ADVANCED PROCESS DIAGNOSIS IN COMPLEX SYSTEMS USING NONLINEAR VARIABLE RECONSTRUCTION

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Abstract: This paper presents a new nonlinear multivariate statistical process control technique for identifying and isolating the root cause of abnormal process behavior. The new technique is a nonlinear extension to the variables reconstruction technique by (Dunia *et al.*, 1996), based on nonlinear principal component analysis (NLPCA). This work demonstrates that the variable reconstruction (i) affects the geometry of the NLPCA model and (ii) alters the NLPCA based monitoring statistics. Incorporating such changes into the NLPCA model using reference data can address these issues. An industrial application study of a glass melter process shows that abnormal events can be identified and isolated earlier than conventional principal component analysis (PCA).

Keywords: Fault diagnosis (detection, identification, isolation), monitoring, neural networks, chemical industry, nonlinear model

1. INTRODUCTION

To guarantee that complex industrial processes operate economically, safely and are environmentally friendly, it is essential to constantly monitor their performance. (MacGregor *et al.*, 1991; Kruger *et al.*, 2001) highlighted that such processes frequently produce a large set of highly correlated process variables. This has led to the evolution of a range of multivariate statistical techniques that are collectively referred to as multivariate statistical process control (MSPC), and represents an extension to more traditional univariate process control (MacGregor and Kourti, 1995).

PCA is one of the most popular MSPC techniques. PCA offers the capability to compress redundant information in the process measurements, resulting from the high degree of correlation, by retaining only essential information that can be exploited to describe the current state of the process operation (Wise and Gallagher, 1996).

(Russell *et al.*, 2000) showed that the diagnosis of anomalous process behavior entails fault detection, fault identification and fault isolation. (Jackson, 1991; Miller *et al.*, 1998) stated that the difficult issue is to determine the root cause responsible for abnormal process behavior. This is because MSPC provides monitoring statistics that only allow such behavior to be detected. (Miller *et al.*, 1998) proposed the use of contribution charts as the "missing link" in multivariate quality control. However, contribution charts only allow the identification of the potential root causes of anomalous behavior.

(Dunia *et al.*, 1996) introduced a variable reconstruction procedure to remove "fault information"

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from the recorded process variables in order to provide a clearer isolation of the fault condition. This technique relies on predicting a set of process variables using the remaining set of variables and the underlying linear PCA model.

This paper presents a nonlinear extension to their linear variable reconstruction technique. This then offers a nonlinear MSPC monitoring approach that addresses the issues of fault detection, identification and isolation. The nonlinear PCA technique is based on recent work by the authors (Antory *et al.*, 2004). (Lieftucht *et al.*, 2004) showed that variable reconstruction in fact alters the underlying PCA model. Consequently, the underlying PCA model must also be "reconstructed" to incorporate the impact of this alteration. The new nonlinear variable reconstruction technique proposed here accommodates the influence of the reconstruction process.

This paper is divided into the following sections. A brief review of PCA/NLPCA is given prior to the introduction of the novel nonlinear variable reconstruction technique. A detailed analysis of the technique is included. This is followed by the application study to an industrial melter process. It is shown that a developing crack could be detected and identified using the NLPCA technique by (Antory *et al.*, 2004) and isolated using the new nonlinear variable reconstruction technique.

2. BACKGROUND TO PCA/NLPCA

In this section, a brief review of the principles of linear and nonlinear PCA is given.

2.1 PCA

For a given vector of n process measurements, $\mathbf{z} \in \mathbb{R}^n$, the application of PCA gives rise to the definition of a reduced set of "artificial" score variables.

PCA describes the measurements in $\mathbf{z}$ as follows:

$$\mathbf{z} = t_1\mathbf{p}_1 + t_2\mathbf{p}_2 + \cdots + t_k\mathbf{p}_k + \mathbf{e}, \qquad (1)$$

$$e_i = \mathbf{d}_i^T\mathbf{z} = z_i - \hat{z}_i, \qquad (2)$$

where $\mathbf{d}_i$ is the i^{th} row of the matrix $\mathbf{D} = \left[\mathbf{I} - \mathbf{P}\mathbf{P}^T\right]$.

where t_1, t_2, $\ldots$, t_k are the score variables, $\mathbf{p}_1$, $\mathbf{p}_2$, $\ldots$, $\mathbf{p}_k$ are PCA loading vectors, $k < n$ is the number of retained principal components (PCs) and $\mathbf{e}$ represents the residuals of the PCA model. The score variables represent *significant process variation*, whilst $\mathbf{e}$ describes *insignificant and redundant variation in* $\mathbf{z}$.

2.2 NLPCA

Nonlinear PCA is a generalisation of linear PCA which describes nonlinear relationships between the recorded process variables. The work presented here relies on the application of autoassociative neural networks (AAN). The architecture of AAN relies on three hidden layers: the mapping, the bottleneck and the de-mapping layers (Kramer, 1992). The input layer receives the measured process variables, while the output layer provides the NLPCA prediction of the process variables. Consequently, this identity mapping encapsulates the important variation of the process variables in a reduced set of nonlinear scores, obtained in the bottleneck layer.

(Antory *et al.*, 2004) proposed an improved NLPCA technique based on first using PCA and subsequent application of an AAN to the linear PCA score variables. This approach has been referred to as the T2T identity mapping network. This enables the removal of linear redundant information from the recorded process data prior to the determination of the AAN architecture. Note that the score variables are (i) fewer in number and (ii) are assumed to be statistically independent (Jackson, 1991), which (iii) gives rise to a pre-conditioning for the identification of the network parameters.

The mathematical description of the T2T network is as follows:

$$\mathbf{t}_{nl} = f\left(\mathbf{t}\right) \qquad (3)$$

$$\widehat{\mathbf{t}} = g\left(\mathbf{t}_{nl}\right) \qquad (4)$$

where $\mathbf{t}_{nl} \in \mathbb{R}^{k_L}$, $k_L < k$, stores the nonlinear score variables, with k_L being the number of bottleneck nodes. $f(\circ)$ and $g(\circ)$ are nonlinear functions that represent the mapping and demapping layers of the T2T network, and $\widehat{\mathbf{t}} \in \mathbb{R}^k$ is the prediction of $\mathbf{t}$.

3. NONLINEAR VARIABLE RECONSTRUCTION

Variable reconstruction was first discussed by (Dunia *et al.*, 1996) in conjunction with linear PCA. Using this technique, a subset of process variables can be reconstructed using the remaining process variables and the identified PCA model (Dunia and Qin, 1998). Recently, (Lieftucht *et al.*, 2004) demonstrated that variable reconstruction alters the confidence limit of the Q statistic and the variance of the score variables. Further, they showed how to incorporate such changes into process monitoring.

The work presented here enhances the variable reconstruction technique by (Dunia and Qin, 1998), so that it can be applied in a nonlinear context. This nonlinear extension is applied in conjunction with NLPCA. They showed that if the Q statistic is significant, the variable reconstruction technique for linear PCA can isolate the fault signature from the recorded process variables. The Q statistic for the NLPCA model is given by:

$$\mathbf{e} = \mathbf{z} - \mathbf{P}f\left(g\left(\mathbf{P}^T\mathbf{z}\right)\right) \quad Q = \mathbf{e}^T\mathbf{e}, \tag{5}$$

with $\mathbf{P} = \left[\, \mathbf{p}_1 \ \mathbf{p}_2 \ \cdots \ \mathbf{p}_k \,\right]$, The principles of nonlinear variable reconstruction to isolate the fault signature using the NLPCA model are outlined next.

3.1 Nonlinear Reconstruction Algorithm

(Dunia *et al.*, 1996) showed that reconstruction of the j^{th} process variable is an iterative process:

$$z_j^{new} = [\, \mathbf{z}_{-j}^T \ z_j^{old} \ \mathbf{z}_{+j}^T \,]\mathbf{c}_j \tag{6}$$

where $\mathbf{c}_j$ is the j^{th} row vector of $\mathbf{C} = \mathbf{P}\mathbf{P}^T$, which can alternatively be formulated as follows:

$$\widetilde{z}_j = \frac{1}{1 - c_{jj}} \sum_{i=1 \neq j}^{n} c_{ji} z_i, \tag{7}$$

where $\widetilde{z}_j$ is the reconstructed value of the j^{th} process variable.

To integrate the above linear variable reconstruction for application in conjunction with NLPCA, the iteration technique of Equation (6) has to be considered. This is because the mapping and demapping of the T2T network are based on nonlinear functions. Using linear PCA, however, these transformations are linear and involve the retained PCA loading vectors, stored in $\mathbf{P}$.

The iterative process of nonlinear reconstruction is as follows:

(i) obtain the nonlinear score variables from the current process measurements *using the mapping layer of the NLPCA model*;
(ii) predict the current process measurements *using the demapping layer of the NLPCA model*;
(iii) replace the measured value of the j^{th} process variable by the predicted one *obtained from step (ii)*; and
(iv) go to step (ii) until the difference between two consecutive values of the predictions of the j^{th} process variable is smaller than a given threshold, e.g. 10^{-8}.

Mathematically, the above procedure can be summarized as follows. The prediction of the current process measurements is given by:

$$\widehat{\mathbf{z}}^{(1)} = \mathbf{P}f\left(g\left(\mathbf{P}\mathbf{z}\right)\right) \tag{8}$$

Replacing the measurement of the j^{th} process variable by its prediction leads to:

$$\mathbf{z}^* = \left(\, z_1 \ z_2 \ \cdots \ \widehat{z}_j \ \cdots \ z_n \,\right)^T \tag{9}$$

Applying Equation (7) again yields:

$$\widehat{\mathbf{z}}^{(i)} = f\left(g\left(\mathbf{z}^*\right)\right) \tag{10}$$

where i represents the actual iteration step. The iterative procedure has converged if

$$\left\| \hat{z}_j^{(i+1)} - \hat{z}_j^{(i)} \right\| < \varepsilon \tag{11}$$

More than one variable can be reconstructed, up to a maximum number equal to the number of bottleneck nodes.

4. APPLICATION STUDY: GLASS MELTER PROCESS

This section presents an application study of NLPCA, and the new nonlinear variable reconstruction technique, to an industrial melter process. The aim is to detect, identify and isolate the influence of a crack based on a historical data.

The melter process is part of the disposal procedure. Waste material is pre-processed by an evaporation treatment leading to the production of powder, which is then clad by a glass layer, provided by the melter process. The melter consists of a vessel, two exit funnels through which the melter load flows out and several induction coils.

The vessel is continuously filled with the powder while raw glass is discretely introduced in the form of glass frit. This binary composition is heated by four induction coils, which are positioned around the vessel. Because of the heating procedure, the glass is melted homogeneously.

The process of filling and heating continues until the desired height of the liquid column is reached. The molten mixture is then poured out through one of the exit funnels. After the contents of the vessel has been emptied to the height of the nozzle, the next cycle of filling and heating begins.

Measurements of 8 temperatures, the power in 4 induction coils and voltage were taken every five minutes. The filling and emptying cycles resulted in a nonlinear relationship between the temperatures, power in the induction coils and voltage.

The melter vessel is made of graphite, which is a brittle material. As a result of the strong temperature variations to which the vessel is frequently exposed, cracks may occur along the regions of high stress. These cracks not only damage the shell of the melter, but also allow the molten content to escape. It is therefore necessary to detect such cracks at an early stage.

Historical data from the melter process was available, which included normal process variation and an abnormal process situation resulting from a developing crack. The recorded data contained 1050 samples, at a sampling frequency of 5 minutes, with the last 50 points corresponded to the development of a crack in the melter vessel.

4.1 Identification of a NLPCA Monitoring Model

A PCA model was identified based on the first 1000 data points of the recorded data set. Previous work by the authors (Antory *et al.*, 2004) showed that the linear PCA model included 10 principal components. By discarding the last three PCs, i.e. $k = 10$, the reconstruction of the 13 process variables revealed that (i) only insignificant variation remained in the PCA residuals and (ii) the emptying and filling cycles were accurately described.

Furthermore, the PCs were assumed to be statistically independent, which provided favorable conditions for the subsequent identification of an AAN architecture. This network included 7 nodes in the mapping layer, 3 bottleneck nodes, i.e. $k_{n_L} = 3$, and 7 nodes in the de-mapping layer. This implies that only 3 nonlinear score variables were required to produce an accurate NLPCA model for a total of 13 process variables.

To monitor this process, the Q statistic and scatter diagrams, for which the confidence regions were obtained using a Kernel Density Estimation (KDE), were used for process monitoring. Using scatter diagrams, the influence of the developing crack was noticed almost 2 hours earlier compared to the application of conventional PCA to the same data (Chen *et al.*, 2000).

4.2 Fault Detection and Identification

Figure 1 shows the influence of the developing crack results in a statistically significant Q statistic from the 33^{rd} data point.

The severity of the crack increases over time and led eventually to the failure of a particular temperature sensor that was closest to it. To identify potential root cases of this event, contribution charts to the Q statistic were used.

Figure 2 illustrates that the contribution chart, evaluated for the 33^{rd} data point, identified the temperature reading of sensor 6 and and the power reading of the 3^{rd} induction coil as the dominant contributors to this event.

This was a correct analysis of the event, since a later investigation showed that the crack indeed developed in the vicinity of the 6^{th} temperature

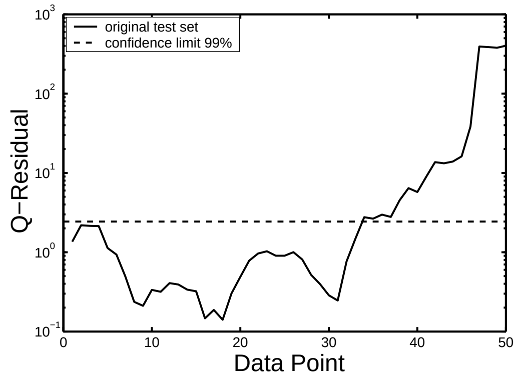

Fig. 1. The Detection of Crack in Melter Process

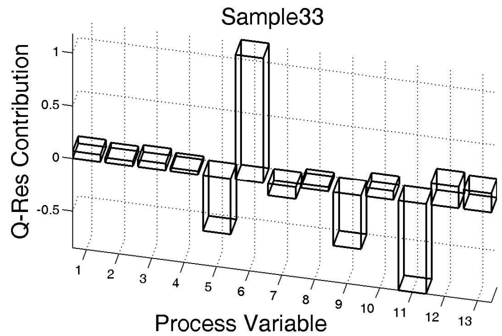

Fig. 2. Variable Contributions to the Fault

sensor. In addition, the change in the temperature profile affected the power consumed by the 3^{rd} induction coil as a result of controller feedback.

4.3 Fault Isolation

Using the new nonlinear variable reconstruction technique, the information from the previous fault identification step is now used to isolate the signature of this event from the recorded data. Given that the 6^{th} temperature sensor shows a significant response, the corresponding variable was reconstructed using the remaining ones.

Figure 3 compares the recorded and reconstructed sequences of the 6^{th} temperature sensor.

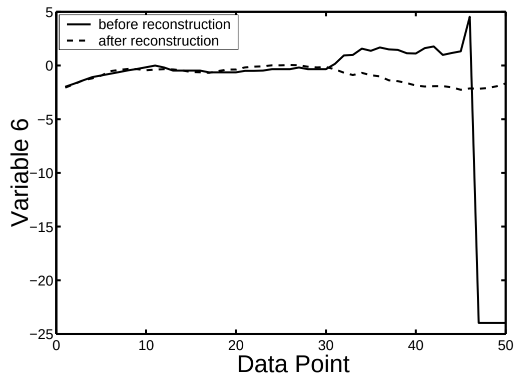

Fig. 3. Temperature Sensor 6 Before and After Reconstruction

This figure demonstrates that the nonlinear reconstruction technique successfully isolates the influence of the developing crack from the recorded sequence. In order to evaluate whether the process was operating "in-statistical-control" after the reconstruction of the 6^{th} temperature sensor, the Q statistic was re-examined. Figure (4) highlights that no violations of the 99% confidence limit arose after the 6^{th} temperature sensor was reconstructed. Consequently, an experienced operator would have been directed to focus attention on this sensor.

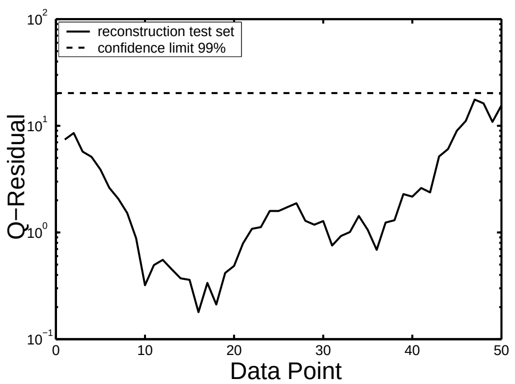

Fig. 4. Fault Detection for a New Reconstructed Test Set

As discussed by (Lieftucht *et al.*, 2004), the confidence limit for the Q statistic must be altered to accommodate the changes of the variable reconstruction on the monitoring model. This was achieved by reconstructing the readings of the 6^{th} temperature sensor in the reference data set, i.e. the first 1000 samples, and recalculating the confidence limit. Figure 5 represents the influence of reconstructing the 6^{th} temperature sensor on the 99% confidence limit of the Q statistic. It should be noticed that after the reconstruction, the confidence limit for the Q statistic increased, as a result of the applied reconstruction process.

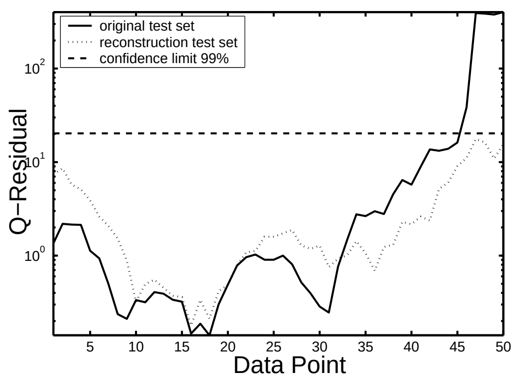

Fig. 5. Comparison of Fault Detection before and after the Reconstruction Process

4.4 Scatter Diagrams for Fault Diagnosis

To show the process variation encapsulated in the nonlinear score variables, (Antory *et al.*, 2004) proposed the use of scatter diagrams for which the confidence regions are identified using KDE. This was motivated by the fact that the nonlinear score variables may not be normally distributed and consequently, the assumptions imposed on the Hotelling's T^2 statistic may be violated.

Figures 6 to 8 show the application of scatter diagrams for fault diagnosis process.

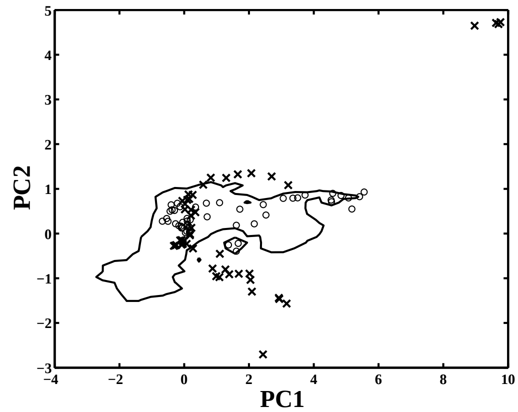

Fig. 6. Scatter Diagram: PC1 vs. PC2

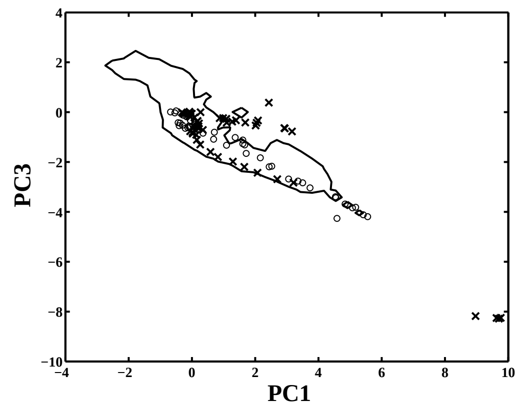

Fig. 7. Scatter Diagram: PC1 vs. PC3

The scatter points corresponding to the measured and reconstructed scatter points are respectively represented by the symbols $\times$ and $\circ$. In a similar fashion to the confidence limit of the Q statistic, the 99% confidence limits were also recalculated on the basis of the reconstruction of the 6^{th} temperature readings in the reference data. Note that a few scatter points remain outside the confidence regions, which would indicate an "out-of-statistical-control" situation. However, these points relate to the instances 46 to 50, i.e. when the sensor failed. The failure of the 6^{th} temperature sensor propagated back to influence to the regulatory control system and consequently adjusted the power in the induction coils. This,

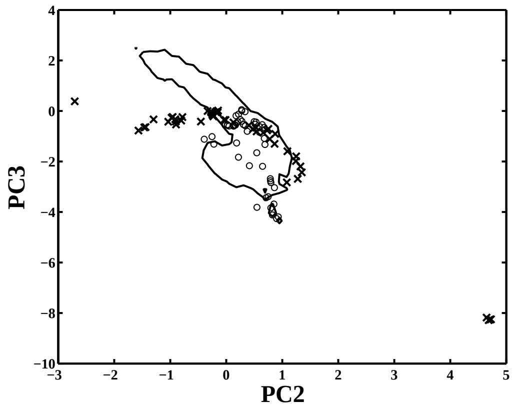

Fig. 8. Scatter Diagram: PC2 vs. PC3

in turn, caused the introduction of an excessive process variation. This excessive process variation produced the "out-of-statistical-control" situation for the last 5 instances. However, the underlying NLPCA model, after the reconstruction of the 6^{th} temperature sensor, could accurately describe the "variation" of the melter process, since Figure 1 represents an "in-the-statistical-control" situation.

5. CONCLUSIONS

This paper presents a novel nonlinear variable reconstruction technique in conjunction with the application of an autoassociative neural network (AAN) based on nonlinear principal component analysis (NLPCA) model for process fault isolation. This reconstruction technique represents a nonlinear extension of the variable reconstruction technique by (Dunia *et al.*, 1996). Based on the findings of (Lieftucht *et al.*, 2004), the confidence limit for the Q statistic and the confidence regions for the scatter diagrams are adjusted to accommodate the changes that the reconstruction process imposes upon the PCA/NLPCA model.

The application study to an industrial melter process demonstrated that (i) a developing crack could be detected and identified using the NLPCA technique by (Antory *et al.*, 2004) and (ii) isolated using the new nonlinear variable reconstruction technique.

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REFERENCES

Antory, D., U. Kruger, G. W. Irwin and G. McCullough (2004). Industrial process monitoring using nonlinear principal component models. *Proceedings of IEEE International Conference on Intelligent Systems (IS'04)*. June 22-24, Varna, Bulgaria.

Chen, Q., R. Wayne and D. J. Sandoz (2000). The application of principal component analysis and kernel density estimation to enhance process monitoring. *Control Engineering Practice* **8**(5), 531–543.

Dunia, R. and S. J. Qin (1998). Joint diagnosis of process and sensor faults using principal component analysis. *Control Engineering Practice* **6**, 457–469.

Dunia, R., S. J. Qin, T. F. Edgar and T. J. McAvoy (1996). Identification of faulty sensors using principal component analysis. *AIChE Journal of Process Systems Engineering* **10**(10), 2797–2812.

Jackson, J. E. (1991). *A Users Guide to Principal Components*. Wiley Series in Probability and Mathematical Statistics. John Wiley. New York.

Kramer, M. A. (1992). Autoassociative neural network. *Computers and Chemical Engineering* **16**(4), 313–328.

Kruger, U., Q. Chen, D. J. Sandoz and R. C. McFarlane (2001). Extended pls approach for enhanced condition monitoring of industrial processes. *AIChE Journal* **47**(9), 2076–2091.

Lieftucht, D., U. Kruger and G. W. Irwin (2004). Improved diagnosis of sensor faults using multivariate statistics. *Proceedings of American Control Conference (ACC'04)*. June 30-July 2, Boston, USA.

MacGregor, J. F. and T. Kourti (1995). Statistical process control of multivariate processes. *Control Engineering Practice* **3**(3), 403–414.

MacGregor, J. F., T. E. Marlin, J. V. Kresta and B. Skagerberg (1991). Multivariate statistical methods in process analysis and control. In: *AIChE Symposium proceedings of the 4^{th} International Conference on Chemical Process Control*. AIChE Publication, No. P-67. New York. pp. 79–99.

Miller, P., R. E. Swanson and C. F. Heckler (1998). Contribution plots: A missing link in multivariate quality control. *Applied Mathematics and Computer Science* **8**(4), 775–792.

Russell, E. L., L. H. Chiang and R. D. Braatz (2000). *Data-Driven Techniques for Fault Detection and Diagnosis in Chemical Processes*. Advances in Industrial Control. Springer-Verlag. London, ISBN 1-85233-258-1.

Wise, B. M. and N. B. Gallagher (1996). The process chemometrics approach to process monitoring and fault detection. *Journal or Process Control* **6**(6), 329–348.