an initial static PCA step will not solve the problem because the linear constraints that span the noise space will remain static.

For a dynamic system, the current values of the variables will depend on the past values. Thus, we need to identify the linear relations between $\mathbf{X}(t)$ and $\mathbf{X}(t-1)$, at least. If all dynamic relationships are first order system, the relation will be the noise subspace of the following equation

$$[\mathbf{X}(k)\,\mathbf{X}(k-1)]\mathbf{b} = 0 \tag{18}$$

In a more general case,

$$\mathbf{X}_A(l)\mathbf{b} = 0 \tag{19}$$

where

$$\mathbf{X}_A(l) = [\mathbf{X}(k)\,\mathbf{X}(k-1)\,\cdots\,\mathbf{X}(k-l)] = \left[\begin{array}{c|c|c|c} \mathbf{x}^{\mathrm{T}}(1) & \mathbf{x}^{\mathrm{T}}(0) & \cdots & \mathbf{x}^{\mathrm{T}}(1-l) \\ \mathbf{x}^{\mathrm{T}}(2) & \mathbf{x}^{\mathrm{T}}(1) & \cdots & \mathbf{x}^{\mathrm{T}}(2-l) \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}^{\mathrm{T}}(m) & \mathbf{x}^{\mathrm{T}}(m-1) & \cdots & \mathbf{x}^{\mathrm{T}}(m-l) \end{array}\right] \tag{20}$$

Note that $\mathbf{X}_A(l)$ has the special form of a Hankel matrix which is widely used in model reduction and system identification [27]. This is essentially the same as the original PCA approach except that the data matrix is composed of time shifted duplicate vectors. By properly choosing of the number l, both the static and dynamic relations should appear in the noise subspace with small singular values. The Q calculated from this noise space will be truly independent and provide a statistical basis for the dynamic system. We will refer to this approach as 'dynamic PCA' or 'DPCA'. The dynamic model which can be extracted from the data is an implicitly multivariate autoregressive (AR) or ARX model if process inputs are included. Processes which contain moving average (MA) terms will be approximated by an AR model. The advantage of this approach is simplicity. The data reduction and model extraction are done in a single step. This method of appending lagged data is not new and has been widely used in system identification [19,20,27]. Identifying multivariate AR models can be done by a least squares method or by canonical analysis [19]. MacGregor and Wong [32] extended the canonical analysis procedure to identify an ARIMA model and then transformed the identified model into state space form for optimal control of a chemical reactor. Our approach is similar to the canonical analysis. However, our approach directly handles static and dynamic relations without problem when the covariance of the data is singular [19].

Let us consider the following noise-free case: an AR(1) process,

$$z(k) = 0.8z(k-1) + u(k-1) \tag{21}$$

by static PCA method,

$$\mathbf{x}_1 = [z(k)\,u(k)]^{\mathrm{T}} \tag{22}$$

where u is a colored noise with 1000 samples generated as follows:

$$u(k) = 0.7u(k-1) + w(k-1) \tag{23}$$

where w is a white noise with variance 1. The singular value decomposition of the covariance matrix of the data matrix $\mathbf{X}_1(k)$, that includes no lagged variables, is:

$$\mathbf{\Sigma}_1 = \begin{bmatrix} 21.47 & 0 \\ 0 & 1.352 \end{bmatrix} \quad \mathbf{V}_1 = \begin{bmatrix} 0.985 & -0.175 \\ 0.175 & 0.985 \end{bmatrix} \tag{24}$$

Attempt to model an inherently 1-dimensional process with PCA, but find that both singular values are significant.

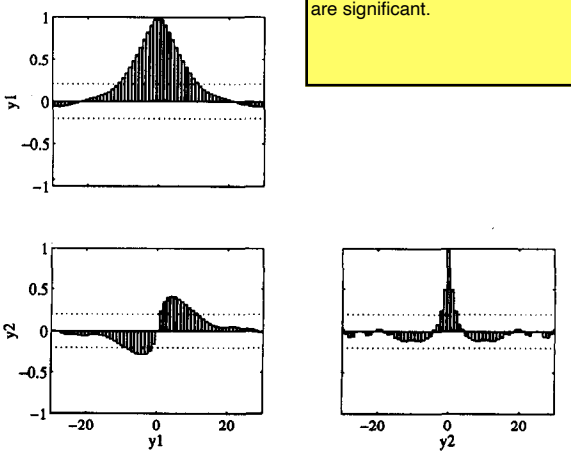

Fig. 1. Cross-correlation functions plots of scores by static PCA: correlated input.

If the data is auto-scaled, then

$$\Sigma_1 = \begin{bmatrix} 1.542 & 0 \\ 0 & 0.458 \end{bmatrix} \quad (25)$$

This result does not reveal any relation between the variables since there is no singular value that is equal or close to zero. Two principal components are significant. The scores are not totally independent as shown in Fig. 1.

If we apply dynamic PCA to this case, the data vector is

$$\mathbf{x}_2 = [z(k)\ u(k)\ z(k-1)\ u(k-1)]^{\mathrm{T}} \quad (26)$$

The result is:

$$\Sigma_2 = \begin{bmatrix} 42.37 & & & \\ & 2.599 & & \\ & & 0.709 & \\ & & & 0 \end{bmatrix}$$

$$\mathbf{V}_2 = \begin{bmatrix} 0.699 & -0.225 & 0.287 & -0.615 \\ 0.110 & -0.633 & -0.766 & 0 \\ 0.692 & 0.452 & -0.274 & 0.492 \\ 0.145 & -0.587 & 0.506 & 0.615 \end{bmatrix} \quad (27)$$

If the data is auto-scaled, then

$$\Sigma_2 = \begin{bmatrix} 2.967 & & & \\ & 0.751 & & \\ & & 0.285 & \\ & & & 0 \end{bmatrix} \quad (28)$$

The single zero singular value shows that there is a linear dynamic relation between the four variables, revealed by the fourth singular vector which implies that

$$-0.615z(k) + 0.492z(k-1) + 0.615u(k-1) = 0 \quad (29)$$

and which can be re-arranged to

$$z(k) = 0.8z(k-1) + u(k-1) \quad (30)$$

which is the same relation given above. The auto- and cross-correlation plots of the scores are shown in Fig. 2. The plots show that the last score is independent from the others. Note that ideally the last score should be zero and correlation plots should be zero also. However, due to the finite computer precision, some low correlations are shown in the plots. The third

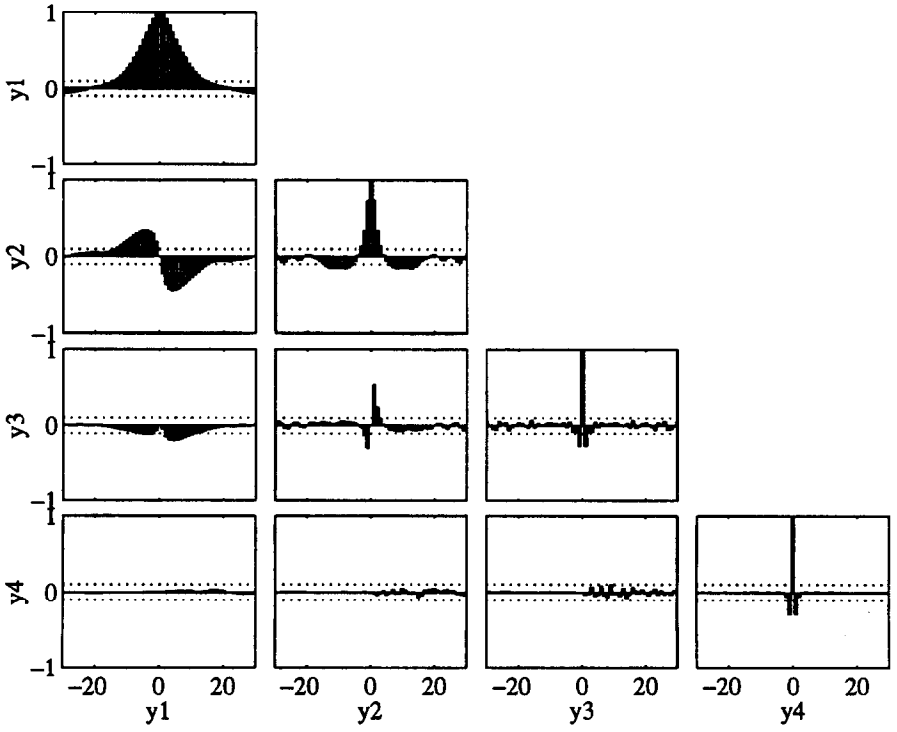

Fig. 2. Correlation plots of scores by dynamic PCA: correlated input.

score shows some correlation with the second one with 30 time lags. Clearly the score corresponding to the first two components show substantial autocorrelation and lagged cross-correlation. This is caused by the autocorrelation of the input $u(t)$, and does not imply that we have the wrong relationship between $z(k)$, $z(k-1)$, and $u(k-1)$.

This noise-free case example is given for the purpose of illustrating how a linear dynamic model can be extracted from the data. For noisy cases, one has to decide the number of singular values that are close to zero and thus determine the number of relationships.

4. The design procedure

To extract the static and dynamic relations from the data by the use of dynamic PCA, one has to determine the necessary number of time lags l and the principal components or the linear relations. The number l usually is 1 or 2 which indicates the order of the dynamic system. For nonlinear systems, l could be higher in order to get a better linear approximation of the actual nonlinear relationships. The following design procedure is proposed to determine the proper number of components and the order of the system.

1. Set $l = 0$.
2. Form data matrix $\mathbf{X} = [\mathbf{X}(k)\mathbf{X}(k-1)\cdots\mathbf{X}(k-l)]$.
3. Perform PCA and calculate all the principal scores.
4. Set $j = n \times (l+1)$ and $r(l) = 0$.
5. Determine if the jth component represents a linear relation. If yes proceed, if no go to step 7.
6. Set $j = j-1$ and $r(l) = r(l)+1$, repeat 5.
7. Calculate the number of new relationships

$$r_{\text{new}}(l) = r(l) - \sum_{i=0}^{l-1} (l-i+1)\, r_{\text{new}}(i) \qquad (31)$$

8. If $r_{new}(l) \leq 0$, go to step 10, otherwise proceed.
9. Set $l = l+1$, go to step 2.
10. Stop.

This procedure assumes that a method for determining the number of the principal components or the

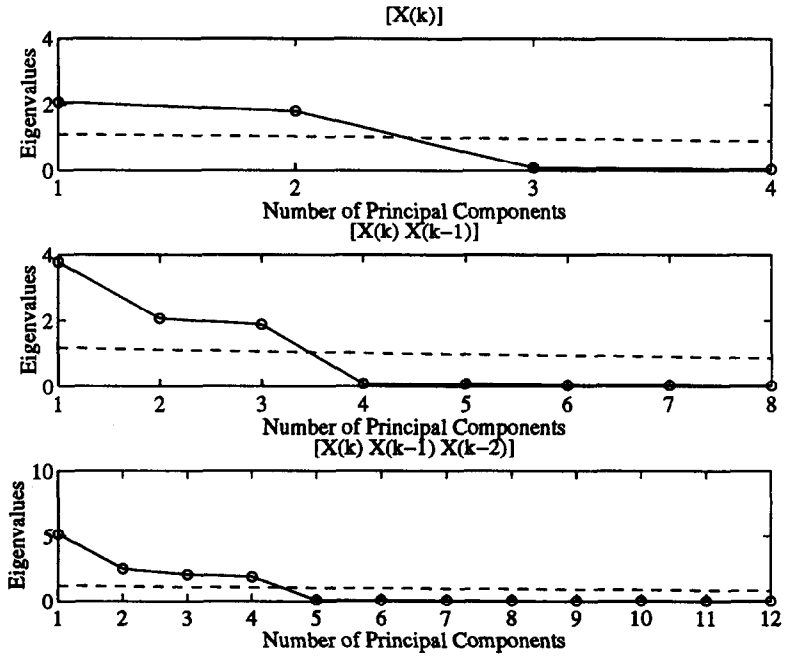

Fig. 3. Parallel analysis on four variable shifted data generated by use of two static and one dynamic relationships.

linear relations has been chosen. We suggest to use parallel analysis and the cross-correlation plots of the scores to determine the number of the principal components. The number of linear relations, r, will be the total number of the variables minus the number of the principal components. Another way is to set a threshold for small singular values. It is important to check if the remaining scores are completely independent using the auto- and cross-correlation plots. At each l-level, r_{new} might have a negative value for some value of l.

Let us consider a four-variable system and assume

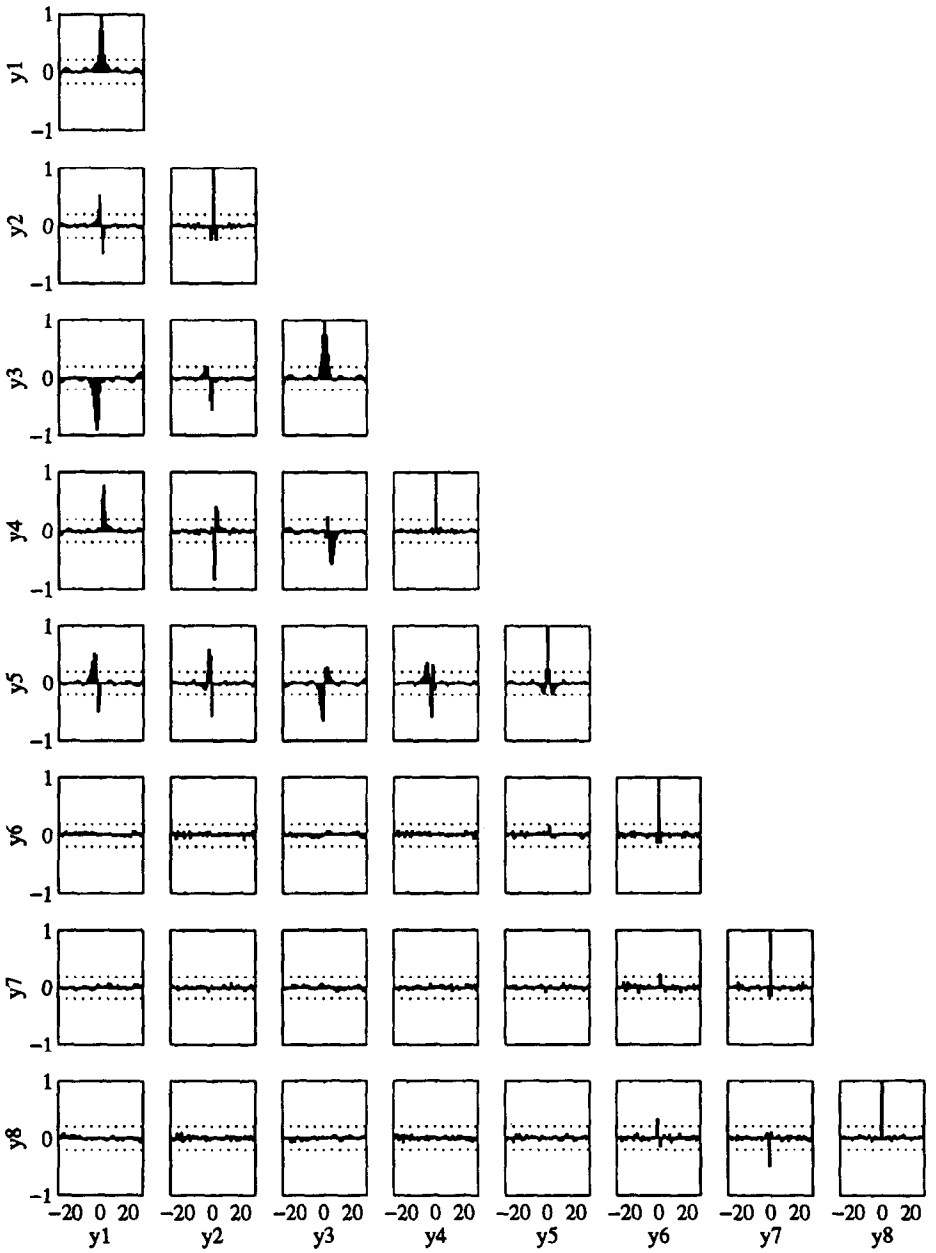

Fig. 4. Auto- and cross-correlation plots of scores by dynamic PCA ($l = 1$).

that all the variables are independent. The singular values of $\mathbf{X}(k)$ and $[\mathbf{X}(k)\ \mathbf{X}(k-1)]$ will be all significant and that no static or dynamic relations will be found. Fig. 3 shows another four-variable system where the variables are inter-dependent. Two of the singular values of $[\mathbf{X}(k)]$ are small which indicates the existence of two linear static relations. Note that these static relations will be repeated $(l+1)$ times in $\mathbf{X}_A(l)$ when dynamic PCA is applied. From the singular values of $[\mathbf{X}(k)\ \mathbf{X}(k-1)]$, we observe that five have small magnitude. This implies that there are five linear relations among the eight variables. Four of them are the two static relations repeated twice and the other one is the new first order dynamic relation in this level $(l=1)$. If we go a level further, $l=2$, the number of relations is 8 which is the static relations repeated three times and the dynamic relation found in level 1 repeated twice. This indicate that no more new information could be found in this level and r_{new} is zero. Therefore, the procedure should stop at level 2 and $[\mathbf{X}(k)\ \mathbf{X}(k-1)]$ will be sufficient to extract the constraining relations between variables and thus the correct PCA model.

5. Application to statistical process monitoring

The PCA method has been widely used in system identification and model reduction for dynamic systems [19,20,27]. However, it is not commonly used in the areas of SPM and only recent studies and publications focus on this use of static PCA [1–5]. Our procedure is used to extract the static and dynamic linear relations which are existing in the data. The main purpose of this paper is not to identify accurate multivariate time series models as this is an active and well-developed area of system identification. Instead, it aims to utilize an easy to use version of these methods to develop multivariate control charts that monitor the principal process variations as well as the process noise characterizing the deviation from the constraining linear relationships in the data. These charts can then be used to detect and isolate process disturbances. We can use dynamic PCA for SPM in a similar way as the static PCA [4] for disturbance detection and isolation. This is done by constructing different dynamic PCA models for normal data and for the disturbance data. For a dynamic system, after properly selecting the number of constraining relations, Q can be calculated from the independent noise space. If data is auto-correlated, T^2 will still be calculated from the correlated variables. Since T^2 represents the movement of the data in the multidimensional space, it contains important information about the process although the variables from which it is calculated are not independent. Adjusting the control limits for T^2 might be necessary when T^2 exhibits strong auto-correlation.

We will demonstrate the use of dynamic PCA for statistical process monitoring purposes first with respect to a simple multivariate process as well as with the much more complex and realistic Tennessee Eastman process.

5.1. Multivariate AR(1) process

Consider the following process:

$$\mathbf{z}(k) = \begin{bmatrix} 0.118 & -0.191 \\ 0.847 & 0.264 \end{bmatrix}\mathbf{z}(k-1) + \begin{bmatrix} 1 & 2 \\ 3 & -4 \end{bmatrix}\mathbf{u}(k-1),$$

$$\mathbf{y}(k) = \mathbf{z}(k) + \mathbf{v}(k) \tag{32}$$

where $\mathbf{u}$ is the correlated input:

$$\mathbf{u}(k) = \begin{bmatrix} 0.811 & -0.226 \\ 0.477 & 0.415 \end{bmatrix}\mathbf{u}(k-1) + \begin{bmatrix} 0.193 & 0.689 \\ -0.320 & -0.749 \end{bmatrix}\mathbf{w}(k-1) \tag{33}$$

The input $\mathbf{w}$ is a random noise with zero mean and variance 1. The output $\mathbf{y}$ is equal to $\mathbf{z}$ plus the random noise, $\mathbf{v}(k)$, with zero mean and variance 0.1. Both input $\mathbf{u}$ and output $\mathbf{y}$ are measured but $\mathbf{z}$ and $\mathbf{w}$ are not. The normal data with 100 samples are used for analysis. Both current and previous values of the measurements are also utilized. The data vector for analysis consists of $[\mathbf{y}^T(k)\ \mathbf{u}^T(k)\ \mathbf{y}^T(k-1)\ \mathbf{u}^T(k-1)]$. Parallel analysis indicates that three of the eight components are principal. However, by examining the correlation plots of all the scores (Fig. 4), the fourth and fifth scores still show certain auto-correlation and cross-correlation. The last three scores are independent of each other. Therefore, 5 principal components are chosen for the dynamic PCA method and the last three components are the dynamic rela-

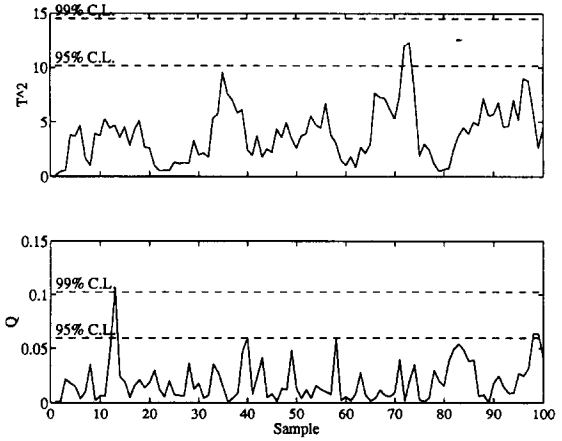

Fig. 5. Dynamic PCA ($l = 1$): T^2 and Q plots of the normal data with 5 PCs.

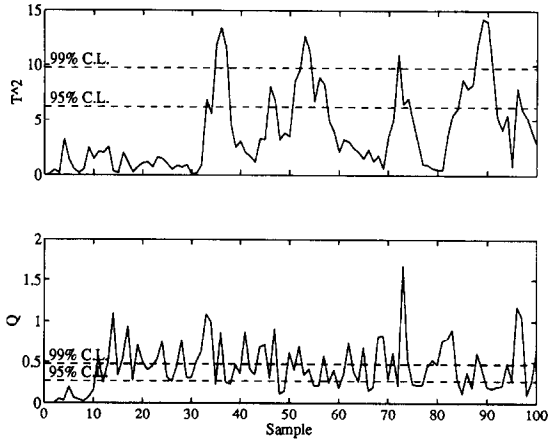

Fig. 7. Static PCA: T^2 and Q plots of the disturbance data with 2 PCs.

tions of the process. The T^2 and Q of the normal operating data are plotted in Fig. 5. The control limits of each of these plots are based on 95% and 99% confidence levels. A disturbance with unit step change of w_1 is introduced at sample 10. Note that this disturbance is not measured but affects the output. The T^2 and Q data collected during the occurrence of the disturbance are plotted in Fig. 6. The Q plot clearly indicates that the process is out of control after sample 10. The T^2 plot also indicates that the process is out of control.

Applying static PCA to a dynamic system might lead to misleading results because data are correlated in time. Specifically, static PCA may not be able to detect small disturbances. Let us use this multivariate AR(1) process with the following changes: static PCA uses 2 principal components and dynamic PCA uses 5 principal components. The level of the disturbance is reduced to 0.5. The T^2 and Q plots are shown in Figs. 7 and 8. Both 95% and 99% control limits are shown on each of the plots. With static PCA, T^2 fails to detect the disturbance and Q goes back and forth across the control limits. With dynamic PCA, the disturbance is well detected by the Q plot. T^2 shows a few out-of-control signals. If we reduce the level of the disturbance to 0.2. The control charts based o

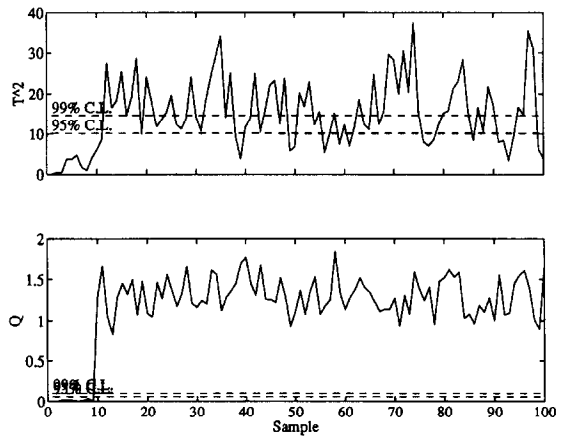

Fig. 6. Dynamic PCA ($l = 1$): T^2 and Q plots of the data with disturbance with 5 PCs.

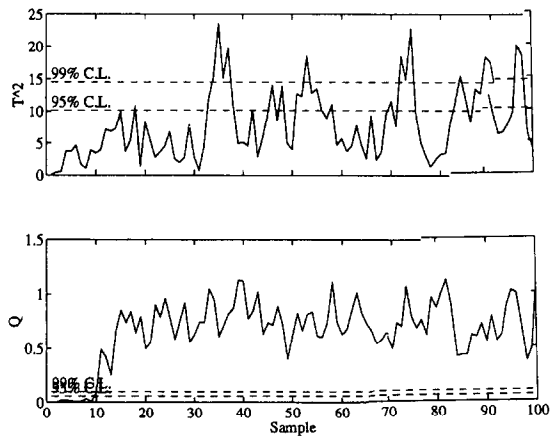

Fig. 8. Dynamic PCA ($l = 1$): T^2 and Q plots of the disturbance data with 5 PCs.

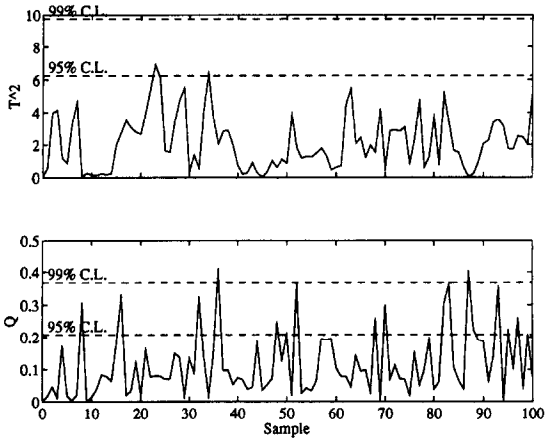

Fig. 9. Static PCA: T^2 and Q plots of the disturbance data with 2 PCs.

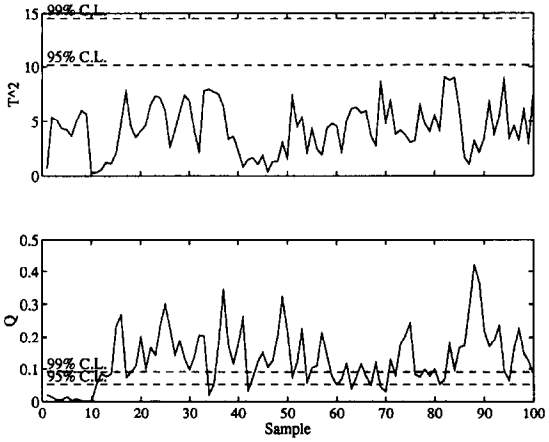

Fig. 10. Dynamic PCA ($l = 1$): T^2 and Q plots of the disturbance data with 5 PCs.

static PCA model are shown in Fig. 9. Both Q and T^2 fail to detect the disturbance. However, the control charts based on dynamic PCA model (as shown in Fig. 10) are still able to detect this disturbance. In general, dynamic PCA should perform better than static PCA when auto-correlation is present.

5.2. *Tennessee Eastman process*

As a more challenging case study we now examine the chemical plant simulation developed by Downs and Vogel of the Eastman Chemical Company (formerly called Tennessee Eastman Company) [7]. This model was presented as an industrial challenge problem in the area of plant-wide control at the Chicago AIChE meeting in November 1990. Lyman [33] and Lyman and Georgakis [34] developed four different control structures for the process. In order to illustrate our procedure, we use data generated from the Tennessee Eastman simulation augmented with the second control structure, that was reported as most effective by Lyman and Georgakis [34]. This process

Table 1
Process disturbances for Tennessee Eastman process

Disturbance	Description	Type
0	No disturbance	None
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	Reactor kinetics	Slow drift
14	Reactor cooling water valve	Sticking
15	Condenser cooling water valve	Sticking
16–20	Unknown	Unknown

was previously used to study static PCA models [4]. In this section, dynamic PCA is applied to this process under the same conditions. There are 41 measurements and 12 manipulated variables from controllers in this process resulting in a total of 53 process variables in the analysis. The simulation includes a set of programmed disturbances which are listed in Table 1. The time period for each simulation used here is 10 hours and the process variables are sampled every 3 minutes. This frequency is decided by the less frequent gas chromatographic measurements. All the disturbances are introduced at hour 1 in our tests.

The use of the Tennessee Eastman Process Simulator imposed some limitations on our simulation study. On the positive side, and with the help of the authors of the simulator, we were able to change random number seeds within the simulator. Thus we were able to generate independent training and test data sets. All runs of the simulator include noise generated from a pseudo-random number generator. This includes the runs in which no disturbance is present. We built PCA models for the nominal (no disturbance) case, and for 15 cases in which various disturbances were present. Later we tested the performance of the PCA models in the detection and isolation of disturbances. In our tests of the models, the random number seeds were changed so that the test data sets were independent of the data sets used to build the models.

On the negative side, we were not able to change the levels or statistical parameters of the disturbances within the simulation. Thus, while training and test sets were independent, the magnitude of the disturbances (i.e. size of the step change in the mean or the rate of random variation) was the same for both data sets. It seems unrealistic to expect that a step change in (say) the condenser cooling water inlet temperature will always be a (say) 10% step change. We were advised against changing the magnitudes of the disturbances by the simulator authors as they believed them to accurately reflect the magnitude of disturbances in their plant.

An additional revealing test would have been to generate several data sets from a particular disturbance over a range of different magnitudes, use all this data to build a PCA model, and then test the ability of the model to detect and isolate disturbances both within and outside this magnitude range. From such a test, the general robustness of the isolation procedure could be quantified. While our inability to alter disturbance magnitude precluded such testing, there is some hint to the robustness of the method in our results. Among the disturbances programmed into the simulation are pairs such as disturbance 5 (condenser cooling water inlet temperature: step), and disturbance 12 (condenser cooling water inlet temperature: random variation), also disturbance 11 (reactor cooling water temperature: random variation) and disturbance 4 (reactor cooling water temperature: step). For these pairs, the disturbance occurred in the same variable within the plant, but with different statistical behavior. As one can observe in Fig. 15, when disturbance 11 occurs, the Q plot associated with the disturbance 11 model is the most likely choice. However, the Q plot from the model based on disturbance 4 is quite closer to being in control than any of the other Q plots. One might say that disturbance 4 would be the second most likely candidate. Similar behavior is observed in Fig. 14 with respect to the disturbance pair 5 and 12. From these observations it appears that the model may be fairly robust, and could be made more so by varying the range of disturbances used to build the models as suggested above.

5.3. Disturbance detection

The process was first run without disturbances to obtain data reflective of normal operating conditions. After auto-scaling, the design procedure given in the last section was applied to the data. We used parallel analysis to initially estimate the number of the principal components and then used correlation analysis to determine the number of linear relations. By parallel analysis, there are 42 static relations and $7 + 2$

Table 2
Parallel analysis on normal data

l	No. of variable	No. of PCs	$r(l)$	$r_{new}(l)$
0	53	11	42	42
1	106	15	91	7
2	159	17	142	2
3	212	22	190	−3

dynamic relations as shown in Table 2. The result shows that choice of $l = 2$ will cover all the linear relations. We decided to choose $l = 2$ and 17 principal components (based on parallel analysis) for the normal data. This result can be verified by the cross-correlation plots as shown in Fig. 11. The small gray scale box in the plots represents the number of the correlation functions above the 99% control limits with ± 30 lags. The darker color indicates that the variables are more correlated. We consider that it is correlated if the number is greater than 1. The plots show that the first 17 principal components are highly correlated and the rest of the principal components are almost independent of each other. Control limits for T^2 and Q are 31.06 and 79.14 respectively which are based on an approximate 95% type I error risk. These two control charts were then used for process monitoring and disturbance detection.

The simulation was run 16 times, once under normal operating conditions, and once under each of the 15 disturbances implemented in the simulation. Disturbances 16–20 were not used here and will be tested later as unknown disturbances. For each simulation, Q charts (Fig. 12) and T^2 charts (Fig. 13) were constructed. When run under normal operating condi-

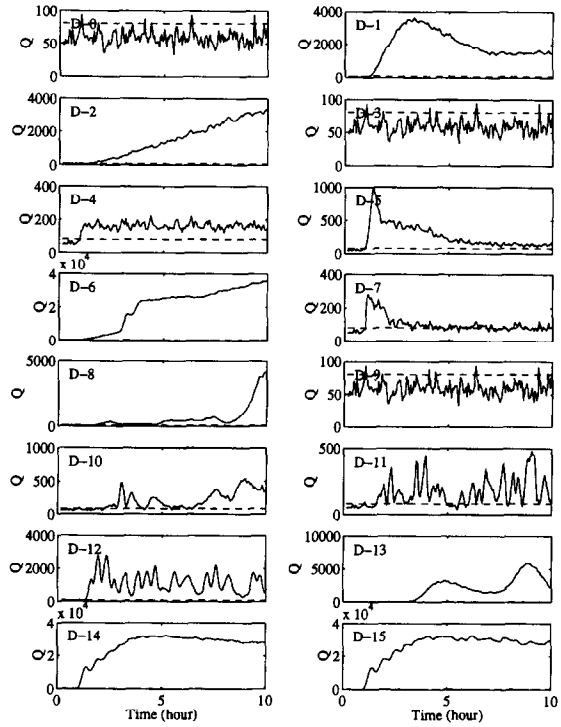

Fig. 12. Q plots of data characterizing different disturbances projected onto the DPCA model ($l = 2$) of normal operating data.

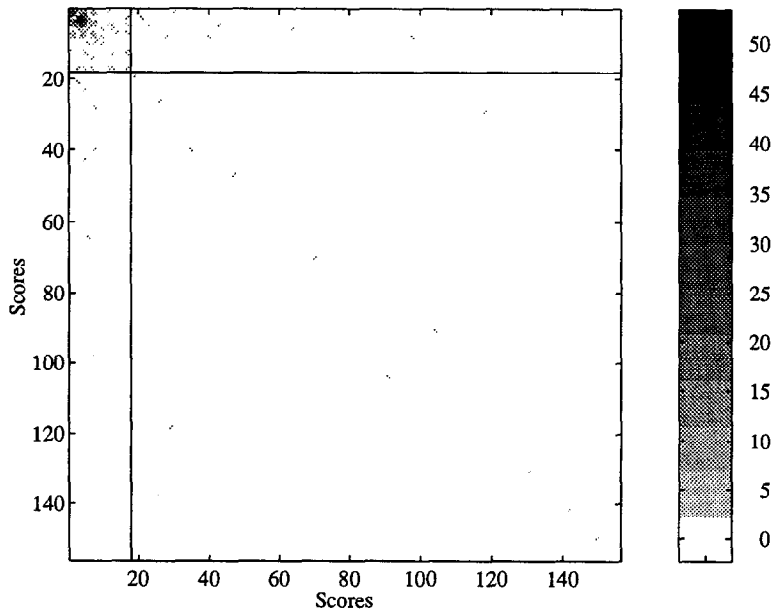

Fig. 11. Cross-correlation plots of the scores with ± 30 lags for dynamic PCA of the TE data with $l = 2$. The gray scale boxes indicate the number of points for each correlation plot that are above the 99% control limits.

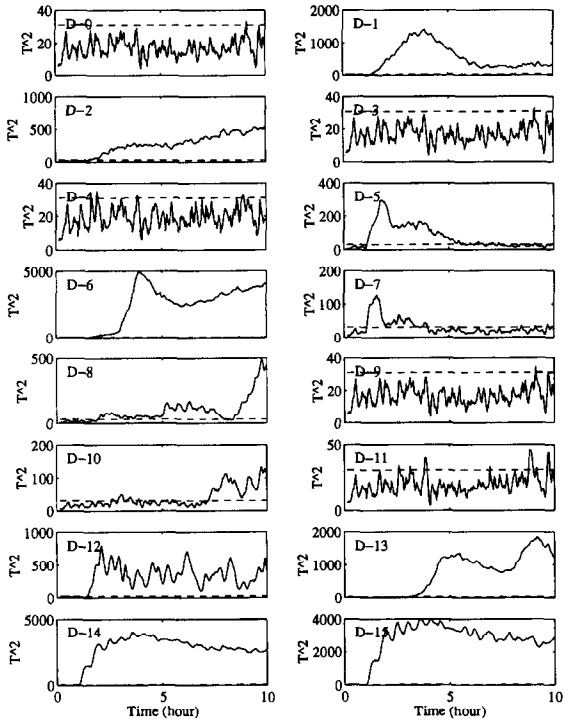

Fig. 13. T^2 plots of data characterizing different disturbances projected onto the DPCA model ($l = 2$) of normal operating data.

tions, the control charts are reflective on an 'in-control' process as they should be. In the presence of disturbances, 13 out of 15 are quickly and easily detected, particularly in the Q charts. The procedure was not able to readily detect disturbances 3 (step change in the temperature of feed stream D) and 9 (random variation in the temperature of feed stream D). This is due to the fact that these disturbances were quite small and had almost no effect on the overall process. The static PCA approach could not detect these disturbances either.

5.4. Disturbance isolation

We next constructed a model bank by building a dynamic PCA model for each of the 15 disturbances (W-1 through W-15) in addition to the model of normal operating conditions (W-0). The disturbance models for isolation are constructed with choice of $l = 2$ for all disturbances. The number of the principal components for each disturbance model is based on parallel analysis. The control limits for Q plots range from 58 to 81. To isolate the disturbances, new observation vectors were projected onto each of the DPCA models and then a Q value was calculated and plotted on a control chart.

In the first example, the process simulator was run so that disturbance 5 occurs after 1 hour of normal operating conditions. The simulation ran for a total of 10 simulated hours. Although both Q and T^2 can be used for isolation, Q charts usually respond faster than T^2 charts. Therefore, Q charts will be sufficient for isolation purpose and only Q charts will be presented in the following analysis. Q charts for each of the 16 potential models appear in Fig. 14. From Fig. 14 it is clear that the only chart showing the data to be consistent with the model is in fact the chart for disturbance 5. Thus the procedure was able to successfully isolate the disturbance in this case.

In the second example we followed the same pro-

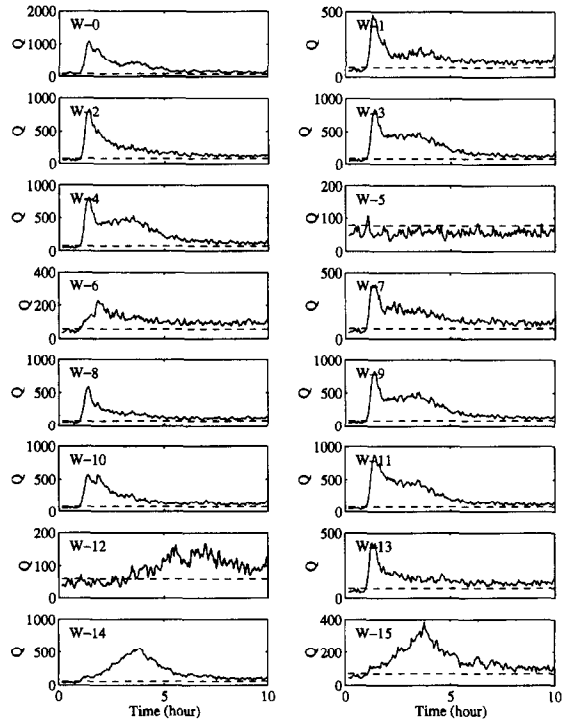

Fig. 14. Q plots of data characterizing disturbance 5 projected onto the DPCA model of the normal operation (W-0) and the DPCA models of the fifteen disturbances (W-1 to W-15).

cedure for disturbance 11 (i.e. disturbance 11 impacts the process after one hour). Q plots for each of the models appear in Fig. 15. In this case, all models except disturbances 4 and 11 are quickly rejected as possible disturbance sources. While the Q plot for disturbance 4 appears to show a higher alarm rate than that of disturbance 11, further investigation may be necessary in this case. However, note that both disturbance 4 and 11 represents a disturbance in the reactor cooling water inlet temperature. The source of the disturbance can be isolated in this case as well. In contrast, the static PCA method could not give a clear isolation among disturbances 4, 11, and 14 [4]. Consequently, the dynamic PCA method shows better isolation in rejection of disturbance models W-4 and W-14 than charts developed by the static PCA method.

In the final example, the process simulation is run so that disturbance 16 impacts the process after one hour. Disturbance 16 is of unknown origin and has not yet been incorporated into the model bank. Q plots for each of the 16 models in the model bank appear in Fig. 16. In this case observations from the process are not consistent with any one model of the known disturbances. The procedure has correctly signaled the presence of a new and previously unaccounted disturbance. Once this disturbance is isolated and identified, then the new model can be added to the model bank for future use.

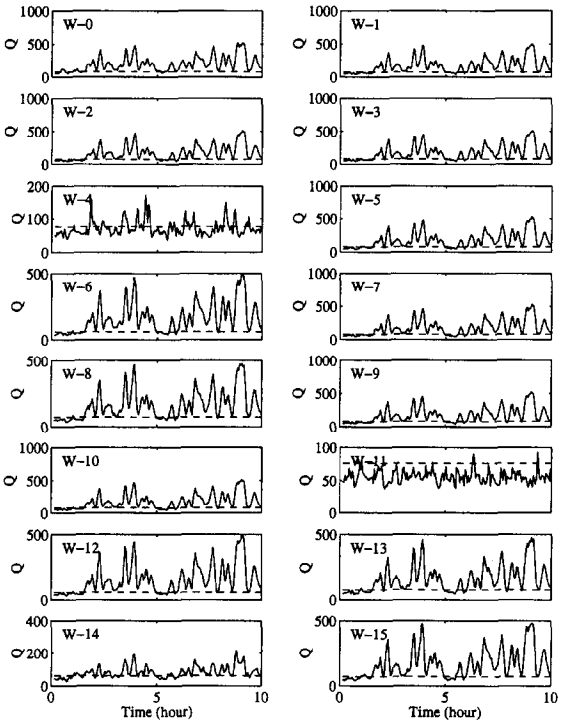

Fig. 15. Q plots of data characterizing disturbance 11 projected onto the DPCA model of the normal operation (W-0) and the DPCA models of the fifteen disturbances (W-1 to W-15).

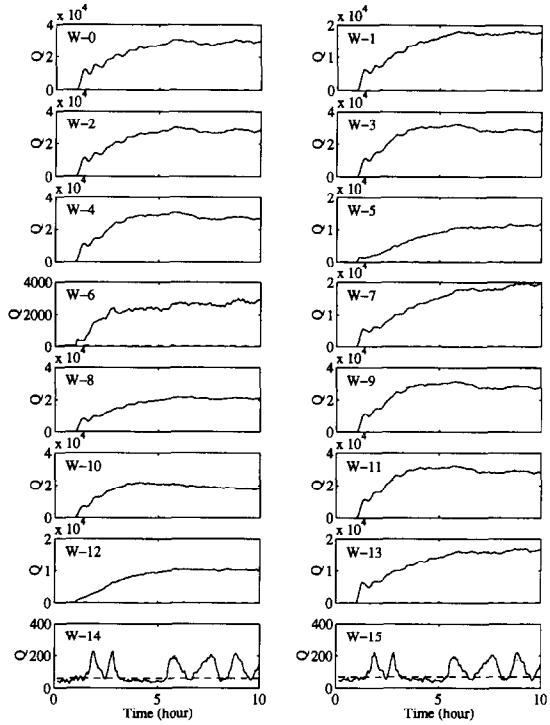

Fig. 16. Q plots of data characterizing disturbance 16 projected onto the DPCA model of the normal operation (W-0) and the DPCA models of the fifteen disturbances (W-1 to W-15).

6. Conclusion

In this paper we have extended the use of PCA models in Statistical Process Monitoring to account for auto-correlation. Using the known approach of augmenting the data matrix $\mathbf{X}(t)$ with time shifted duplicates $\mathbf{X}(t-l)$, we then developed PCA models which incorporate both static and dynamic process characteristics. The developed statistical, denoted by DPCA, charts correctly identify and isolate the several disturbances of the Tennessee Eastman Process.

Motivated by the analysis of some simple dynamic systems, we have also argued that the components related with the smallest amount of variations, usually denoted as noise in the development of the PCA model, are related to static and/or dynamic linear relationship that constrain the different measured variables. Guided by such insight we have proposed a design procedure for developing such DPCA models that focuses attention on the auto- and cross-correlation of the components with the smallest singular values. The data block is shifted further in time until this auto- and cross-correlation is minimized. Use of these charts for the detection and isolation of process disturbances was also demonstrated with the simulated Tennessee Eastman process. Dynamic PCA charts were shown to be better than static PCA charts in detecting the occurrence of small disturbances in a simulated dynamic process as well as in the Tennessee Eastman process.

7. Nomenclature

$\mathbf{A}$	data matrix without noise
$\mathbf{E}$	noise matrix
F	F distribution
$\mathbf{I}$	identity matrix
m	number of samples
n	number of variables
Q	sum of squares of the residuals
r	rank or number of relations
r_{new}	number of new relations
$\mathbf{S}$	covariance matrix
T^2	Hotelling's T-squares
t	time
$\mathbf{U}$	matrix of left singular vectors
$\mathbf{u}$	input vector
$\mathbf{u}_k$	left singular vector
$\mathbf{V}$	matrix of right singular vectors
$\mathbf{v}_k$	right singular vector
$\mathbf{W}$	eigenvectors, loading vectors
$\mathbf{W}_k$	reduced eigenvectors, loading vectors
$\mathbf{w}$	random noise
$\mathbf{X}$	data matrix
$\mathbf{x}$	data vector
$\mathbf{y}$	scores
$\mathbf{z}$	output vector

Greek letters

Λ	eigenvalues matrix
Σ	singular values matrix
σ_k	singular value
σ^2	variances

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