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Chemical Engineering Journal 67 (1997) 181–189

Chemical Engineering Journal

Process monitoring using non-linear statistical techniques

J. Zhang [a,*], E.B. Martin [b], A.J. Morris [a]

[a] *Centre for Process Analysis, Chemometrics and Control, Department of Chemical and Process Engineering, University of Newcastle, Newcastle upon Tyne NE1 7RU, UK*

[b] *Department of Engineering Mathematics, University of Newcastle, Newcastle upon Tyne NE1 7RU, UK*

Received 21 August 1996; revised 14 April 1997; accepted 17 April 1997

Abstract

A large number of process variables are usually measured and stored in computer data base during process operation. These variables are usually highly correlated and the real dimensionality of the monitored process is considerably less than that represented by the number of process variables collected. Successful process performance monitoring requires the efficient handling of large amounts of monitored plant data. Principal component analysis reduces the dimensionality of the process by creating a new set of variables, principal components, which attempt to reflect the true underlying system dimension. Process performance can then be monitored in a low dimensional principal component space. Linear process performance monitoring is based upon plots of scores and squared prediction errors from a principal component model. However, for highly non-linear processes, this form of monitoring may not be efficient since the process dimensionality cannot be represented by a small number of linear principal components. Non-linearly correlated process variables can be reduced to a set of non-linear principal components, through the application of non-linear principal component analysis. Efficient process monitoring can then be performed in a low dimensional non-linear principal component space. In parallel with the conventional multivariate plots, the use of accumulated scores provides a significant breakthrough in the separation of different operating conditions/faults, leading to robust early warning of potential plant malfunctions. An application to the condition monitoring of a polymerisation reactor demonstrates the effectiveness of the non-linear monitoring approach. © 1997 Elsevier Science S.A.

Keywords: Process monitoring; Fault diagnosis; Multivariate statistics; Non-linear principal component analysis; Polymerisation

1. Introduction

Process equipment is subject to breakdowns and malfunctions during its operational life time. Malfunctions can have a major impact on process behaviour. They can reduce the efficiency and consistency of production, lead to equipment damage, or even result in hazardous situations arising. Prompt detection and diagnosis of faults is becoming increasingly important owing to the increasing economic, safety, and environmental demands. Several techniques for process fault detection and diagnosis have been developed and these include state and parameter estimation based approaches [1–4], knowledge based approaches [5–8], neural network based approaches [9–12], and statistical data analysis based approaches [13–25].

During process operation, typically a large number of process variables are routinely monitored and stored in computer data base. For some complex processes where the first principles models describing the processes are not well understood, or alternatively too complicated to model, then process measurement data could be the only sources for gaining a deep understanding of the processes. These processes have the characteristic of ''data rich and knowledge poor''. Process monitoring based on multivariate statistical analysis of process data has recently been investigated by a number of researchers [13–25]. These approaches use the techniques of principal component analysis (PCA) or projection to latent structure (PLS). The aim of these approaches is to reduce the dimensionality of the correlated process data by projecting them down onto a lower dimensional latent variable space. In practice, there are only a small number of events driving a process at any one time. Thus the true dimensionality of a process is typically low. PCA and PLS aim to realise the true dimensionality of the monitored process. Process performance monitoring can then be carried out in this reduced latent variable space. An envelope of normal operation can be defined from the nominal process operating data. The detection and classification of process malfunctions can be undertaken through the inspection and analysis of plots of

* Corresponding author. Tel.: +44 191 222 6000; fax: +44 191 222 5292; e-mail: jie.zhang@newcastle.ac.uk

PII S1385-8947(97)00048-X

the squared prediction error (SPE) and the scores from the PCA or PLS model.

These multivariate statistical performance monitoring techniques are based on linear statistical techniques. In some processes where severe non-linear correlation exists among process variables, linear statistical techniques are not very effective in reducing process data dimension. If linear PCA is used in these processes, a large number of principal components are required to explain sufficient data variance. In this case, the PCA approach becomes cumbersome because too many plots are needed. For non-linearly correlated data, the results from linear PCA may be inadequate because minor components can contain important information on non-linearity [26]. By discarding the minor components, this important information is lost. However, if these minor components are kept, the linear methods may contain too many components to be useful. For processes with severely non-linear correlation, non-linear statistical techniques for data dimension reduction should be used. This paper presents a technique for process performance monitoring using non-linear statistical technique for PCA. Non-linear PCA can effectively reduce the dimensionality of non-linearly correlated process data. A technique for improved fault classification using accumulated non-linear principal component scores is also proposed in this paper. The proposed non-linear statistical process performance monitoring technique has been applied to a polymerisation process.

This paper is organised as follows. Section 2 presents process condition monitoring based on linear multivariate statistic techniques and discusses their limitations. Section 3 presents non-linear PCA using the principal curve method. Application of non-linear PCA based process monitoring to a polymerisation reactor is described in Section 4. The last section contains some concluding remarks.

2. Statistical process performance monitoring

2.1. Principal component analysis

PCA is one of the most widely used multivariate statistical techniques. By considering all the noisy and highly correlated measurements on a process, a reduced set of latent variables are calculated through the application of PCA. These latent variables summarise all the relevant information by projecting the original information down onto a low dimensional subspace.

Let $X=(x_1, x_2, \ldots, x_m)$ be an m-dimensional data set. The first principal component is the line that best approximates the data, that linear combination of the columns of X which describes the greatest amount of variability $t_1=p_1^{\mathrm{T}}X$ subject to $\|p\|=1$. The direction of the line is determined by the loading vector p_1, and the co-ordinates of the point i are t_{i1}, the scores. The second principal component then explains the greatest amount of variability in the residual data: $t_2=p_2^{\mathrm{T}}E_1$ where $E_1=X-p_1^{\mathrm{T}}t_1$. This procedure is essentially repeated until m principal components are calculated. In effect PCA decomposes the observation matrix, X, as

$$X=TP^{\mathrm{T}}=\sum_{i=1}^{m} t_i P_i^{\mathrm{T}} \tag{1}$$

where p_i is the eigenvector of the covariance matrix of X. The matrix P is defined as the principal component loading matrix and T is defined as the matrix of principal component scores. The loadings provide information as to which variables contribute the most to individual principal components. They are the coefficients on the principal components model.

PCA depends critically on the scales used to measure the variables. If there are large differences between these variables, then those variables whose magnitudes are large will tend to dominate the first a few principal components. Thus the results of PCA vary with the scales used for different variables. The lack of scale invariance implies that care needs to be taken when scaling the data. Different scaling routines can produce different results. A commonly used scaling method is the so called ''auto-scaling'' where each variable is scaled to zero mean and unit variance.

One feature of PCA is that the less important components often describe noise in the data. If the process variables are collinear, k principal components ($k<m$) will explain the majority of the data variability, i.e. a smaller number of principal components than original variables are sufficient to explain the major variability in the data. It is therefore desirable to exclude these less important principal components. The data matrix X can be written as

$$X=\sum_{i=1}^{k} t_i P_i^{\mathrm{T}}+E \tag{2}$$

where E is the residual matrix due to the omission of the less important principal components. The number of components to include in a model can be identified using techniques such as cross-validation [27]. By disregarding E, noise filtering can be achieved. In practice, there are only a small number of events driving a process at any one time. Thus the true dimensionality of a process is typically low, i.e. $k \ll m$. The process performance can then be monitored by using a small number of principal components.

2.2. Performance monitoring charts

Statistical process control (SPC) charts such as the Shewart charts are well established statistical procedures for monitoring stable univariate processes. The assumption behind them is that a process subjects only to its normal variability will remain in a state of statistical control unless a special event occurs. Control charts represent statistical hypothesis testing procedures aimed at detecting the occurrence of a special event as quickly as possible. However, with the advent of new computer systems, a large number of process variables are now monitored. Plotting SPC charts for individual variables therefore becomes excessive and unmanageable for the process operator to successfully monitor process performance. Multivariate monitoring strategies will circumvent such problems.

Development of a monitoring strategy using projection techniques commences with the development of a PCA representation, from nominal process operation data, with an envelope of nominal operation being defined [13,14,20]. Once the nominal model has been defined, the fitted values can be calculated for each new multivariate observation. These values can then be used to evaluate the squared prediction error, SPE, for each new observation, i.e. the squared difference between the observed values and the predicted values from the nominal or reference model. Process monitoring charts can then be set up using the first two or three principal components and the SPE from the PCA model. Figs. 1–3 show a number of performance monitoring charts involving plots of SPE and scores [13]. In Fig. 1 the principal components T1 and T2 form the x and y-axes of the monitoring chart, respectively, with the SPE defining the z-axis. Fig. 2 gives three possible two-dimension representation of scores and the SPE. Fig. 3 can be used to monitor the SPE at each sampling time point. Malfunctions within a process are generally identified by one of the following two scenarios. In the first case, the fault will affect the correlation structure among the measured process variables. The nominal PCA model will cease to be valid and the calculated predictions will result in the SPE being significantly different from zero. This can be detected from the SPE plot and is represented by $\triangle$ in Figs. 1–3. In the second situation, the fault has no impact on the correlation structure between process variables and the SPE will remain within its control limit but, the scores from the PCA model will move outside the envelope of normal operation. This situation is represented by $\times$ in Figs. 1–3. Acceptable process performance would fall within the envelope of normal operation and is represented by $\bigcirc$ in Figs. 1–3. Confidence bounds for the normal operating region can be calculated based upon statistical distribution theory [20,21,23].

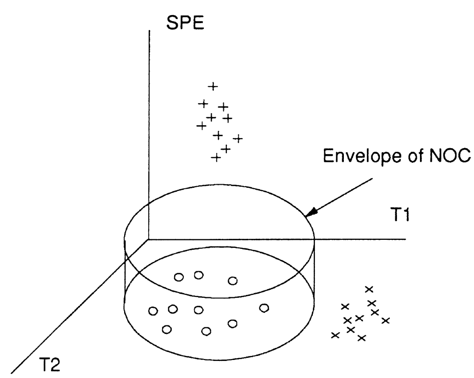

Fig. 1. Three dimensional representation of SPE and scores.

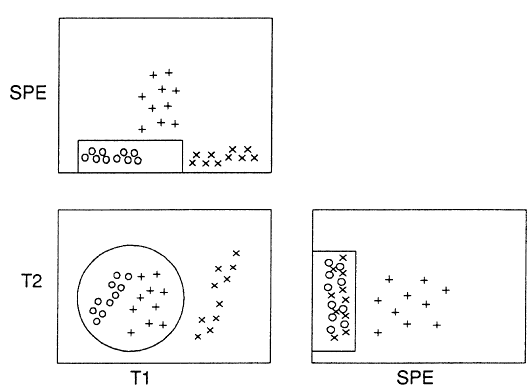

Fig. 2. Various two-dimensional representations of scores and SPE.

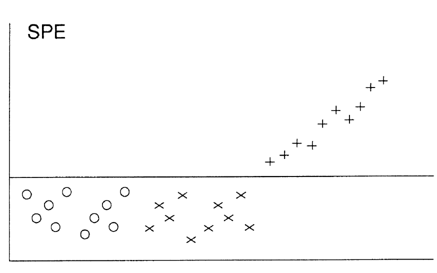

Fig. 3. SPE against time.

It is a common practice to limit the number of latent variables to no more than three, for the convenience of visual inspection [14]. However, for some processes which exhibit non-linear behaviour, such as batch processes and some continuous processes with product grade changes, a small number of linear principal components cannot adequately explain a sufficient level of variability in the data. If a small number of principal components are still used in this case, a large value for the SPE can be observed even when the process is under normal operation. The large SPE may not be due to a fault but may be a consequence of having an insufficient number of principal components retained in the PCA model. Furthermore, the results of using linear PCA on a non-linear process may be inadequate because minor components can contain important information on non-linearity [26]. By discarding the minor components, this important information on non-linearity is lost. On the other hand, if too many components are kept the advantage of PCA in reducing data dimension is lost. To overcome these problems, non-linear principal component analysis can be used.

3. Non-linear principal component analysis

Several approaches for non-linear principal component analysis have been proposed. Gnanadesikan and Wilk [28] suggested a generalised principal component analysis approach. Hastie and Stuetzle [29] developed the concept of principal curve which has subsequently been incorporated into a neural network topology by Dong and McAvoy [30] to create non-linear principal components. The use of autoassociative neural networks was proposed by Kramer [31] to extract non-linear features from within a data set. In this paper, the principal curve approach is adopted to monitor process operation.

The main difference between PCA and non-linear PCA is the introduction of non-linear mappings between the original and reduced dimensional space. A linear principal component minimises the sum of the orthogonal deviations between a straight line and the data whilst the non-linear approach summarises the data by a smooth curve which is determined by the non-linear relationships between all the variables. The curve minimises the orthogonal deviations between the data and the curve. If a non-linear function can be used to express this curve, then the function is equivalent to the principal loadings in linear PCA, whilst if we project the data down onto the curve and find indexes to express the projected points, these indexes are equivalent to the principal scores for linear PCA.

Hastie and Stuetzle [29] presented a possible solution for solving the non-linear principal component problem, principal curves. A principal curve is a smooth one-dimensional curve that passes through the middle of an m-dimensional data set. Its shape is determined by the structure of the data. A one-dimensional curve in an m-dimensional space is a vector $f(\lambda)$ of m functions of a single variable λ. These functions are called co-ordinate functions. The variable λ parameterises the curve and provides an ordering along it. There is a natural parameterisation for curves in terms of the arc length.

Let $X \in R^m$ be a random vector, then the curve f is called a principal curve of X if

$$E(X \mid \lambda_f(X) = \lambda) = f(\lambda) \qquad (3)$$

where λ_f is defined as a projection index of $R^m \to R^1$

$$\lambda_f(X) = \sup_{\lambda}\{\lambda: \|X - f(\lambda)\| = \inf_{\mu}\|X - f(\mu)\|\} \qquad (4)$$

So the projection index $\lambda_f(X)$ of X is the value of λ for which $f(\lambda)$ is closest to X. If there are several such values, the largest is used. It is proven in [29] that, if the principal curve is a straight line, then it is a linear principal component.

Calculation of principal curve using Eq. (3) requires that the distribution of X be known. In practical applications, we usually work with a finite multivariate data set, X, and its distribution is unknown. Hastie and Stuetzle [29] show that $E(X \mid \lambda_f(X) = \lambda)$ can be estimated by means of scatter-plot smoothing and locally weighted regression using neighbourhoods of each point defined by their projections onto the current estimate of the principal curve. For every iteration, the algorithm consists of two steps, a projection step and a smoothing step. The calculation is generally started with the linear principal component as the initial curve. In the projection step, data points are projected down onto the curve. Then each data point is assigned a parameter value λ_i, which is the arc length measured from the curve starting point. The data are then ordered according to the parameter values. In the smoothing step, the curve is smoothed using a technique such as the locally weighted regression smoother [32] or kernel smothers [33]. After each iteration, the distance between the data set and the estimated principal curve is calculated and if its relative change is below a pre-defined threshold, the algorithm is assumed to be converged. The procedure is iterated between the two steps till convergence results. If one principal curve cannot explain sufficient data variance then the second principal curve is calculated from the residual data. This procedure is repeated until sufficient number of principal curves are found. Detailed calculation procedure for principal curves can be found in [29,30].

In linear PCA, the principal loading vectors can be used as a model to generate principal scores for new data. However, the principal curve procedure does not give any non-linear loadings. In industrial process applications, it is usually desirable to have a non-linear principal component model which can be used to generate non-linear principal components for new data. Dong and McAvoy [30] proposed using neural networks to learn non-linear principal component models. Two networks are required. One is used to learn the mapping between the data and the non-linear scores and the other is used to learn the mapping between the non-linear scores and the corrected data.

The following example demonstrates the power of non-linear PCA over linear PCA. In this example, data are generated from the following equations:

$$x_1 = 0.5t^2 - 2t + 0.5 \qquad (5)$$

$$x_2 = t^2 + t + \sin(\pi t) \qquad (6)$$

$$x_3 = 2t^2 - t - 2\cos(\pi t) \qquad (7)$$

with t taking random values in the range $[-1, 1]$. The three variables are correlated in a non-linear manner with the intrinsic dimensionality of the variables being one. Two hundred data points were generated and random noise in the range $(-0.3, 0.3)$ was added to these data. The noise accounts for 1.55% of data variability in the noisy data set. Fig. 4 compares the results of linear PCA and non-linear PCA using principal curves. It can be seen that the first linear principal component can only explain about 60% of the data variance whereas the principal curve can explain about 98% of the data variance. Linear PCA indicates that the data dimension cannot be

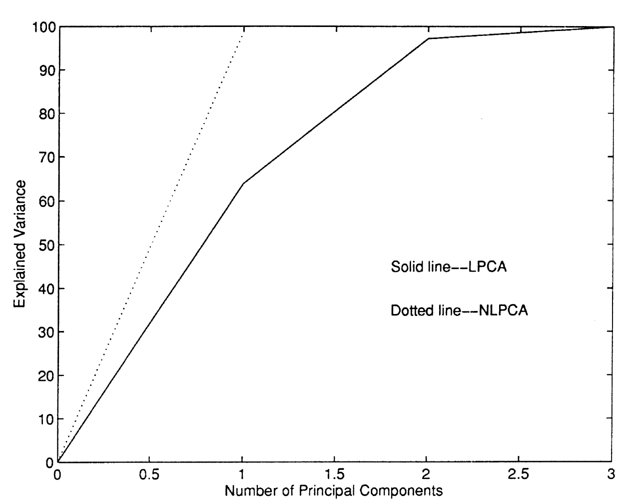

Fig. 4. Data variance explained.

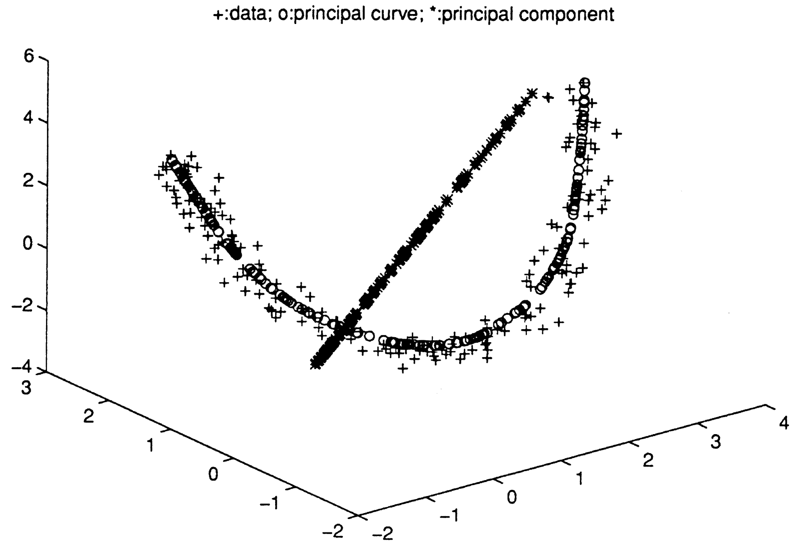

Fig. 5. Reconstruction based on linear and non-linear principal components.

reduced to its true intrinsic dimension since that will lead to a significant loss in the explained data variance. However, the principal curve based non-linear PCA reveals that the data dimension can be reduced from three to one. Fig. 5 compares the reconstruction from a linear principal component and that from a non-linear principal component. In Fig. 5, the original data points are represented by $+$, data reconstruction from the first linear principal component is represented by $*$, and that from the first non-linear principal component is represented by $\bigcirc$. It can be seen that the principal curve lies smoothly on top of the data in sharp contrast to the linear principal component.

4. Application to a polymerisation reactor

4.1. The polymerisation reactor

A low density continuous polyethylene reactor is used to demonstrate the methodology. A simulation programme based on detailed reaction kinetics has been developed by the Department of Chemical Engineering, University of Thessaloniki, Greece. There are 14 measured variables and 5 quality variables which are not measured. The simulation programme is capable of simulating the reactor under various operating conditions.

The economic operation of a polymerisation process usually requires that unreacted species be recovered and recycled back into the process. Associated with the recycle of solvent and unreacted monomers is also the recycle of reactive impurities which are introduced into the system in the fresh feed or as byproduct of chemical reactions. The levels of reactive impurities can be built up to the point where the reacting system is severely affected. Almost all types of polymerisation are sensitive to reactive impurities. In polymerisation processes, reactive impurities are usually traces of inhibitors or oxygen. The studies of Penlides et al. [34] show that impurities in an emulsion system consume rapidly reactive free radicals, thus preventing particle generation and decelerating the growth of any polymer particles already present.

Another problem affecting polymerisation is reactor fouling. Many polymers are viscous and can accumulate on the wall of a reactor vessel during polymerisation. Most of the polymerisation processes are operated under controlled temperature profiles, either constant or time varying.

Reactor temperature is usually controlled by manipulating the flow rate or temperature of coolant through the reactor jacket. The accumulation of polymer particles on the reactor wall will reduce the heat transfer capability of the reactor and is known as reactor fouling. Reactor fouling will make the reactor temperature control system less effective. In this study, four fault situations are studied and they are: reactive impurities, reactor fouling, problems with solvent, and combined reactive impurities and reactor fouling. Process operating data for normal and faulty operating conditions are generated from simulation.

4.2. Process monitoring using non-linear PCA

Linear PCA of the normal reactor operation data shows that two principal components can explain 49% of the data variance with three principal components explaining 65%. In this case, there is a substantial amount of data variance which cannot be explained by the first two or three principal components. Process monitoring based on the first two or three linear principal components may therefore give unreliable results due to the inadequate linear PCA models. A non-linear PCA model should be used to monitor the process.

Non-linear PCA based on principal curves was used to analysis the normal reactor operation data. Two non-linear principal components explain 75% data variance and three non-linear principal components explain 90% of the data variance. This suggests that non-linear PCA is more appropriate in this situation, with fewer components required to explain the variability in the data. One of the major advantages of this result is that the operators monitoring the behaviour of the process would only be required to supervise a small number of charts. A non-linear principal component model with three principal components was developed. The neural network model for the non-linear scores had the structure (14–15–3) whilst that for the principal curves had the structure (3–15–14). The structures for these network models are determined from cross validation studies. The reactor data were split into a set of training data and a set of testing data. The network structures giving the best performance on the testing data were selected.

The non-linear principal component model, developed from the normal operation data, is used to monitor the operation of the process. At each sampling instance, the non-linear scores and SPE for the new observations are calculated. The non-linear scores and SPE are monitored to detect any abnormalities in the process. When there is no fault in the process, the SPE is expected to be small and the scores should be within the nominal region. A fault in the process can change the data correlation structure or change the range of certain process variables. This can be detected by large SPE or variations in the non-linear scores.

In this study, four different fault situations are studied and they are reactor fouling, reactive impurity, solvent problems, and combined reactor fouling and reactive impurities. The SPE plot for the four different fault situations are presented in Fig. 6. In each of these plots, the fault occurs at the 51st sampling time. It can be seen from Fig. 6 that the SPE from the non-linear PCA model is very small when there is no fault. Once a fault occurred the SPE becomes very large. Fig. 6 indicates that, for all four fault situations, the occurrence of the fault can be detected by monitoring the SPE.

Score plots have been used to distinguish different faults [14]. The motivation behind this approach is that different faults can result in different process measurement values which could be projected to different areas of the score space. In this study, it has also been attempted to use non-linear score plots to localise the four different fault situations. The score plots are presented in Fig. 7 where nsc1, nsc2, and nsc3 represent the first three non-linear principal components. It can be seen that the faults cannot be distinguished from the score plots.

Different faults usually cause process variables to move in different directions. The directions of the process variable movement can be monitored by studying the projected score movement in the score space. Here we propose using the accumulated scores to distinguish between different fault situations. The accumulated scores are defined as follows:

$$A(n) = \sum_{i=1}^{n} (x(i) - \bar{x}) \tag{8}$$

where $x(i)$ is the non-linear score for the ith observation, $\bar{x}$ is the mean of the nominal non-linear score, and $A(n)$ is the accumulated non-linear score till time n. By definition, the accumulated non-linear scores will remain around the origin when there is no fault in the process. Once a fault occurs, the accumulated non-linear scores will move away from the origin. Different faults could cause the accumulated non-linear scores moving in different directions.

Fig. 8 shows the plot of the accumulated scores. In Fig. 8, as1, as2, and as3 represent the accumulated first, second, and third non-linear scores, respectively. It can be seen that the fault situations can be clearly distinguished. The upper left diagram shows the plot of the accumulated first and second scores. From this diagram, it can be seen that reactor fouling

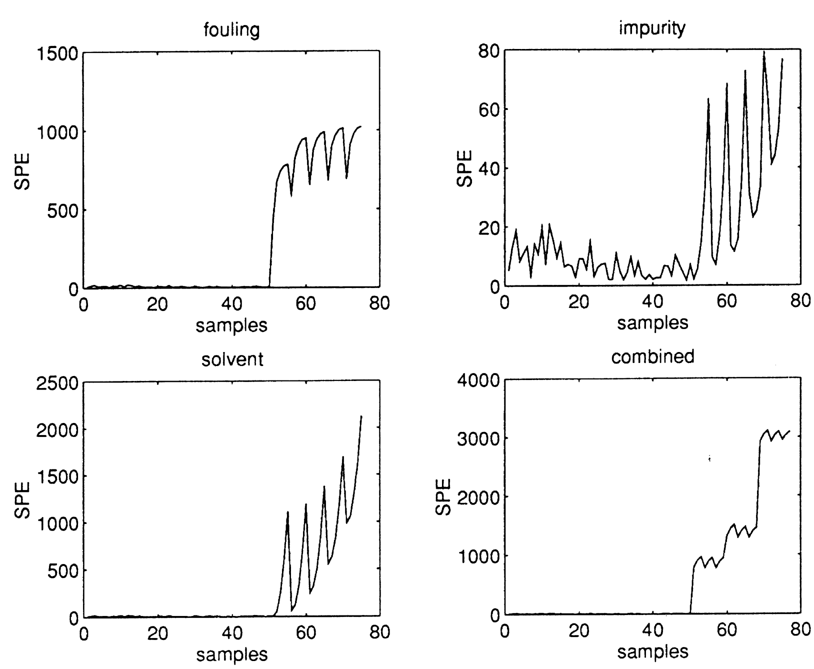

Fig. 6. SPE plots for different faults.

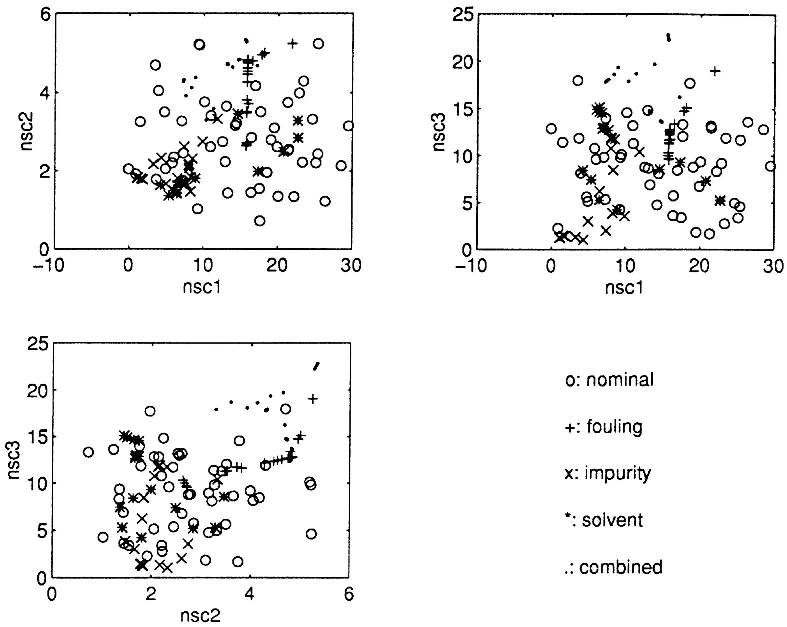

Fig. 7. Non-linear score plots for different faults.

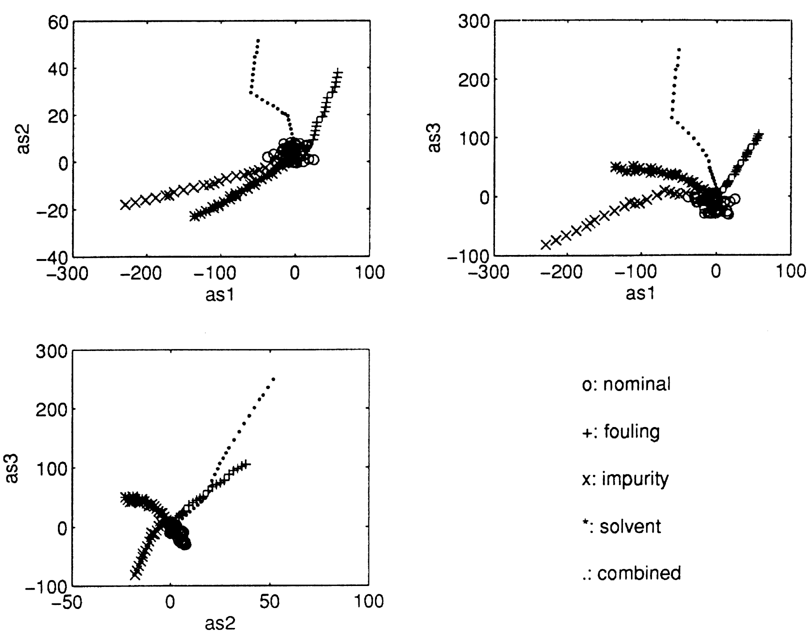

Fig. 8. Accumulated non-linear score plots.

is characterised by the score movement in the north-east direction while the combined fault of reactive impurity and reactor fouling is characterised by the score movement in the north-west direction. Both reactive impurity and solvent problems result in the score move in the south-west directions. However, they can be clearly differentiated between from the lower left plot which plots the accumulations of the second and the third non-linear scores. In this plot, reactive impurity corresponds to the score movement in a south-west direction whilst the solvent problem corresponds to the score movement in a north-west direction. The results clearly indicate that the accumulated scores due to different faults move away from the origin along different directions.

Fig. 9 shows the accumulated non-linear score plots for two different realisations of reactive impurities. It can be seen that the movements of the accumulated non-linear scores due to the two different realisations follow the same pattern. Fig. 10 shows the accumulated non-linear score plots for two different realisations of reactor fouling. The movements of accumulated non-linear scores due to the two different realisations are also very similar. Thus the accumulated score plots can be used to classify different fault situations. The

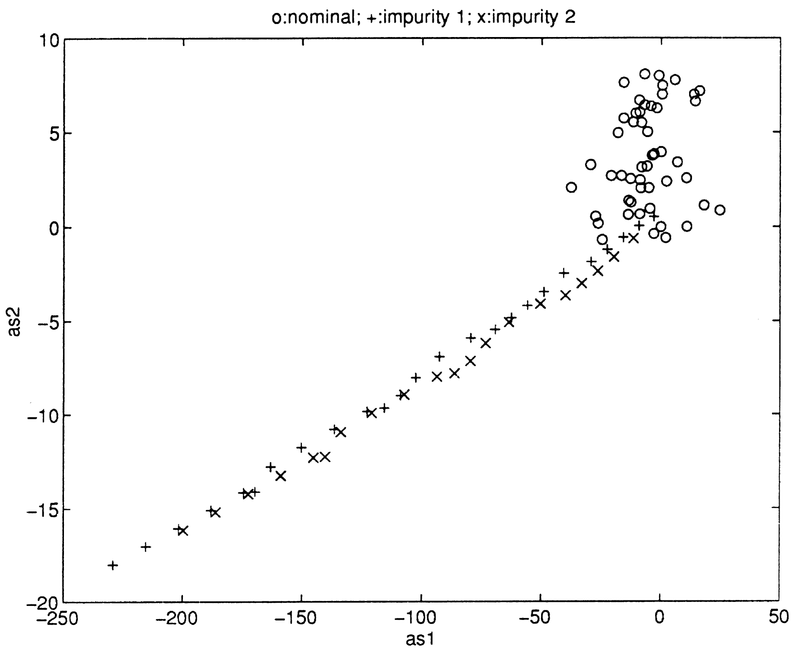

Fig. 9. Accumulated non-linear score plots for impurities.

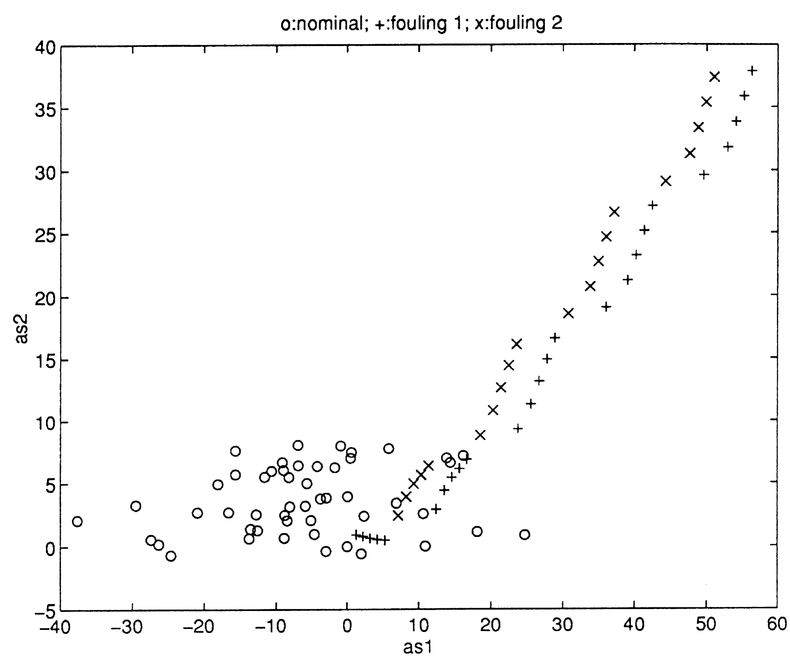

Fig. 10. Accumulated non-linear score plots for fouling.

proposed non-linear statistical monitoring technique can also be combined with other fault diagnosis techniques, such as knowledge based approaches, to improve fault identification.

5. Conclusions

Non-linear PCA can provide more effective and robust data compression than linear PCA for processes with non-linearly correlated variables. Studies have shown that fewer non-linear components than linear principal components are required to explain the same percentage of variance in a non-linear process, hence its appeal in a performance monitoring context, fewer charts are required to be managed by the operator. For the monitoring of processes with non-linearly correlated variables, non-linear statistical techniques are more appropriate. Non-linear score plots do not always identify problems in the process. A new approach using accumulated non-linear scores has been shown to be a powerful approach for the detection and identification of faults, with plots of the trajectory of the integrated scores being associated with different faults. Application studies demonstrate that the proposed technique is very effective.

Acknowledgements

This work is supported by an European Community BRITE EURAM Project (Project No. BE-7009). The authors thank Prof. C. Kiparissides for providing the polymerisation data.

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