Applied Mathematics & Information Sciences
An International Journal

http://dx.doi.org/10.12785/amis/090421

New Adaptive Kernel Principal Component Analysis for Nonlinear Dynamic Process Monitoring

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Received: 22 Oct. 2014, Revised: 22 Jan. 2015, Accepted: 23 Jan. 2015
Published online: 1 Jul. 2015

Abstract: In this paper a new algorithm for adaptive kernel principal component analysis (AKPCA) is proposed for dynamic process monitoring. The proposed AKPCA algorithm combine two existing algorithms, the recursive weighted PCA (RWPCA) and the moving window kernel PCA algorithms. For fault detection and isolation, a set of structured residuals is generated by using a partial AKPCA models. Each partial AKPCA model is performed on subsets of variables. The structured residuals are utilized in composing an isolation scheme, according to a properly designed incidence matrix. The results for applying this algorithm on the nonlinear time varying processes of the Tennessee Eastman shows its feasibility and advantageous performances.

Keywords: Kernel PCA, dynamic process, fault detection and isolation, residual structuration, partial PCA model.

1 Introduction

Engineers are often confronted with the problem of extracting information about poorly-known processes from data [1]. Recently, with the development of measurement and data storage equipment, it is strongly required to use multivariate statistical method for extracting useful information from a large amount of process data [2]. Principal Component Analysis (PCA) is a multivariate statistical method that can be used for process monitoring. The basic strategy of PCA is to extracts linear structure from high dimensional data by finding new principal axes. PCA divides data systematically into two parts, the first part is the data with wide variation and the second part is the data with the least variance, which is noisy. A major limitation of PCA based monitoring is that the model, once built from the data, is time invariant, while most real industrial processes are time varying. The time varying characteristics of industrial processes include: (i) changes in the mean, (ii) changes in the variance, and (iii) changes in the correlation structure among variables, including changes in the number of significant principal components (PCs).

To address the challenge, several adaptive PCA schemes have been proposed [30,13]. The principle behind the moving window (MW) is well known. As the window slides along the data, a new process model is generated by including the newest sample and excluding the oldest one. Recursive techniques, on the other hand, update the model for an ever increasing data set that includes new samples without discarding old ones. It offers efficient computation by updating the process model using the previous model rather than completely building it from the original data. Recursive PCA (RPCA) allows older samples to be discarded in favor of newer ones that are more representative of the current process operation. Wold et al [31] and Gallagher et al [29] introduced the use of exponentially weighted moving average (EWMA), exponentially weighted moving covariance (EWMC), and exponentially weighted moving PCA (EWM-PCA). This is achieved by updating the process model at each time when a new vector of measurements becomes available. The past vectors of process measurements are then exponentially weighted in time so that the influence of the most recent measurements is the greatest.

In some complicated cases in industrial processes with particular nonlinear characteristics, PCA performs poorly due to its assumption that the process data are linear. Principal Component Analysis is in its nature a linear transformation, which degrades its performance for handling non linear systems. To cope with this problem, several non linear extensions of PCA have been

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developed, which allows extracting both linear and non linear correlation among process variables. An elegant and one of the most widely used non linear generalization of the linear PCA is the kernel principal component analysis (KPCA), which was proposed in 1998 by Scholkopf et al. in [3] and first employed as a monitoring tool by Lee et al. in [14]. It has the following advantages over previous versions of nonlinear PCA: (i) unlike nonlinear PCA methods based on neural networks, it does not include the determination of the number of nodes, layers and approximation for the nonlinear function. (ii) kernel PCA does not involve a nonlinear optimization procedure. Despite recently reported KPCA-based monitoring applications, the following problems arise : the monitoring model is fixed which may produce false alarms if the process is naturally time-varying, and the fault isolation step is a much more difficult problem in nonlinear PCA than in linear PCA [8,9]. The first problem has been addressed by a recursive KPCA formulation to overcome the same problems of the linear case, presented in the previous paragraph.

The kernel PCA method based process monitoring have recently shown to be very effective for online monitoring nonlinear processes. Similar to the linear case, two methods are presented in the literature for nonlinear adaptive process monitoring. As the moving window kernel PCA (MWKPCA) and the recursive kernel PCA (RKPCA) approaches, where, little research have been presented on this issue. A variable moving window kernel PCA scheme is presented by Khediri et al. in [11]. This method is then applied in a monitoring procedure with a variable window size model that can provide a flexible control strategy. Recursive kernel PCA algorithm is presented by Liu et al. in [15], the proposed technique incorporates an up-and down-dating procedure to adapt the data mean and covariance matrix in the feature space.

In this work, a new adaptive kernel principal component analysis (AKPCA) algorithm is introduced to monitor and diagnose nonlinear dynamic systems. The AKPCA algorithm allow to update recursively the kernel PCA model and its corresponding control limits for monitoring statistics. The basic idea of the proposed algorithm refers to a paradigm where, at each time instant, a new observation is available, and the covariance matrix in the feature space (Gram matrix) need to be recursively updated according to the newly available data. The adaptive KPCA algorithm update the covariance matrix in the feature space with the degree of change in the operating process, which depend on the magnitude of the forgetting factor.

The paper is organized as follows : In section 2 linear principal component analysis and kernel principal component analysis are presented. Section 3 gives the adaptive version of the proposed KPCA approach. Section 4 gives the residual generation based on the AKPCA for fault detection and isolation. Results of simulation studies performed on the Tennessee Eastman process are presented in section 5. Finally, conclusions are given in section 6.

2 Preliminaries

2.1 Principal Component Analysis (PCA)

PCA is a powerful dimension-reducing technique. It produces new variables that are uncorrelated with each other and are linear combinations of original variables [6]. Let X represent a $N\times m$ matrix of data. PCA is an optimal factorization of X into matrix T (principal components $N\times l$) and P (loadings $m\times l$) plus a matrix of residuals E ($N\times m$).

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

where l is the number of factors $(l < m)$. The Euclidean norm of the residual matrix E must be minimized for a given number of factors. This criterion is satisfied when the columns of P are eigenvectors corresponding to the l largest eigenvalues of the covariance matrix of X. PCA can be viewed as a linear mapping from $\Re^m$ to a lower dimensional space $\Re^l$. The mapping has the form :

$$t = P^T X \tag{2}$$

When using linear PCA the variables involved should be linearly correlated. If they are correlated nonlinearly it is more powerful to use the nonlinear principal component analysis (NLPCA) for data modeling [19].

2.2 Kernel PCA (KPCA)

As a nonlinear extension of PCA, kernel PCA was proposed in [5] to generalize PCA to the nonlinear case by nonlinearly mapping input samples to a higher or infinite dimensional feature space F and performing PCA there. The feature space F is nonlinearly transformed from input space and implicitly defined by a kernel function. However, unlike other forms of nonlinear PCA, the implementation of kernel PCA relies on linear algebra. We may therefore think of kernel PCA as a natural extension of ordinary PCA.

Let vector $\Phi(X_j)$ denote the image of an input vector (X_j) induced in a feature space defined by the nonlinear map : $\Phi : R^{m_0} \rightarrow R^{m_1}$, where m_0 is the dimensionality of the input space and m_1 is the dimensionality of the feature space. Given the set of examples $\{X_i\}_{i=1}^N$, where the a corresponding set of feature vectors $\{\Phi(X_i\}_{i=1}^N$. Accordingly, we may define an $m_1 - by - m_1$ correlation matrix in the feature space, denoted by $\tilde{R}$, as follows :

$$\tilde{R} = \frac{1}{N}\sum_{i=1}^{N} \Phi(X_i)\Phi^T(X_i) \tag{3}$$

As with ordinary PCA, the first thing we have to do is to ensure that the set of feature vectors $\{\Phi(X_i\}_{i=1}^{N}$ has zero mean :

$$\frac{1}{N}\sum_{i=1}^{N}\Phi(X_i)=0 \tag{4}$$

To satisfy this condition in the features space is a more difficult proposition than it is in the input space. A principal component v is then computed by solving the eigenvalue problem :

$$\tilde{R}\tilde{q}=\tilde{\lambda}\tilde{q} \tag{5}$$

where $\tilde{\lambda}$ is an eigenvalue of the correlation matrix $\tilde{R}$ and $\tilde{q}$ is the associated eigenvector. Now we note that all eigenvectors that satisfy Eq.(5) for $\tilde{\lambda}\neq 0$ lie in the span of the set of feature vectors $\{\Phi(X_j\}_{j}^{N}$.

$$\tilde{q}=\sum_{j=1}^{N}\alpha_j\Phi(X_j) \tag{6}$$

Thus substituting Eq.(3) and Eq.(6) into (5), we obtain :

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_j\Phi(X_i)K(X_i,X_j)=N\tilde{\lambda}\sum_{j=1}^{N}\alpha_j\Phi(X_j) \tag{7}$$

Where $K(X_i,X_j)$ is an inner-product kernel defined in terms of the feature vectors by :

$$K(X_i,X_j)=\Phi^T(X_i)\Phi(X_j) \tag{8}$$

We need to go one step further with Eq.(7) so that the relationship is expressed entirely in terms of the inner-product kernel. To do so, we pre-multiply both sides of Eq.(7) by the transposed vector $\Phi^T(X_k)$.

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_jK(X_k,X_i)K(X_i,X_j)=N\tilde{\lambda}\sum_{j=1}^{N}\alpha_jK(X_k,X_j) \tag{9}$$

Accordingly, we my recast Eq.(9) in the compact matrix form :

$$K^2\alpha\simeq N\tilde{\lambda}K\alpha \tag{10}$$

All solution of this eigenvalue problem that are of interest are equally well represented in the simpler eigenvalue problem :

$$K\alpha=N\tilde{\lambda}\alpha \tag{11}$$

Where the coefficient vector α plays the role of the eigenvector associated with the eigenvalue λ of the kernel matrix K. For extraction of principal components, we need to compute the projection onto the eigenvectors $\tilde{q}_k$ in feature space, as shown by :

$$\tilde{q}_k{}^T\Phi(X)=\sum_{i=1}^{N}\alpha_{k,j}\Phi(X_j)\Phi(X)=\sum_{i=1}^{N}\alpha_{k,j}K(X_j,X) \tag{12}$$

Kernel principal component analysis method have recently shown to be very effective for monitoring nonlinear processes. However, their performance largely depend on the kernel function and currently there is no general rule for kernel selection. Existing methods simply choose the kernel function empirically or experimentally from a given set of candidates. The kernel function plays a central role in KPCA, and a poor kernel choice may lead to significantly impaired performance [20,21]. Regarding the kernel functions, they can be chosen for instance as follows:

- ***Polynomial kernel,***

$$K(x_i,x_j)=(x_i\,.x_j+1)^d \tag{13}$$

where d is a positive integer;

- ***Radial basis function (RBF),***

$$K(x_i,x_j)=\exp(-\left\|x_i-x_j\right\|^2/2\delta^2) \tag{14}$$

where $2\delta^2$ =w is the width of the Gaussian kernel.

The above kernel functions give similar results if appropriate parameters are chosen. The radial basis function may present advantages owing to its flexibility in choosing the associated parameter. For instance, the width of the Gaussian kernel can be very small (<1) or quite large [7].

A major limitation of KPCA-based monitoring is that the KPCA model, once built from the data, is time-invariant, while most real industrial processes are time-varying. The time-varying characteristics of industrial processes include: (i) changes in the correlation structure among variables, (ii) including changes in the number of significant principal components (PCs). When a time-invariant KPCA model is used to monitor processes with the aforementioned normal changes, false alarms often result, which significantly compromise the reliability of the monitoring system.

3 Adaptive Kernel PCA (AKPCA)

When the process operating condition change either, gradually or abruptly, the covariance matrix will not be constant and will need to be updated. In the existing recursive methods, only linear methods were proposed [23,24,25,26]. Because the kernel function is unknown, it is difficult to describe the nonlinear dynamic data structure. Moving Window PCA (MWPCA) as in [23,24], and Exponentially Weighted PCA (EWPCA) as in [25] are two representative adaptive PCA methods. Similar to the linear case, in the moving window kernel PCA algorithm, a data window of fixed length is moved in real time to update the kernel PCA model once a new normal sample is available (see Figure 01).

In [11], the study proposes a variable window real-time monitoring system based on a fast block adaptive KPCA scheme. On the other hand, Li et al in

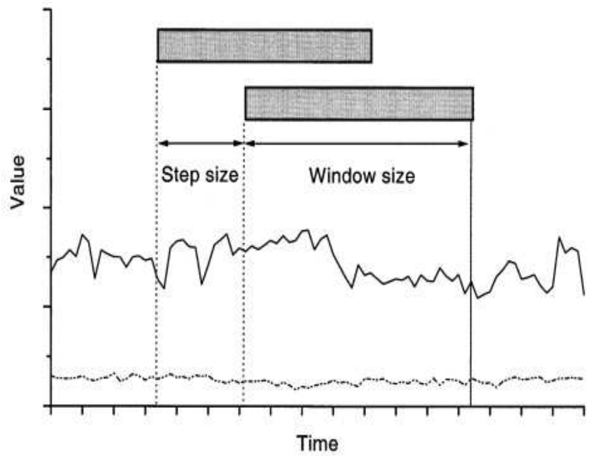

Fig. 1: MWKPCA

[27] introduced a new recursive PCA technique. In this work, we present the same development of WPCA approach and adapt it in the feature space, nonlinear adaptive KPCA. However, the updating rule of the covariance matrix for the linear case $(X^T X)_t$ is carried out as follows :

$$(X^T X)_t = \lambda (X^T X)_{t-1} + (1-\lambda)(x^T x)_t \qquad (15)$$

Here the scaling of the new online vector of process measurements x_t by the factor $(1-\lambda)$ is more in keeping with the traditional multivariate exponentially weighted moving average control chart. An important issue in EWPCA is the choice of the weighting factor. The weighting factor determines the influence that the older data has on the model. The most model updating approaches have used an empirical constant forgetting factor.

When the process changes rapidly, the updating rate should be high, whereas when the change is slow and thus the essential process information is valid for a long period, it should be low. However, it is likely that the rate of process change or variation in real processes vary with time. Choi et al in [13] for the linear case propose a new algorithm to adapt the forgetting factor. In this algorithm two forgetting parameters α and β are used to update the sample mean vector and covariance (or correlation) matrix, respectively. The forgetting factor α for updating the mean vector is calculated as:

$$\alpha_t = \alpha_{\max} - (\alpha_{\max} - \alpha_{\min}) \left[1 - \exp(-k(\frac{\|\Delta m_{t-1}\|}{\|\Delta m_{nor}\|})^n) \right] \qquad (16)$$

Similarly, the forgetting factor β for updating the covariance (or correlation) matrix is given by:

$$\beta_t = \beta_{\max} - (\beta_{\max} - \beta_{\min}) \left[1 - \exp(-k(\frac{\|\Delta R_{t-1}\|}{\|\Delta R_{nor}\|})^n) \right] \qquad (17)$$

Where $\alpha_{\min}$, $\alpha_{\max}$, $\beta_{\min}$, $\beta_{\max}$ are the maximum and minimum forgetting value, respectively, k and n are function parameters, and $\|\Delta x\|$ is the Euclidean vector norm of the difference between two consecutive mean vectors or covariance (correlation) matrix. Here $\|\Delta x_{nor}\|$ is the averaged $\|\Delta x\|$ obtained using historical data.

The proposed AKPCA algorithm combine the MWKPCA and the recursive WPCA algorithms to update online the kernel PCA model and its corresponding control limits. Similarly to the linear case, the covariance matrix in the feature space (gram matrix) is updated as in the equation (15), and the forgetting factors are calculated according to the equation (17). The gram matrix is updated with the degree of change in the model structure being dependent on the magnitude of the forgetting factors [22]. The proposed adaptive kernel PCA algorithm uses the same procedure developed in the linear case of adaptive PCA and adapt it in the feature space of the KPCA. The main idea and the core of the proposed algorithm is described in the algorithm 1.

4 Fault Isolation and Control Chart

4.1 Control Chart (SPE)

For slowly time-varying processes, the confidence limits for the detection indices will change with time, making adaptation of these limits necessary for online monitoring. A complete implementation of AKPCA also requires recursive determination of the number of significant principal components. In this study, the cumulative percent variance (CPV) method is used, which has been usually applied for the determination of the number of principal component (PCs) retained in the model. The CPV is a measure of the percent variance explained by the first PCs [4]:

$$CPV(n_{pc}) = \frac{\sum_{i=1}^{n_{pc}} \lambda_i}{\sum_{i=1}^{M} \lambda_i} \times 100\% \qquad (20)$$

where λ_i is the eigenvalue for each eigenvector. The number of PCs is chosen such that CPV reaches a predetermined value, e.g. 95%.

The *SPE* (squared prediction error) is a statistic that measures the lack of fit of the KPCA model to the data in the feature space. It is a measure of the amount of variation not captured by the principal component model. The *SPE* indicate the extent to which each sample conforms to the KPCA model.

Algorithm 1 Adaptive kernel PCA algorithm

1. ***Off-line Learning :***
   (a)Given an initial standardized block of training data, set PC numbers and kernel parameter.
   (b)Construct the kernel matrix K and scale it $(\bar{\mathsf{K}}_0)$.
   (c)Estimate the initial KPCA model (the eigen values and vectors of the $\bar{\mathsf{K}}_0$).
   (d)Calculate the initial control limit of the monitoring statistic.
2. ***On-line Learning and monitoring :***
   (a)Obtain the next testing sample x, calculate the PC numbers and kernel parameter.
   (b)Compute k_{new} and scale it $(\bar{\mathsf{K}})$.
   (c)Project $\bar{\mathsf{K}}$ into KPCA to obtain $\hat{\mathsf{K}}$.
   (d)Calculate the monitoring statistic.
   (e)Test if $SPE_t <$ The control limit; the testing sample is not an outlier and the system operate properly, go to step 3. Otherwise, consider the current condition to be abnormal and go to step 2.
3. If updating condition is satisfied, do:
   (a)Calculate the adaptive gram matrix.

$$\mathbf{K} = \lambda_t \times \bar{\mathsf{K}}_{t-1} + (1-\lambda_t) \times \bar{\mathsf{K}}_t \tag{18}$$

   Where λ_t is a flexible forgetting factor.

$$\lambda_t = (\lambda_{\max} - (\lambda_{\max} - \lambda_{\min})[1 - \exp(-ß(\|\Delta R\|)\ )]) \tag{19}$$

   $\lambda_{min} = 0.9$, $\lambda_{max} = 0.99$, $\|\ \Delta R\ \|$ is the Euclidean vector norm of the difference between two consecutive gram matrix and the parameter *ß* control the sensitivity of the change in λ_t.
   (b)Find the number of principal components (l).
   (c)Update the KPCA model: calculate the new eigenvalues and vectors of the new covariance matrix in the feature space (gram matrix).
   (d)Update the forgetting factor λ_t.
   (e)Recalculate the monitoring statistics and the corresponding controls limits.
   (f)Return to step 2.

The calculation procedure of the detection index *SPE* in KPCA method is clearly presented in [17]. First, for an observation vector x, KPCA performs a nonlinear mapping $\Phi(\cdot)$ from an input space $(Step1)$. Then, a linear PCA is performed in this high dimensional space, which gives rise to score vector t in a lower p dimensional space $(Step2)$.

In order to compute SPE in feature space, we need to reconstruct a feature vector $\Phi(x)$ from t. This is done by projecting t into the feature space via eigenvectors v $(Step3)$. Thus, the reconstructed feature vector can be written as :

$$\hat{\Phi}_p(x) = \sum_{i=1}^{p} t_i v_i \tag{21}$$

Therefore, SPE in feature space F is defined as

$$SPE = \left\|\Phi(x) - \hat{\Phi}_P(x)\right\|^2 = \sum_{j=1}^{n} t_j^2 - \sum_{j=1}^{p} t_j^2 \tag{22}$$

where n is the number of nonzero eigenvalues. The confidence limit for the *SPE* can be computed from its approximate distribution:

$$SPE_\alpha \approx \eta \chi_h^2 \tag{23}$$

where α is the confidence level, $\eta = b/2a$ and $h = 2a\,2/b$, a and b are the estimated mean and variance of the *SPE*.

4.2 Fault Diagnosis Based on The Structured Residual Approach

When a faulty condition is detected, one needs to determine the root cause of this problem. AKPCA is used in monitoring, its performed on the full data set. The sum of squared residuals can be used as a metric in detecting faults. However, there is no indication of the location of the fault [18]. The partial AKPCA is an AKPCA performed on reduced vector, where some variable in the data are left out. When data is evaluated against a properly designed partial AKPCA subspace, the residual will only be sensitive to faults associated with the variables that are present in the reduced vector. Faults associated with variables eliminated from the partial AKPCA will leave the residuals within the nominal thresholds. With the selectivity of partial AKPCA to subsets of faults, it is possible to design an incidence matrix for a set of such partial AKPCAs, resulting in a structure with same fault isolation properties as parity relations (show figure 2).

The procedure for structuring the residuals is as follow [12]:

– Perform a standard AKPCA to determine the number of relations m,
– Construct a matrix of incidence strongly isolable (matrix of theoretical signatures),
– Construct a group of partial adaptive kernel PCA models, according to the incidence matrix,
– Determine the thresholds beyond which abnormality is indicated.

After the structured partial KPCA subspace set is obtained, it can be used in on-line monitoring and fault isolation. New observation are evaluated against the structured set as follows (show figure 3):

The localization test can be done online, for each time:

– Run the observed data against each partial AKPCA subspace and compute the residuals,

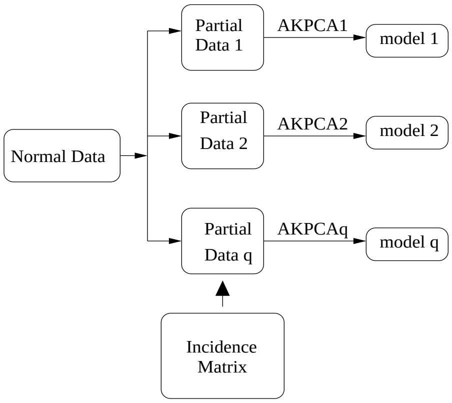

Fig. 2: The modeling procedure of structured partial AKPCA

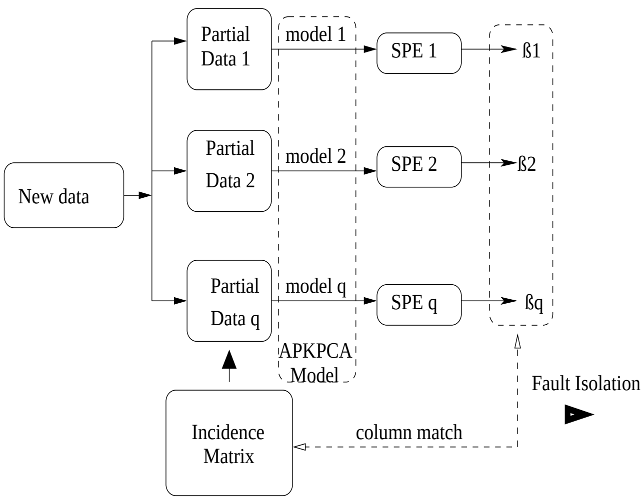

Fig. 3: The fault isolation procedure by structured partial AKPCA.

- –Compare the indices to appropriate thresholds and from the fault code S_{ei} according to: $S_{ei} = 0$ if $SPE_i \leqslant$ control limit(i) and, $S_{ei} = 1$ if $SPE_i >$ control limit(i),
- –Compare the fault code to the columns of the incidence matrix to arrive at an isolation decision.

5 Experimental part

In this section, in order to investigate the potential application of AKPCA method, it was applied to online monitoring in the simulation benchmark of Tenesses Estman and the monitoring performance of AKPCA was compared with the MWKPCA algorithm proposed by Liu et al in [15].

5.1 Tennessee Eastman Process (TEP) data

The TEP was developed by Downs and Vogel of the Eastman Company to provide a realistic simulation for evaluating process control and monitoring methods. It has become perhaps the most important and commonly used benchmark simulation for the development of plant-wide control. There are five major units in TEP simulation (as shown in (fig.04)) a reactor, separator, stripper, condenser, and a compressor. The process has 12 manipulated variables, 22 continuous process measurements, and 19 composition measurements sampled less frequently [9]. Corresponding to different production rates, there are six modes of process operation.

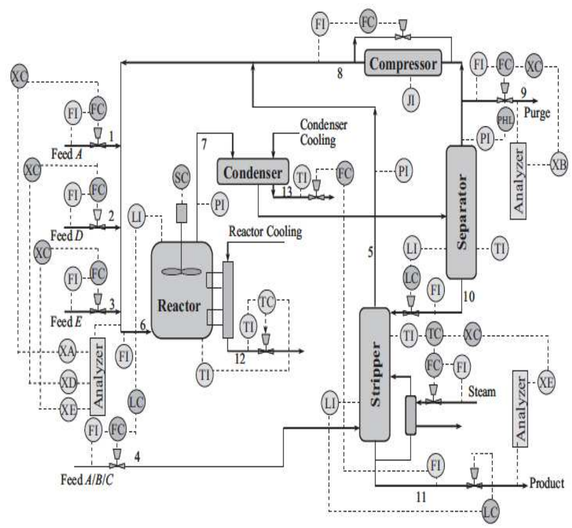

Fig. 4: Tennessee Eastman Process

5.2 Simulation results

The Tennessee Eastman process was run for 1/2 hours, and we collected 600 samples from 16 measurements (show Table 1). An important issue concerning the proposed adaptive monitoring technique is to evaluate it with respect to most current KPCA process control strategies. Analysis of monitoring performances for the different adaptive approaches AKPCA can be reported by using the false alarm rate and the detection rate criterion. The first criteria gives information about the robustness of the adopted method against normal system changes whilst the second criteria gives information about the sensitivity and efficiency of detecting faults.

In this study we propose, to compare performances of the proposed Adaptive KPCA (flexible forgetting factor) with Moving Window KPCA (MWKPCA) of Liu et al. [15], and the proposed adaptive KPCA with different fixed

$N^{\circ}var$	variables
1	A feed
2	Reactor temperature
3	E feed
4	A and C feed
5	Recycle flow
6	Reactor feed rate
7	D feed
8	Purge rate
9	Product separator temperature
10	Product separator pressure
11	Product separator under flow
12	Stripper pressure
13	Stripper temperature
14	Stripper steam flow
15	Reactor cooling water outlet temperature
16	Separator cooling water outlet temperature

Table 1: The measurements used for monitoring

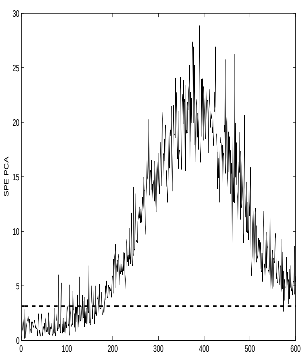

Fig. 5: SPE PCA with fixed model.

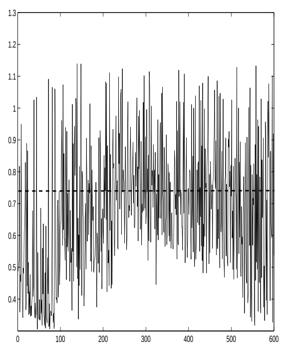

Fig. 6: SPE KPCA with fixed model.

values of forgetting factor. Firstly, for the value σ of the radial kernel function is tuned based on the method of Park and Park [31], which proposes to select $\sigma = C * Averd$, where *Averd* is the mean distance between all observations in feature space and C is a predetermined value. In this study, the C value is set to be equal to the square root of the number of process variables.

The first 100 samples were utilized to build the initial PCA and KPCA models, and the adaptive monitoring is started using forgetting factor combined with a Moving Window, the size of this Moving window is 70 samples. The proposed AKPCA algorithm is used to monitor online the TEP system. We use the parameters described earlier in the algorithm. For the forgetting factor, we choose these values of parameters : $\lambda_{max} = 0.99$, $\lambda_{min} = 0.9$, k=0.05.

In the identification step of the APCA model, the number of significant PCs is selected by using CPV method, such that the variance explained is approximately 95% of the total variance (see Fig. 13). Thus, for greater

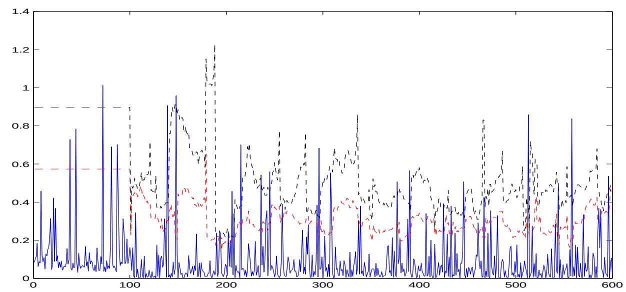

Fig. 7: Evolution the SPE Moving Window Kernel PCA

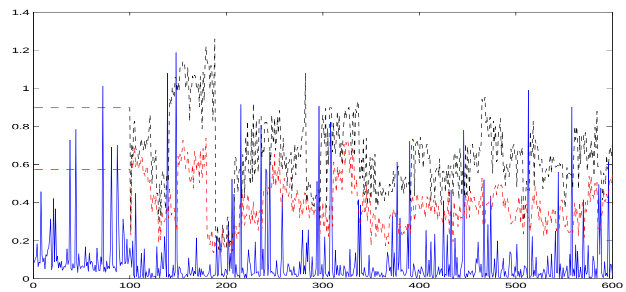

Fig. 8: Evolution the SPE AKPCA with fixed forgetting factor 0.9

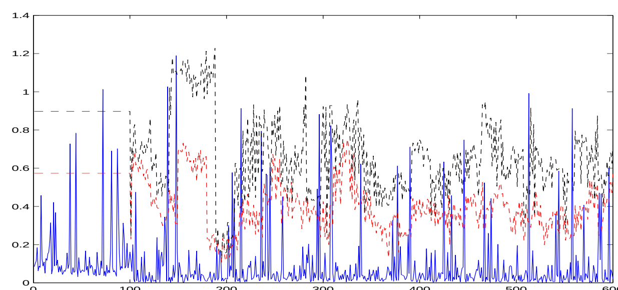

Fig. 9: Evolution the SPE AKPCA with fixed forgetting factor 0.95

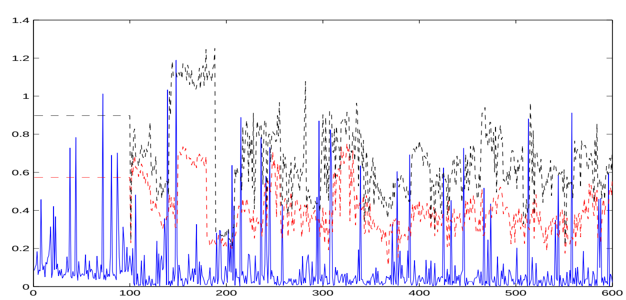

Fig. 10: Evolution the SPE AKPCA with fixed forgetting factor 0.97

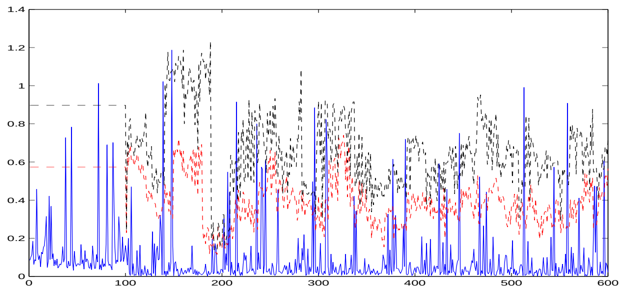

Fig. 11: Evolution the SPE Adaptive kernel PCA

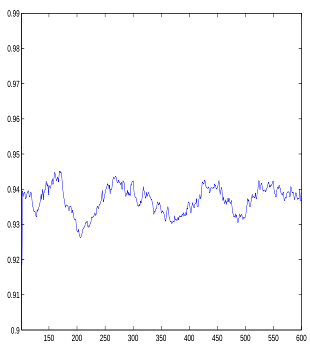

Fig. 12: The flexible forgetting factor.

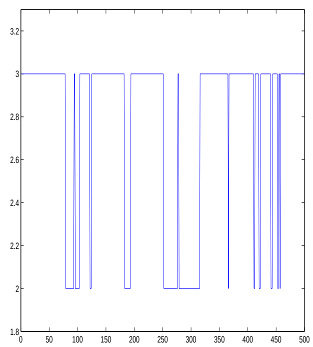

Fig. 13: Number of principal components.

flexibility to adapting with the evolution of the system, an adaptive forgetting factor is used to update the covariance matrix in the feature space in real time according to the change of the system (shows in Fig.12).

In order to show that Batch PCA and KPCA models are not appropriate for monitoring of non-stationary processes, Fig. 5 and Fig. 6 show monitoring performances of both methods when the process is operating under normal condition. The false alarm rate provided by PCA and KPCA approaches is undesirable. In this case the detection index SPE PCA and SPE KPCA shows that the system is faulty, knowing that the system works properly in this simulation part. The analysis of the detection performance of these methods is not performed, since these control charts are not adequate for monitoring of non-stationary processes. However, as shown in (Fig. 7,8,9,10 and 11) and in contrast to the fixed models, applying adaptive PCA based control charts to the same data set, allows better capabilities of adaptation to the nonlinear non-stationary behavior of the process.

Figure. 7 shows that the MWKPCA is less robust to false alarms. Where as AKPCA using forgetting factor is more robust to false alarms. Figures 8, 9, 10 and 11 show that bigger forgetting factors result in a more robustness to false alarms. For example a forgetting factor of 0.9 means according to equation (19) in the adaptive algorithm KPCA that:

$$\mathbf{K} = \lambda_t \times \bar{\mathsf{K}}_{t-1} + (1-\lambda_t) \times \bar{\mathsf{K}}_t \tag{24}$$

$$\mathbf{K} = 0.9 \times \bar{\mathsf{K}}_{t-1} + 0.1 \times \bar{\mathsf{K}}_t \tag{25}$$

The adaptive model of AKPCA takes 10% of its information from the new window and 90% of its information from the previous window. The robustness is related to the way the window is moving. If the moving window collect simple wise, the problem is less serious, but when the window is updated with block wise where the KMWPCA model undergoes an abrupt changes in a more or less rapid system, it will generate a very high rate of false alarms, and sometimes even instability and divergence of detection index (Q statistics) comparing with control threshold. Our algorithm adapts to this problem by the introduction of old information of the system using the forgetting factor in the moving window. This will result in a better adaptation to abrupt changes of the systems and hence a good robustness to false alarms.

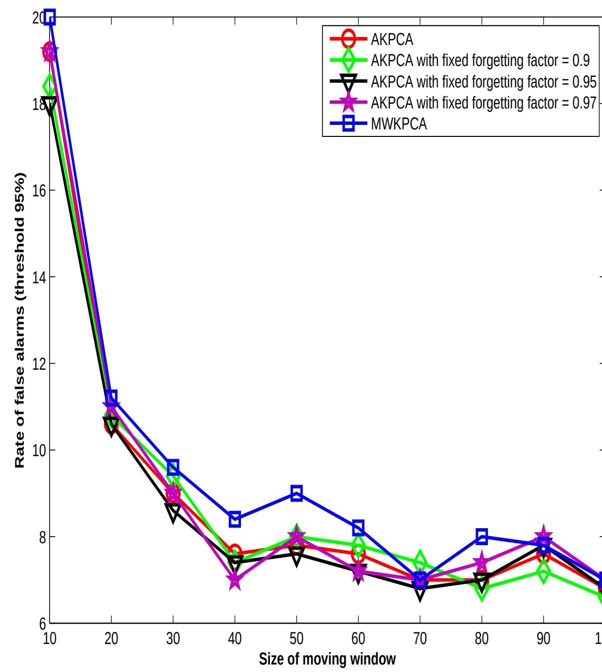

Fig. 14: Rate of false alarms (threshold 95%)

Fig. 12 and Fig. 13 show the evolution of the flexible forgetting factor and the number of principal component PCs with the degree of change in the system, respectively. For better representation, Figures 14 and 15 show a graphical representation of the rate false alarms evolution with different value of thresholds and different moving window size. The figures show that the adaptive KPCA

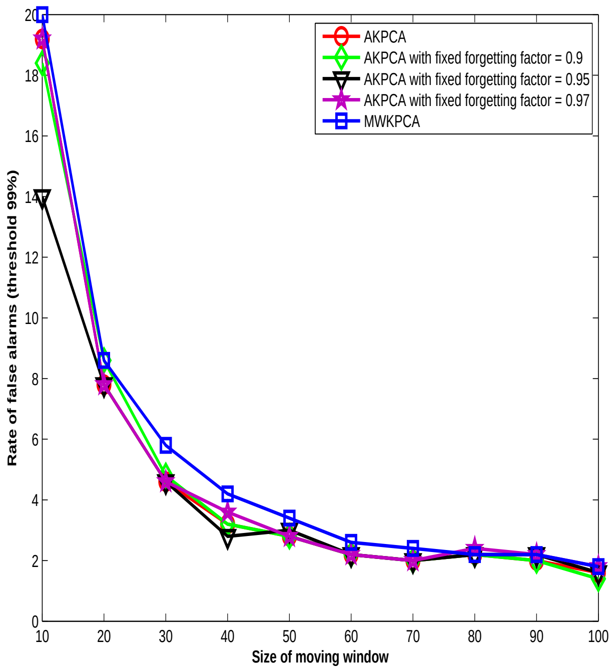

Fig. 15: Rate of false alarms (threshold 99%)

(with flexible forgetting factor) and the adaptive KPCA with different value of forgetting factor are more robust to false alarms than the moving window kernel PCA method. This robustness is the outcome of the previously observation, which is considered in the new built model.

A fault affecting the variable x_2 is simulated between samples 500 and 600 with the magnitude of 35% of the range of variation of the reactor temperature sensor, which is represented with the variable x_2. Control limits are calculated at the confidence level 95%.

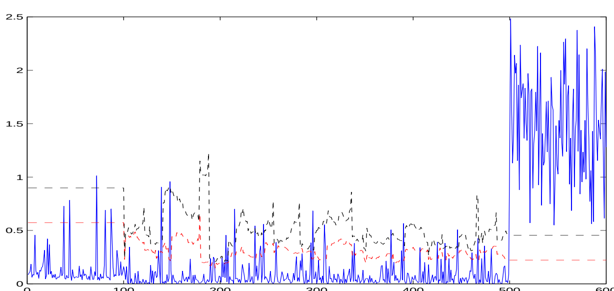

Fig. 16: Evolution the SPE Moving Window Kernel PCA

After time point $k = 500$, it is found that the monitoring indices continuously exceed their thresholds, which indicates a fault has been successfully detected (show figures 16-20). Consequently, the model updating is terminated.

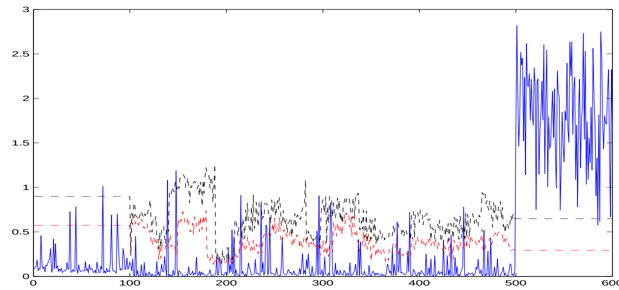

Fig. 17: Evolution the SPE AKPCA with fixed forgetting factor 0.9

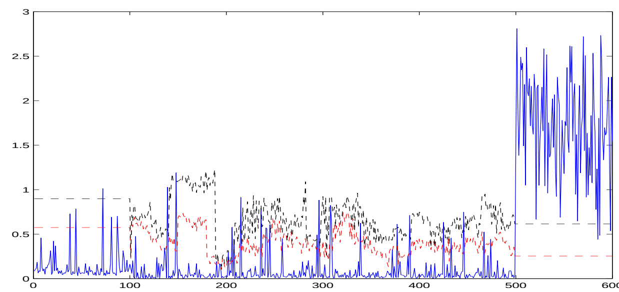

Fig. 18: Evolution the SPE AKPCA with fixed forgetting factor 0.95

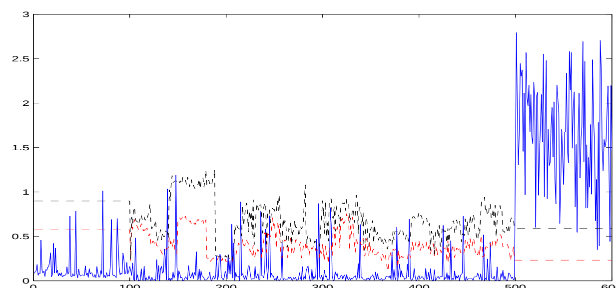

Fig. 19: Evolution the SPE AKPCA with fixed forgetting factor 0.97

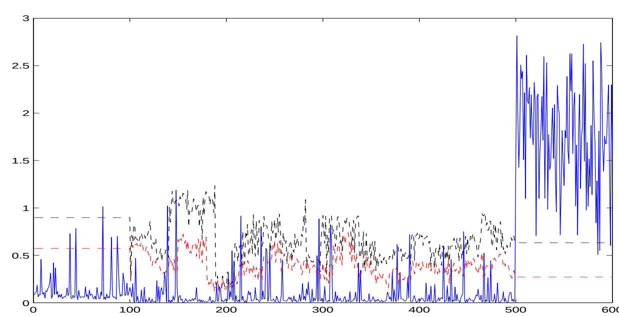

Fig. 20: Evolution the SPE Adaptive kernel PCA

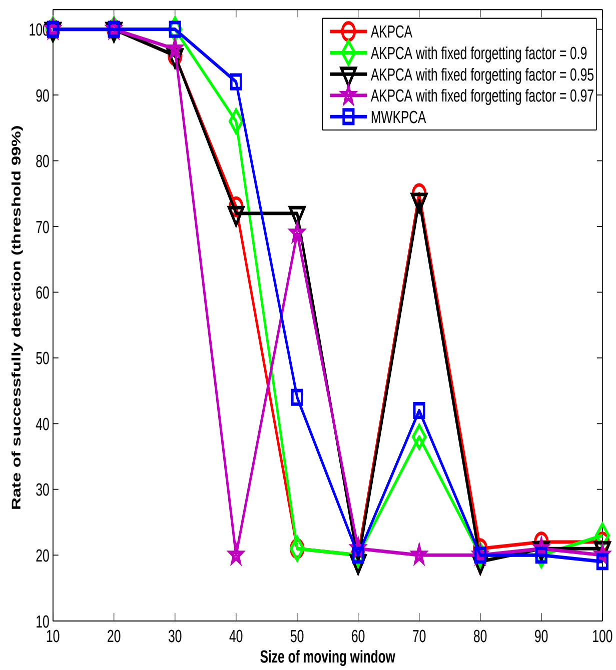

Fig. 21: Rate of successfully detection with a magnitude of the fault = 30%

Figure 21 show a graphical representation of the rate of successfully detection with different value of moving window size. There is clear in the figure that if the size of the moving window is small, the sensitivity of fault detection is greater. Thus that, the adaptive kernel PCA algorithms have more sensitivity of fault detection than the moving window PCA algorithm if the moving window size is greater than 60 samples.

5.3 On-line fault isolation case

When a faulty condition is detected, we need to determine the root cause of this problem. The adaptive partial kernel PCA method is used to diagnose the provenance of this faulty. This technique allows the structuring of the residuals by building a set of models, so that each model is sensitive to certain variables and insensitive to others. The models are built according to the following incident matrix (Table 2 which is the table of theoretical signatures).

In this approach, we built 16 models of KPCA. Each model is insensitive to (06) variables (sensors or actuators) as it is illustrated in the table of theoretical signatures which shows the structuring of the chosen models. Figures 23 and 24 shows the evolution of the experimental signatures when a default is introduced to the variables (sensor/actuator) of the system. The

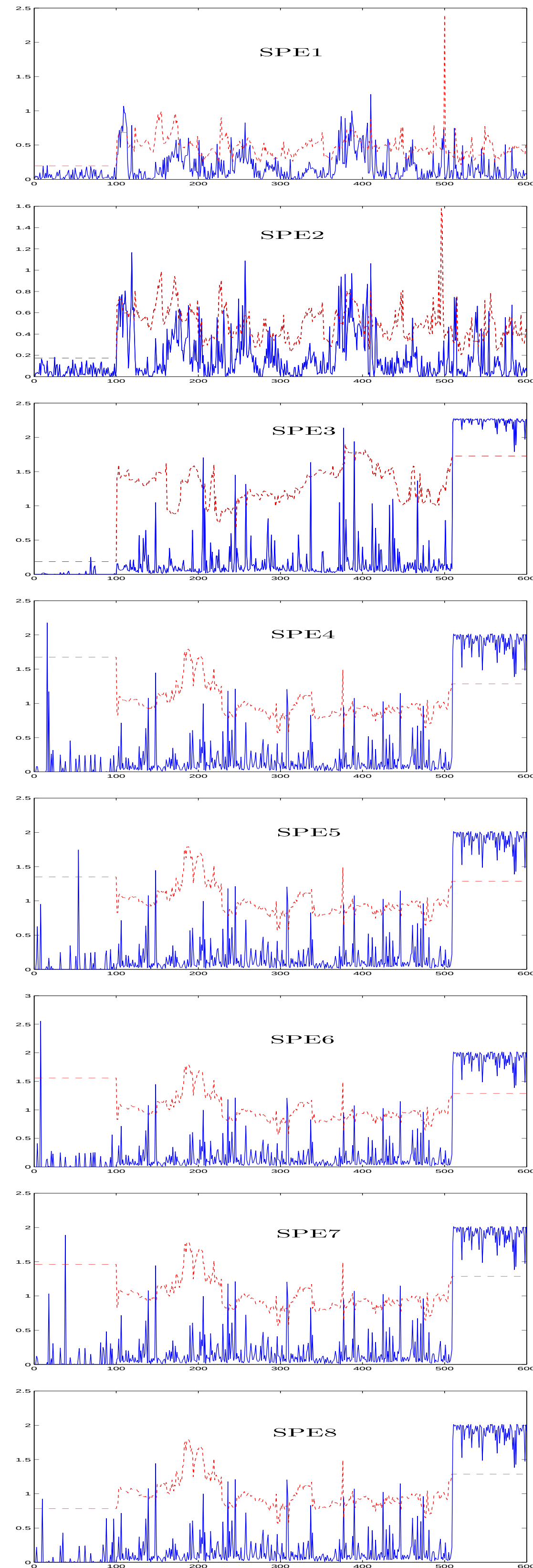

Fig. 22: Evolutions of SPE corresponding to the first Eight different partial AKPCA models.

Partial models	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{16}
SPE_1	0	0	0	0	0	0	×	×	×	×	×	×	×	×	×	×
SPE_2	×	0	0	0	0	0	0	×	×	×	×	×	×	×	×	×
SPE_3	×	×	0	0	0	0	0	0	×	×	×	×	×	×	×	×
SPE_4	×	×	×	0	0	0	0	0	0	×	×	×	×	×	×	×
SPE_5	×	×	×	×	0	0	0	0	0	0	×	×	×	×	×	×
SPE_6	×	×	×	×	×	0	0	0	0	0	0	×	×	×	×	×
SPE_7	×	×	×	×	×	×	0	0	0	0	0	0	×	×	×	×
SPE_8	×	×	×	×	×	×	×	0	0	0	0	0	0	×	×	×
SPE_9	×	×	×	×	×	×	×	×	0	0	0	0	0	0	×	×
SPE_{10}	×	×	×	×	×	×	×	×	×	0	0	0	0	0	0	×
SPE_{11}	×	×	×	×	×	×	×	×	×	×	0	0	0	0	0	0
SPE_{12}	0	×	×	×	×	×	×	×	×	×	×	0	0	0	0	0
SPE_{13}	0	0	×	×	×	×	×	×	×	×	×	×	0	0	0	0
SPE_{14}	0	0	0	×	×	×	×	×	×	×	×	×	×	0	0	0
SPE_{15}	0	0	0	0	×	×	×	×	×	×	×	×	×	×	0	0
SPE_{16}	0	0	0	0	0	×	×	×	×	×	×	×	×	×	×	0

Table 2: Table of theoretical signatures

experimental signature is obtained after codifying the residual. Where exceeding the threshold of detection is represented by 1, and less than the threshold is represented by 0. This gives the following experimental signature (0 0 1 1 1 1 1 1 1 1 1 1 0 0 0 0). This signature is identical to the second column in the theoretical table, which means that the suspect variable (sensor/actuator) is x_2.

6 Conclusion

In this work, a new adaptive kernel PCA algorithm is proposed for dynamic process modeling. The proposed AKPCA model is then performed on subsets of variables to generate a structured residuals for sensor and actuator fault detection and isolation. The proposed algorithm is applied for sensor and actuator fault detection and isolation of Tennessee Eastman process.

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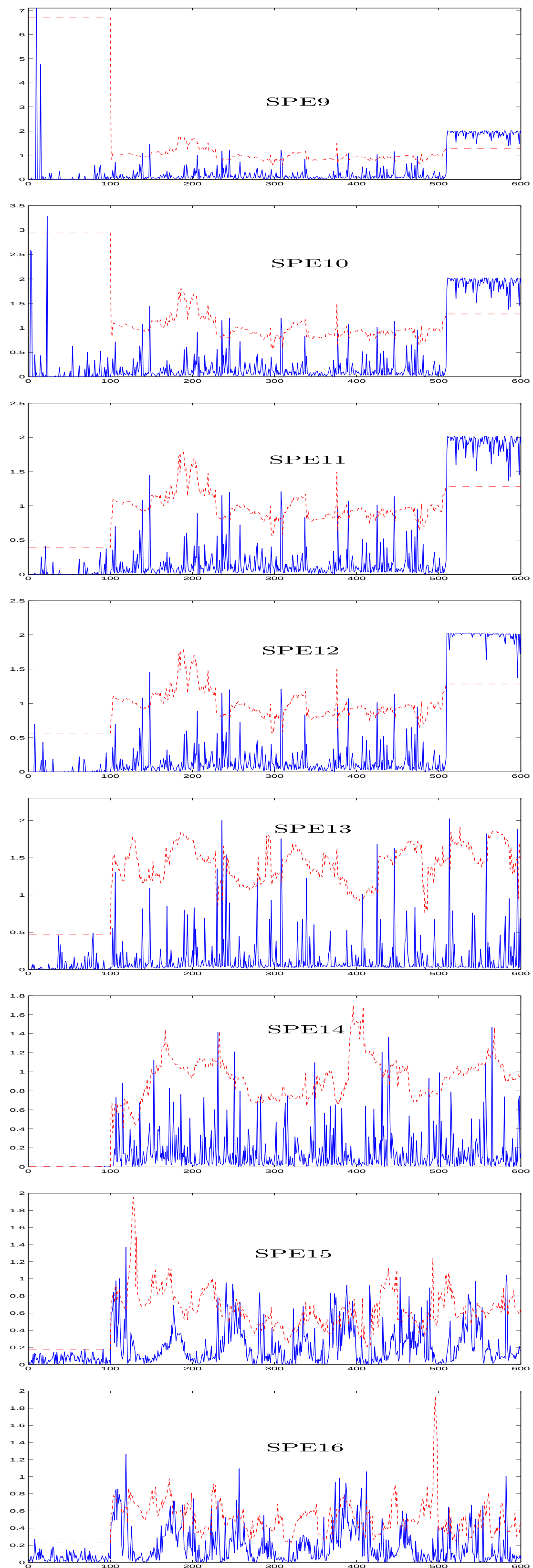

Fig. 23: Evolutions of SPE corresponding to the last Eight different partial AKPCA models.

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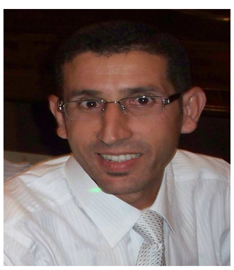

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