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Recursive partial least squares algorithms for monitoring complex industrial processes

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Abstract

The monitoring of processes that exhibit non-stationary and/or time varying behaviour is discussed in this paper. It is shown that the application of recursive partial least squares (RPLS) algorithms together with adaptive confidence limits can lead to a considerable reduction in the number of false alarms. The integration of these algorithms into the multivariate statistical process control (MSPC) framework is introduced and its extensions to multi-block approaches is discussed. Example studies are given with respect to a simulation of a fluid catalytic cracking unit and the analysis of data obtained from an industrial distillation process.
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1. Introduction

Modern industrial processes, often present a large number of measured variables, such as temperatures, pressures, flow-rates and compositions, which are sampled at appropriate time intervals, typically 1 min. This creates huge amounts of process data (MacGregor, Marlin, Kresta, & Skagerberg, 1991), which must be analysed on-line or archived for subsequent analysis. Identifying and troubleshooting abnormal operating conditions by direct observation of the process variables is difficult with such large amounts of data, particularly since the variables are usually highly correlated (Piovoso & Kosanovich, 1992).

Multivariate statistic process control (MSPC) methods are known to be effective for detecting and diagnosing abnormal operating conditions in the above circumstances (MacGregor et al., 1991; Martin & Morris, 1996; Wise & Gallagher, 1996). Two of the most commonly used MSPC methods are principal component analysis (PCA) and partial least squares (PLS), (Kresta, MacGregor, & Marlin, 1991; MacGregor & Kourti, 1995; Kourti & MacGregor, 1995). Applications of PCA or PLS for process monitoring are based on a predefined PCA or PLS model that has been produced from the analysis of reference data on the process. Both methods are able to reveal linear relationships between the process variables by utilising a reduced set of "artificial" (or "latent") variables, (Wise & Gallagher, 1996; Martin & Morris, 1996). Based on these "artificial" variables, univariate statistics that relate to the squared prediction error (SPE) and the Hotelling's T^2 statistic can be generated to monitor the process. In order to discriminate normal from abnormal behaviour, statistical confidence limits for each of the univariate statistics must be calculated. Violations of these limits are considered to be indicative of abnormal behaviour. The confidence limits relate generally to the statistical properties of the process variables and are defined typically in terms of the percentage (often 5% or 1%) of data points that fall outside certain thresholds in a given time interval.

Gallagher, Wise, Butler, White, and Barna (1997) highlighted that most industrial processes are time varying and thus require an adaptive rather than a fixed model. For the monitoring of such processes, it is required that the model can be updated to accommodate time varying behaviour while still being able to detect

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abnormal behaviour defined according to confidence limits which may also have to vary with time.

Another problem that frequently arises is that of non-stationary process behaviour. A potential cause of such behaviour is a varying throughput. Examples of such behaviour are considered in the application studies presented in this paper.

Whilst several approaches have been developed to address time varying process behaviour, little consideration has been given to non-stationary process behaviour. This paper introduces a novel approach that can be applied in cases where the process is non-stationary and/or time varying. A brief review of approaches that tackle time varying process behaviour is presented and analysed below.

Qin (1998) discussed the integration of a moving window approach into the recursive PLS algorithm. This approach gives rise to the identification of a PLS model on the basis of a data set that is within a selected window. Problems that may arise are as follows:

(i) the process monitoring results can be different for different window sizes,
(ii) previous data that is representative of normal process behaviour is discounted in favour of new data which may not be as representative
(iii) a heavy computational effort may be required for updating the model.

Wold (1994) developed an exponentially weighted moving average (EWMA) approach for PCA and PLS. For EWMA models, more recent observations receive a larger weighting than earlier ones. In order to avoid unwarranted adaptation of the PCA/PLS model, Wold (1994) proposed a technique in which older PCA/PLS models are conserved and utilised for the determination of updated PCA/PLS models. Particularly for time varying process behaviour, however, older process models do not accurately represent the relationships between the process variables and hence, conserving older process models may not be useful in this context. An additional problem of this EWMA technique is that of the parameter selection. If the parameters are chosen are so that the EWMA technique can accommodate strong variations of the process, it may not be sensitive in detecting abnormal process behaviour and vice-versa. Therefore, the EWMA PCA or PLS approach may be difficult to implement in practice unless sufficient a priori knowledge of abnormal process behaviour is provided so that the parameter and/or the integration of "old conserved" models can be chosen and/or incorporated.

A recursive algorithm for PLS was presented first by Helland, Berntsen, Borgen, and Martens (1991). When new observations become available, the PLS model is updated recursively. Improvements of the recursive PLS (RPLS) approach are discussed in (Dayal & MacGregor, 1997; Qin, 1993, 1998).

In this paper, the application of RPLS is considered to address non-stationary and time varying process behaviour. The application of RPLS to monitoring industrial processes has not received significant attention in the research literature. Whilst the RPLS approach can address the problem of time varying process behaviour, it will not overcome the problem of non-stationary process behaviour as will be demonstrated in this paper.

A recursive PCA (RPCA) approach has been presented by Li, Yue, Valle-Cervantes, and Qin, (2000) for adaptive process monitoring. In addition, the confidence limits of the monitoring statistics have also been generated adaptively. In an application study concerned with an annealing process in semiconductor processing it was observed that PCA led to an unacceptable number of false alarms. In contrast, RPCA in conjunction with adaptive confidence limits could eliminate false alarms while events that are considered abnormal could still be detected. It is shown in this paper that time varying process behaviour can be adequately accommodated by adapting the linear relationships between the process variables. However, the approach by Li et al. (2000) may run into difficulties if the process shows non-stationary process behaviour that naturally occurs.

The contributions of this paper are as follows. Firstly, the RPLS modelling technique is integrated into the MSPC framework. Secondly, the inclusion of an offset term for the RPLS approach, as proposed by Qin (1998), is revisited and further analysed. Thirdly, the RPLS algorithm is further developed into a recursive multi-block PLS (MBPLS) algorithm. Fourthly, an adaptation of the confidence limits is presented. On the basis of the recursive adaptation of the process model and the adaptation of confidence limits, a novel monitoring approach is finally introduced and applied to two application studies.

MBPLS, discussed for instance in (Wangen & Kowalski, 1988; Westerhuis, Kourti, & MacGregor, 1998; Qin, Valle, & Piovoso, 2001) is designed to further divide the process variables, for example to represent individual operating units, of the process. The recursive MBPLS or RMBPLS algorithm can therefore estimate the contribution of individual operating units to an abnormal process event and hence simplify the diagnosis of that behaviour (MacGregor, Jaeckle, Kiparissides, & Koutoudi, 1994).

It should be noted that the recursive monitoring approach, presented in this paper, differs from the RPCA approach by Li et al. (2000), as the confidence limits are not determined on the updated PCA model. The new approach adapts the confidence limits

using a moving window technique. The length of the moving window, however, is crucial to the adaptation of the confidence limits. If the window length is too short, the approach may adapt to abnormal behaviour, which should be detected. In contrast, if the window length is too long, the approach may lead to false alarms.

The paper is divided into six sections. Section 2 presents a review of the PLS and the MBPLS algorithm and their associated monitoring statistics. Section 3 then demonstrates how conventional PCA/PLS approaches give rise to false alarms when the process behaves non-stationary or the process is time varying. This demonstration is based on two simplified examples. Section 4 is concerned with how to utilise a recursive process model for process monitoring, how to develop an RMBPLS model on the basis of a given RPLS model, how to determine univariate statistics for RPLS and RMBPLS and how to adapt the confidence limits for each univariate statistic. This is followed by a presentation of a realistic simulation of a fluid catalytic cracking unit and data obtained from an industrial distillation process in Section 5. Conclusions are drawn in Section 6 along with suggestions for further work.

2. Process monitoring using PLS and MBPLS

Wold (1966) pioneered the PLS approach in the mid 1960s and the first multiblock extensions to PLS were introduced in the late 1970s and early 1980s (Gerlach, Kowalski, & Wold, 1979; Frank, Feikema, Constantine, & Kowalski, 1994).

For PLS, the process data are divided into two blocks, one block containing the process input or predictor variables and the other block containing the output or response variables. In contrast, for applications of MBPLS, the process data are divided into three or more blocks, each of which represents an operating unit of the process (MacGregor et al., 1994).

2.1. Partial least squares

The PLS approach relies on decomposing the predictor matrix, $\mathbf{X}\in\mathbb{R}^{K\times M}$, and the response matrix, $\mathbf{Y}\in\mathbb{R}^{K\times N}$, to sums of rank one component matrices, (Geladi & Kowalski, 1986). K is the number of measurements, N is the number of response variables and M is the number of predictor variables. Typically, $\mathbf{X}$ and $\mathbf{Y}$ are mean centred and appropriately scaled prior to the identification procedure. The PLS decomposition of $\mathbf{X}$ and $\mathbf{Y}$ results in the following:

$$\begin{aligned}\mathbf{X} &= \sum_{i=1}^{n}\tilde{\mathbf{X}}_i + \mathbf{F}_n = \sum_{i=1}^{n}\mathbf{t}_i\mathbf{p}_i^{\mathrm{T}} + \mathbf{F}_n\\ &= \mathbf{T}_n\mathbf{P}_n^{\mathrm{T}} + \mathbf{F}_n = \mathbf{X}_n + \mathbf{F}_n,\\ \mathbf{Y} &= \sum_{i=1}^{n}\tilde{\mathbf{Y}}_i + \mathbf{E}_n = \sum_{i=1}^{n}\hat{\mathbf{u}}_i\mathbf{q}_i^{\mathrm{T}} + \mathbf{E}_n\\ &= \hat{\mathbf{U}}_n\mathbf{Q}_n^{\mathrm{T}} + \mathbf{E}_n = \hat{\mathbf{Y}}_n + \mathbf{E}_n,\end{aligned} \tag{1}$$

where n is the number of rank one component matrices, $\tilde{\mathbf{X}}_i = \mathbf{t}_i\mathbf{p}_i^{\mathrm{T}}$ and $\tilde{\mathbf{Y}}_i = \hat{\mathbf{u}}_i\mathbf{q}_i^{\mathrm{T}}$, retained in the decomposition. The vectors $\mathbf{t}_i$ and $\hat{\mathbf{u}}_i$ are referred to as the t-score vector and the predicted u-score vector, the vectors $\mathbf{p}_i$ and $\mathbf{q}_i$, are loading vectors, $\boldsymbol{X}_n$ and $\hat{\mathbf{Y}}_n$ represent the sum of n the rank one component matrices to reconstruct the predictor matrix and predict the response matrix, respectively, and $\mathbf{E}_n$ and $\mathbf{F}_n$ are residual matrices. The predicted u-score vectors, $\hat{\mathbf{u}}_i$, can be estimated from the t-score vectors as follows:

$$\hat{\mathbf{U}}_n = [\hat{\mathbf{u}}_1 \vdots \ \dots \ \vdots \hat{\mathbf{u}}_n] = [\mathbf{t}_1 b_1 \vdots \ \dots \ \vdots \mathbf{t}_n b_n] = \mathbf{T}_n\mathbf{B}_n, \tag{2}$$

where $\mathbf{B}_n$ represents a diagonal matrix containing the regression coefficients of the score model, b_i, determined by the PLS algorithm.

Several algorithms have been proposed to determine the score and loading vectors, among which the NIPALS (Geladi & Kowalski, 1986) and the SIMPLS (de Jong, 1993) algorithms are the most popular ones.

Most industrial processes present strongly correlated variables and often only a few t-score vectors are needed to describe most of the process variation. The number of retained t-score vectors is typically determined by cross-validation or the analysis of variance, as demonstrated for example by (MacGregor et al., 1991; MacGregor & Kourti, 1995; Morud, 1996). Note that the scores are often referred to as latent variables, i.e. each score vector represents instances of a particular latent variable or LV.

2.2. Multiblock partial least squares

The multiblock extension of PLS leads to a division of the predictor and response variables into blocks as schematically shown in Fig. 1 for grouping predictor variables only. These blocks may correspond to individual operating units of the process and therefore multiblock PLS or MBPLS simplifies the monitoring task by reducing the number of variables to be considered.

The example that is presented in Fig. 1 illustrates that the u-score vector is regressed on each "predictor block" to determine the weight vectors for each block:

$$\mathbf{w}_b = \frac{\mathbf{X}_b^{\mathrm{T}}\mathbf{u}}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}, \tag{3}$$

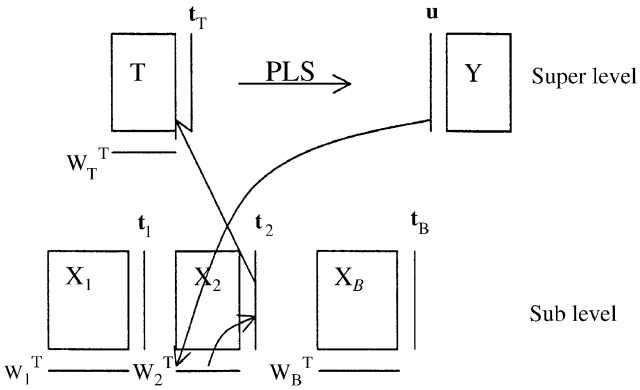

Fig. 1. MBPLS method with multiple predictor blocks and a single response block.

where $\mathbf{X}_b$ and $\mathbf{w}_b$ represents the bth predictor block and its associated weight vector, respectively. Subsequently, the t-score vectors for each predictor block are calculated as the matrix-vector product of the bth predictor matrix and bth weight vector. The t-score vectors for each block are then stored into a block score matrix, $\mathbf{T}$, i.e. $\mathbf{T} = [\mathbf{t}_1, \ldots, \mathbf{t}_B]$, where B is the total number of predictor blocks. This is followed by determining a regression vector for predicting the u-score vector on the basis of the block score matrix by applying the least squares solution:

$$\hat{\mathbf{u}} = \mathbf{T}\mathbf{w}_T. \tag{4}$$

The predicted u-score vector is often referred to as "super" t-score vector $\mathbf{t}_T$. In a similar fashion to the PLS algorithm, the above procedure may also be carried out iteratively, initiated by selecting the u-score vector as some column of $\mathbf{Y}$. The iteration procedure has converged when the difference between two successively determined u-score vectors is negligible. In this paper, the division of the predictor variables into predictor blocks is considered and the corresponding MBPLS algorithm is presented in the appendix. After calculating each latent variable, the super score is deflated from each predictor block and response block.

It was shown that the above MBPLS approach and the conventional PLS algorithm provide equivalent results when the division of the predictor matrix into "predictor blocks" is inverted, (Westerhuis et al., 1998; Qin et al., 2001). More precisely, the super-score vectors $\mathbf{t}_T$ obtained from MBPLS are equivalent to the t-score vectors obtained from PLS.

2.3. Monitoring statistics for PLS and MBPLS

The monitoring of industrial processes usually relies on univariate statistics such as the Hotelling's T^2 or in short T^2 statistic and the SPE statistic, (Wise & Gallagher, 1996; Martin & Morris, 1996). For PLS, the T^2 statistic is constructed from the t-score variables and residuals of both, the predictor variables and the response variables, give rise to individual SPE statistics (MacGregor et al., 1991). The definition of these statistics is as follows:

$$\begin{aligned} T_k^2 &= \boldsymbol{\tau}_k^{\mathrm{T}} \boldsymbol{\Lambda}_n^{-1} \boldsymbol{\tau}_k, \\ \mathrm{SPE}_k^{(X)} &= \|\boldsymbol{\xi}_k - \boldsymbol{\xi}_k^{(n)}\|_2^2, \\ \mathrm{SPE}_k^{(Y)} &= \|\boldsymbol{\psi}_k - \hat{\boldsymbol{\psi}}_k^{(n)}\|_2^2, \end{aligned} \tag{5}$$

where $T_k^2, \mathrm{SPE}_k^{(X)}$ and $\mathrm{SPE}_k^{(Y)}$ represent the T^2 and the SPE statistics of the predictor and the response variables, respectively, $\boldsymbol{\tau}_k, \boldsymbol{\xi}_k$ and $\boldsymbol{\psi}_k$ are vectors that store the calculated values of the t-score variables and the measured values of the predictor and response variables of the kth data point, respectively. Furthermore, $\boldsymbol{\xi}_k^{(n)}$ and $\hat{\boldsymbol{\psi}}_k^{(n)}$ are vectors that store the predicted values of the predictor and response variables of the kth data point, $\boldsymbol{\Lambda}_n$ is the covariance matrix of the n retained t-score variables and $\| \ \|_2^2$ represents the squared norm of a vector.

With these statistics, the overall process variation, incorporated in the T^2 statistic, can be observed as well as departures of the model prediction from the current process behaviour, represented by the SPE statistics.

With MBPLS, each of the predictor blocks presents a T^2 statistic and a SPE statistic so that an individual monitoring of operating units can be achieved. Additionally, the residuals of the response variables present a SPE statistic.

Abnormally large T^2 values represent an excessive or abnormal variation of the predictor variables (or some of the predictor variables) and therefore an excessive or abnormal variation of the entire process. In contrast, large $\mathrm{SPE}^{(X)}$ values indicate a change in the relationship between the predictor variables (or some of the predictor variables) and abnormally large $\mathrm{SPE}^{(Y)}$ values correspond to a mismatch between past process operation, when the PLS or MBPLS process model was determined, and present process operation.

3. Non-stationary and time varying process behaviour

In this section, the difficulties of monitoring non-stationary and time varying processes with conventional PLS are demonstrated on the basis of two simple examples in which two predictor and two response variables are considered. In order to simulate non-stationary process behaviour, the signals of both predictor variables are initially equal and constructed from the following AutoRegressive Integrated Moving Average (ARIMA) signal (Box & Jenkins, 1970):

$$\upsilon_{\mathrm{ARIMA}}(z^{-1}) = \frac{1 + az^{-1}}{(1 + bz^{-1})(1 - z^{-1})} \varepsilon(z^{-1}), \tag{6}$$

where $\upsilon_{\mathrm{ARIMA}}(z^{-1})$ represents the ARIMA signal in the z-transform domain, $\varepsilon(z^{-1})$ represents a normally distributed random signal of zero mean and unit variance, i.e. $\varepsilon(z^{-1}) \in \mathcal{N}\{0,1\}$, a and b are parameters and z^{-1} is the back-shift operator. A normally distributed random signal of zero mean and a variance of $0.2, \mathcal{N}\{0, 0.2\}$, is then superimposed on each of the predictor variables and hence both predictor variables are highly correlated. The response variables are then determined as linear combinations of the predictor variables:

$$\begin{pmatrix} \psi_{1k} \\ \psi_{2k} \end{pmatrix}_t = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{pmatrix} \xi_{1k} \\ \xi_{2k} \end{pmatrix}_t ; \begin{pmatrix} \xi_{1k} \\ \xi_{2k} \end{pmatrix}_t = \begin{pmatrix} \upsilon_k \\ \upsilon_k \end{pmatrix} + \begin{pmatrix} \varepsilon_{1k} \\ \varepsilon_{2k} \end{pmatrix}, \tag{7}$$

where ξ_{1k}, ξ_{2k} and ψ_{1k}, ψ_{2k} are the values of the predictor and response variables and $\upsilon_k, \varepsilon_{1k}$ and ε_{2k} are the value of the ARIMA signal and the two superimposed random signals for the kth instance in time, respectively. The subscript t refers to the true values of the predictor and the response variables and c_{11} to c_{22} are constant parameters.

After the true predictor and response signals are computed, each process variable is augmented by adding a normally distributed random signal of zero mean and a variance of $0.1, \mathcal{N}\{0, 0.1\}$ to account for measurement noise:

$$\begin{pmatrix} \xi_{1k} \\ \xi_{2k} \end{pmatrix}_m = \begin{pmatrix} \xi_{1k} \\ \xi_{2k} \end{pmatrix}_t + \begin{pmatrix} \varepsilon_{3k} \\ \varepsilon_{4k} \end{pmatrix} \text{ and } \begin{pmatrix} \psi_{1k} \\ \psi_{2k} \end{pmatrix}_m = \begin{pmatrix} \psi_{1k} \\ \psi_{2k} \end{pmatrix}_t + \begin{pmatrix} \varepsilon_{5k} \\ \varepsilon_{6k} \end{pmatrix}, \tag{8}$$

where m denotes the measured values and ε_{3k} to ε_{6k} are the kth instances of added random signals to the predictor and the response variables. Given the described construction of the predictor variables, it is clear that only one LV is required to determine a sufficiently accurate process model.

A second data set, simulating stationary and time varying process behaviour, was constructed as follows. Both predictor variables were initially equivalent and obtained from a single AutoRegressive Moving Average (ARMA) signal (Box & Jenkins, 1970):

$$\upsilon_{\mathrm{ARMA}}(z^{-1}) = \frac{1 + az^{-1}}{1 + bz^{-1}} \varepsilon(z^{-1}), \tag{9}$$

where $\upsilon_{\mathrm{ARMA}}(z^{-1})$ represents the ARMA signal. Both predictor variables were then augmented by adding uncorrelated normally distributed random signals of zero mean and a variance of $0.2, \mathcal{N}\{0, 0.2\}$. The response variables were then obtained as linear combinations of the predictor variables as shown in Eq. (7). In order to represent measurement noise, the true signals received a normally distributed random signal of zero mean and a variance of $0.1, \mathcal{N}\{0, 0.1\}$ as shown in Eq. (8). The time varying process behaviour was achieved by adding a ramp signal to c_{22} after a certain number of data points were recorded. Each of the simulated data sets contained 1000 data points and an initial process model was obtained using the first 200 data points. The parameters a and b for both, the ARIMA and the ARMA signal, were selected to be 0.5 and the parameters c_{11}, c_{12}, c_{21} and c_{22} were chosen to be -0.2, 0.3, 0.1 and -0.05, respectively. The ramp signal with an increment of 0.005 was added to c_{22} after 500 data points were simulated.

3.1. Non-stationary process behaviour

The results of monitoring the non-stationary process with conventional PLS are illustrated in Fig. 2. For the SPE statistics, the number of violations of the 99% confidence limit is less than 10 and the number of violations of the 95% confidence limit is less than 50. Therefore, less than 1% and 5% of the data points violate their respective confidence limits. However, the T^2 statistic indicates violations of the confidence limits for long sequences of the data points after the first 380 data points whereas they are in fact due to the non-stationary character of the process. Note that the relationships between the process variables did not change throughout the simulation. In contrast, the process variation is excessive; thus the process variables manoeuvre into operating regions that were not present when the confidence limits were established. Consequently, the T^2 statistic violates the confidence limits shortly after their determination.

The RPCA approach by Li et al. (2000) adapts the confidence limit of the T^2 statistic based on a varying number of retained PCs. Hence, this approach may not

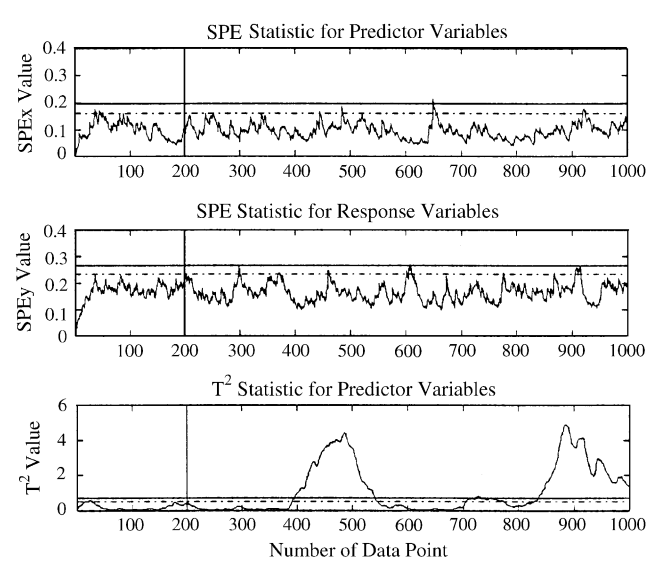

Fig. 2. Process monitoring of a non-stationary process using PLS.

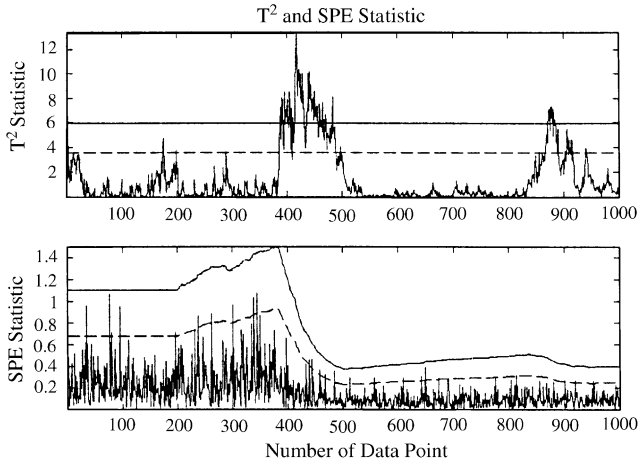

Fig. 3. Process monitoring of a non-stationary process using RPCA.

eliminate false alarms when the process behaves in a non-stationary way. An example is presented in Fig. 3 for which the approach by Li et al. (2000) is applied to the same data set. A strong violation of the 99% confidence limit is evident between the 380th and the 500th data point and around the 880th data point although the process does not behave abnormally. Consequently, the confidence limits of the T^2 statistic need to be adapted to accommodate non-stationary process behaviour. Note that the decrease in the *SPE* statistic is a consequence of the sharp increase in the variance of process variable after the 380s data point. An adaptation of the confidence limits for the PLS monitoring statistics is proposed in this paper and presented in Section 4.3.

3.2. Time varying process behaviour

The results of monitoring the time varying process with conventional PLS are shown in Fig. 4. It can be seen from this figure that the $SPE^{(Y)}$ statistic violates its confidence limits shortly after the step change of one of the linear coefficients is superimposed with a ramp signal after the 500th data point was recorded. This implies that the process gradually deviates from its behaviour when the PLS model and the confidence limits were established.

The response of the $SPE^{(Y)}$ statistic is to be expected, as the predictor variables, and consequently the T^2 and $SPE^{(X)}$ statistics, are not affected by the changes in the process behaviour. This example highlights that an adaptation of the process model has to be considered, which is proposed in the next section.

4. Process monitoring using recursive PLS algorithms

As discussed in the previous section, adaptation of the process model is required to address time varying

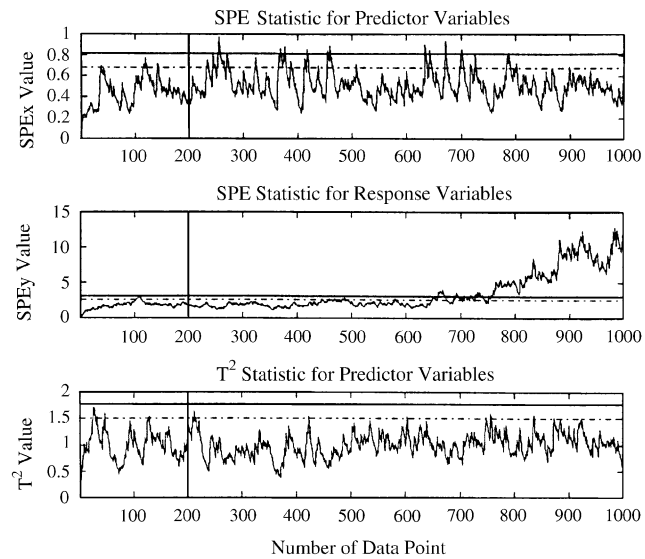

Fig. 4. Process monitoring of a time varying process using PLS.

process behaviour. In this section, recursive applications of the PLS algorithm are reviewed, which are designed to adapt the process model when new data points become available. Qin (1998) suggested the incorporation of an offset term as an additional predictor variable to compensate for changes in the mean value of each process variable. This is revisited and analysed with the introduction of a novel way of recursively updating a MBPLS model.

4.1. Recursive PLS

Recursive PLS algorithms were first reported in the early 1990s, (Helland et al., 1991) and improvements are presented in (Dayal & MacGregor, 1997; Qin, 1993, 1998). RPLS algorithms allow an existing PLS model to be updated as new observations become available. Qin (1998) showed that: "given a PLS model $\{\mathbf{X},\mathbf{Y}\} \rightarrow^{PLS} \{\mathbf{T},\mathbf{W},\mathbf{P},\mathbf{B},\mathbf{Q}\}$ and a new data pair $\{\mathbf{x}_1,\mathbf{y}_1\}$, performing PLS regression on data pair $\begin{bmatrix}\mathbf{P}^{\mathrm{T}}\\ \mathbf{x}_1\end{bmatrix}, \begin{bmatrix}\mathbf{BQ}^{\mathrm{T}}\\ \mathbf{y}_1\end{bmatrix}$ results in the same regression model as performing PLS regression on data pair $\begin{bmatrix}\mathbf{X}\\ \mathbf{x}_1\end{bmatrix}, \begin{bmatrix}\mathbf{Y}^{\mathrm{T}}\\ \mathbf{y}_1\end{bmatrix}$". This leads to a considerable reduction in the computational effort required to identify an updated RPLS model. Note that the weight vectors of the PLS model are stored as column vectors in $\mathbf{W}$ and that each of the above PLS matrices contain the maximum number of LVs (Qin, 1998). Qin (1998) further highlighted that introducing an offset term as an additional predictor variable may accommodate changes in the mean value. This is revised below.

4.1.1. Considerations for augmenting a set of predictor variables by an offset term

Given the following assumptions:

1. over the operating region which is to be monitored, there are linear relationship between the predictor and the response variables and,
2. if each predictor variable is equal to zero (plant shutdown) then the response variables are also equal to zero,

the true steady state relationship of the process is as follows:

$$\boldsymbol{\psi} = \mathbf{A}\boldsymbol{\xi}, \tag{10}$$

where $\boldsymbol{\xi} \in \mathbb{R}^M$ and $\boldsymbol{\psi} \in \mathbb{R}^N$ store the predictor and response variables, respectively, and $\mathbf{A} \in \mathbb{R}^{N \times M}$ represents the linear steady-state relation between these variables. Introducing mean centring and scaling of $\boldsymbol{\xi}$ and $\boldsymbol{\psi}$ gives rise to:

$$\boldsymbol{\xi}^* = \boldsymbol{\Sigma}_\xi(\boldsymbol{\xi} - \overline{\boldsymbol{\xi}}) \quad \text{and} \quad \boldsymbol{\psi}^* = \boldsymbol{\Sigma}_\psi(\boldsymbol{\psi} - \overline{\boldsymbol{\psi}}) \tag{11}$$

for which $\boldsymbol{\xi}^*$ and $\boldsymbol{\psi}^*$ represent the mean centred and scaled predictor and response variables, respectively, $\overline{\boldsymbol{\xi}}$ and $\overline{\boldsymbol{\psi}}$ are vectors storing the mean values and $\boldsymbol{\Sigma}_\xi$ and $\boldsymbol{\Sigma}_\psi$ are diagonal matrices storing the scaling factors of the predictor and response variables. Note that $\boldsymbol{\xi}^*$ and $\boldsymbol{\psi}^*$ are obtained prior to the determination of the steady-state process model. Substituting Eq. (11) into Eq. (10) leads to:

$$\boldsymbol{\Sigma}_\psi^{-1}\boldsymbol{\psi}^* + \overline{\boldsymbol{\psi}} = \mathbf{A}(\boldsymbol{\Sigma}_\xi^{-1}\boldsymbol{\xi}^* + \overline{\boldsymbol{\xi}}) \text{ or}$$
$$\boldsymbol{\psi}^* = \boldsymbol{\Sigma}_\psi\mathbf{A}\boldsymbol{\Sigma}_\xi^{-1}\boldsymbol{\xi}^* + \boldsymbol{\Sigma}_\psi(\mathbf{A}\overline{\boldsymbol{\xi}} - \overline{\boldsymbol{\psi}}). \tag{12}$$

The expression $\mathbf{A}\overline{\boldsymbol{\xi}} - \overline{\boldsymbol{\psi}}$ is clearly zero if the steady-state relationships, $\mathbf{A}^* = \boldsymbol{\Sigma}_\psi\mathbf{A}\boldsymbol{\Sigma}_\xi^{-1}$, between the predictor and response variables remains time invariant. Therefore, an offset term is not required if the process is non-stationary but time-invariant. In contrast, an offset term, that represents $\boldsymbol{\Sigma}_\psi(\mathbf{A}\overline{\boldsymbol{\xi}} - \overline{\boldsymbol{\psi}})$ is required if the process exhibits time varying behaviour, i.e. the elements of $\mathbf{A}$ change with time.

Each time the PLS model is recursively updated, the number of retained LVs has to be determined. Since the RPLS algorithm requires the maximum number of LVs to be retained (Qin, 1998), the number of LVs for the RPLS algorithm may be selected on the basis of the variance captured by each LV in the predictor and the response block as advocated by MacGregor et al. (1991). In fact, the number of LVs determines how many degrees of freedom are incorporated in the predictor variables that influence the response variables. Since the predictor variables are assumed to be correlated, the number of retained LVs is usually smaller than the number of predictor variables (MacGregor et al., 1991). Even under the assumption that the process is time varying and/or shows non-stationary behaviour, the number of degrees of freedom within the predictor variables that influence the response variables is unlikely to change unless the process behaviour changes drastically. It is therefore assumed that the number of LVs is not time varying. In this paper, the number of LVs is determined on the basis of a sufficiently large reference data set recorded from the process under investigation.

4.2. Recursive MBPLS

Since the conventional MBPLS model can be converted into an equivalent PLS model, (Westerhuis et al., 1998; Qin et al., 2001), it is possible to use the RPLS approach as discussed in the previous section and then divide the predictor variables into blocks that represent individual operating units of the process. In this paper, the MBPLS algorithm that is discussed in Westerhuis et al. (1998) is used along with the RPLS algorithm that is presented by Qin (1998). It should be noted that an RMBPLS algorithm could also be established without the integration of the RPLS algorithm. This, however, would be computationally less efficient, as discussed by Westerhuis et al. (1998) and Qin et al. (2001), for integrating conventional PLS into the MBPLS algorithm. The integration of RPLS into MBPLS forms a recursive MBPLS or RMBPLS algorithm that can provide multiple predictor blocks and a single response block and is illustrated in Table 1.

The iteration process is initiated by calculating a PLS model at first using a small reference data set, which contains 200 sampling points for instance. The w-weight and the p-loading matrices is then separated into the corresponding predictor blocks to form the initial MBPLS model. If a new sample point becomes available, the initial PLS model is recursively updated as discussed in the previous section and the resultant w-weight and p-loading matrices are again divided into the corresponding predictor blocks.

The process of recursively updating the PLS model and the successive division of the w-weight and p-loading matrices into the corresponding predictor blocks is applied for every new sample that is obtained from the process.

4.3. Adaptive confidence limits

Li et al. (2000) introduced an adaptation of the confidence limits for the monitoring statistic on the basis of a recursive PCA approach. However, the simplified applications study in Section 3 demonstrated that non-stationary process behaviour requires an improved adaptation of the confidence limits, particularly for the T^2 statistic. Such an approach is introduced below.

MacGregor and Kourti (1995) highlighted that, under the assumption that the process variables are normally distributed, the univariate statistics, introduced in

Table 1
Illustration of the RMBPLS algorithm

1. Scale the data matrices $\{\mathbf{X},\mathbf{Y}\}$.
2. Derive a PLS model using the algorithm presented by Qin (1998): $\{\mathbf{X},\mathbf{Y}\} \rightarrow \{\mathbf{T},\mathbf{W},\mathbf{P},\mathbf{B},\mathbf{Q}\}$. Separate the PLS model into a corresponding MBPLS model $\{[\mathbf{X}_b],\mathbf{Y}\} \rightarrow \{[\mathbf{T}_b,\mathbf{T}_T],[\mathbf{W}_b,\mathbf{W}_T],[\mathbf{P}_b],\mathbf{B},\mathbf{Q}\}$ and obtain corresponding statistic limits.
3. When a new pair of data $\{\mathbf{x}_1,\mathbf{y}_1\}$ is available, scale it the same way as step 1. Let $\mathbf{X} = \begin{bmatrix} \mathbf{P}^{\mathrm{T}} \\ \mathbf{x}_1 \end{bmatrix}, \mathbf{Y} = \begin{bmatrix} \mathbf{B}\mathbf{Q}^{\mathrm{T}} \\ \mathbf{y}_1 \end{bmatrix}$ and return to step 2.

Eq. (5), follow a central Chi-Squared distribution. As each of the univariate statistic represents a sum of squared values, the confidence limits can be obtained on the basis of the theorems developed by Box (1954). Given a univariate statistic, $\zeta > 0$ along with its mean value $\bar{\zeta}$, and its variance σ_ζ, the confidence limits that represent a confidence of $(1-\alpha)$ is as follows:

$$\zeta^{(1-\alpha)} = g\chi^2(\alpha, h), \tag{13}$$

where $\zeta^{(1-\alpha)}$ represents the confidence limit, $g = (\sigma_\zeta/2\bar{\zeta}), h = (2\bar{\zeta}^2/\sigma_\zeta)$ and χ^2 denotes the Chi-Squared distribution function. The confidence $(1-\alpha)$ is typically selected to be 95% and 99%, i.e. $\alpha = 0.05$ or 0.01.

In order to adapt the confidence limits, the following approach may be applied. Consider a section of measured data that is close to the current instance, k, the confidence limits can be estimated on the basis of this portion by applying Eq. (13). Given that the number of data points that are considered is L, this section is defined as:

$$S_k = \{\zeta_{k-L}, \ldots, \zeta_{k-1}\}, \tag{14}$$

where S_k represents the section of contiguously determined values of the univariate statistic ζ that is used to determine the confidence limits for the kth value, $\zeta_k^{(1-\alpha)}$. Since the most currently obtained values of ζ correspond to the present performance of the process more closely than those values of ζ that are obtained earlier, the selection of S_k is expedient. The confidence limits for ζ_k can then been determined by calculating g_k and h_k—see Eq. (13) on the basis of S_k.

If a new data point becomes available, the previous value of ζ, ζ_k, is added as an extra element to S_k and the element ζ_{k-L} is eliminated. This forms the section of S_{k+1} for obtaining the confidence limits for the $(k+1)$th value of the univariate statistic, $\zeta_{k+1}^{(1-\alpha)}$, by calculating g_{k+1} and h_{k+1}. This procedure is similar to a moving window approach, however, the estimated statistical parameter $\zeta_k^{(1-\alpha)}$ is to be applied outside S_k.

The size of S_k clearly determines how slowly the confidence limits are updated. Thus, L can be seen as a parameter that "tunes" the speed of adaptation. It is important to guarantee that the confidence limits are not adapted too quickly so that abnormal but slowly progressing process behaviour is adapted and thus, making the introduced monitoring approach invalid. In contrast, if the confidence limits are adapted too quickly, false alarms may consequently occur. Therefore, the recorded data set (reference data set) must be large enough to capture variation that naturally occurs so that L can be selected accordingly. The length L is further referred to as window length.

4.4. Implementation of the introduced adaptive monitoring approach

The procedure for implementing the introduced monitoring scheme is summarised below with respect to RPLS, followed by its multiblock extension (RMBPLS).

4.4.1. Step 1 for RPLS: initialisation of the monitoring scheme

The initial PLS model can be calculated from a small data set that is part of the reference data set. It has to be ensured, however, that this small data set captures enough process variation to reveal the correlation structure within the predictor variables so that the significant LVs can be determined accordingly. After that, the confidence limits can be computed by applying Eq. (13). It is now required to apply a recursively-updated model to the rest of the reference data in order to select the window length L for each univariate statistic. Note that L might vary for each univariate statistic. This can be seen from the simple application study corresponding to the non-stationary process behaviour presented in Fig. 2. Note that the T^2 statistic shows much more significant variation than the SPE statistics, which may lead to a different "L" for each statistic.

4.4.2. Step 2 for RPLS: recursive adaptation of the process model and the confidence limits

Given that the kth data point is available, compute T_k^2, $SPE_k^{(X)}$ and $SPE_k^{(Y)}$ on the basis of the $(k-1)$th process model. This is followed by calculating the thresholds for each of the univariate statistics, i.e. ${}_{(1-\alpha)}T_k^2, {}_{(1-\alpha)}SPE_k^{(X)}$ and ${}_{(1-\alpha)}SPE_k^{(Y)}$ on the basis of $S_k^{(T^2)}, S_k^{(SPE^{(X)})}$ and $S_k^{(SPE^{(Y)})}$, respectively. Then, update the associated monitoring charts by plotting the values of the univariate statistics along with their thresholds. The last step is to recursively adapt the $(k-1)$th process model by applying the RPLS algorithm, presented in Section 4.1, in order to obtain the kth process model and to establish $S_{k+1}^{(T^2)}, S_{k+1}^{(SPE^{(X)})}$ and $S_{k+1}^{(SPE^{(Y)})}$.

4.4.3. Step 1 for RMBPLS: initialisation of the monitoring scheme

For the application of RMBPLS, the predictor variables of the initial PLS model are divided to form predefined predictor blocks. The corresponding monitoring statistics, i.e. ${}_jT^2_{1:m}$ and $SPE^{(X_j)}_{1:m}$ for the jth predictor block and $SPE^{(Y)}_{1:m}$ for the response block are then determined along with the confidence limits for each univariate statistic on the basis of the initial model and the data set, containing m data points, from which the initial model was obtained. As for the RPLS implementation, the window length, L, needs to be determined for each univariate statistic.

4.4.4. Step 2 for RMBPLS: recursive adaptation of the process model and the confidence limits

Given that the kth data point is available, the corresponding monitoring statistics, ${}_jT^2_k, SPE^{(X_j)}_k$ for the jth predictor block and $SPE^{(Y)}_k$ for the response block are established on the basis of the $(k-1)$th RMBPLS model. Then, the confidence limits for each univariate statistic are determined by applying Eq. (13), utilising $S^{({}_1T^2)}_k, S^{(SPE^{(X_1)})}_k, \ldots, S^{(SPE^{(Y)})}_k$. This is then followed by updating the corresponding monitoring charts by plotting ${}_1T^2_k, SPE^{(X_1)}_k, \ldots, SPE^{(Y)}$ along with their confidence limits. Now, the RMBPLS model is updated by dividing the predictor variables and the associated weight and loading matrices of the kth RPLS model into the predefined blocks and define $S^{({}_1T^2)}_{k+1}$, $S^{(SPE^{(X_1)})}_{k+1}, \ldots, S^{(SPE^{(Y)})}_{k+1}$.

The introduced monitoring approach does not require a substantial amount of data in order to determine the initial model. In fact, only two data sets are required, one for obtaining the initial model and the other to determining the window length, L, as discussed above. In contrast, the conventional MSPC approach requires a sufficiently large amount of data to ensure that naturally occurring variation is adequately represented otherwise false alarms may occur even when the process behaves normally, (Kourti & MacGregor, 1995; Kruger, Chen, Sandoz, & McFarlane, 2001).

4.5. Non-stationary process behaviour

The application of the introduced monitoring approach to the data that are used in Section 3.1 to describe non-stationary process behaviour is presented in Fig. 5. The length of data section for adaptively determining the confidence limits was selected to be 50. Comparing Fig. 5 with Fig. 2, which shows the application of the conventional monitoring approach, reveals that the number of violations of the respective confidence limits is less than 1% and 5%. Therefore, the number of violations is greatly reduced so that no out of statistical confidence situation arises for the entire data set.

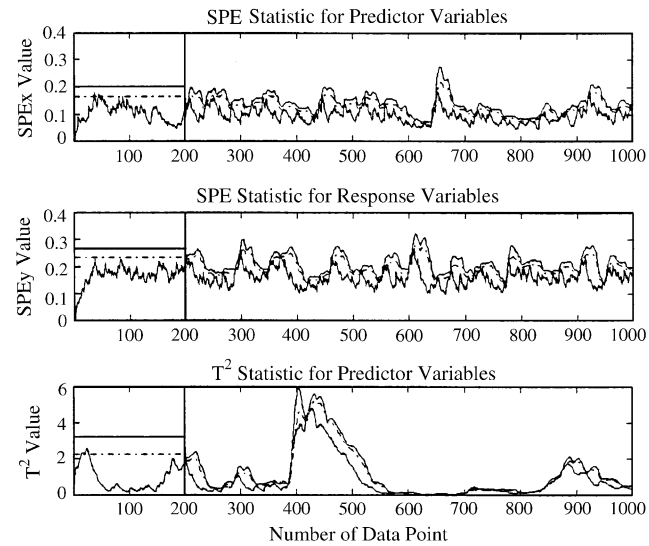

Fig. 5. Process monitoring of a non-stationary process using RPLS and adaptive determination of the thresholds.

Fig. 6 shows that the RPCA approach by Li et al. (2000) can accommodate non-stationary process behaviour if the confidence limits of the T^2 limits are adapted, in this example with a window length of 50, as discussed in Section 4.3. The choice of RPLS in this paper is based on the partitioning of the process variables into predictor and response variables. This can provide initial information to assist the diagnosing of abnormal events as discussed in Section 5. In particular, the application of RMBPLS can present valuable information about the contribution of individual process units to an abnormal event.

4.6. Time varying process behaviour

Fig. 7 presents the application of the introduced monitoring scheme to the data that describe time varying process behaviour, see Section 3.2. The superimposed ramp to one of the linear parameters for determining the response variables can clearly be accommodated by the recursive PLS algorithm. Additionally, the adaptation of the confidence limits for each univariate statistic can accommodate variations that occur as a consequence of the time varying process behaviour and cannot be recursively adapted.

In cases where the RPLS model cannot adapt the influence of time variant process behaviour rapidly enough, a forgetting factor can be incorporated to down-weight older data points and to give more emphasis to newer data points. In contrast, if time variant process behaviour is slowly progressing the forgetting factor may also be selected to down-weight

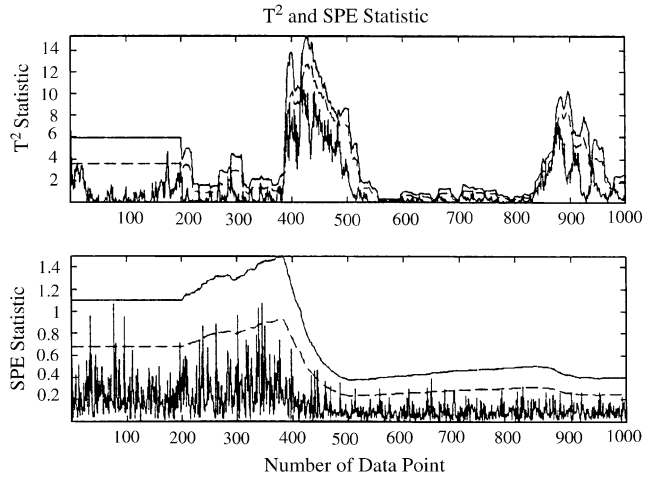

Fig. 6. Process monitoring of a non-stationary process using RPCA with adaptive determination of both thresholds.

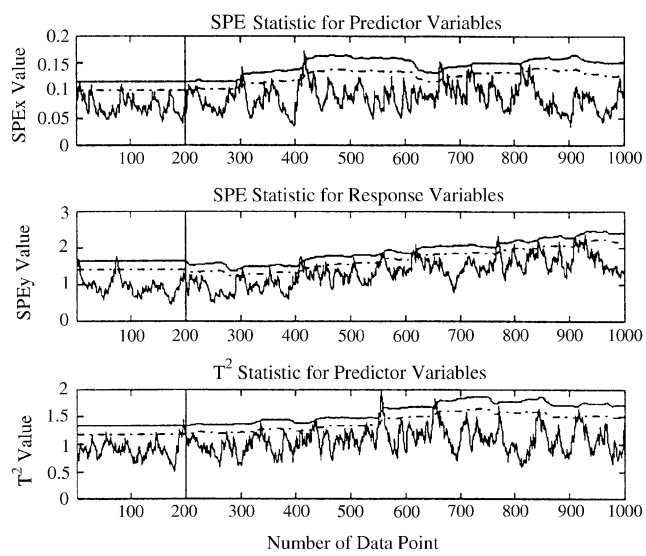

Fig. 7. Process monitoring of a time varying process using RPLS and adaptive determination of the thresholds.

newer samples in order to give more emphasis on older samples. Introducing a forgetting factor along with the length L, however, requires considerably a priori knowledge otherwise the monitoring approach may be insensitive in detecting abnormal process behaviour. In this paper, no forgetting factor was considered in any of the presented application studies.

5. Application studies

In this section, two application studies are considered to illustrate the benefits of the recursive PLS and recursive MBPLS approaches along with an adaptation of the confidence limits. The processes are firstly a simulation of a fluid catalytic cracking unit (FCCU), published by McFarlane, Reineman, Bartee, and Georgakis (1993), and secondly an industrial distillation process for purifying butane. The next subsection introduces the principles of the processes. This is followed by the details of how recursive PLS was applied to both processes and how recursive MBPLS was applied to the FCCU. Note that the ordinates of each monitoring chart are presented logarithmically. This is to reduce the sharp increase in corresponding statistics, which occurs with the injection of occurrence of abnormal process behaviours.

5.1. Description of the processes

5.1.1. The simulation of a fluid catalytic cracking unit

A fluid catalytic cracking unit or FCCU is an important economic unit in refining operations. It typically receives several different heavy feedstocks from other refinery units and cracks these streams to produce lighter, more valuable components that are eventually blended into gasoline and other products. The particular Model IV unit described by McFarlane et al. (1993) is illustrated in Fig. 8. The principal feed to the unit is gas oil, but heavier diesel and wash oil streams also contribute to the total feed stream. Fresh feed is preheated in a heat exchanger and furnace and then passed to the riser, where it is mixed with hot, regenerated catalyst from the regenerator. Slurry from the main fractionator bottoms is also recycled to the riser. The hot catalyst provides the heat necessary for the endothermic cracking reactions. The gaseous cracked products are passed to the main fractionator for separation. Wet gas at the top of the main fractionator is increased to the pressure of the downstream separation by the wet gas compressor. Separation of light components occurs in this downstream separation section. As a result of the cracking process, a carbonaceous material, coke, is deposited on the surface of the catalyst, which depletes its catalytic property. For this reason, spent catalyst is recycled to the regenerator where it is mixed with air in a fluidised bed for regeneration of its catalytic properties. Oxygen reacts with the deposited coke to produce carbon monoxide and carbon dioxide. Air is pumped to the regenerator with a high-capacity combustion air blower and a smaller lift air blower. In addition to contributing to the combustion process, air from the lift air blower assists with catalyst circulation. Complete details of the mechanistic simulation model for this particular model IV FCCU can be found in (McFarlane et al., 1993). This was simulated in C.

The selected process variables for the FCCU case study are given in Table 2. In order to obtain from the simulation typical signals that exhibit non-stationary character, various different ARIMA and ARMA signals

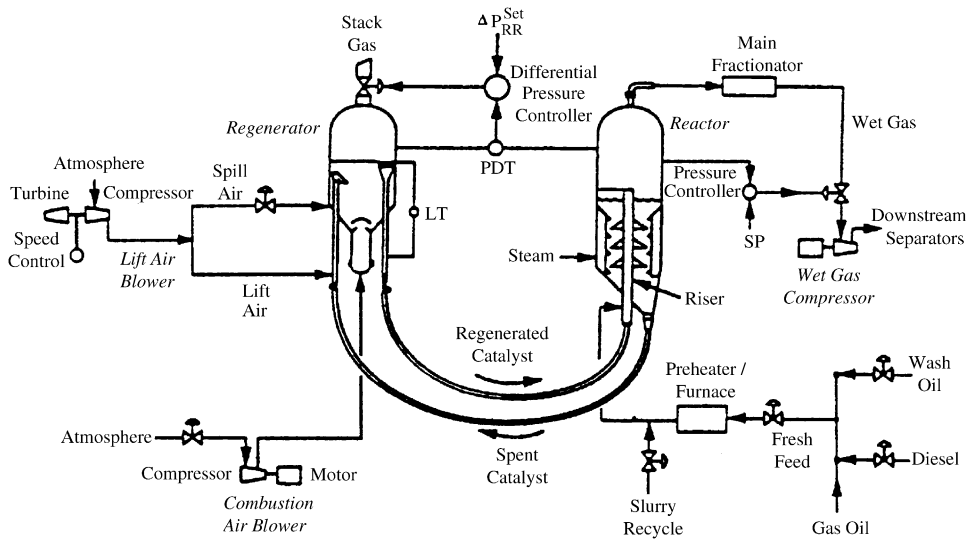

Fig. 8. Schematic diagram of the fluid catalytic cracking unit.

Table 2
Considered process variables of the FCCU case study

	Variable No.	Description
Predictor variables	1	Wash oil feed flowrate
	2	Total fresh feed flowrate
	3	Slurry flowrate
	4	Preheater outlet temperature
	5	Fresh feed temperature to riser
	6	Furnace firebox temperature
	7	Combustion air blower suction flowrate
	8	Combustion air blower throughput
	9	Combustion air flowrate
	10	Lift air blower suction flowrate
	11	Lift air blower speed
	12	Lift air blower throughput
Response variables	13	Riser temperature
	14	Wet gas compressor suction pressure
	15	Wet gas compressor suction flowrate
	16	Wet gas flowrate to vapour recovery unit
	17	Regenerator bed temperature
	18	Regenerator stack gas temperature
	19	Regenerator pressure
	20	Standpipe catalyst level
	21	Stack gas O_2 concentration
	22	Combustion air blower discharge pressure
	23	Wet gas composition suction valve position

were superimposed on the initial or calculated values of the predictor variables as indicated in Table 3. The predictor variables represent the feed section and the air blower units of the FCCU.

In order to achieve time varying process behaviour, two parameters within the model, i.e. the coke formation factor and the ambient air temperature were modified by the addition of an ARIMA signal. Both these parameters are not among the measured predictor variables but clearly influence the performance of the FCCU. The variation of the coke formation factor influenced the amount of coke deposited on the catalyst whereas changes in the ambient air temperature influenced the performance of the air blowers and subsequently the reaction conditions of the regenerator.

The response variables are listed in Table 2. A complete list of measured variables of the FCCU system may be found in (McFarlane et al., 1993). To simulate measurement noise, an ARMA signal was added to each of the process variables.

Table 3
Selected predictor variables for FCCU case study

No	Predictor variable	Added signal	Initial value
1	Wash oil feed flowrate	ARMA sequence	13.8 lb/s
2	Total fresh feed flowrate	ARIMA sequence	126.0 lb/s
3	Slurry flowrate	ARIMA sequence	5.25 lb/s
4	Preheater outlet temperature	ARIMA sequence	460.9°F
5	Fresh feed temperature to riser	ARMA sequence	667.261°F
6	Furnace firebox temperature	ARMA sequence	1607.55°F
7	Combustion air blower suction flowrate	ARMA sequence	Calculated
8	Combustion air blower throughput	ARMA sequence	Calculated
9	Combustion air flowrate	ARMA sequence	Calculated
10	Lift air blower suction flowrate	ARMA sequence	Calculated
11	Lift air blower speed	ARMA sequence	Calculated
12	Lift air blower throughput	ARMA sequence	Calculated

The FCCU simulator included several pre-programmed faults that could be applied on command. The first was a 5% loss in combustion air blower capacity. The second simulated a degradation in the flow of regenerated catalyst between the regenerator and riser, which is typically caused by partial or complete plugging of steam injectors located in this line. The third fault considered was a 5% decrease in the heat exchanger coefficient, which simulates fouling in the furnace. For each of these faults, a data set was simulated containing 1150 data points at sampling intervals of 1 min. Each fault was injected after 950 data points of the recorded data set. This produced three data sets, which will be referred to as Fault1, Fault2 and Fault3.

5.1.2. An industrial distillation process

This distillation process, schematically shown in Fig. 9, is designed to purify Butane from a fresh feed comprising of a mixture of hydrocarbons, mainly Butane and Hexane and impurities of Propane. The distillation tower includes 33 trays with which the separation is achieved. A purified Butane stream leaves the distillation process as the top product and consequently, the Hexane and impurities of Propane leave the distillation process with the bottom draw.

The process operates at a single operating point and the product quality refers to Hexane concentration in the top draw. More precisely, the Hexane concentration should be kept below a predefined limit. Furthermore, to achieve an economic operation, it is desirable to maintain the Butane concentration of the bottom draw also below a specified limit.

Since there is no respective controller to regulate the top and bottom concentrations of Hexane and Propane, the process operation will be affected by changes in the feed and the feed-temperature. It is clear that any variation of these variables will eventually result in undesired variation of the top and bottom draw concentrations.

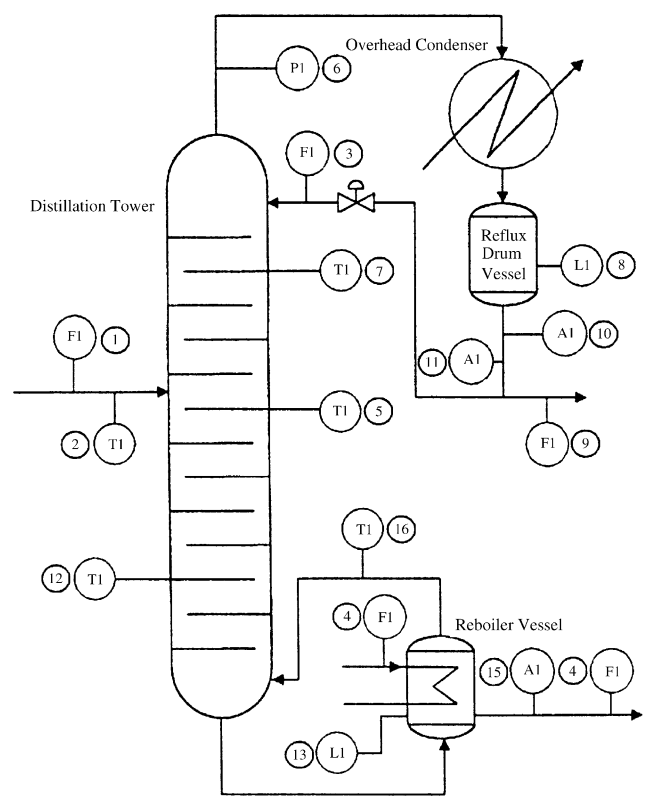

Fig. 9. Schematic diagram of the industrial distillation process.

The predictor variables of this process are the flow and the temperature of the fresh feed, the reflux flow and the fuel flow within the reboiler. As response variables, the temperatures, pressures, flow-rates and compositions are selected and the process variables are as listed in Table 4. Note that the circled numbers in Fig. 9 correspond to the process variables listed in Table 4.

5.2. Application of recursive PLS to the fluid catalytic cracking unit

Before the recursive PLS approach can be applied to the unit, an initial PLS regression model has to be

established. The number of latent variables retained was selected as advocated by MacGregor et al. (1991), i.e. the contribution of the rank one component matrices to the response matrix was analysed and the most dominant LVs were selected and insignificantly contributing LVs were discarded.

For the FCCU example study, the first 500 sampling points of the data set Fault1 were used to identify the initial regression model. The contribution of the rank one component matrices to the predictor and the response matrices are summarised in Table 5. Whilst the first 2 LVs contribute significantly to the response matrix, the remaining LVs are only marginally contributing, thus 2 LVs were retained. The "window" size for determining the thresholds for each univariate statistic was selected to include the past 50 values.

5.2.1. Fault 1: loss of combustion air blower capacity

The procedure described in Section 4.4 was applied to the first data set (Fault1). The RPLS monitoring charts representing the loss of combustion air blower capacity are given in Fig. 10, which shows that each of the univariate statistics are strongly affected by this event. The strongest response is observed in the $SPE^{(X)}$ statistic. A much smaller response is seen in the T^2 statistic, and the $SPE^{(Y)}$ statistic shows still a significant response. This makes physical sense as a loss of combustion air blower capacity reduces the airflow into the regenerator and hence reducing the regenerator pressure. There are a number of consequences that are associated with the reduction in regenerator pressure. Firstly, the lift air blower increases its level of air pumped into the spent catalyst line, secondly, less oxygen is available for recycling the catalyst, which

Table 4
Considered process variables for the industrial distillation process

	Variable No.	Description
Predictor variables	1	Fresh feed flow
	2	Temperature of fresh feed
	3	Reflux flow
	4	Reboiler steam flow
Response variables	5	Tray 14 temperature
	6	Column overhead pressure
	7	Tray 2 temperature
	8	Reflux vessel level
	9	Butane product flow (top draw)
	10	Percentage of C3 in C4
	11	Percentage of C5 in C4
	12	Tray 31 temperature
	13	Reboiler vessel level
	14	Bottom draw
	15	Percentage of C4 in C5
	16	Reboiler temperature

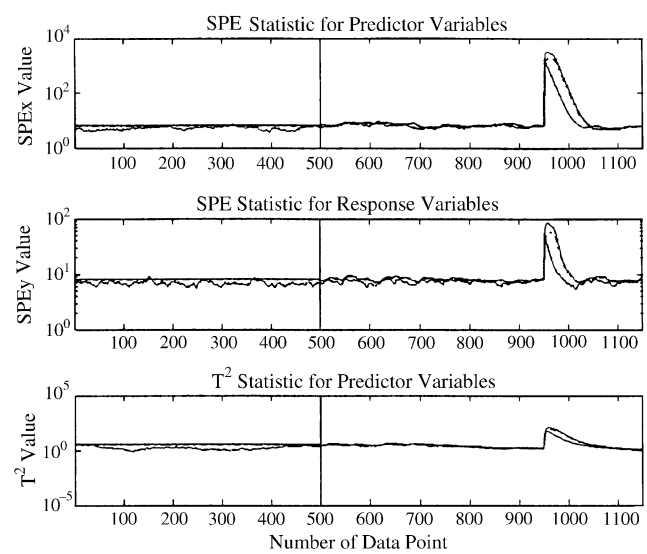

Fig. 10. RPLS monitoring charts representing the loss in combustion air blower capacity (FCCU).

Table 5
Contribution of the rank one component matrices to the predictor and response matrices (FCCU case study)

LV	Predictor variables		Response variables	
	This LV	Total	This LV	Total
1	48.45	48.45	28.41	28.41
2	11.92	60.37	5.39	33.81
3	6.95	67.32	0.84	34.64
4	2.87	70.19	1.01	35.65
5	4.45	74.65	0.50	36.15
6	4.54	79.19	0.37	36.52
7	4.19	83.38	0.26	36.78
8	5.44	88.82	0.13	36.91
9	1.29	90.11	0.56	37.46
10	4.38	94.49	0.19	37.66
11	4.93	99.43	0.11	37.77
12	0.57	100	0.04	37.80

thirdly leads to a deterioration of the reaction conditions in the riser.

Given the above discussion, most of the predictor variables contribute to this event leading to a considerable change in the relationship between them. This change gives rise to a considerable increase of the $SPE^{(X)}$ statistic. Since the reaction conditions in the regenerator and the riser are clearly affected, the $SPE^{(Y)}$ statistic is also significant. Since the variables of the air blowers in particular vary excessively, the overall variation of the predictor variables is significant and thus, the T^2 statistic variation is significant too.

5.2.2. Fault 2: degradation in the flow of regenerated catalyst

The corresponding RPLS monitoring charts for this event, as seen in the data set Fault 2, are presented in Fig. 11. It can be seen from this figure that the $SPE^{(Y)}$ statistic is most dominantly responding to this event. Physically, any change in regenerated catalyst flow will primarily affect catalyst-to-feed ratio in the riser, resulting in a change in the amount of coke deposited on spent catalyst and subsequently the level of oxygen usage in the regenerator. Further consequences are related to the material balance in the standpipe, and hence its level as well as the reaction conditions in the reactor.

Given the above discussions, most of the response variables were affected which explains the dominant response of the $SPE^{(Y)}$ statistic. An increase in the T^2 and the $SPE^{(X)}$ statistic can, however, be noted too. This is explained by a pressure change in the regenerator as a consequence of the excess production of carbon monoxide and carbon dioxide, which leads to a reduction of the air-flow of the combustion as well as the lift air blower. A change of the relationship between the predictor variables is the consequence, which leads to a significant $SPE^{(X)}$ statistic. Since the variation of the air blower variables is excessive, the T^2 statistic is significant too.

5.2.3. Fault 3: decrease in the heat exchanger coefficient of the furnace

Fig. 12 presents the RPLS monitoring charts corresponding to the performance degradation of the furnace, as seen in the data set Fault 3. This figure shows that the $SPE^{(X)}$ statistic is strongly affected by this event followed by the T^2 statistic. Small but insignificant response can also be noticed from the $SPE^{(Y)}$ statistic. A decrease of the heat exchanger coefficient reduces the amount of heat exchanged with the consequence of a lower temperature of the outlet stream. Therefore, fresh feed stream entered the riser with a lower temperature than expected. This did not lead to a significant change in the reaction conditions as the hot catalyst provided the necessary heat for the endothermic reactions. However, the parametric model between the predictor and the response variables cannot be updated with immediate effect and hence, a small contribution of the $SPE^{(Y)}$ statistic can be noticed.

Given the above discussion, the relationships between the predictor variables changed considerably leading to a significantly increased $SPE^{(X)}$ statistic. Since the drop in the fresh feed temperature represents an excessive variation of that variable, the T^2 statistic is also significant.

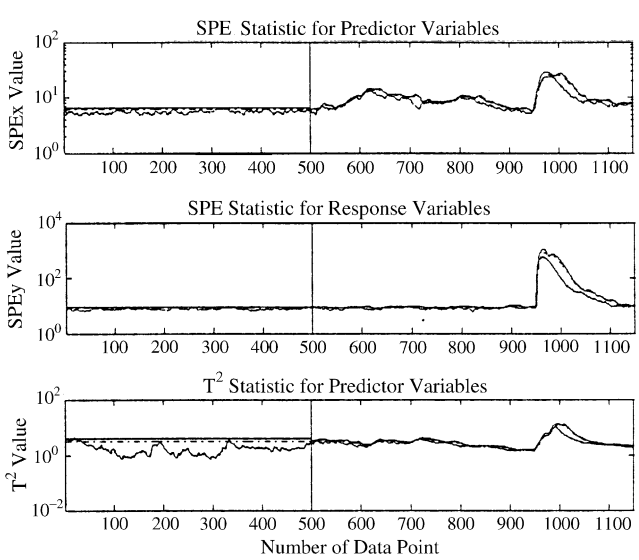

Fig. 11. RPLS monitoring charts representing the degradation in the flow of regenerated catalyst (FCCU).

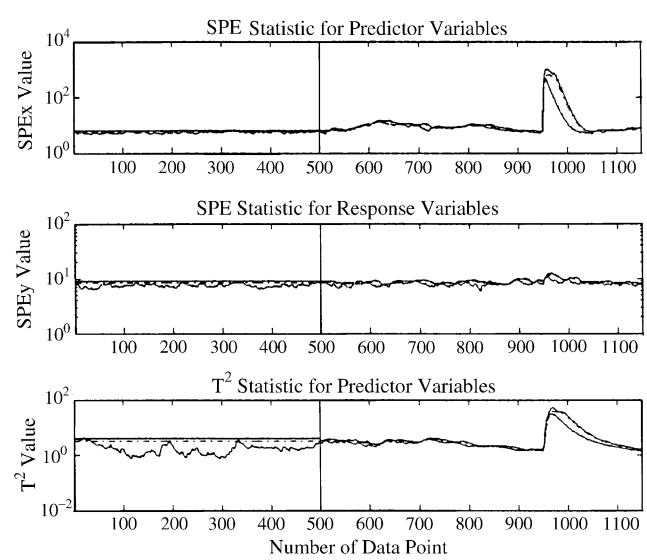

Fig. 12. RPLS monitoring charts representing the decrease in the heat exchanger coefficient (FCCU).

5.3. Application of recursive PLS to the distillation process

Two data sets were considered to demonstrate the performance of the introduced monitoring scheme. The first data set illustrates that this process is time varying and behaves non-stationary. The second data set presents an example of a severe drop in feed flow and feed temperature that led eventually to an upset of the process performance, i.e. the concentration of Hexane in the top draw and Butane in the bottom draw exceeded their predefined limits. The first data set contains 2400 data points and the second data set contains 980 data points that were recorded at a sampling interval of 30 s.

The first 450 sampling points were used to identify an initial regression model for the first data set. The contribution of the rank one component matrices to the predictor and response matrices is presented in Table 6. It can be seen that the first 3 LVs contribute significantly to the response variables, whilst the 4th LV makes negligible difference. Hence, 3 LVs are selected for this process. The window size for determining the confidence limits for each univariate statistic was selected to include the past 50 values.

The resultant monitoring statistics are established on the first data set and presented in Fig. 13. It can be seen that the $SPE^{(X)}$ statistic did not show significant variations and hence the residuals of the predictor variables are insignificant at any time. This also implies that the relationships between the predictor variables did not change significantly. However, the T^2 statistic presents non-stationary behaviour, which can also be noticed by the variations of the confidence limits. That the process is time varying can be seen from the $SPE^{(Y)}$ statistic, which does not show the character of stochastic Chi-Squared distributed signal. In fact, the variations of the confidence limits indicate that residuals of the response variables vary with time, compare the value of the $SPE^{(Y)}$ statistic at the 600th sample with that of the 700th sample for instance.

Since the abnormal process behaviour was recorded about 350 data points into the data set, the first 300 data points were used to identify an initial model for the second data set. This drop in feed and feed temperature led to a drop in the liquid level at the bottom of the distillation tower and consequently an increase in its temperature. Consequently, more Hexane was evaporated and the concentration of Hexane in the top draw exceeded the predefined limit.

The RPLS monitoring charts are presented in Fig. 14. The drop of the fresh feed occurred 2 h and 55 min (equal to 350 data points) after the recording began. At first, the T^2 and the $SPE^{(X)}$ statistic respond to this event. With a delay of about 20 min (40 data points), the $SPE^{(Y)}$ statistic shows a considerably increasing response to this event with a duration of approximately 25 min until it settles to show very large $SPE^{(Y)}$ values thereafter.

The observations from the monitoring charts describe a physically correct representation of the progression of this event. The reduced flow of fresh feed as well as the drop in fresh feed temperature lead gradually to an increasing temperature of the liquid at the bottom of the distillation column. Therefore, the temperature measurements in the distillation tower follow the increase in specific enthalpy at first, followed by a considerable increase of the Hexane concentration in the top draw. It should be noted that heat-exchanging processes within

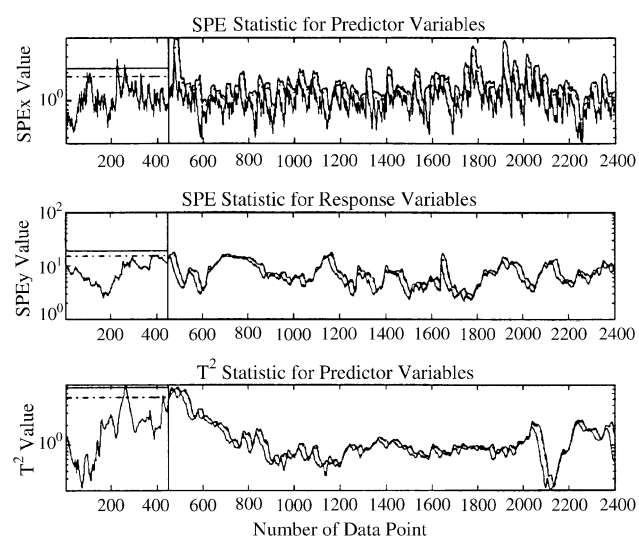

Fig. 13. RPLS monitoring charts representing non-stationary process behaviour (Distillation process).

Table 6
Contribution of the rank one component matrices to the predictor and response matrices (industrial distillation process)

LV	Predictor variables		Response variables	
	This LV	Total	This LV	Total
1	35.43	35.43	20.21	20.21
2	45.01	80.43	11.09	31.30
3	18.69	99.13	8.39	39.69
4	0.87	100	1.08	40.78

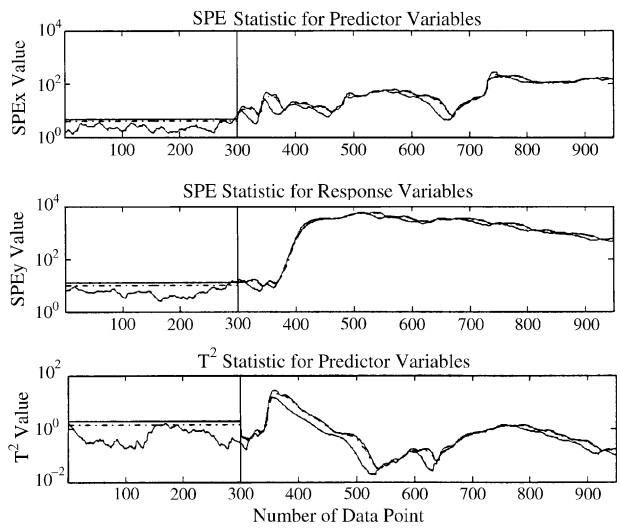

Fig. 14. RPLS monitoring chart representing the drop in feed and feed temperature (Distillation process).

the distillation unit could not be initiated instantly and therefore a gradual response to the alterations of the feed conditions occurred.

5.4. Application of recursive MBPLS to the fluid catalytic cracking unit

The operation of the FCCU suggests dividing the predictor variables into a block that represent the feed section and a block that is associated with the air blowers. The block in which the variables of the feed section are stored is referred to as block 1 and the block in which the variables that are associated with the air blowers are stored is denoted as block 2.

The proposed division of the predictor variables is expedient since the 6 variables of the feed section influence primarily the reaction condition in the riser. Furthermore, the remaining 6 variables of the air blowers influence mainly the regenerator. Fig. 8 and Table 3 give a list of the predictor variables. The catalyst flow connects the reactor with the regenerator and vice versa. Thus these process units are clearly shown to be highly interactive. The resultant diagnosis of each of the three abnormal events is individually presented in the following subsections.

5.4.1. Loss of combustion air blower capacity

The corresponding monitoring statistics of block 1 and block 2, i.e. the T^2 and the $SPE^{(X)}$ statistics, are presented in Figs. 15 and 16, respectively and the $SPE^{(Y)}$ statistic is shown in Fig. 17. From these figures, it can be seen that the most dominant response to this event is associated with the $SPE^{(X)}$ and T^2 statistics of block 2 and the $SPE^{(Y)}$ statistic. In contrast, the T^2 and the $SPE^{(X)}$ statistics of block 1 show a small but noticeable response to this event.

As the variables of the combustion air blower are stored in block 2 and the variables of the lift air blower are also affected by this event, the large response of the block 2 statistics would assist an experienced plant operator in narrowing down potential causes of this event. A more detailed discussion of this abnormal conditions is presented in Section 5.2.

5.4.2. Degradation in the flow of regenerated catalyst

The $SPE^{(X)}$ and T^2 statistics of block 1 and block 2 are presented in Figs. 18 and 19, respectively, and the $SPE^{(Y)}$ is shown in Fig. 20. A strong response to the degradation of the regenerated catalyst flow is apparent from the $SPE^{(Y)}$ statistic. Furthermore, a small response is also noticeable from the T^2 statistic of block 2 and the remaining statistics do not show a significant response.

As discussed in Section 5.2, this abnormal event affects mainly the response variables and subsequently the variables of the air blowers. The provided RMBPLS monitoring charts therefore give a correct representation of this event as they reveal a considerable mismatch between the measured and the predicted response variables and excessive variation of the variables corresponding to the air blowers. This would assist an experienced operator in identifying potential root causes of this event.

5.4.3. Decrease in the heat exchanger coefficient of the furnace

The corresponding monitoring charts for this fault are presented in Figs. 21 and 22 (T^2 and $SPE^{(X)}$ statistics for blocks 1 and 2, respectively) and Fig. 23 ($SPE^{(Y)}$ statistic). A strong response to this event comes from the $SPE^{(X)}$ statistics of both predictor blocks. In contrast, the T^2 statistic of both predictor blocks and the $SPE^{(Y)}$ statistic only show a small but noticeable response. The fact that both predictor blocks show responses to this event is a consequence of the super t-scores being determined on the basis of the whole set of predictor variables, which can be seen from the multi-block algorithm in the appendix. Since the p-loading vectors for each block are determined with respect to the super t-scores, an abnormal process behaviour that affects primarily a single predictor block may propagate through to affect other predictor blocks too. This can also be observed from the other two examples above, however, to a much lesser degree. Though both predictor blocks appear to respond to the performance deterioration of the furnace, it should be noted that the response of block 1 is much more significant (by a factor of 10). On the basis of the RMBPLS monitoring charts, an experienced operator would be advised to trace the

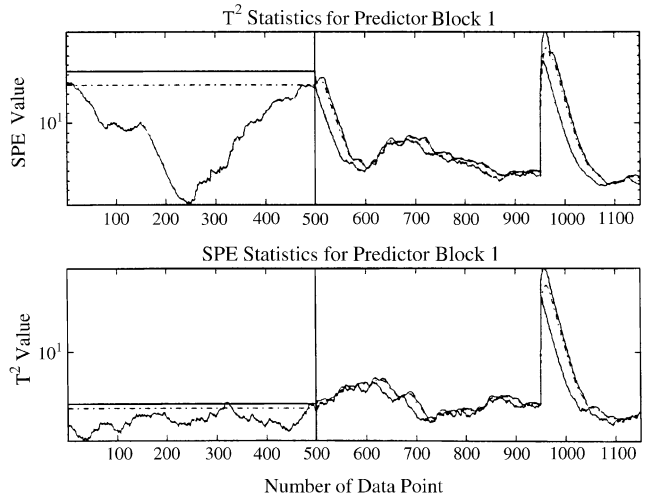

Fig. 15. RMBPLS monitoring chart for Block 1 (feed section) representing the loss in combustion air blower capacity (FCCU).

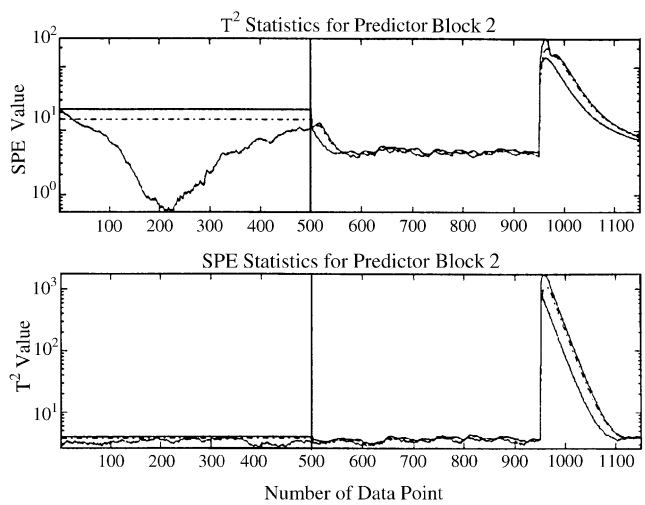

Fig. 16. RMBPLS monitoring chart for Block 2 (air blowers) representing the loss in combustion air blower capacity (FCCU).

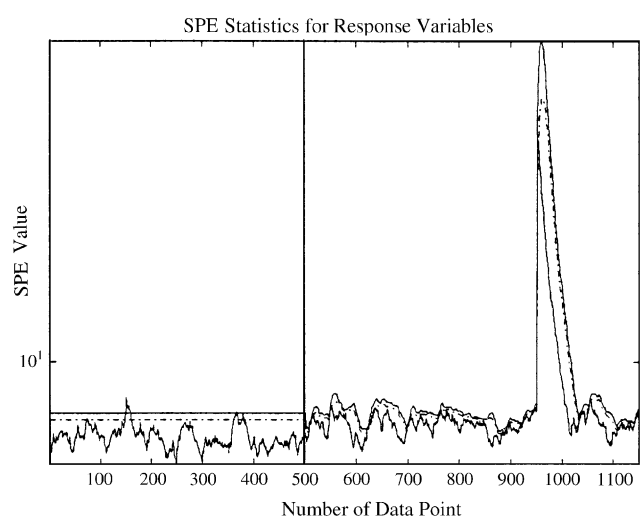

Fig. 17. RMBPLS monitoring chart for response block representing the loss in combustion air blower capacity (FCCU).

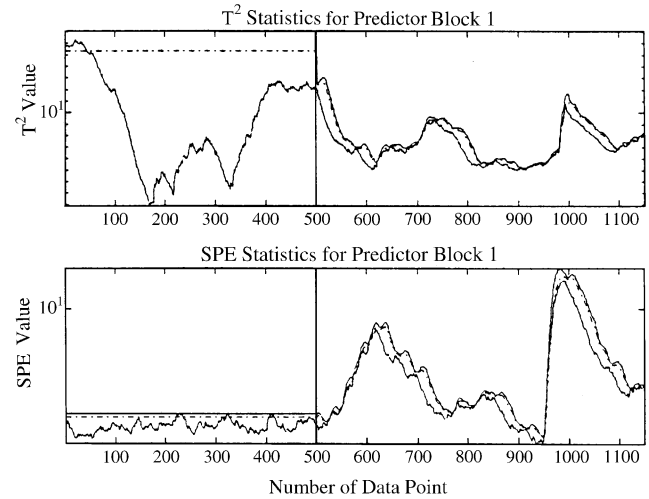

Fig. 18. RMBPLS monitoring chart for Block 1 (feed section) representing the degradation if the flow of regenerated catalyst (FCCU).

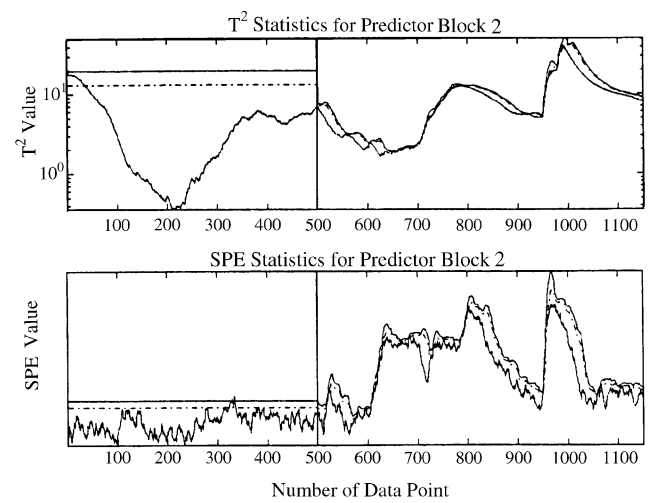

Fig. 19. RMBPLS monitoring chart for Block 2 (air blowers) representing the degradation of the flow of regenerated catalyst (FCCU).

root cause of this event to a problem within the feed section of the FCCU.

6. Conclusions

In this paper, the monitoring of complex industrial processes that exhibit non-stationary and time varying behaviour is discussed. It is shown that monitoring methods that fall under the conventional MSPC framework give rise to false alarms, thus rendering the practical implementation of such methods a difficult task. This is illustrated using two simplified examples.

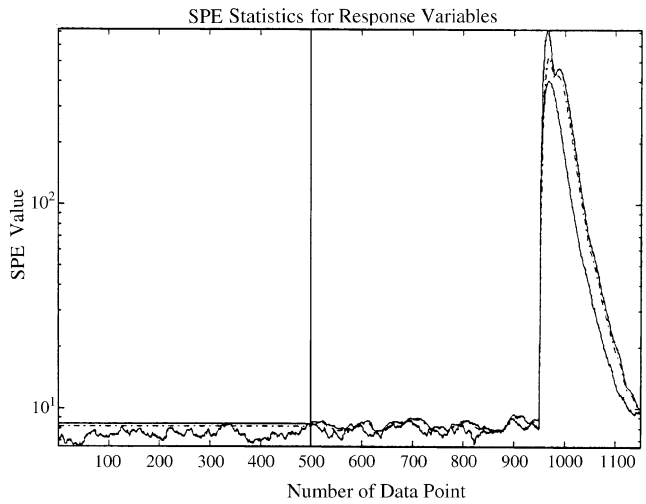

Fig. 20. RMBPLS monitoring chart for the response block representing the degradation if the flow of regenerated catalyst (FCCU).

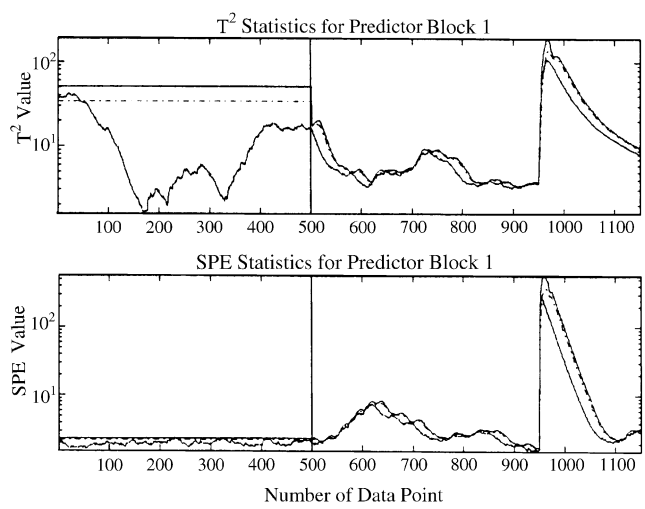

Fig. 21. RMBPLS monitoring chart for Block 1 (feed section) representing the decrease in the heat exchanger coefficient of the furnace (FCCU).

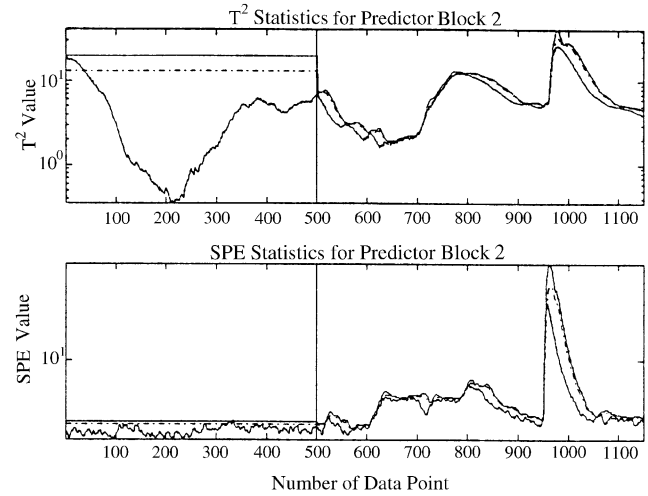

Fig. 22. RMBPLS monitoring chart for Block 2 (air blowers) representing the decrease in the heat exchanger coefficient of the furnace (FCCU).

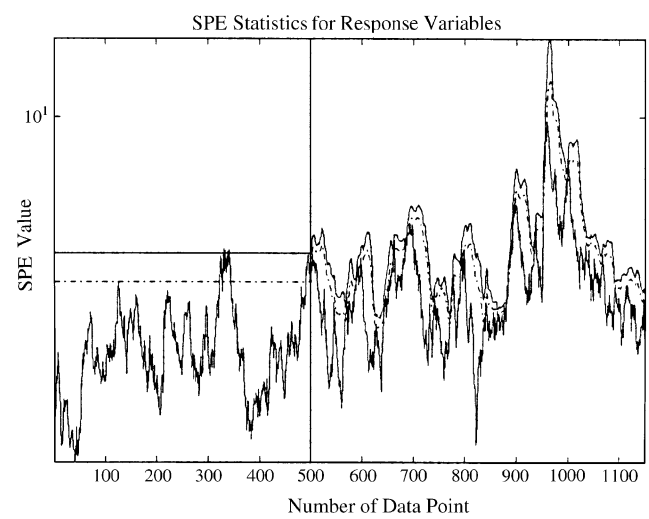

Fig. 23. RMBPLS monitoring chart for response block representing the decrease in the heat exchanger coefficient of the furnace (FCCU).

Furthermore, it is also shown that a recursive adaptation of the employed MSPC model alone, as proposed by Li et al. (2000), does not necessarily reduce the number of false alarms if the process shows non-stationary process behaviour.

To overcome the deficiency of conventional MSPC, recursive PLS algorithms are considered along with an adaptation of the confidence limits for each of the utilised univariate statistics. RPLS is advocated to RPCA because the process variables are divided into predictor and response variables, which provides an enhanced initial diagnosis. The inclusion of an offset term, as proposed by Qin (1998), as an additional predictor variable is re-considered and it is concluded that such an offset term must be included if the process is time variant. In contrast, non-stationary process behaviour does not require the inclusion of such an offset term.

On the basis of the two simple examples, it is concluded that the application of recursive PLS and the adaptation of the confidence limits can reduce the number of false alarms considerably-presumably whilst still being able to detect faults. As a further contribution of this paper, it is demonstrated that the recursively updated PLS model can be integrated into the modified multi-block PLS algorithm.

The introduced monitoring scheme is applied to a simulation of a fluid catalytic cracking unit (FCCU) and an industrial distillation process. The FCCU simulator was programmed to include several pre-programmed

faults of which a 5% loss of combustion air blower capacity, a degradation of the flow of regenerated catalyst and a 5% decrease in the heat exchanger coefficient of the furnace are considered in this paper. The feed of the industrial distillation process can drop drastically and hence affect the concentrations of impurities within the product stream. An example of such an event was recorded and investigated.

Both application studies demonstrated that the introduced monitoring approach did not raise false alarms and that the investigated abnormal conditions were detected. With RPLS, the monitoring charts gave a clear indication as to where the predictor and/or the response variables corresponded to the abnormal events under investigation. Furthermore, the application of RMBPLS showed that division of the predictor variables of the FCCU led to a correct diagnosis of the contributing blocks. Hence, an experienced operator could be assisted to reduce the number of possible causes of the abnormal events.

An additional benefit of the introduced monitoring approach is that only a relatively small number of data are required to identify an initial process model. In contrast, applications of conventional MSPC approaches require a substantial amount of operating data to guarantee that normal process variation is captured in sufficient detail, otherwise, false alarms may be the consequence. Furthermore, the sensitivity of this monitoring approach can be influenced by the basis of the forgetting factor used for updating the PLS model and the window size for computing the confidence limits for the monitoring charts. This allows the "speed" of adaptation to be adjusted so that abnormal process behaviour is still detectable by the monitoring approach.

It should be noted that the window length for an adaptive estimation of the confidence limits has to be selected with care. If the window length is too short, the confidence limits are adapted very quickly and even abnormal behaviour may be adapted, which, in fact, should be detected. In contrast, if the window length is too long, the adaptation of the confidence limits is very slow and consequently, false alarms may occur. The method proposed in this paper is to apply the RPLS and the RMBPLS approach to a second reference data set. The number of violations of the adaptive confidence limits can then be recorded versus the window length and form a criterion to determine the window length.

Future work is focused on utilising contribution charts for improving the diagnosis of abnormal process behaviour and to further compare the introduced monitoring approach with the RPCA approach by Li et al. (2000). Another aspect that requires attention is that of auto-correlated process data, which often occur in industrial processes. Therefore, further work is focused on how to treat auto-correlated process data.

Acknowledgements

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Appendix. Modification of the MBPLS algorithm

The multi-block PLS algorithm is presented below. The changes to achieve super t-score vectors of unit length are summarised in the box (Westerhuis et al., 1998).

1	Mean centre and appropriately scale $\mathbf{X}_1$, $\mathbf{X}_2$ and $\mathbf{Y}$	
2	Set $\mathbf{u}$ to the first column of $\mathbf{Y}$	
3	Loop until convergence of $\mathbf{u}$	
3.1	Determine block weight vector for $\mathbf{X}_1$ block:	$\mathbf{w}_1 = \dfrac{\mathbf{X}_1^{\mathrm{T}}\mathbf{u}}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}$
3.2	Scale first block weight vector to unit length:	$\mathbf{w}_1 = \dfrac{\mathbf{w}_1}{\lVert \mathbf{w}_1 \rVert_2}$
3.3	Calculate t-score vector for $\mathbf{X}_1$ block:	$\mathbf{t}_1 = \mathbf{X}_1\mathbf{w}_1$
3.4	Determine block weight vector for $\mathbf{X}_2$ block:	$\mathbf{w}_2 = \dfrac{\mathbf{X}_2^{\mathrm{T}}\mathbf{u}}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}$
3.5	Scale second block weight vector to unit length:	$\mathbf{w}_2 = \dfrac{\mathbf{w}_2}{\lVert \mathbf{w}_2 \rVert_2}$
3.6	Calculate t-score vector for $\mathbf{X}_2$ block:	$\mathbf{t}_2 = \mathbf{X}_2\mathbf{w}_2$
3.7	Combine block t-score vectors to super block $\mathbf{T}$:	$\mathbf{T} = [\mathbf{t}_1 \vert \mathbf{t}_2]$
3.8	Determine block weight vector:	$\mathbf{w}_T = \dfrac{\mathbf{T}^{\mathrm{T}}\mathbf{u}}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}$

3.9	Determine super t-score vector:	$\mathbf{t}_T = \mathbf{T} \cdot \mathbf{w}_T$
3.10	Adjust length of super block weight vector:	$\mathbf{w}_T = \dfrac{\mathbf{w}_T}{\lVert \mathbf{t}_T \rVert_2}$
3.11	Set super t-score vector to unit length:	$\mathbf{t}_T = \dfrac{\mathbf{t}_T}{\lVert \mathbf{t}_T \rVert_2}$
3.12	Calculate loading vector for response block:	$\mathbf{q} = \dfrac{\mathbf{Y}^{\mathrm{T}} \cdot \mathbf{t}^{\mathrm{T}}}{\lVert \mathbf{Y}^{\mathrm{T}} \cdot \mathbf{t}_T \rVert_2}$
3.13	Calculate new score vector of response block:	$\mathbf{u} = \mathbf{Y} \cdot \mathbf{q}$
4	Determine loading vector for $\mathbf{x}_1$ block:	$\mathbf{p}_1 = \mathbf{X}_1^{\mathrm{T}} \mathbf{t}_T$
5	Determine loading vector for $\mathbf{x}_2$ block:	$\mathbf{p}_2 = \mathbf{X}_2^{\mathrm{T}} \mathbf{t}_T$
6	Calculate regression coefficient for score model:	$b = \mathbf{u}^{\mathrm{T}} \mathbf{t}_T$
7	Deflate $\mathbf{X}_1$ block using super t-score vector:	$\mathbf{X}_1 = \mathbf{X}_1 - \mathbf{t}_T \mathbf{p}_1^{\mathrm{T}}$
8	Deflate $\mathbf{X}_2$ block using super t-score vector:	$\mathbf{X}_2 = \mathbf{X}_2 - \mathbf{t}_T \mathbf{p}_2^{\mathrm{T}}$
9	Deflate response block:	$\mathbf{Y} = \mathbf{Y} - b \mathbf{t}_T \mathbf{q}^{\mathrm{T}}$
10	Goto step 2 or terminate algorithm	

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