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Monitoring and Fault Detection in a Reverse Osmosis Plant using Principal Component Analysis

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Abstract— **This paper presents a monitoring and fault detection system based on principal component analysis techniques (PCA) for a simulated reverse osmosis desalination plant.**

The classical fault detection techniques based on PCA are not suitable for the type of plants studied in this work due to the cleaning cycles necessary for correct plan running. These cleaning cycles periodically change the operating mode of the plant and these changes could be detected as faults. So a well-known PCA approach designed for monitoring batch processes (U-PCA) has been adapted and applied in order to monitor this type of processes.

The developed technique has been tested with several types of faults, obtaining good results. The ratio of false alarms has also been reduced in the nominal behaviour.

I. INTRODUCTION

Two of the most important aims of the industry are the best quality products and safe operation. The control and automation theory has solved an important number of problems with optimal results from the point of view of the quality. Unfortunately, special causes can appear in the industrial processes and normal operation and quality can be altered. These special causes can even put the security and health of the plant operators and the final users at risk . This problem can be solved by implementing monitoring schemes.

One approach widely extended in monitoring, fault detection and diagnosis tasks is the multivariate statistical process control (MSPC) [1], replacing the traditional univariate charts such as the Shewart, CUSUM and EWMA charts.

One of the most widely used MSPC methods is the Analysis of Principal Components (PCA). These techniques use historical databases to build empirical models. The models obtained are able to describe the system's trend. PCA models extract useful information from the historical data. This extraction is based on the calculation of the relationship between the measured variables. When a fault appears, these special causes can change the covariance structure captured by the PCA model and this situation can be detected.

Some processes with continuous behaviour can go through several operating modes due to, for example, changes in the final product specifications, feed flow-rate compositions or set-points. These changes can be detected as faults because they can produce substantial changes in the covariance structure captured by the PCA model. So, many authors have applied different solutions to deal with these lacks [2], [3].

This work presents a monitoring and fault detection method based on the PCA approach applied to a simulated reverse osmosis desalination plant. The simulated plant is based on small and medium real plants placed in remote areas. The remote localization of this kind of plants makes the application of monitoring and fault detection tools very suitable, since the staff cannot be present during all the day or they may even only be able to be present one day per week. Using the current technologies could make it very easy to monitor the state of plants from a remote centralised operation centre.

The plant studied in this work is a continuous process, but here the monitoring is applied using a batch monitoring PCA-based scheme (U-PCA). This approach is used due to the necessary cleaning phases for the correct plant operation that produces a significant amount of false alarms. Also, the upper limits of the typical monitoring statistics used in control charts take high values when the training data do not have a stationary behaviour. High values in the upper limits of the statistics can detract from the detectability of the fault detection method.

So, the aim of this paper is to test the adaptation of the U-PCA monitoring and fault detection approach in a continuous process to reduce false alarms and improve the detectability.

Other works related with the monitoring of reverse osmosis desalination plants can be found in [4] and [5].

Theoretical aspects of PCA are described in section II. Section III describes the techniques used to monitor batch processes. The simulated reverse osmosis desalination plant, with the results of applying both PCA and U-PCA methods to monitor the system are presented in section IV. The conclusions obtained are presented in section V.

The notation used in this paper is the following: bold capitals for matrices, bold lower case for vectors and cursive for scalars.

II. PRINCIPAL COMPONENT ANALYSIS

One of the most widely used multivariate statistical techniques is probably the Principal Component Analysis (PCA). PCA has been used in MSPC [6] and in Fault Detection and Isolation (FDI) tasks [1] with good results. PCA basically produces a linear transformation that generates new uncorrelated variables, also called components, from the variables measured from the process, which are usually highly correlated. This transformation is based on a dimensional reduction of the original data, which means that only a few

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of these components are sufficient to represent appropriately the hidden sources of variability in the studied process.

PCA calculates the correlation structure of the process variables. The data collected from an industrial plant can be arranged into a matrix $\mathbf{X} \in \Re^{K \times J}$, where J is the number of process variables and K is the number of samples, also called individuals. The data used to perform the PCA model for a fault detection or monitoring scheme must be collected under normal plant operation.

Mathematically, PCA estimates an approximation of the matrix $\mathbf{X}$ as the product of two new matrices $\mathbf{T}$ and $\mathbf{P}^T$. The columns ($\mathbf{t}_R$) of the matrix $\mathbf{T}$ are known as score vectors and the rows ($\mathbf{p}_R^T$) of the matrix $\mathbf{P}^T$ are known as the loading vectors [7]. This calculation is performed through the covariance matrix:

$$\mathbf{S} = \frac{1}{K-1}\mathbf{X}^T\mathbf{X} \tag{1}$$

X has to be previously normalized to zero mean and unit variance. Then, the singular value decomposition SVD is performed over the covariance matrix $\mathbf{S}$ obtaining [8]:

$$\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T \tag{2}$$

The transformation from the original space of the correlated measured variables to the uncorrelated reduced space of the scores is performed using the transformation matrix $\mathbf{P}_{1:A} \in \Re^{J \times A}$:

$$\mathbf{T} = \mathbf{X}\mathbf{P}_{1:A} \tag{3}$$

The matrix $\mathbf{P}_{1:A}$ is arranged choosing the A eigenvectors or columns of $\mathbf{V}$ that correspond to the greatest A eigenvalues. The eigenvalues are the diagonal of the matrix $\mathbf{\Lambda}$ sorted in decreasing order.

The scores can be transformed into the original space operating in equation 3:

$$\widehat{\mathbf{X}} = \mathbf{T}\mathbf{P}_{1:A}^T \tag{4}$$

The difference between the original measured data $\mathbf{X}$ and that estimated using the PCA model $\widehat{\mathbf{X}}$ is known as the residuals:

$$\mathbf{E} = \mathbf{X} - \widehat{\mathbf{X}} \tag{5}$$

The original data space can be obtained by taking into account the estimated data and the residuals:

$$\mathbf{X} = \mathbf{T}\mathbf{P}_{1:A}^T + \mathbf{E} \tag{6}$$

The PCA model can also be calculated using the NIPALS algorithm [7].

There are several rules for choosing the correct number of principal components A; several of these techniques are heuristic, but the most popular procedure is the cross validation [9], [10]. This approach consists of the selection of the components which maximize the goodness of fit and the goodness of prediction.

A. Monitoring and Fault Detection

When a PCA model has been established using nominal data, the monitoring statistics are used in order to monitor and detect faults in a new data set of the plant or in a real-time scheme connected to the plant. The monitoring statistics are drawn in control charts, the faults and special causes are detected when the value of the monitoring statistics are greater than a specific threshold. The most common statistics used in fault detection and monitoring are Hotelling's T^2 statistic and the square prediction error (SPE or Q) statistic.

The Hotelling's T^2 statistic is calculated as follow:

$$T^2 = \mathbf{x}^T\mathbf{P}_{1:A}\mathbf{\Lambda}_A^{-1}\mathbf{P}_{1:A}^T\mathbf{x} \tag{7}$$

where Λ_A is a squared matrix formed by the first A rows and columns of Λ.

The process is considered *normal* for a given significance level α if:

$$T^2 \leq T_\alpha^2 = \frac{(K^2-1)A}{K(K-A)}F_\alpha(A, A-K) \tag{8}$$

where $F_\alpha(A, K-A)$ is the critical value of the Fisher-Snedecor distribution with A and $K-A$ degrees of freedom and α is the level of significance. α takes values between 90% and 95%.

Hotelling's statistic uses only the A principal components and is able to detect deviations in the latent variables. The Q statistic is based on the rest of the components and can be used as a test to detect deviations in the residuals.

$$Q = \mathbf{r}^T\mathbf{r} \tag{9}$$

with:

$$r = (\mathbf{I} - \mathbf{P}_{1:A}\mathbf{P}_{1:A}^{\mathbf{T}})\mathbf{x}$$

The upper limit of this statistic can be computed as follows:

$$Q_\alpha = \theta_1\left[\frac{h_0 c_\alpha\sqrt{2\theta_2}}{\theta_1} + 1 + \frac{\theta_2 h_0(h_0-1)}{\theta_1^2}\right]^{\frac{1}{h_0}} \tag{10}$$

with:

$$\theta_i = \sum_{j=R+1}^{J}\lambda_j^i \qquad h_0 = 1 - \frac{2\theta_1\theta_3}{3\theta_2^2}$$

where c_α is the value of the normal distribution, with α being the level of significance.

III. U-PCA

All the described PCA approaches can be applied when the process presents a linear behaviour. This implementation cannot be suitable for processes with a non-linear behaviour. So, for non-linear processes a special configuration of the PCA must be applied. These variations of the classical PCA configuration is called multi way PCA (MPCA) or unfolded PCA (U-PCA) [11] [12] and it is usually applied to batch processes or transitory states and start-ups [13] [14].

The PCA approach is mainly used as a fault detection tool in stationary processes. When a process presents several stationary states, some variations of the classical PCA approach can be applied, for example, the adaptive PCA approach [3], the recursive PCA approach [15] or the exponentially weighted PCA approach [16].

The plant considered in this paper presents a behaviour similar to batch processes and U-PCA will be applied.

In the configuration of this approach, the database is made up of data from past normal batches or transitions. In every $i = 1, 2, \ldots, I$ correct past batches $j = 1, 2, \ldots, J$ variables are measured at $k = 1, 2, \ldots, K$ time intervals. All these datasets are arranged into a three-way matrix $\underline{\mathbf{X}}(I \times J \times K)$ (following the notation of [17]) as shown in the left part of the Fig. 1.

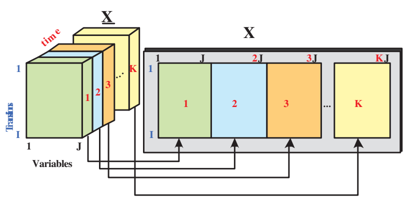


Fig. 1. Matrix unfolding

The three-way matrix must be unfolded into a two-way matrix structure in order to apply the PCA formulation. There are several ways to perform the unfolding of the three-way matrix. In this work, the direction of the batches is maintained and the trajectory of all process variables of the first sample time are arranged into the unfolded matrix, and then the next sample time, and so on, as shown in Fig. 1. This formulation is used in [11], but there are other options as discussed in [18].

In this configuration of PCA, when a batch monitoring method is applied to a continuous process, two tasks have to be considered: the data alignment and the data imputation.

A. Data alignment

When the data is collected from the process, it is arranged into the three-way matrix, but in the example presented in this work, it is normal that the events which produce the activation of the filters and membrane cleanings do not always trigger an alarm with the same frequency, so the datasets do not have the same length. In these cases, the three-way matrix cannot be arranged, so it is necessary to use the same alignment technique to align the trajectories to the same length.

There are principally two alignment techniques. One is the indicator variable approach [11] [19]. This technique is applied when the progress of the process variables in a batch or transitory state is a complex function of different phenomena and it is not simply a function of time. When this approach is applied, a monotonically increasing or decreasing variable has to be found. This variable leads the data collection instead of time. For example, in cases where a reagent is added, an indicator variable can be used if the accumulated flows are monotonically increasing variables.

In the plant studied in this work, it is not possible to find indicator variables to align the data, so the indicator variable is not a suitable approach. In this case, the method used is dynamical time-warping (DTW) [20]. Basically, for two multivariate trajectories of two different implementations between the cleaning cycles, $\mathbf{A}$ and $\mathbf{B}$, both matrices of dimensions $K_1 \times J$ and $K_2 \times J$, where the number of samples K_1 and K_2 is not equal, DTW aligns both trajectories to the length of one of these or to a reference trajectory, created by eliminating some points. These processes of compression or expansion of the time scales must be performed to minimize the dissimilarity between the two trajectories. Also, a real-time version of the DTW methodology has been developed to allow *on-line* monitoring.

B. Imputation

When the plant is monitored *on-line* at each time t, as figure 2 shows, the future values of the variables are necessary in order to calculate the corresponding score. The matrix $\mathbf{P}_{1:A}$ was built using data along the whole past nominal trajectories. There are several methods to deal with this missing future data problem. These methods impute the missing data and estimate the scores using different strategies. In [21], the principal missing data imputation methods are presented, explained and compared. In this work, two methods will be used: Trimmed score method (TRI) and Trimmed score regression method (TSR).

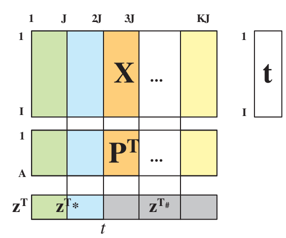


Fig. 2. Imputation

The data matrix $\mathbf{X}$ is a collection of column vectors $\mathbf{x}_j$ (variables) or row vectors $\mathbf{z}_i^T$ (observations). Columns of the loading matrix $\mathbf{P}$ are $\mathbf{p}_j$. The score matrix $\mathbf{T}$ will be considered as a set of row vectors $\boldsymbol{\tau}_i^T$ (scores in the ith observation) or column vectors $\mathbf{t}_i$ (latent variables). A new observation at a particular time instant is partitioned as following:

$$\mathbf{z} = \begin{bmatrix} \mathbf{z}^* \\ \mathbf{z}^\# \end{bmatrix} \tag{11}$$

where $\mathbf{z}^*$ is the known past and current process variable values and $\mathbf{z}^\#$ is the unknown future data values.

The loadings matrix $\mathbf{P}$ is partitioned, separating the known and the unknown data, separating the significant A principal components and leaving $K - A$ components, as equation in 12:

$$\begin{aligned}\mathbf{P} &= \begin{bmatrix} \mathbf{P}^* \\ \mathbf{P}^{\#} \end{bmatrix} = \begin{bmatrix} \mathbf{P}_{1:A} & \mathbf{P}_{A+1:K} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{P}^*_{1:A} & \mathbf{P}^*_{A+1:K} \\ \mathbf{P}^{\#}_{1:A} & \mathbf{P}^{\#}_{A+1:K} \end{bmatrix}\end{aligned} \tag{12}$$

The trimmed score method (TRI) substitutes every missing value by its mean, as the statistics are calculated using centred data, where the mean value is zero. In short, this method substitutes the future unknown data by zeros $\mathbf{z}^{\#} = 0$. The scores can be calculated as [21]:

$$\begin{aligned}\boldsymbol{\tau}_{1:A} &= \mathbf{P}^T_{1:A}\mathbf{z} = \begin{bmatrix} \mathbf{P}^{*T}_{1:A} & \mathbf{P}^{\#T}_{1:A} \end{bmatrix} \begin{bmatrix} \mathbf{z}^* \\ \mathbf{z}^{\#} \end{bmatrix} \\ &= \mathbf{P}^{*T}_{1:A}\mathbf{z}^* + \mathbf{P}^{\#T}_{1:A}\mathbf{z}^{\#} = \mathbf{P}^{*T}_{1:A}\mathbf{z}^*\end{aligned} \tag{13}$$

The trimmed score regression (TSR) method reconstructs $\mathbf{T}_{1:A}$ from the trimmed scores using the following regression model $\mathbf{T}_{1:A} = \mathbf{T}^*_{1:A}\mathbf{B} + \mathbf{U}$. The scores are estimated as follows [21]:

$$\boldsymbol{\tau}_{1:A} = \boldsymbol{\Lambda}_A \mathbf{P}^{*T}_{1:A}\mathbf{P}^*_{1:A}\left(\mathbf{P}^{*T}_{1:A}\mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^{*T}\mathbf{P}^*_{1:A}\right)^{-1}\mathbf{P}^{*T}_{1:A}\mathbf{z}^* \tag{14}$$

C. *Control limits*

The T^2 monitoring statistic and the upper limit in this adaptation of PCA are calculated using equations 7 and 8. The number of individuals in the unfolded matrix $\mathbf{X}$ is the number of past I instead of the number of process samples K.

The Q statistic is calculated as the squared prediction error SPE in every particular instant k [11]:

$$SPE_k = \sum_{(k-1)J+1}^{kJ} e(c)^2 \tag{15}$$

instead of the squared residuals over all time periods Q, as this measurement does not represent the instantaneous perpendicular distance to the reduced space.

The upper limit for these statistics can be calculated by approximating the value every instant to a *chi squared* distribution, as as explained in [11].

IV. STUDY CASE

The approach presented in this paper has been applied to a simulated reverse osmosis desalination plant. The description of the plant can be found in [22]. The plant has been simulated using the simulation environment EcosimPro©. EcosimPro© is an object-oriented and dynamic simulation tool that allows first principles models to be built. Every component is modelled in correlation with the real component principles and such related parameters as the quality of feed water, salinity, temperature, type of filter, membrane characteristics, etc.

The simulated plant presented in this work is based on real small or medium plants placed in remote areas. The aim of the simulated plant is to test different control and monitoring and fault detection techniques in order to facilitate the autonomous functioning and reduce the human maintenance and operation.

This type of plants are based on the reverse osmosis separation process that uses high pressure to force the water through a semi-permeate membrane that retains the salt. Two filters are placed before this membrane, first a sand filter and then a cartridge filter. Both filters are necessary in order to remove particles which can break the membranes.

A typical problem in this kind of plants is the decrease in performance of the membranes and filters during the operation. This decrease is due to deposits such as silt, scale, organic components, etc. Thus, cleaning cycles are performed to reduce the amount of deposits.

The accumulation of deposits in the filters and membranes and the cleaning cycles mean that the plant does not have a strictly stationary behaviour, due to the differences in measurements of pressures and concentrations when the plant has just been cleaned and when the plant was cleaned long ago, as Fig. 3 shows. All these factors mean that the classical PCA approach for monitoring and fault detection in this kind of processes is not the most effective. The monitoring by the T^2 statistic (Fig. 4(a)) and the Q statistic (Fig. 4(b)) clearly shows a high number of false alarms in different zones corresponding to the different cleaning cycles. The PCA model used in this monitoring was built with nominal data from 10 variables during several cleaning cycles. The monitoring was run over new data from the plant.

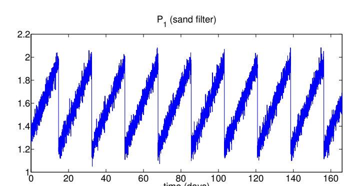
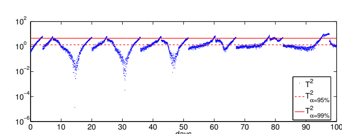
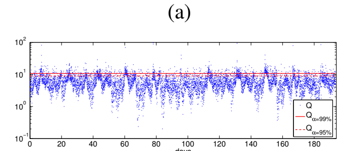


Fig. 3. Pressure measured in the sand filter output



(a)



(b)

Fig. 4. Monitoring using classical PCA (a) T^2 monitoring statistic, (b) Q monitoring statistic

A. *Plant monitoring using U-PCA*

To apply the U-PCA configuration, first of all, a data base of past implementations between the cleaning phases under normal operation is necessary. In this work, each batch is the implementation between the cleaning phases.

Ten variables was selected to monitor the plant presented in this paper. Principally, these variables were concentrations, pressures and flows related with the two filters and the membrane.

All these variables were arranged into the same matrix in order to apply U-PCA in a first approximation. But the cleaning frequency is not the same in the filters and in the membrane, so, in the same way as when the classical PCA was applied, the changes in the behaviour due to the cleaning phases were detected by the monitoring statistics as faults. It is not possible to select a citerion for arranging the data into the three-way matrix.

The solution taken to deal with this drawback consists of building three U-PCA models: two models for the filters and another model for the membrane. Some of the variables, which are not affected by the cleaning phases, were included in several models. The variables affected by a specific cleaning phase are only selected in the model related with the filter or membrane related with that cleaning phase. This configuration is suitable for reducing the number of false alarms.

The sand filter model was performed using six variables, the dimension of the unfolded matrix was 18×5094 and 8 principal components were extracted. The carriage filter unfolded matrix dimension was 27×1821 (three variables were selected) and 13 principal components were extracted. In the case of the membrane, the dimension of the unfolded matrix was 21×2313, the number of variables in this case was three. The number of principal components extracted in this case was 10. In all cases, the number of principal components was calculated using the cross validation approach cited in section II.

Table I shows the false alarms percentage observed using the classical PCA approach and the U-PCA in the different sections. The U-PCA approach, using the TRI imputation method, drastically reduces the amount of false alarms in the case of the T^2 monitoring statistic. This reduction is not so significant when the monitoring statistic applied is the Q or SPE. In this case, the biggest reduction is more effective when the selected imputation method is TSR. However the amount of false alarms in the membrane section really obtains an important improvement.

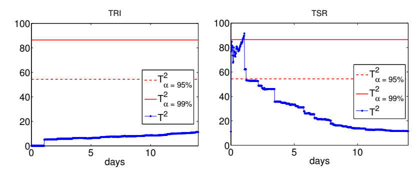
Method	Percentage			
	T^2		Q or SPE	
Classical PCA	6.7%		16.3%	
U-PCA	TRI	TSR	TRI	TSR
Sand filter	0%	1.6%	16.3%	16.2%
Cartridge filter	0%	2.6%	13.0%	11.3%
Membrane	0%	1.0%	21.9%	4.0%

TABLE I

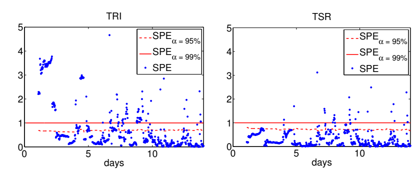
FALSE ALARMS PERCENTAGE

Fig. 5(a) shows the T^2 monitoring of the membrane section using U-PCA, the control chart on the left is the monitoring using the TRI imputation method and on the right is the same monitoring, but using the TSR imputation method. The percentage of false alarms using the TSR imputation only appears in the first stages while in the rest of the monitoring the statistic remains under the upper limits. This is due to the $\mathbf{P}^{*T}_{1:A}\mathbf{P}\mathbf{\Lambda}\mathbf{P}^{*T}\mathbf{P}^{*}_{1:A}$ term in Eq. 14 possibly being an ill conditioned matrix when the known data is scare.

On the other hand, Fig. 5(b) shows the SPE monitoring. The 99% upper limits are equalled to one. So, the 95% upper limit and the statistics are divided by 99% upper limit to normalize these charts because the thresholds in the SPE statistic are not contsant. The results obtained with the TSR imputation method are more acceptable than the results obtained using the TRI imputation method as the percentage of false alarms is lower.



(a)



(b)

Fig. 5. Monitoring using U-PCA in the membrane section (a) T^2 monitoring statistic, (b) SPE monitoring statistic

Looking at the results presented in Table I and Fig. 5(a) and 5(b), one can conclude that the best option to monitor this particular process, using U-PCA, is to use the TRI imputation method for the T^2 statistic and the TSR imputation method for the SPE statistic.

B. Fault Detection

The main results obtained with different sizes of faults can be seen in Table II. The types of faults induced in this work were offsets in the pressure, temperature and concentration sensors, blockages in the filters and breakages in the membranes. Every cell in the table is evaluated with one of three possible values: lowly detectable (LD), when the percentage of alarms after the occurrence of the fault, has a value lower than 33%, partially detectable (PD) when the percentage of alarms is between 33% and 66% and highly detectable when this value is greater than 66%. When the size of the fault is greater than 20%, the method detects faults with a high level of detectability.

Figs. 6(a) and 6(b) show an example of fault detection using the approach presented in this work. The fault consists of an offset in a pressure sensor in the sand filter section. The fault appeared on the second day. The SPE monitoring quickly detects the fault because the statistic using both the imputation methods raises the upper limit practically

Phase	Sensor Offset	Blockage	Breakage
10%	LD	LD	LD
20%	HD	HD	HD
40%	HD	HD	HD
60%	HD	HD	HD

TABLE II

FAULT DETECTION RESULTS

without delay. However the T^2 statistic in several of the tested faults did not raise the upper limits as quickly as the SPE statistic. The delay committed by this statistic was very high, principally in the smallest faults, so the T^2 statistic cannot be very suitable in this type of systems.

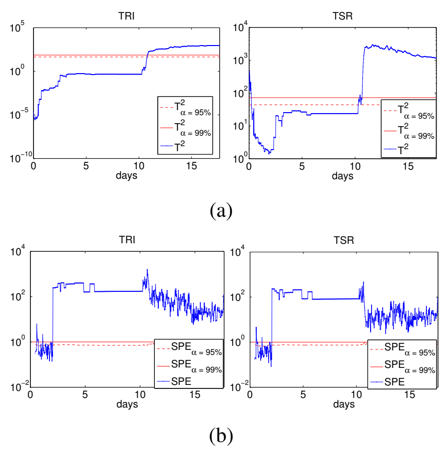


Fig. 6. Fault detection of a 20% offset in a pressure sensor (a) T^2 monitoring statistic, (b) SPE monitoring statistic

V. CONCLUSIONS

A. Conclusions

This work presents a configuration for monitoring and fault detection in continuous processes based on an approach for batch processes.

The monitoring system is applied to a reverse osmosis desalination plant, which needs cyclical cleaning phases that changes slightly the plant behaviour. The little changes are detected as faults, so it is necessary to use a monitoring tool that explores not only the stationary state of the plant, but the dynamics that these cleaning phases introduces into the process nature.

The approach presented in this article: the adapted U-PCA for the continuous process, reduces the ratio of false alarms and is able to detect faults in several components in the plant with good results.

B. Future Works

The next logical step in a monitoring and fault detection system is the diagnosis stage. When a multivariate statistical method like PCA is applied, a very suitable option for fault diagnosis is the contribution plots [6].

Another issue that can considered is to use some of the modifications proposed to PCA, such as recursive PCA (RPCA), exponentially weighted (EWPCA) or adaptive PCA (APCA).

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