MULTIVARIATE STATISTICAL MONITORING OF NONLINEAR BIOLOGICAL PROCESSES USING KERNEL PCA

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Abstract: In this paper, a new nonlinear process monitoring technique based upon kernel principal component analysis (KPCA) is developed. In recent years, KPCA has been emerging to tackle the nonlinear monitoring problem. KPCA can efficiently compute principal components in high dimensional feature spaces by the use of integral operator and nonlinear kernel functions. The basic idea of KPCA is to first map the input space into a feature space via nonlinear mapping and then compute the principal components in that feature space. In comparison to other nonlinear PCA techniques, KPCA requires only the solution of an eigenvalue problem without any nonlinear optimization. Based on T^2 and *SPE* charts in the feature space, KPCA was applied to fault detection in the simulation benchmark of the biological wastewater treatment process (WWTP). The proposed approach can effectively capture the nonlinear relationship in process variables and its application for process monitoring shows better performance than PCA.

Keywords: Biological wastewater treatment; Fault detection; Fault diagnosis and monitoring; Feature space; Kernel principal component analysis (KPCA); Kernel function; Nonlinear process monitoring

1. INTRODUCTION

Monitoring and fault diagnosis of chemical or environmental processes are very important in process system engineering since the goal of them is 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 these variables are recorded in abundance per day. Such data sets are highly correlated and are subject to considerable noise. In the absence of an appropriate processing method, only limited information is extracted, which causes the plant operators to badly understand the process and leads to unstable operation. However, if properly treated, this data can provide a wealth of information leading to keep the plant operators understand the status of the process and assist them to make appropriate actions to remove abnormalities resulting from the process.

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 and Gallagher, 1996; Dong and McAvoy, 1996). PCA is the most widely used data-driven technique for process monitoring since it can handle high dimensional, noisy, and highly correlated data by projecting the data onto a lower dimensional subspace which contains most of the variance of the original data (Wise and Gallagher, 1996). The lower-dimensional representations of the data produced by PCA can improve

the proficiency of detecting and diagnosing faults using multivariate statistics. However, for some complicated cases in industrial chemical and environmental processes which especially have nonlinear characteristics, PCA exhibits bad behavior because of its linearity assumption (Dong and McAvoy, 1996).

One classic way of including nonlinearity in the PCA is to include cross-products of variables as well as nonlinear transformations of variables. The nonlinear mapping function would be ideal to be a linearising transform which reflects the process with first exploiting one's knowledge of the physics and chemistry of the process to create meaningful. But this method needs to specify a nonlinearity shape in advance which has a specific transformation to each process. Kramer (1991) presented a nonlinear principal component analysis based on auto-associative neural networks. However, the network is difficult to train since it has five layers. To determine the number of nodes in each layer is difficult, too. Dong and McAvoy (1996) have developed a nonlinear PCA approach based on principal curves and neural networks. However, the principal curve method assumes that the nonlinear function can be approximated by a linear combination of several univariate functions and thus it can be decomposed as the sum of the functions of the individual variables. These mappings only represent a limited class of nonlinear models and thus the principal curve algorithm is restricted to identifying structures which exhibit additive type behavior (Jia *et al*., 2001).

In recent years, a new nonlinear PCA technique, called kernel principal component analysis (KPCA) has been emerging to tackle the nonlinear problem (Schölkopf *et al.*, 1998). The basic idea of KPCA is to first map the input space into a feature space via nonlinear mapping and then compute the principal component in that feature space. Given any algorithm which can be expressed solely in terms of dot products, i.e. without explicit usage of the variables themselves, this kernel method enables us to construct different nonlinear versions of it (Christianini and Shawe-Taylor, 2000). Compared to other nonlinear methods, KPCA has the main advantage that no nonlinear optimization is involved (Schölkopf *et al.*, 1998). It is essentially linear algebra, as simple as standard PCA. It requires only the solution of an eigenvalue problem, and by the possibility to use different kernels, it comprises a fairly general class of nonlinearities that can be used. In addition, KPCA does not require that the number of components to be extracted be specified prior to modeling. Based on these merits, KPCA has shown better performance than linear PCA in feature extraction and classification including nonlinearity (Schölkopf *et al.*, 1998).

As shown in Fig. 1 (Romdhani *et al.*, 1999), conceptually, KPCA performs a nonlinear mapping $\Phi(\cdot)$ from an input vector $\mathbf{x}$ to a high dimensional feature space F. Then, a linear PCA is performed in this feature space, which gives score values t_k in a lower p dimensional KPCA space. However, the KPCA method of Schölkopf *et al.* (1998) provides only nonlinear principal components and does not provide any reconstruction method of the data in the feature space. Thus, there is a problem to apply it directly to process monitoring since the monitoring chart based on squared prediction error (*SPE*) can not be considered.

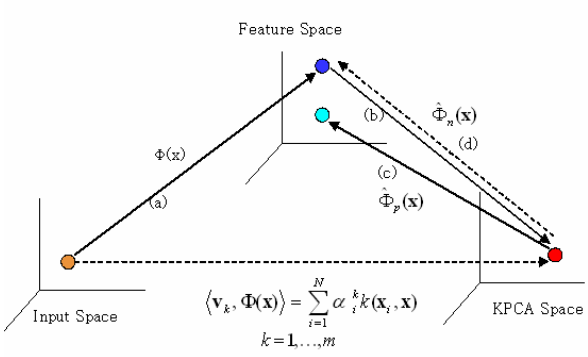

Fig. 1. Conceptual diagram of KPCA.

In this paper, we propose a new nonlinear process monitoring technique based upon KPCA. The monitoring charts of T^2 and *SPE* are made in the feature space. The superiority of process monitoring using KPCA is illustrated through an example of the wastewater simulation benchmark.

2. THEORY

2.1 Kernel principal component analysis (KPCA)

The key idea of KPCA is both intuitive and generic. In general, PCA can only be effectively performed on a set of observations that vary linearly. When the variations are nonlinear, they can always be mapped into a higher dimensional space which is again linear. This higher dimensional linear space is referred to as the *feature space* (F). KPCA finds a computationally tractable solution through a simple kernel function which intrinsically constructs a nonlinear mapping from the input space to the feature space. As a result, KPCA performs a nonlinear PCA in the input space (Romdhani *et al.*, 1999).

If a PCA is aimed at decoupling nonlinear correlations among a given set of data (with zero mean) in the input space, $\mathbf{x}_k \in R^m$, $k = 1, \ldots, N$ through diagonalising their covariance matrix, the covariance can be expressed in a linear feature space F instead of the nonlinear input space, i.e.

$$\mathbf{C}^F = \frac{1}{N} \sum_{j=1}^{N} \Phi(\mathbf{x}_j) \Phi(\mathbf{x}_j)^T \qquad (1)$$

where $\Phi(\cdot)$ is a nonlinear mapping function which projects the input vectors from the input space to the *feature space*, F. Note that the feature space could have an arbitrarily large or possibly infinite dimensionality (Schölkopf *et al.*, 1998). To diagonalise the covariance matrix, one has to solve the eigenvalue problem in the feature space

$$\lambda \ \mathbf{v} = \mathbf{C}^F \mathbf{v} \tag{2}$$

where eigenvalues $\lambda \geq 0$ and $\mathbf{v} \in F \setminus \{\mathbf{0}\}$. The $\mathbf{v}$ along with the largest λ obtained by Eq. (2) become the first principal component and the $\mathbf{v}$ along with the smallest λ become the last principal component in feature space, F. Here, $\mathbf{C^F v}$ can be represented as follows

$$\mathbf{C}^F \mathbf{v} = \left(\frac{1}{N} \sum_{j=1}^{N} \Phi(\mathbf{x}_j) \Phi(\mathbf{x}_j)^T \right) \mathbf{v} = \frac{1}{N} \sum_{j=1}^{N} \left\langle \Phi(\mathbf{x}_j), \mathbf{v} \right\rangle \Phi(\mathbf{x}_j) \tag{3}$$

where $\langle \mathbf{x}, \mathbf{y} \rangle$ means dot product between $\mathbf{x}$ and $\mathbf{y}$. This implies that all solutions $\mathbf{v}$ with $\lambda \neq 0$ must lie in the span of $\Phi(\mathbf{x}_1), \ldots, \Phi(\mathbf{x}_N)$. Hence, $\lambda \ \mathbf{v} = \mathbf{C}^F \mathbf{v}$ is equivalent to

$$\lambda \ \left\langle \Phi(\mathbf{x}_k), \mathbf{v} \right\rangle = \left\langle \Phi(\mathbf{x}_k), \mathbf{C}^F \mathbf{v} \right\rangle, \quad k = 1, \ldots, N \tag{4}$$

and there exist coefficients $\alpha_i \ (i = 1, \ldots, N)$ such that

$$\mathbf{v} = \sum_{i=1}^{N} \alpha_i \ \Phi(\mathbf{x}_i) \tag{5}$$

Combining Eq. (4) and Eq. (5), we have

$$\lambda \sum_{i=1}^{N} \alpha_i \left\langle \Phi(\mathbf{x}_k), \Phi(\mathbf{x}_i) \right\rangle = \frac{1}{N} \sum_{i=1}^{N} \alpha_i \left\langle \Phi(\mathbf{x}_k), \sum_{j=1}^{N} \Phi(\mathbf{x}_j) \right\rangle \left\langle \Phi(\mathbf{x}_j), \Phi(\mathbf{x}_i) \right\rangle \tag{6}$$

for all k=1,…,N. Note that the eigenvalue problem in Eq. (6) only involves dot products of mapped shape vectors in the feature space. In general, the mapping $\Phi(\cdot)$ may not always be computationally tractable, although it exists. However, it need not be explicitly computed; only dot products of two vectors in the feature space are needed.

Now, let's define an $N \times N$ matrix $\mathbf{K}$ by $[\mathbf{K}]_{ij} = K_{ij} = \left\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \right\rangle$. Then the left term of Eq. (6) can be described as

$$\lambda \sum_{i=1}^{N} \alpha_i \left\langle \Phi(\mathbf{x}_k), \Phi(\mathbf{x}_i) \right\rangle = \lambda \sum_{i=1}^{N} \alpha_i K_{ki} \tag{7}$$

Since $k = 1, \ldots, N$, Eq. (7) becomes $\lambda \mathbf{K}\boldsymbol{\alpha}$. The right term of Eq. (6) can be written as

$$\frac{1}{N} \sum_{i=1}^{N} \alpha_i \left\langle \Phi(\mathbf{x}_k), \sum_{j=1}^{N} \Phi(\mathbf{x}_j) \right\rangle \left\langle \Phi(\mathbf{x}_j), \Phi(\mathbf{x}_i) \right\rangle = \frac{1}{N} \sum_{i=1}^{N} \alpha_i \sum_{j=1}^{N} K_{kj} K_{ji} \tag{8}$$

Since $k = 1, \ldots, N$, Eq. (8) becomes $\mathbf{K}^2\boldsymbol{\alpha}/N$. Combining Eq. (7) and Eq. (8), we have

$$\lambda \ N\mathbf{K}\boldsymbol{\alpha} = \mathbf{K}^2\boldsymbol{\alpha} \tag{9}$$

where $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_N]^T$. To find solutions of Eq. (9), we solve the eigenvalue problem

$$N\lambda \ \boldsymbol{\alpha} = \mathbf{K}\boldsymbol{\alpha} \tag{10}$$

for nonzero eigenvalues. A justification of this procedure is given in Schölkopf's paper (1998). Now, performing PCA in the feature space F is equal to resolving the eigen-problem of (10). This yields eigenvectors $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_N$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$. Dimensionality can be reduced by retaining only the first p eigenvectors. We normalize $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_p$ by requiring that the corresponding vectors in F be normalized, i.e.,

$$\left\langle \mathbf{v}_k, \mathbf{v}_k \right\rangle = 1 \ \text{ for all } k=1,\ldots,p. \tag{11}$$

Using $\mathbf{v}_k = \sum_{i=1}^{N} \alpha_i^k \ \Phi(\mathbf{x}_i)$, Eq. (11) leads to

$$1 = \left\langle \sum_{i=1}^{N} \alpha_i^k \Phi(\mathbf{x}_i), \sum_{j=1}^{N} \alpha_j^k \Phi(\mathbf{x}_j), \right\rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^k \alpha_j^k \left\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \right\rangle \tag{12}$$
$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i^k \alpha_j^k K_{ij} = \left\langle \boldsymbol{\alpha}_k, \mathbf{K}\boldsymbol{\alpha}_k \right\rangle = \lambda_k \left\langle \boldsymbol{\alpha}_k, \boldsymbol{\alpha}_k \right\rangle$$

The principal components $\mathbf{t}$ of a test vector $\mathbf{x}$ are then extracted by projecting $\Phi(\mathbf{x})$ onto eigenvectors $\mathbf{v_k}$ in F where k=1,…,p.

$$t_k = \left\langle \mathbf{v}_k, \Phi(\mathbf{x}) \right\rangle = \sum_{i=1}^{N} \alpha_i^k \left\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}) \right\rangle \tag{13}$$

To solve the eigen-problem of Eq. (10) and to project from the input space to the KPCA space using Eq. (13), one can avoid the needs for performing the nonlinear mappings and computing both the dot products in the feature space through introducing a *kernel function*, that is, $k(\mathbf{x}, \mathbf{y}) = \left\langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \right\rangle$ (Schölkopf *et al.*, 1998; Romdhani, Gong, and Psarrou, 1999).

There exist a number of kernel functions. According to Mercer's theorem of functional analysis, there exists a mapping into a space where a kernel function acts as a dot product if the kernel function is a continuous kernel of a positive integral operator. So the requirement on the kernel function is to satisfy Mercer's theorem (Christianini and Shawe-Taylor, 2000). Representative kernel functions are as follows

Polynomial kernel: $k(\mathbf{x}, \mathbf{y}) = \left\langle \mathbf{x}, \mathbf{y} \right\rangle^d$ (14)

Sigmoid kernel: $k(\mathbf{x}, \mathbf{y}) = \tanh\left(\beta_0 \left\langle \mathbf{x}, \mathbf{y} \right\rangle + \beta_1 \right)$ (15)

Radial basis kernel: $k(\mathbf{x}, \mathbf{y}) = \exp\left(- \frac{\|\mathbf{x} - \mathbf{y}\|^2}{c} \right)$ (16)

where d,β_0, β_1 and c are specified a priori by the user. The polynomial kernel and radial basis kernel always satisfy Mercer's theorem while the sigmoid kernel satisfies it only for some values of β_0 and β_1 (Hasykin, 1999). These kernel functions effectively provide a low dimensional KPCA subspace which represents the distributions of the mapping of the training vectors in the feature space. A specific choice of kernel function implicitly determines the mapping and the feature space F. If one have a nonlinear information (shape) of process, it could be used to select the kernel function among kernels in KPCA.

Before applying KPCA, mean centering in high-

dimensional space should be performed. This can be done by substituting the kernel matrix **K**with

$$\widetilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N \quad (17)$$

where $\mathbf{1}_N = \frac{1}{N}\begin{vmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{vmatrix} \in R^{N\times N}$. For details, see the paper of Schölkopf *et al.*(1998).

2.2 On-line monitoring strategy of KPCA

Based on the merits of KPCA, a new monitoring method is presented in this section. The monitoring method of KPCA is similar to that of PCA, i.e. Hotelling's T^2 statistic and the Q-statistic in the feature space can be interpreted in the same way.

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

$$T^2 = [t_1,\ldots,t_p]\Lambda^{-1}[t_1,\ldots,t_p]^T \quad (18)$$

where t_k is obtained from Eq. (13) and $\mathbf{\Lambda}^{-1}$ is the diagonal matrix of the inverse of the eigenvalues associated with the retained principal components. The confidence limit for T^2 is obtained using the *F*-distribution.

$$T^2_{p,N,\alpha} \sim \frac{p(N-1)}{N-p}F_{p,N-p,\alpha} \quad (19)$$

where *N* is the number of samples in the model and *p* is the number of principal components.

On the other hand, the measure of goodness of fit of a sample to the PCA model is the squared prediction error (*SPE*), also known as the *Q* statistic. Unfortunately, the KPCA method of Schölkopf *et al.*(1998) only provides nonlinear principal components and does not provide any reconstruction method of the data in the feature space. So, there is a problem to make *SPE* monitoring chart. In this paper, a simple calculation of *SPE* in the feature space is suggested.

In order to reconstruct a feature vector $\Phi(\mathbf{x})$ from t_k, t_k is projected into the feature space via $\mathbf{v}_k$ giving a reconstructed feature vector $\hat{\Phi}_n(\mathbf{x}) = \sum_{k=1}^{n} t_k\mathbf{v}_k$. Then *SPE* in the feature space is defined as $SPE = \left\|\Phi(\mathbf{x}) - \hat{\Phi}_p(\mathbf{x})\right\|^2$. Here, $\Phi(\mathbf{x})$ is identical to $\hat{\Phi}_n(\mathbf{x}) = \sum_{k=1}^{n} t_k\mathbf{v}_k$ if *p* equals *n* where *n* is the number of nonzero eigenvalues generated from Eq. (10) among *N*. The confidence limit for the *SPE* can be computed from its approximate distribution

$$SPE_\alpha \sim g\chi^2_h \quad (20)$$

The control limits for the *SPE* are based on Box's equation and are obtained by fitting a weighted χ^2-distribution to the reference distribution obtained from the normal operating condition data. In Eq. (20), parameter *g* represents the weight to account for the magnitude of *SPE* and parameter *h* for the degrees of freedom. Let *a* and *b* be the estimated mean and variance of the *SPE*, then the *g* and *h* are approximated by $g = b/2a$ and $h = 2a^2/b$. Note that the method of matching moments may go wrong when the number of observations is small and there are outliers in the data. So, it is necessary to select the reference data carefully and abundantly. Furthermore, the use of the chi-square distribution implicitly assumes normality of the errors, which may not always be true in practice.

2.3 Outline of on-line KPCA monitoring

<u>*Developing the normal operating condition (NOC) model*</u>

1) Acquire normal operating data and normalize the data using the mean and the standard deviation of each variable.

2) Given a set of *m*-dimensional scaled normal operating data $\mathbf{x}_k \in R^m$, $k = 1,\ldots,N$, we compute the kernel matrix $\mathbf{K} \in R^{N\times N}$ by $[\mathbf{K}]_{ij} = K_{ij} = \langle\Phi(\mathbf{x}_i),\Phi(\mathbf{x}_j)\rangle = [k(\mathbf{x}_i,\mathbf{x}_j)]$.

3) Carry out mean centering in the feature space

$$\widetilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N \quad (21)$$

where $\mathbf{1}_N = \frac{1}{N}\begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \in R^{N\times N}$.

4) Solve the eigenvalue problem $N\lambda\,\boldsymbol{\alpha} = \widetilde{\mathbf{K}}\boldsymbol{\alpha}$ and normalize $\boldsymbol{\alpha}_k$ such that $\langle\boldsymbol{\alpha}_k,\boldsymbol{\alpha}_k\rangle = \frac{1}{\lambda_k}$.

5) For normal operating data $\mathbf{x}$, extract a nonlinear component via

$$t_k = \left\langle \mathbf{v}_k, \widetilde{\Phi}(\mathbf{x})\right\rangle = \sum_{i=1}^{N}\alpha_i^k\left\langle\widetilde{\Phi}(\mathbf{x}_i),\widetilde{\Phi}(\mathbf{x})\right\rangle = \sum_{i=1}^{N}\alpha_i^k\widetilde{k}(\mathbf{x}_i,\mathbf{x}) \quad (22)$$

6) Calculate the monitoring statistics (T^2 and *SPE*) of the normal operating data

7) Determine control limits of the T^2 and *SPE* charts

<u>*On-line monitoring*</u>

1) Obtain new data for each sample and scale it with the mean and the variance obtained at step 1 of the modeling procedure.

2) Given the *m*-dimensional scaled test data $\mathbf{x}_t \in R^m$, compute the kernel vector $\mathbf{k}_t \in R^{1\times N}$ by $[\mathbf{k}_t]_j = [k_t(\mathbf{x}_t,\mathbf{x}_j)]$ where $\mathbf{x}_j$ is the normal operating data $\mathbf{x}_j \in R^m$, $j = 1,\ldots,N$.

3) The test kernel vector $\mathbf{k}_t$ is mean centered as follows;

$$\widetilde{\mathbf{k}}_t = \mathbf{k}_t - \mathbf{1}_t\mathbf{K} - \mathbf{k}\mathbf{1}_N + \mathbf{1}_t\mathbf{K}\mathbf{1}_N \quad (23)$$

where $\mathbf{K}$ and $\mathbf{1}_N$ are obtained from step 2 of the modeling procedure and $\mathbf{1}_t = \frac{1}{N}[1,\ldots,1] \in R^{1\times N}$.

4) For the test data $\mathbf{x}_t$, extract a nonlinear component via

$$t_k = \left\langle \mathbf{v}_k, \tilde{\Phi}(\mathbf{x}_t) \right\rangle = \sum_{i=1}^{N} \alpha_i^k \left\langle \tilde{\Phi}(\mathbf{x}_i), \tilde{\Phi}(\mathbf{x}_t) \right\rangle = \sum_{i=1}^{N} \alpha_i^k \tilde{k}_t(\mathbf{x}_i, \mathbf{x}_t) \quad (24)$$

5) Calculate the monitoring statistics (T^2 and *SPE*) of the test data.
6) Monitor whether T^2 or *SPE* exceeds its control limit calculated in the modeling procedure.

3. RESULTS

In this section, the proposed monitoring method was applied to fault detection in the simulation benchmark of the biological wastewater treatment process (WWTP) and monitoring results of PCA and KPCA are compared. In this paper, a radial basis kernel function, is selected as a kernel function with $c = rm\sigma^2$, where r is a constant value which should be determined according to the considered process, m equals the dimension of the input space and σ^2 is the variance of the data (Schölkopf *et al*., 1998). After testing the monitoring performance for different values of r, we have found that $c = 10m\sigma^2$ is most appropriate to monitor a process with various faults. Although the value c is dependent upon the system under study, we recommend the radial basis kernel function as a representative kernel function for the KPCA process monitoring.

When designing the PCA model, we must determine the number of principal components. This number should be determined considering both the curse of dimensionality and loss of data information. For linear PCA, we used a cross validation method (Wise, 1996) based on PRESS to determine the number of PC in this research. The cross validation method may also be available for KPCA but it needs a high computational load. For KPCA, the cut-off method using the average eigenvalue is used to determine the number of PCs due to its simplicity and robustness. This criterion accepts all eigenvalues with values above the average eigenvalue and rejects those below the average (Valle *et al.*, 1999). In general, the selected number of PCs for KPCA is larger than the number of PCs for linear PCA since KPCA extracts the major PCs from the infinite high dimensional feature space while the linear PCA extracts major PCs from the finite input dimensional space. According to Schölkopf *et al*. (1999), KPCA has the potential to utilize more PCs to code structure rather than noise; hence, KPCA outperforms linear PCA in denoising if a sufficiently large number of PCs is used.

The KPCA monitoring algorithms proposed here was tested for its ability to detect small internal disturbances in simulated data obtained from a '*benchmark simulation*' of the WWTP (Spanjer *et al.*, 1998).The Activated Sludge Model No. 1 (ASM1) and a ten-layer settler model were used to simulate the biological reactions and the settling process, respectively. The training model was based on a normal operation period of one week of dry weather and validation data was used on data set for two weeks dry weather condition. The sampling time was 15 minutes and hence each daily period consists of 96 samples. Seven variables of influent ammonia, influent flow rate, total suspended solids in reactor 4, dissolved oxygen in reactor 3 and 4, oxygen transfer coefficient in reactor 5 and nitrate concentration in reactor 2 were selected to build the monitoring system among the many variables used in the benchmark because they are typically monitored and important variables in real WWTP systems.

In the present work, deterioration of nitrification was simulated as the internal disturbance (Yoo *et al*., 2002). A deteriorating nitrification rate can strongly affect the performance of the activated sludge, and it is important to detect it early on. Although other methods exist to measure the nitrification rate, *e.g.* by respirometry, this parameter cannot be measured in an easy way (Vanrolleghem and Gillot, 2001). However, PCA or KPCA can be used to monitor the process since this drift affects process measurements. The internal disturbance was imposed by decreasing the nitrification rate in the biological reactor through a decrease in the specific growth rate of the autotrophs bacteria (μ_A). Two types of disturbance are considered: a step decrease and a linear decrease. In the step decrease case, at sample 288 the autotrophic growth rate was decreased rapidly from 0.5 to 0.44 day^{-1}. In the linear decrease case, from sample 288 the autotrophic growth rate changed from 0.5 to 0.4 over 2 days (192 samples) and the value of 0.4 lasted to the end.

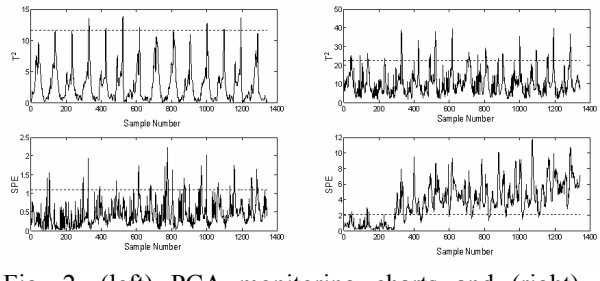

Fig. 2. (left) PCA monitoring charts and (right) KPCA monitoring charts for the case of a step decrease in the nitrification rate.

Fig. 2 compares the monitoring results of linear PCA and KPCA for a step decrease case. The linear PCA model was able to capture most of the variability of the **X**-block by three PCs selected from cross validation. However, it is clear from the T^2 and *SPE* charts shown in Fig. 2(left) that the PCA method with 3 PCs fails to detect the internal disturbance because the periodic and nonlinear features of the wastewater treatment plant dominate. The T^2 and *SPE* charts of the PCA method show periodic and non-stationary features originating from the fluctuations in the influ-

ent load, which is characterized by strong diurnal changes in the flow rate and composition of the feed waste stream. This non-stationary (periodic) behavior of T^2 score values in the PCA model is the cause of false alarms and missed faults due to the resulting widened confidence limit (Yoo *et al*., 2002). In contrast to the PCA result, the *SPE* chart of the KPCA monitoring with 9 PCs selected from the average eigenvalue approach, given in Fig. 2(right), successfully detects the internal disturbance from sample 288 onwards, which represents almost 100% detection without a delay. In contrast, the T^2 chart detects the disturbance only at some samples.

Fig. 3 shows the monitoring results for the case of a linear decrease of nitrification rate. The T^2 chart of PCA in Fig. 3(left) hardly reveals the change while the *SPE* chart shows a distinct change from about sample 390, a delay of about 102 samples. Furthermore, in the *SPE* chart, there are some samples below the 99% control limit even when the fault is already present. The KPCA monitoring charts are shown in Fig. 3(right) for the case of the same disturbance. The *SPE* chart of the KPCA can detect it from about sample 318, which is faster than that of PCA by 72 samples. Furthermore, in the *SPE* chart, there are few samples for the fault data below the 99% control limit. Abnormality is also detected in the T^2 chart of KPCA though the detectability is lower than that of the *SPE* chart. Overall, the scores extracted from KPCA efficiently distinct a fault from normal operating data.

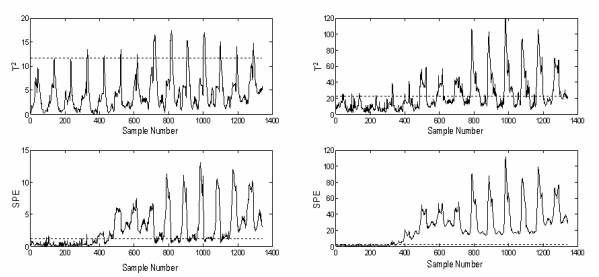

Fig. 3. (left) PCA monitoring charts and (right) KPCA monitoring for the case of a linear decrease in the nitrification rate.

4. CONCLUSIONS

This paper proposes a new approach to process monitoring that uses KPCA to achieve multivariate statistical process control. KPCA can efficiently compute principal components in high dimensional feature spaces by the use of integral operator and nonlinear kernel functions. Compared to other nonlinear methods, KPCA has the following main advantages: no nonlinear optimization is involved, it involves simple calculations as in standard PCA and the number of PCs needs not to be specified in advance. The simulation result demonstrates that KPCA can effectively capture the nonlinear relationship in process variables and its application for process monitoring shows better performance than PCA. If the process has serially correlated (dynamic) as well as nonlinear data, a dynamic KPCA monitoring that uses an augmenting matrix with time-lagged variables (Ku et al., 1995) can be used.

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