FAULT DETECTION AND ROOT CAUSE DIAGNOSIS USING SPARSE PRINCIPAL COMPONENT ANALYSIS (SPCA)

By

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Abstract

Data based methods are widely used in process industries for fault detection and diagnosis. Among the data-based methods multivariate statistical methods, for example, Principal Component Analysis (PCA), Projection to Latent Squares (PLS), and Independent Component Analysis (ICA) are most widely used methods. These methods in general are successful in detecting process fault, however, diagnosis of the root cause is always not very accurate. The primary goal of the thesis is to improve the fault diagnosis ability of PCA based methods. In PCA, each Principal Component (PC) is a linear combination of all the variables, therefore makes it difficult to identify the root cause from the violation of a PC. Sparse Principal Component Analysis (SPCA) is one version of PCA that gets a sparse description of the PCA loading matrix making it more suitable for fault diagnosis. The present research aims to devise novel strategies to find the sparse description of loading matrix, more aligned with process fault detection and diagnosis. The thesis also looks into improving the fault diagnosis of PCA using clustering methods. The entire thesis can be divided into three major tasks.

First, a novel fault detection and diagnosis method is proposed based on the Sparse Principal Component Analysis (SPCA) approach. This approach incorporates a new criterion based on the Fault Detection Rates (FDRs) and False Alarm Rates (FARs) into Zou et al.'s (2006) SPCA algorithms. The objective here is to find appropriate the (Number of Non-Zero Loadings) NNZLs for SPCs that can result in low FARs and high FDRs. A comparison between PCA and four SPCA-based methodes for FDD using a

continuous stirred tank heater (CSTH) as a benchmark system is also carried out. The results indicate that shortcomings of the PCA can be overcome using the Sparse Principal Component Analysis (SPCA) that uses the novel NNZL criterion. The FDR-FAR SPCA approach gives the highest FDRs for the *SPE* statistic (93.8%).

The second task focuses on developing statistical methods to decide on the non-zero elements of the loading elements of SPCA. Rather than using heuristics, the proposed methods use the distribution of the loading elements to decide if an element should be set to zero. Two SPCA algorithms are proposed to find the NNZL and its position of each PC. The first algorithm is based on bootstrapping of the data, and the second approach is based Iterative Principal Component Analysis (IPCA). The proposed methods are implemented on a CSTH process to test the performance with PCA- and other SPCA-based methods for fault detection and diagnosis. The results reveal that the approaches have superior performance in fault detection, as well as diagnosis of the root cause of fault. Both the Bootstrap-SPCA and Sparse-IPCA methods give the highest FDRs for fault 1 for the *SPE* statistic (99.3% and 95.76%, respectively)

As the third task, this research combines the clustering (k-means) algorithm and PCA algorithm to improve the detection and diagnosis of the fault. PCA has the advantage of detecting the fault without the need for data labelling, while clustering is able to distinguish data from different fault groups into separate clusters. By combining these two algorithms we are able to have better detection and diagnosis of fault and eliminate the need for data labelling. The performance of the proposed method is demonstrated in simulated and large-scale industrial case studies.

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List of Abbreviations

AHU	Air-Handling Units
ANN	Artificial Neural Network
AR	Analytical Redundancy
AV	Adjusted Variance
BBN	Bayesian Belief Networks
BN	Bayesian Network
CBCR	Case Based Reasoning
CC	Cluster center
CFM	Critical Fault Magnitude
CPRA	Clustering and Pattern Recognition Analysis
CSTH	Continuous Stirred Tank Heater
CUSUM	Cumulative Sum.
DAG	Directed Acyclic Graphs
DPCA	Dynamic Principal Components Analysis
DPLS	Discriminant Partial Least Squares

EFK	Extended Kalman Filter
EWMA	Exponentially Weighted Moving Average
FAR	False Alarm Rates
FCCU	Fluid Catalytic Cracking Unit
FDA	Fisher’s Discriminate Analysis
FDD	Fault Detection and Diagnosis
FDR	Fault Detection Rates
FTA	Fault Tree Analysis
FTC	Fault Tolerant Control
GA	Genetic Algorithm.
GSPCA	greedy sparse Principal Components Analysis
ICA	Independent Component Analysis
IGCC	Integrated Gasification & Combined Cycle
IPCA	Iterative Principal Component Analysis
IPCA	Iterative Principal Component Analysis
IS	Index of Sparseness

KF	Kalman Filter
KICA	Kernel Independent Components Analysis
KPCA	Kernel Principal Components Analysis
LASSO	Least Absolute Shrinkage and Selection Operator
LSPCA	Laplace Sparse Principal Component Analysis
MBPCA	Multi-block Principal Components Analysis
MPC	Model Predictive Control
MSPM	Multivariate Statistical Process Monitoring
MWPCA	Moving Window Principal Components Analysis
NL	Normalization
NLGBN	Nonlinear Gaussian Belief Network
NNZL	Number of Non-Zero Loadings
PCA	Principal Component Analysis
PCEG	Possible Cause and Effect Graph
PI	Proportional Integral
PLS	Partial Least Squares

PM–FD	Process Monitoring and Fault Diagnosis
QTA	Qualitative Trend Analysis
RNSPCA	Robust, Nonlinear, and Sparse Principal Components Analysis
RPCA	Recursive Principal Components Analysis
SCoT	Simplified Component Technique
SDG	Signed Digraph
SDP	Semi-Definite Programming
ShPCA	Shrinking Principal Component Analysis
SJSPCA	Structured Joint Sparse Principal Component Analysis
SMI	Subspace Model Identification
SPCA	Sparse Principal Component Analysis
SPCA	Sparse Principal Component Analysis
SPE	Squared Prediction Error
SVD	Singular Value Decomposition
T	Principal Component
TEP	Tennessee Eastman Process

UCL	Upper Control Limit
UIO	Unknown input observer
UKF	Unscented Kalman Filter
WWTP	Water Waste Treatment Plant

List of symbols

μ	Mean.
σ	Standard deviation.
Λ	Diagonal matrix
e_i	Residual vector
P_l	Loading vector
γ	Covariance matrix for SPC scores
Σ^*	Covariance matrix for both PC/SPC scores
$\widetilde{X}$	Noise-free data matrix
X	Noisy data matrix
ε	Measurement noise
Σ_ε	Error covariance matrix
ν_i	Random noise vector
C_α	Normal deviate associated with 1-α percentile

Chapter 1

Introduction

1.1. Background

Regulations and requirements for product quality and process safety are being stricter day by day. Monitoring is a key to maintain quality and ensure safety. In general, process monitoring can be categorized into two distinct areas: fault detection and fault diagnosis. Fault detection serves to provide users with early warnings of process faults (e.g., operational errors), whereas fault diagnosis attempts to find their underlying reasons. Fault diagnosis is necessary to facilitate troubleshooting responses to the faults (Luo et al., 2017).

Recently, several Multivariate Statistical Process Monitoring (MSPM) methods have drawn the interest of researchers and industry personnel in the process monitoring field. In particular, data-driven methods are drawing increased attention in relation to monitoring of complex chemical plants. In these environments, building sufficiently accurate, fundamental law-based mathematical models that include all relevant operational data can be challenging and time-consuming.

Although univariate statistical techniques are simple to implement, these methods cannot correctly distinguish between normal and abnormal changes, which significantly increases the number of false alarms. Furthermore, the necessity of separately monitoring each variable can easily overwhelm an operator and, hence, it is only possible to monitor a few quality variables using the univariate techniques. The multivariate statistical process monitoring (MSPM) techniques eliminate some of the limitations of the univariate techniques. The multivariate techniques can transform high-dimensional process data into lower dimensional space making it possible to monitor high dimensional process systems (Kourti and MacGregor, 1995; Bakdi & Kouadri, 2017; Ge et al., 2013; Alaei et al., 2013; Jiang et al., 2013). Most of the multivariate techniques are very successful in detection of fault. However, diagnosis of the root cause of the fault is usually not very precise. In a process system usually process variables are highly correlated due to material recycle, heat integration and feedback control. A fault originated at any particular location in the process plant quickly impacts many variables in the unit and makes diagnosis difficult. Therefore, the goal of this thesis is to improve the diagnosis ability of the commonly used fault detection diagnosis techniques, we specifically focus on principal component analysis (PCA). Nowadays, principal component analysis (PCA) has become the most commonly applied data-driven approach to monitor process plants. In highly correlated process data, the original data is projected to a feature space where variables, called principal components (PCs), are uncorrelated to each other. Usually only the first few PCs in the transformed domain is sufficient to express most of the variability in the data. These transformed variables are linear combinations of the original variables. Instead of monitoring the large dimensional variables it is possible to monitor the first few PCs in the transformed domain (Chiang et al., 2000). Interpreting outcomes for PCA-based monitoring methods can, however, prove challenging, especially with regard to fault diagnosis. This is because each of these PCs is a linear combination of all the original variables. Usually, weights of the variables to a PC, called loading vector, is used to determine the root cause of the variable. However, typically all the elements of the loading vector will be non-zero with several of them very close in the values. Consequently, loading vector values are unable to provide sufficiently accurate information on what is causing the fault (Luo et al., 2017; Xie et al., 2013). To overcome the problem, sparse principal component analysis (SPCA) has been proposed. In the SPCA a sparse structure of the loading matrix is obtained. In a loading vector several of the elements would be "0", which makes it easier to diagnose the root cause of a fault by looking at the weights of a PC. However, most of these SPCA methods have been developed with a goal to have the sparsest structure, without an objective of fault detection and diagnosis. In this thesis we bring the focus of SPCA to fault detection and diagnosis and demonstrate the utility of the SPCA method in fault diagnosis. Subsequently we propose several SPCA algorithms to further improve the fault detection and diagnosis capabilities of PCA based methods.

1.2. Objectives

The goal of the thesis is to improve the fault detection and diagnosis capabilities of PCA based methods. We have taken two routes to achieve the better performance in fault detection and diagnosis: (i) through improving the performance of SPCA methods for fault detection and diagnosis, and (ii) combining PCA with clustering algorithm. The main objectives set for the thesis are as follows:

1. Improve the fault detection and diagnosis ability of the SPCA algorithm through calibration of the SPCA method for fault detection and diagnosis. We propose a new SPCA method called FDR-FAR SPCA where the sparse structure of the loading matrix of the SPCA algorithm were optimized for maximizing fault detection and diagnosis performance.
2. Develop a method to find the distribution of the loading elements and use sound statistical basis to determine the "zero" and "non-zero" elements of the loading matrix. We propose two new SPCA algorithms that are based on bootstrap methods to calculate confidence intervals of the loadings.
3. Compare the FDD performances of the benchmark SPCA namely, IS [index of sparseness], AV [Adjusted variance], NL [Normalization], and the proposed SPCA algorithms with the traditional PCA.
4. Improve the fault diagnosis capabilities of PCA method by combining it with clustering algorithm. We propose a method by combining PCA with k-means clustering algorithm to detect and diagnose process faults. The proposed method also eliminates any need for pre-labelled normal and abnormal data typically needed for most machine learning methods.

1.3. Thesis Structure

This research is presented in a manuscript styled thesis which involves one published journal article and two submitted manuscripts. This thesis includes six chapters as described below. Chapter 1 briefly explains the main aim of fault detection and diagnosis (FDD) as well as the benefits of using data-driven methods such as PCA, followed by the limitation of the traditional PCA and the motivations of the proposed SPCA approach and the objectives of this research. Chapter 2 introduces a comprehensive literature review related to various FDD approaches with their advantages and disadvantages. Chapter 3 proposes a fault detection and diagnosis (FDD) method based on SPCA; in this approach, the number of non-zero loadings (NNZL) of SPCAs is selected based on both the false alarm rate (FAR) and the fault detection rate (FDR). The criterion is to have lower FAR and higher FDR. This was published in the Canadian Journal of chemical Engineering. Chapter 4 provides two new SPCA algorithms based on the bootstrap method to calculate confidence intervals of the loadings. Sparse principal component analysis using the bootstrap method is the subject matter of the second manuscript. This paper was published in Chemical Engineering Science. It went through the first review, currently undergoing a second round of review. In chapter 5, a fault detection and diagnosis method based on clustering (K-means) and principal component analysis (PCA) is proposed to detect and diagnose the root cause of the process faults. This paper is ready to be submitted. Finally, the summary of the outcomes of this thesis is covered and some future directions are provided in chapter 6.

1.4. Software Used

All calculations done in the thesis were done on Matlab platform. All the codes are written in Matlab for the proposed algorithms. We did extensive Matlab coding in custom m-files as well as used built-in Matlab functions to carry out the calculations. The CSTH system built in Matlab Simulink to generate both the normal and faulty data sets.

1.5. Authorship Statement

Chapter 3:

"I (Abdalhamid Ahmad Rahoma) have contributed to Conceptualization, Methodology, Formal Analysis, Software, Investigation, Writing - Original Draft, and Writing - Review & Editing of this research article. Dr. Syed Imtiaz contributed to Conceptualization, Methodology, Formal Analysis, Writing - Review & Editing, Supervision, and Project Administration; Dr. Salim Ahmed contributed to Methodology, Formal Analysis, Writing - Review & Editing, Supervision, and Project Administration. A version of chapter 3 (article 1) is published in the Canadian Journal of Chemical Engineering, January 2021, https://doi.org/10.1002/cjce.24026."

Chapter 4:

I (Abdalhamid Ahmad Rahoma) have contributed to Conceptualization, Methodology, Formal Analysis, Software, Investigation, Writing - Original Draft, and Writing - Review & Editing of this research article. Dr. Syed Imtiaz contributed to Conceptualization, Methodology, Formal Analysis, Writing - Review & Editing, Supervision, and Project Administration; Dr. Salim Ahmed contributed to Methodology, Formal Analysis, Writing - Review & Editing, and Supervision. A version of chapter 4 (article 2) is published in Chemical Engineering Science.

Chapter 5:

I (Abdalhamid Ahmad Rahoma) have contributed to Conceptualization, Methodology, Formal Analysis, Software, Investigation, Writing - Original Draft, and Writing - Review & Editing of this research article. Dr. Syed Imtiaz contributed to Conceptualization, Methodology, Formal Analysis, Writing - Review & Editing, Supervision, and Project Administration; Dr. Salim Ahmed contributed to Methodology, Formal Analysis, Writing - Review & Editing, and Supervision; Dr. Faisal Khan contributed to Methodology, Formal Analysis, Writing - Review & Editing, and Supervision. A version of chapter 5 (article 3) has been submitted to Canadian Journal of Chemical Engineering.

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Chapter 2

Literature review

In recent years, fault detection and diagnosis (FDD) have become important research topics in process industries because they can help to ensure normal operation, enhance process safety, and maintain product quality. FDD methods are mainly classified into two categories: model-based methods, which may be subdivided into qualitative and quantitative methods, and process history-based methods (Chiang et al., 2001; Venkatasubramanian et al., 2003b, 2003c). This chapter briefly discusses these methods.

2.1. Quantitative Model-Based FDD Approaches

2.1.1 The general procedure

Quantitative model-based methods are based on a fundamental understanding of the physics underlying the process being studied. This is used to express the relationships between the inputs and outputs of the system using explicit mathematical equations, typically based on material- and energy-balance equations (first-principles models).

Current FDD approaches model the monitored system primarily using analytical redundancy (AR) (Willsky, 1976; Frank, 1990), and employ a mathematical model of the monitored system. The residual generator and residual evaluator are generally two modules in a model based FDD system. The measurements of the system are compared with the process model outputs and the differences are reported as residuals by the residual generator, which are received by the residual evaluator which makes decision about the faulty or normal state of the process (Isermann, 2005; Chow and Willsky, 1984). Although the residual should equal zero under an ideal condition, noise, and modeling uncertainly in the industrial processes typically result in a non-zero residual even during a normal operation. In quantitative model-based tools, the most commonly used techniques include diagnostic observers, parity relations, Kalman filters, state-space models, input-output relationship, first-principal models, and frequency response models (Venkatasubramanian et al., 2003c). A number of papers have evaluated model-based FDD approaches (Frank, 1996; Gao et al., 2015; Gertler, 1991, 2015; Isermann, 1997, 2006; Isermann and Balle, 1997; Katipamula and Brambley, 2005; Simani et al., 2003; Venkatasubramanian et al., 2003c).

2.1.2 Observer-based FDD

The observer-based FDD schemes function by decoupling the effects of the faults from disturbances and diagnosis is performed by combining analytical- and knowledge-based redundancy (Frank, 1990). These schemes use a bank of observers by the observer based FDD algorithms to generate residuals (Frank and Ding, 1997), each of which is sensitive to a specific fault. Although Observers track the process closely, residuals from unknown inputs will be minimal during normal operating conditions. It is assumed that when a fault occurs, all observers that are insensitive to the fault will continue to generate small residual, whereas those sensitive to the fault will significantly deviate from their normal trends and produce residuals of large magnitudes. After these observers are designed for specific faults, fault isolation becomes easier; this observer-based methodology was successfully implemented by (Yoon and MacGregor, 2000) for a CSTR plant for detecting fault.

Another way called unknown input observer (UIO) is used to remove the effect of disturbances. A bank of UIOs was used by (Sotomayor and Odloak, 2005) under model predictive control (MPC) to diagnose different types of faults in inputs, outputs, and model parameters. A technique was proposed by (Zarei and Poshtan, 2010) to design non-linear UIO, where the gain of the observer was estimated using an unscented transformation.

2.1.3 Kalman filter and its variants

In chemical industries, the Kalman filter (KF) is also used as a state estimator. A general procedure for Kalman filtering is to estimate all process states; then residuals can be evaluated to indicate the presence of a fault by comparing the estimated process states with their measured values (Benkouider et al., 2009, Chang and Chen, 1995, Hanlon and Maybeck ,2000; Arasaratnam & Haykin,2009; Hwang et al., 2009; Simani et al.,2000).

However, classical KFs are not optimal when the system is non-linear and so the extended KF (EFK) and unscented KF (UKF) were developed. Using the Taylor series expansion, EKF linearizes the model, while UKF determines a set of sigma points and transform each through the non-linear function to compute a Gaussian distribution from the transformed and weighted points (LaViola, 2003). The results obtained by these approaches indicate that UKF has better performance with highly non-linear system compared to the KF and EKF (Wan and Van Der Merwe, 2000).

2.1.4 FDD using parity relations

Examining parity equation relation came early as a common model based fault detection approach. It forms residuals as the difference between the system and model outputs, with the assumptions that there is no process uncertainty or modelling errors; the parity relations are linear, and the explicit model can explain all faults (Patton and Chen, 1991). However, it is difficult to build an explicit model, and noise causes uncertainty in the measurements, which may make the residuals non-zero. Several studies have investigated parity relation- or equation-based fault detection techniques (Patton and Chen, 1994; Gertler, 1997; Odendaal and Jones, 2014; Zhong et al., 2015).

Parity relation-based fault detectors for multiple sensors generate residuals from a fully decoupled parity equation that is only sensitive to a particular sensor fault; the relations are used to estimate faults using a recursive least-squares method (Song and Zhang,2002; Chan et al.,2006). However, because the parity relation approach is only valid when operating conditions are approximately linear, it is difficult to apply this approach to batch or nonlinear processes where operating conditions continuously vary.

2.1.5 Limitations of model-based FDD

The model based FDD approaches use parameter estimation wherein unmeasurable process parameters and/or state variables are estimated to diagnose the fault (Isermann, 1984). The parameters of the physical system under normal operating conditions are initially modelled and compared to those obtained from the on-line process measurements, with the assumption that any significant change from the former denotes a fault (Isermann, 1997). The parameter estimation approach has been applied to detect faults in various situations (e.g., Che Mid and Dua, 2017) and has been combined with the parity relation-based approach for optimal fault detection (Höfling and Pfeufer 1994). However, this approach requires precise dynamic models that are difficult to obtain in large scale industrial processes and its diagnostic performance is complex and often misleading (Venkatasubramanian et al., 2003c).

A list of review articles on the model based FDD methods can be found in the literature (Frank, 1996; Gao et al., 2015; Gertler, 1991; Isermann, 2006; Isermann and Balle, 1997; Katipamula and Brambley, 2005; Venkatasubramanian et al., 2003c). The elimination of costly hardware redundancy is the most important benefit of the model based FDD approaches. However, it is often difficult to obtain an explicit mathematical model of the system that is required to generate the residual for diagnosis purpose. Most approaches impractically assume the process to be linear, and typically some modelling error is present. These limitations drastically reduce the effectiveness of the model-based approach and make it unsuitable for monitoring of large scale processes (Venkatasubramanian et al., 2003c).

2.2. Qualitative Knowledge-Based FDD

2.2.1 The general procedure

In knowledge-based FDD, fundamental understanding of process dynamics is used to develop knowledge-based models and prior process knowledge is required to build the model. They are often computer-aided programs consisting of various logics and conditional reasoning (If-else) (Venkatasubramanian et al., 2003a). A number of related studies have applied knowledge based FDD approaches for fault diagnosis. Expert system, fault tree analysis (FTA), case-based reasoning (CBR), signed digraph (SDG), possible cause and effect graph (PCEG) and Bayesian network (BN) are the most common knowledge based FDD techniques.

2.2.2 The expert systems

Diagnosis of the fault and suggestion on how the human operator can handle the faulty state and bring the system to normal condition is the main purpose of the expert system (Chen and Modarres, 1992). For example, the CATDEX is a well-known approach that uses simple AND-OR decomposition strategy to diagnose the root cause of a fault in the fluid catalytic cracking unit (FCCU) (Venkatasubramanian and Chan, 1989). Although the expert system is used as a diagnostic technique with important benefits such as the simplicity of development and explanation of the provided solutions, they are not adaptable to new fault conditions.

2.2.3 Fault tree analysis

Fault tree analysis (FTA) is a popular method for analyzing system reliability and risk analysis (Lee et al., 1985). It is a top-down deductive failure analysis that combines Boolean logic and lower-level events to analyze a fault in the system (Sklet, 2004). Basic events propagation up to top-events are described using logical "AND" and "OR" and the qualitative structure of a fault is analyzed using cut set analysis. The fewest events that lead to a top event (i.e., the minimal cut set) is used to diagnose the root cause of a fault (Woodward and Pitbaldo, 2010). Although FTA is easily implemented, it is generic in nature, cannot assess interdependency among the variables, and a perfect FT model is difficult to build due to complicated interdependency among the variables for large scale processes. Thus, this method it is hardly applied to diagnose a process fault.

2.2.4 Signed diagraphs

Signed digraphs (SDG) can also be used to represent the cause-effect relationship between the process variables or models (Iri et al., 1979). In SDG, each cause and effect node represent the steady state of a process variable and the directed arcs between them may be positive or negative. SDG is beneficial, as it is relatively easy to implement, and the causal information can readily be converted into rules. SDG can be obtained from the mathematical model of the process, the operational data, or the differential equation of the process model (Umeda et al., 1980). Conditional arcs have been used in SDG to improve the ability of diagnosis (Shiozaki et al., 1985) and a SDG modelling technique based on cross-correlation analysis of the process data and transfer entropy validated using prior knowledge has been proposed (Yang et al., 2012). To overcome some of the limitations of SDG, the possible cause effect graph (PCEG) was developed, which is unrestricted and provides more explicit information about the states of a variable to achieve root cause diagnosis (Leung and Romagnoli, 2000; Wilcox and Himmelblau, 1994a, 1994b). Although the previous methods are easily implemented, they do not measure uncertainty in the diagnostic information. Since process measurements are extremely noisy and diagnosis involves compiling this noisy uncertain evidence to reach a conclusion, the diagnostic tool needs to be robust.

2.2.5 Bayesian network

Bayesian belief networks (BBNs) can overcome some of these limitations and their use as a fault diagnosis tools has been comprehensively reviewed elsewhere (Guo and Hsu, 2002; Weber et al., 2012).

A Bayesian belief network (BBN) is a graphical model that represents the probabilistic relationships between variables. Specifically, the conditional dependence between random variables is calculated using a conditional probability table. These relationships are depicted in directed acyclic graphs (DAGs), the nodes of which represent random variables and the edges represent dependencies/independencies, which are calculated using a conditional probability table (Neapolitan and Jiang, 2010; Neapolitan, 2004).

In FDD, BBNs are used to diagnose the root cause of abnormal conditions and have been employed in a number of studies (Azhdari and Mehranbod, 2010; Dey and Stori, 2005; Mehranbod et al. 2003, 2005; Zerrouki and Smadi, 2017; Wilson and Huzurbazar, 2007). BBN are developed from the process knowledge of the system and although they can successfully diagnose known faults, they assume that faults do not occur simultaneously. Regardless, BBNs have been used to combine various fault detection and diagnosis methods (e.g., Huang, 2008).

2.3. History-Based FDD Approaches

2.3.1 The general procedure

With the expanding complexity of modern process, data-based methods are being increasingly popular. These are also known as process history-based methods because they train the monitoring scheme to extract features using a large amount of historical process data. According to the extraction process, history based FDD approaches are divided into quantitative and qualitative methods. Methods that depend on qualitative information include expert systems and qualitative trend analysis (QTA) whereas quantitative methods include neural networks and statistically derived models, such as those based on principal component analysis (PCA) and partial least squares (PLS) (Venkatasubramanian et al., 2003b). History-based methods also contain both univariate and multivariate methods. Univariate techniques include the $\bar{x}$ chart, Exponentially Weighted Moving Average (EWMA) control chart, and Cumulative Sum (CUSUM) control chart.

2.3.2 Univariate control charts

Originally proposed by Shewhart (1930), the $\bar{x}$ chart is the most widely used univariate control chart. Samples that exceed the upper control limit (UCL) or lower control limit

(LCL) – which are typically calculated as three standard deviations from the mean ($\mu \pm 3\sigma$), are identified as faults.

Cumulative sum (CUSUM) is another statistical procedure for monitoring stable univariate processes (Woodward & Goldsmith, 1964), wherein the variables are compared to a predetermined reference value, and the cumulative sum of their deviations from this value is calculated. A change in the mean level of the variables is evidenced if the cumulation reaches or exceeds a predetermined decision interval. The exponentially weighted moving average (EWMA) chart is another univariate monitoring technique that can quickly detect small and moderate shifts in a process over time (Roberts ,1959). Univariate monitoring approaches such as CUSUM and EWMA are very simple to implement compared to multivariate techniques; however, they are more expensive and highly based on the tuning parameter (Montgomery &Runger, 2010). Also, a separate control chart is required to monitor each variable, making the system more complicated and it is therefore impractical to monitor all the process variables in a system. Although univariate statistical techniques are simple to implement, they cannot distinguish between normal and abnormal changes which significantly increases the number of false alarms. Furthermore, the necessity of separately monitoring each variable can easily overwhelm an operator and, hence, it is only possible to monitor a few quality variables using univariate techniques (Kourti and MacGregor, 1995).

2.3.3 Multivariate control charts

Compared to the univariate analysis, multivariate statistical process monitoring (MSPM) techniques eliminate some of these limitations. Two statistical indices are typically used, Hotelling'sT^2 and squared prediction error (*SPE*), which represent the process data in a lower dimensional space and reduce the monitoring cost. Another important feature of MSPMs is that they capture the correlations among process variables, thus reducing false alarms when operating condition changes.

2.3.4 Techniques for dimension reduction

Dimensionality reduction techniques, such as principal component analysis (PCA), partial least squares (PLS), independent component analysis (ICA), and Fisher's discriminant analysis (FDA), can improve the efficiency of FDD. PCA, in particular, has been commonly applied for monitoring multivariate processes because it transforms higher dimensional data onto lower dimensional representation with the most variance of the original data (Luo et al.,2014). In the following section we provide brief discussions on PCA and its variants.

2.4 Principal component analysis

2.4.1 The approach, general procedure, and limitations

In general, PCA aims to project the variables onto the principal component space and derives a new set of variables known as the principal components (PCs) (Dunia et al., 1996). The PCs are ordered based on the amount of variance; the most variance is the first PC, the second most variance is the second PC, and so forth. In PCA-based process monitoring, Hotelling'sT^2 and squared prediction error (*SPE*) are commonly used to detect process abnormalities. The distance between the sample space and center of the feature space can be estimated by Hotelling'sT^2 while *SPE* is used as indicator of the lack of goodness of fit of sample data from the residual space. On-line samples that violate the threshold of Hotelling'sT^2 or *SPE* are detected as faults. To diagnose the fault, the multivariate contribution plots of every variable to T^2 and *SPE* statistics are used to identify the root-cause variable, which indicates that the variable has the maximum contribution is the responsible causing fault. However, it is not always the variable with the highest contribution is the correct the root cause of the fault. Thus, the diagnosis task will be incomplete and complex (Joe Qin, 2003; Xie et al.,2013). Furthermore, it is important to select the appropriate number of PCs to represent the system, because an insufficient amount will generate a poor model that incompletely represents the process and an excessive amount will result in an over-parameterized model and include noise (Valle et al.,1999). PCA is able to provide the best solution if process data follow a Gaussian distribution (Rhoads and Montgomery, 1996) and this technique assumes that a monitored process behaves linearly. A number of variants of the PCA method have been developed to achieve different needs for process monitoring as shown in Table 2.1.

Table 2.1: Summary of the relevant literature review of using PCA.

Reference	**Methodology**	**Critical Analysis & Classification**	**Application and Result**
(Dunia and	-Principal component	-Assesses the adequacy of *SPE* as	-The proposed approach was tested using data from a simulated process plant where

Qin. 1998)	analysis (PCA)	an indicator for fault detection	two separation columns are used to obtain three different products.
(Kassidas et al.,1998)	-Principal component analysis (PCA)	-PCA was incorporated into the feature extraction stage	-The method was tested on data simulated using the TEP and was implemented off-line under the assumption that the control system will react to a fault and drive the plant to a new steady-state condition. -This may not be true for faults which will cause a plant shutdown
(Chiang et al.,2000)	-Principal component analysis (PCA) - Discriminant partial least squares (DPLS). - Fisher's discriminant analysis (FDA)	-Develops an information criterion to automatically determine the order of the dimensionality reduction for FDA, DPLS and PCA	-These techniques were applied to simulated data collected from the Tennessee Eastman process (TEP) - FDA and PLS are better dimensionality reduction techniques than PCA analysis for fault diagnosis
(Wang et al., 2002)	-Principal component analysis (PCA)	- Critical fault magnitude (CFM) was introduced as a new performance index for PCA, providing insight into the root causes of faults	-A simulated double-effective evaporator process was monitored to illustrate and verify the results
(Lu et al., 2003)	-Principal Component and Wavelet Analysis for Multivariate Process	-PCA-based methods were improved by extending the time-domain process features into time-frequency information, and their	- The efficiency of the proposed process to monitor and diagnose faults was demonstrated using a three-tank system and data simulated using the TEP -The proposed method not only detected abnormal conditions, but also differentiated

	Monitoring and Fault Diagnosis	ability to process features for on-line process monitoring and fault diagnosis were compared using a similarity measure	faults with similar time-domain characteristics
(Joe Qin., 2003)	- Principal component analysis	-PLS models were used for process monitoring in a similar manner to PCA models	-The PLS models were tested in a polyester film process monitoring example with many variables -The difficulty of interpreting contribution plots when monitoring many variables is effectively overcome using multi-block analysis and hierarchical contribution plots.
(Xiao and Wang., 2003)	-Principal component analysis (PCA)	-The Q-statistic and Square Prediction Error (*SPE*) as indexes of fault detection	-The PCA method was modified to accommodate the characteristics of the air-handling units (AHUs) and is a useful tool for process monitoring, fault detection and isolation in these systems
(Srinivasan et al., 2004):	-Principal component analysis (PCA)	-Presents a two-step clustering method based on PCA that first classifies process states into modes corresponding to quasi steady states and transitions; then historical data is segmented into modes and transitions using a novel multivariate algorithm	-The proficiency of the proposed method is demonstrated through extensive testing on a fluidized catalytic cracking unit and data simulated using the TEP
(Wang and Xiao., 2006)	Principal component	-Two PCA models are developed corresponding to the heat balance and	-A robust FDD detection strategy for typical air-handling units (AHUs) was proposed. -The results show that the PCA method

	analysis (PCA)	pressure-flow balance of the air-handling process, respectively.	effectively and reliably diagnoses sensor faults while the outputs of the PCA model are more meaningful and understandable
(Tamura and Tsujita et al., 2007)	principal components analysis (PCA)	-Because the number of PCs differ depending on the number of faults, the Fault signal-to-noise ratio (Fault SNR) was proposed to determine the number of PCs that provide the maximum sensitivity in order to identify a sensor fault	-Fault SNR was tested using data simulated using TEP, and easily determined the optimum number of PCs needed to identify a sensor fault
(Kettunen et al., 2008)	-Principal component analysis (PCA), partial least squares (PLS) and subspace model identification (SMI)	-The closed-loop trained PCA, PLS and SMI monitoring methods were embedded in a MPC-based control system.	-The methods were tested using a heavy oil fractionator - The fault detection and fault compensation rates of the different fault tolerant control (FTC) system performed well with both the MPC and the set of PI controllers. -FTC systems are effective, fast and can identify different types of fault regardless of the control system used
(Garcıa-Alvarez.,2009)	-Principal component analysis (PCA)	-A PCA model for detecting faults and the thresholds of the T^2 and Q statistics were developed using data collected from the plant under normal conditions	-The proposed approach was tested in a simulated water waste treatment plant (WWTP) based on the COST benchmark and performed well
(Zanoli et	- A new	-Based on Clustering	-FCC was tested on experimental data from

al.,2010)	approach to fault detection and isolation that combines Principal Component Analysis (PCA), Clustering and Pattern Recognition	and Pattern Recognition Analysis (CPRA), the Fuzzy Faults Classifier (FFC) was proposed	an IGCC (Integrated Gasification & Combined Cycle) section of an oil refinery plant and was effective at detecting and isolating faults while monitoring a compressor
(Lubin et al.,2011)	Principal component analysis (PCA)	-Based on structural residuals, a novel multi-level approach is proposed to isolate complex faults	-The proposed approach was applied to 18 fault scenarios of the TEC process and the multi-level approach is advantageous for identifying complex faults compared to the traditional approach.
(Yin et al. 2012)	-Principal component analysis (PCA), partial least squares (PLS), independent component analysis (ICA), fisher discriminant analysis (FDA), and subspace aided approach (SAP)	-Multiple techniques were used to further study process monitoring and fault diagnosis (PM–FD) on large-scale nonlinear dynamic industrial processes	-The methods were tested using data generated by the TEP.
(Wang et al., 2015)	-Principal component analysis (PCA) and partial least squares (PLS)	-PCA was combined with PLS regression to reduce the dimensionality of the data and detect and	-The proposed method was applied to data simulated using the TEP and successfully detected faults pertaining to individual process variables and units

	regression	isolate faults.	
(Gajjar and Palazoglu., 2016)	- principal component analysis (PCA)	-To allow the operator to constrict the root causes of a fault, a method was developed that applies a control limit to each PC	-The proposed method was tested using data simulated using TEP, and had considerable higher fault detection rates relative to classic approaches
(Ahmed et al.,2017)	principal component analysis (PCA)	PCA based methodology was developed to not only identify the fault variable but also estimate the path of fault propagation in the system	-The proposed PCA model was applied to NGL fractionation process and quickly detected the fault variable without using fault detection indices that assume the variable with the highest variation is likely the fault variable

2.4.2 PCA variants for nonlinear processes

For nonlinear processes, several approaches have been developed, including Kernel PCA (KPCA), which improves the dimensionality reduction performance (Choi et al., 2005; Choi and Lee, 2004; Lee et al., 2004). KPCA technique can efficiently select the number of PCs in high dimensional spaces that are correlated to the input space during minimal nonlinear mapping. However, since PCA still plays a key part in this technique, KPCA is unable to extract non-Gaussian features from the noisy process data. Unlike PCA, ICA retains the non-Gaussian features of the process (Yu et al.,2015), and Kernel ICA (KICA) has been proposed to relax the limitation of linear projection, which first use KPCA to perform Kernel whitening and centering on the mapped process data. Recently, the kernel method has found increasing numbers of applications in the chemical industry (Schölkopf et al., 1998; Cho et al., 2005; Mika et al.,1999; Romdhanietal.,1999; Alcala and Qin. 2010; Zhang and Qin., 2008; Lee et al.,2004; Wang and Yao., 2015).

A Nonlinear Gaussian Belief Network (NLGBN) fault diagnosis technique has also been proposed for industrial processes that outperforms conventional nonlinear techniques such as KPCA, KICA, SPA, and Moving Window KPCA (Yu et al.,2015). The traditional PCA may lead to higher false alarm rate or miss detection rate due to highly time dependence in process data (Bakdi & Kouadri.2017). Therefore, the dynamic PCA (DPCA) method is used to detect the presence of disturbances as well as to isolate their sources (Ku et al., 1995). More details of DPCA can be found in (Russell et al.,2000; Rato & Reis.,2013; Huang and Yan. 2015).

2.4.3 PCA variants for high dimensional data

Multi-block PCA (MBPCA) have also been developed to block the appropriate process variables and limit the root cause of the faults in different systems, thus providing better diagnostic information than single PCA (Hong et al., 2014; Qin, 2001; Westerhuis et al., 1998). Furthermore, because the interpretation of the normal changes in the process as faults when the process data often experience gradual deviation that may cause significant false alarms, the recursive PCA (RPCA) algorithm (Li et al., 2000; Elshenawy et al.,2010) and Moving Window PCA (MWPCA) method (Jeng, 2010) were developed to continuously update the monitoring model with time.

In order to make the PCA algorithm invariant to scaling, Iterative PCA (IPCA) was developed which uses standard deviation of the measurement error to scale the data set. Covariance of error matrix is calculated from the data by minimizing a log likelihood function. The method involves iteration to more accurately estimate the error covariance as well as the loading matrix, which gives it the name Iterative PCA (IPCA) (Imtiaz et al., 2004; Narasimhan & Shah, 2008).

Some other variants are multi-way PCA (Nomikos and MacGregor, 1994; Abd Majid et al., 2011) and multi-scale PCA (Bakshi, 1998; Misra et al., 2002; Zhang et al., 1999; Lau et al.,2013; Sheriff et al., 2017) which were developed to monitor the multi dimensional data in batch processes.

2.4.4 PCA variants for enhanced fault diagnosis

The results of PCA are difficult to interpret the physical meaning of principal components being extracted because each PC is a linear combination of all original variables, instead of just among a few of them and loading vector elements typically are rated as nonzero. Another issue is that PCA essentially gives little to no support in instances of fault isolation (Xie et al.,2013). A number of solutions have been proposed to improve PCA interpretation issues (Qi et al.,2013; Ning et al., 2015; Adachi & Trendafilov ,2016; d'Aspremont et al.,2008; Witten et al., 2008).

For example, the PC rotation technique has been used to more specifically associate PCs with the original variables, although there is some question as to how many components should be rotated (Jolliffe, 1989). A thresholding method that resets PC loadings to zero in cases where the absolute values are less than a predestinated limit has also been explored (Cadima and Jolliffe, 1995). Several normalization approaches used to rotate PCs to better interpret their components have been reviewed (Jolliffe,1995). The simplest involves overlooking (i.e., reducing to zero) the absolute value of the component loadings that fall below a certain threshold. All of these led to the approach known as the sparse PCA.

2.4.5 Sparse PCA

The essential sparseness of the PCs dictates the simplification of the instructor to improve interpretability (Trendafilov,2014). Another method, called the simplified component technique (SCoT), imposes a penalty function to encourage sparsity in PC loadings, and although it performed better than the rotated PCA, it is difficult to apply (Jolliffe & Uddin,2000). Finally, the SCoTLASSO method applies a least absolute shrinkage and selection operator (LASSO) constraint to the simplified component technique (SCoT) to reduce a portion of the components' loadings until they reach zero, thus rendering them more attractive in variable selection (Jolliffe et al.,2003).

Over the years, other methods were proposed for simplifying PCA interpretation to produce modified PCs with sparse loadings (Luo et al.,2017; Liu et al.,2017; Gajjar et al.,2016; Banerjee et al., 2008). DSPCA is one such algorithm that uses semi-definite programming (SDP) to obtain sparse PCA (D'Aspremont et al.,2005). The greedy sparse PCA (GSPCA) algorithm (Moghaddam et al.,2006), regression-type sparse PCA(SPCA) (Zou et al.,2006) method, and a normalized singular value decomposition (SVD) method (Shen and Huang,2008) have also been proposed to obtain sparse PCs.

The connection between SCoTLASSO and SPCA has also been introduced (Witten et al.,2009). A generalized power (GPower) algorithm that considers specific constraints (cardinality or LASSO) is currently the computationally fastest (Journée et al.,2010). In another approach, the difference of convex (DC) function was applied to PCA in what is known as the DC-PCA algorithm (Sriperumbudur et al.,2011). (Qi et al.2013) also proposed a novel SPCA method that replaces the norm position of the conventional eigenvalue problem with a 'mixed-norm', whereas (Xie et al.,2013) introduced a shrinking principal component analysis (ShPCA) method without information loss in PCs. Finally, (Yu et al., 2016) developed a robust, nonlinear, and sparse PCA (RNSPCA) technique and (Liu et al.,2015) demonstrated how their adaptive sparse PCA approach functioned much better than the classical PCA technique.

The choice of the number of non-zero loadings (NNZL) for the principal component is another important consideration in terms of sparseness. In one approach, a genetic algorithm (GA) is utilized to determine the NNZL for the SPCs that would optimize the Index of Sparseness (IS) (Gajjar et al.,2017). In another method, if the degree of variance in SPC is maintained as the corresponding PC in ordinary PCA, the structure is chosen (Gajjar et al.,2018).

In (Liu et al., 2018), the authors use a structured joint sparse principal component analysis (SJSPCA) method to develop a new type of fault detection and isolation technique as a means to enhance fault isolation. The proposed technique resulted in enhanced fault-isolation performance for both a gas flow fault from an industrial blast furnace and a simulation example. (Zhai et al., 2020) presented the novel approach of Laplace sparse principal component analysis (LSPCA), which they achieve through the addition of the Laplace penalty term in SPCA. The proposed method was illustrated by a simulation example and a case study of a distillation process.

2.5 Concluding remarks

Many algorithms have been presented in the literature, and most studies have focused on the degree of sparseness and level of variance explained by PCs. While these are good indicators of performance, for FDD it is important to evaluate how well these algorithms perform when detecting and, especially, diagnosing a fault in a system.

2.6 Bootstrapping technique

One of the main drawbacks that should be mentioned here about the PCA algorithm is its descriptive nature. Because of this characteristic, no verifiable method exists that can be used to estimate the scores or PCs' sampling variability, or the variance proportion explained by each PC. According to (Girshick, 1939; Tipping & Bishop,1999), PC-based asymptotic confidence intervals (CIs) that are analytically derived usually assume normally distributed data.

Bootstrapping represents a method of resampling that was introduced by (Efron, 1979). In bootstrapping approach, the original dataset undergoes numerous realizations via resampling and replacement. Note that each resampled dataset retains the same dimensions (sizing) as the original one, but due to replacement, one data point could undergo several samplings whereas another one could be entirely left out of the dataset.

In this way, every new realization is different, even though they are all derived from the same original dataset.

As an analytical asymptotic CI alternative (Diaconis & Efron, 1983) introduced bootstrap-based CIs intended for use in PCA results. A decade later, (Mehlman et al., 1995) applied a small dataset in a novel bootstrap resampling method with the aim of providing CIs for eigenvector loading estimates. The new method demonstrated that this could happen via a reflection from eigenvectors for bootstrap samples, as a means to enhance the probability around accurately interpreting significant axes numbers. More recently, (Hall & Hosseini-Nasab, 2006) provided theoretical justification for applying bootstrap confidence regions in estimating functional PCA output sampling variability. At the same time, (Salibián-Barrera et al., 2006) employed bootstrap for a robust PCA process, where the authors used eigenvalue decomposition to estimate a population shape matrix, i.e., a population covariance matrix as a scaled version. (Goldsmith et al., 2013) used bootstrap in functional PCA as a way to estimate confidence bands of underlying functions. In so doing, they took into account additional uncertainty within the PC decomposition.

(Babamoradi et al., 2013) published a case study showing the steps for developing bootstrap confidence limits (CLs) for values of score and loading; they also applied their method to examine global score clusters using PCA, intending to boost the application of bootstrap in uncertainty estimations. A few years later, (Karoui & Purdom, 2016) tested bootstrap performance with simulations in PCA, examining the bootstrap properties through high dimensional covariance matrices' spectral analysis. It is worth mentioning that for high-dimension matrices, the data-generating process is not mimicked by bootstrapping. From this, it can be assumed that conventional bootstraps only function in low-dimensional problems.

2.7 Supervised vs. Unsupervised learning methods

Diagnosis of the root cause of a fault is essentially a classification problem. For classification, the type may be either supervised or unsupervised. For supervised classifications, well labeled historical data containing both normal and faulty data is utilized for training a model. The trained model is used to classify new measured data for fault diagnosis. The learning methods currently most popular are BN and ANN. Conversely, for the unsupervised learning approach, no previous knowledge of fault information, or labeled data is required. Examples of unsupervised learning strategies include PCA, PLS, control chart, k-means algorithm (Tidriri et al., 2016).

Most data-driven strategies employ historical data to derive the mapping relationships of fault features and fault modes. However, in the majority of fault detection/diagnosis methods, the quality of the training data determines the performance (Yin et al., 2012).

The main data driven techniques are principal component analysis (PCA), partial least squares (PLS), Independent Component Analysis (ICA), and Fisher Discriminant Analysis (FDA). These approaches are standard in process industries (Chiang et al., 2000; Huang & Yan, 2015). More recently, machine learning techniques are gaining in popularity, such as support vector machine and artificial neural network. A major issue of the mentioned supervised approaches is that they need large training datasets that should include normal and abnormal data at different fault conditions. Process data tend to be large and unlabeled, sourcing training datasets suitable for supervised learning methods often limits the supervised methods' utility.

A data partitioning technique often used for data mining is cluster analysis (CA). During the process of CA, sample datasets are divided, so that samples from one cluster group share more similarities with others in their own group than they do with samples from other groups (Li & Hu, 2018). CA enables the main operating variables which impact a system to be grouped (i.e., clustered). At its core, CA utilizes the distance between data points, and best applied in analyzing big complex data which feature a broad range of variables that are interrelated. In the classification and grouping process, CA designates as a cluster variable groups which have features that are alike. This form of clustering enhances the accuracy of the dataset behavior. Data clustering has been used to improve the fault detection and diagnosis performance of multivariate analysis. (Sebzalli & Wang, 2001) utilized PCA to achieve dimension reduction and find operational zones in Fluid Catalytic Cracking (FCC) processes. This work was followed by another study, which employed a fuzzy c-means algorithm for validating PCA-obtained clusters and also to find the centers of the clusters (Srinivasan et al., 2004). The authors used clustering and PCA as a means for classifying dynamic system data into various related states and operational modes. To achieve this, the authors first reduced the data dimension using PCA and then applied the clustering algorithm to the resultant scores in order to find the modes and states. The system's operational, i.e., transition state vs steady state, is found via the heuristic rule known as "dwelling time". In this approach, when the system remains in a specific state longer than the so-called dwelling time, it is deemed to be in a steady state. Then, when the state is determined, the data are segmented as various operational modes. The technique is validated by an FCC unit along with simulations performed using the Tennessee Eastman process.

(Imtiaz et al., 2006) utilized a clustering algorithm as a means to find different operational zones in a data set from a pulp and paper mill. Such mills are typically characterized as having multiple product grades and frequent change-overs from product to product. The authors found that the clustering algorithm validated how basis weight (a core operating parameter) provided a useful indicator for classification of data as separate operational zones (i.e., clusters). Based on this finding, several PCA models were built for the clusters and then applied to sheet-break fault detection and diagnosis at the mill.

A few years later, (Lam et al., 2008; 2009) utilized clustering and PCA for classifying days-of-the-year as clusters according to weather characteristics. The authors developed regression models from these climate data for predicting probable consumption of chiller system power. Similarly, (Li & Hu, 2018) proposed a novel technique for fault detection/diagnosis and estimation (FDD&E). The strategy combined PCA and density-based clustering. More specifically, Density-Based Spatial Clustering of Applications with Noise (DBSCAN) is able to categorize data as clusters automatically, while also recognizing related operational conditions. The authors employed sub-PCA models in their work instead of just one PCA model so they could better characterize standard operating conditions. Their innovation improved the sensitivity as well as the reliability of fault detection/diagnosis efforts; it also enhanced the accuracy of the sensor fault estimation. The authors validated their method through field operation data gleaned from a screw chiller plant. The data were applied across various sensor faults at different magnitudes, with the results indicating better sensor FDD&E in comparison with traditional PCA-based sensor FDD&E using single PCA models (Li & Hu, 2018).

(Du et al., 2017) tested a refrigeration compressor system firstly by classifying the data for the test as clusters and secondly by building PCA models of the individual clusters in order to detect sensor faults. The outcomes of the tests indicated substantial increases in detection levels of the sensor faults for sub-PCA models. (Zanoli et al., 2010) also presented a fault detection technique, which incorporated an isolation strategy using clustering and PCA. It also used pattern recognition analysis. The authors applied their novel approach to data acquired from an oil refinery (the Integrated Gasification & Combined Cycle section) to monitor the compression process.

More recently, k-nearest neighbor (kNN) has been applied in fault detection efforts, with some success. In a study by (He et al., 2010), the authors employed a PC-kNN approach that hosts original data within a PC subspace. Then, to build the fault detection model, the kNN rule is included in the score matrix. This technique brings a substantial reduction in both storage space and time (He et al., 2010). A few years later, (Guo et al., 2014) proposed a novel approach to process-monitoring known as FS-kNN. In this method, data samples are projected onto feature space, from which the indicators squared prediction error (*SPE*) and principal components may be extracted. The indicators have the capability of capturing pertinent information about raw data, making the detection accuracy of FS-kNN better than that of PC-kNN.

From the above literature review, we can see that clustering algorithms and PCA can be used in combination in data mining and to delineate operational modes. We can also see from the review that PCA has carried out online fault detection and diagnosis, whereas clustering is mostly used for improving PCA model performance and to segment data as various operational modes. That being said, we are convinced that the clustering algorithm technique can do more, and that it can in fact be used for online fault detection and diagnosis by itself, without the assistance of another tool. Therefore, in the present work, we combine PCA with the k-means clustering algorithm, using PCA in the training of the clustering algorithm based on unlabeled data. After the training is finished, the k-means clustering algorithm successfully performs online fault detection and diagnosis.

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Chapter 3

A new criterion for selection of non-zero loadings for sparse principal component analysis (SPCA)

Abstract: Sparse Principal Component Analysis (SPCA) has recently emerged as an approach aimed at producing compact principal component loadings by suppressing spurious values and thus overcoming some limitations of the traditional Principal Component Analysis. This paper proposes a fault detection and diagnosis (FDD) method based on SPCA; in this approach, the number of non-zero loadings (NNZL) of SPCAs is selected based on both the false alarm rate (FAR) and the fault detection rate (FDR). The criterion is to have lower FAR and higher FDR. This new feature makes SPCA better suited for FDD, which is demonstrated by comparing its performance with that of three other methods for finding loadings. The overall FDD performances of both PCA and SPCA-based techniques are illustrated using the benchmark continuous stirred tank heater (CSTH) process. The results show that the PCs derived based on the proposed NNZL criterion has a better fault diagnosis ability.

KEYWORDS

false alarm rate, fault detection rate, principal component analysis, sparse principal component analysis

3.1. Introduction

Process monitoring has emerged as a necessary tool for ensuring process safety. Process monitoring consists of two main stages: fault detection and fault diagnosis. In combination fault detection and diagnosis (FDD) work to ensure process safety, which results in a decrease in financial losses, fewer accidents, and fewer problems with equipment. Multivariate statistical process monitoring (MSPM) approaches are fast becoming popular in industry. MSPM is beneficial in that it requires marginal process knowledge and relies more on process data. As it is primarily data driven, MSPM is simple to implement and use. It is also ideal for highly advanced and complex industrial processes where either the knowledge base or mechanistic models are difficult to build. MSPM approaches such as principal component analysis (PCA) have proven highly successful across a number of applications. PCA presents a linear combination of the original variables of a super-sized dataset and is mainly applied for process data dimension reduction and fault detection in different applications. However, interpretation of the outcomes of PCA-dependent monitoring approaches can be incredibly difficult, particularly in fault diagnosis (Qin.,2012; Ge et al.,2013; Chen & Jiang., 2020; Venkatasubramanian.et al.,2003 b; Chen et al., 2018). The difficulty arises mainly because the projection matrix (or loading) is usually dense. Each principal component (PC) is a combination of all variables. Therefore, the values of the loading vector do not give a definitive indication of the root cause of a fault (Chiang et al.,2000; Xie et al.,2013).

Several studies have applied various techniques to deal with the interpretation of PCA issues (Ning et al., 2015; Qi et al., 2013; Liu et al., 2017; Adachi & Trendafilov.,2016; d'Aspremont et al.,2008; Witten et al.,2009). (Jolliffe., 1989) used the PC rotation technique to interpret the components with some drawbacks related to whether to rotate some or all the components. In another review, (Jolliffe., 1995) discussed several normalization approaches that could be used to rotate PCs in order to better interpret the components.

The simplest approach involves overlooking (ie, reducing to zero) the absolute value of the component loadings less than a certain threshold. In this way, the simplicity of the PCs' and the ease of their interpretation are related to their essential sparseness (Cadima & Jolliffe.,1995; Trendafilov.,2014). The literature suggests additional approaches for enhancing PC interpretability by imposing more constraints. In these instances, PC loading sparsity can be achieved, but the variance is usually sacrificed. One such approach is the simplified component technique (SCoT), in which a penalty function encourages sparsity in PC loadings. Every component gained through SCoT is constrained as either orthogonal or uncorrelated to other components in order to achieve the required sparsity. (Jolliffe and Uddin.,2000) found SCoT showed much better results compared to rotated PCA with regard to the varimax factor (Kaiser., 1958). However, SCoT also suffers from some difficulty in application. The penalty function applied to the solution is problem-specific (ie, different penalty values are required for different cases; there is no one solution for all (Jolliffe & Uddin.,2000; Jolliffe et al.,2002). (Jolliffe et al.,2003) introduced an approach called the simplified component technique – LASSO (SCoTLASS) that includes a least absolute shrinkage and selection operator (LASSO) constraint on the SCoT. The constraint reduces a portion of the components' loadings until they reach zero, thus rendering them more attractive in variable selection.

Over the years, various other techniques have been presented in the literature regarding ways to achieve the desired sparse loadings (Luo et al.,2017; Journée et al.,2010; Gajjar et al., 2016; Banerjee et al.,2008). (D'Aspremont et al.,2005) for example, discussed an algorithm called DSPCA, which uses semi-definite programming (SDP) to obtain sparse PCA. (Moghaddam et al.,2006) introduced a bi-directional greedy search method and named it the greedy sparse PCA (GSPCA) algorithm. (Shen and Huang.,2008) suggested that the sparse structure of PCs could be attained through a normalized SVD method. Accordingly, they implemented normalization penalties in order to encourage sparsity for PC loadings. In addition, these researchers pointed to the usefulness of cross-validation as well as imposing a more systematic tuning strategy in choosing sparsity levels. (Journée et al.,2010) introduced a generalized power (GPower) approach in order to handle sparse PCA through specific constraints (cardinality or LASSO) to obtain the desired sparse loading vectors. Regarding computational speed, GPower appears to be faster than all other currently used algorithms. (Sriperumbudur et al.,2011) debuted what they referred to a DC-PCA algorithm. This approach resolves sparse PCA by applying DC (difference of convex functions) programming. (Xie et al.,2013) introduced a shrinking principal component analysis (ShPCA) method. They showed how classical PCA can be modified such that all loadings would achieve simplified interpretation and nearly zero information loss in PCs. (Yu et al.,2016) developed a "robust, nonlinear, and sparse PCA"(RNSPCA) technique that extracts sparse PCA. The results showed that the detection performance of the SPCA method was better compared to traditional PCA. (Liu et al.,2015) showed how their adaptive sparse PCA approach functioned much better than the PCA technique.

Overall, the choice of the number of non-zero loadings (NNZL) for the principal component is important. (Gajjar et al.,2017) utilized a genetic algorithm (GA) to determine the NNZL for the SPCs that would optimize the Index of Sparseness (IS). (Gajjar et al.,18) highlighted another approach for choosing the number of non-zero loadings in SPCA, while keeping approximately the same degree of variance in the corresponding PC as in ordinary PCA. They found that the ideal amount of NNZL in PCs decreases if more constraints are introduced into SPCs to maintain at least 90% of the variance gains in corresponding PCs while keeping CPV above a particular cut-off point. Thus, the NNZL for one PC would vary, but the remainder of the PCs would remain the same. Overall, because SPCA is easier to interpret compared to PCA, its application potential is very high for FDD (Luo et al.,2017). Though many algorithms have appeared in literature, these mainly focus on the degree of sparseness and level of variance explained the by PCs. While these are good indicators of performance in the context of FDD, it is important to evaluate how well the algorithm performs in detecting a fault, and especially diagnosing the fault. False alarm rate (FAR) and fault detection rate (FDR) are two important performance indicators for FDD algorithms.

The main contribution of this study is to develop an SPCA algorithm that delivers better FDD performance. Here, FDR and FAR criteria were combined with the LASSO technique for choosing the right NNZL in SPCs that provides high FDRs and low FARs. In addition, a comparison between PCA and four SPCA-based strategies is also provided with regard to FDD on the benchmark continuous stirred tank heater (CSTH) process. The remainder of the article is organized as follows: The preliminaries section introduces PCA and SPCA concepts. FDD using PCA and SPCA, and LASSO SPCA with (FDR) and (FAR)are presented in Section 3.2. The benchmark process simulation case study (CSTH) is introduced next in Section 3.4. The complete results and discussion of the proposed sparse PCA and three SPCA methods compared to classical PCA are then presented in detail in the results and discussion section 3.5. Finally, the conclusions of this study are summarized in Section 3.6.

3.2. Preliminaries

3.2.1. Principal component analysis (PCA)

PCA is a dimensionality reduction technique that converts a large set of correlated variables to a concise set of uncorrelated variables, called principal components that capture most of the variability of the original data. PCA is widely used in process industries for detecting process abnormalities.

Consider an auto scaled data set $X \in R^{n\times m}$ where n is the number of observations and m is the number of variables. In order to transform the data to PCA, singular value decomposition (SVD) is performed on the data set, which gives a_{mxm} set of projection vectors called loadings$\mathrm{P}_{\mathrm{m\times m}} = [\mathrm{P}_1\mathrm{P}_2 \ldots\ldots \mathrm{P}_\mathrm{m}]$. The principal components $T^{n\times m} = [\mathrm{t}_1\, \mathrm{t}_2 \ldots\ldots \mathrm{t}_\mathrm{m}]$are obtained as follows:

$$T = XP \tag{3.1}$$

The transformed variables T have the same dimension as the original set of variables. Interestingly, the first few variables of T capture most of the covariance information of the data. Therefore, only the first PCs $T^{n\times l} = [t_1\, t_2 \ldots\ldots t_l], (l < m)$ are required to capture the information necessary for a concise representation of the data. More details about PCA and its implementations steps can be found elsewhere (Chiang et al.,2000; Yin et al.,2014; Bakshi.,1998; Mallick & Imtiaz.,2013).

3.2.2. LASSO Sparse principal component analysis (SPCA)

(Zou et al.,2006) used LASSO (elastic net) constraints on loadings in the PCA to obtain a sparse description of PCA. In this, the estimation of loading vectors *A* is formulated as a constrained regression problem. Suppose $A^{m\times l} = [\alpha_1 \alpha_2 \ldots\ldots \alpha_l]$ is the indicator variable for the non zero values of the loading matrix $P_l^{m\times l} = [P_1\; P_2 \ldots\ldots P_l]$. For any $\lambda > 0$, simultaneous estimates of the indicator matrix and loading matrix are calculated as follows (Gajjar et al.,2017).:

$$(\hat{A}, \hat{P}) = \underset{A,P}{\arg\min} \sum_{i=1}^{n} || x_i - AP^T x_i ||^2 + \lambda \sum_{j=1}^{l} ||P_j||^2 \tag{3.2}$$

Subject to $A^T A = I_{l\times l}$

For known n, indicator matrix is calculated as follows:

$$(\hat{P}) = \underset{A,P}{\arg\min} \sum_{i=1}^{n} \|x_i - AP^T x_i||^2 + \lambda \sum_{j=1}^{l} ||P_j||^2 + \lambda_{1,j} \sum_{j=1}^{l} ||P_j||_1 \tag{3.3}$$

3.2.3. Index of sparseness (IS)

The IS method defines a new indicator to select optimum NNZL structure. IS indicator is defined as follows (Trendafilov.,2014):

$$IS = \frac{V_a V_s}{V_o^2} \times \frac{\neq_o}{ml} \quad (3.4)$$

where V_a is the adjusted variance, V_s is the unadjusted variance, V_o is the ordinary total variance, and $\neq_o$ indicates all the zero loadings for a specific SPCA loadings matrix.

First, the LASSO algorithm creates m^l combinations of the sparse loading matrices with different specifications of the NNZL by placing 'zeros' in the loading vectors. In the next step, the (IS) is calculated for each sparse loading matrix, the sparse loading set that gives the maximum (IS) can be selected as the optimal NNZL.

3.2.4. Adjusted Variance (AV)

Adjusted variance (AV) is another criterion to select the optimal structure from a set of sparse structures by substituting zeros in the loadings obtained from the LASSO algorithm. This will generate m^l sets of sparse loading matrices that have different NNZL. Next, the AV is calculated for each sparse loading matrix and then compared to the corresponding PC for ordinary PCA. If the AV captured by SPC retains 90% of the variance explained by the corresponding PC in the regular PCA, then the structure is selected (Gajjar et al.,2018).

3.2.5. Fault detection and diagnosis using PCA and SPCA

In order to detect the fault, two statistics, including the squared prediction error (*SPE*) or *Q* statistic, and the *T*-squared statistic (T^2), are calculated using the loading matrix, $\mathrm{P}_{\mathrm{m}\times\mathrm{l}} = [\mathrm{P}_1 \mathrm{P}_2 \ldots\ldots \mathrm{P}_\mathrm{l}]$.The *SPE* represents the Euclidean distance of the residuals in the residual space. *SPE* is calculated as follows:

$$e_i = (I - PP^T)x_i \quad (3.5)$$

$$Q_i \quad or \;\; SPE \; = e_i^T e_i \tag{3.6}$$

where e_i is the residual vector and $P_l = [P_1 \; P_2 \; \ldots\ldots P_l]$contains first *l* loading vectors. The threshold for the *SPE* is given by:

$$J_{th,SPE} = \theta_1 \left[\frac{C_\alpha \sqrt{2\theta_2 h_\circ^2}}{\theta_1} + 1 + \frac{\theta_2 h_\circ (h_\circ - 1)}{\theta_1^2} \right]^{1/h_\circ} \tag{3.7}$$

where C_α indicates a normal deviate associated with 1-α percentile and

$$\theta_i = \sum_{j=i+1}^{m} (\lambda_i)^2 \quad i = 1,2,3, \;\; h_\circ = 1 - \frac{2\theta_1\theta_3}{3\theta_2^2}$$

While *SPE* detects the breakdown of correlation in the data, theT^2 statistic is sensitive to any shift in the operating conditions. TheT^2statisticis calculated as follows:

$$T^2 = t_i \Lambda^{-1} t_i^T = x_i P_l \Lambda^{-1} P_l^T x_i^T \tag{3.8}$$

where Λ is a diagonal matrix that contains the largest eigenvaluesλ_i.

Hotelling'sT^2 follows a F- distribution and the threshold for the T^2statistic at significance level αis formulated as:

$$J_{th,}T^2 = \frac{l(N^2 - 1)}{N(N - l)} F_\alpha(l, N - l) \tag{3.9}$$

For typical PCAs, PCs remain unassociated and have orthogonal loadings. However, sparse PCs (SPCs) are not necessarily uncorrelated in SPCAs, and sample covariance's can be altered to consider the correlation in the Hotelling'sT^2measure for SPCA T^2 as follows:

$$T_{SPCA}^2 = t_i \gamma^{-1} t_i^T \tag{3.10}$$

where γ denotes a covariance matrix for SPC scores.

Fault diagnosis is crucial in process monitoring, as determining the root cause of a fault is highly desirable. Contribution plots are commonly used for fault diagnosis along with PCA models, in which contributions of all process variables to the *SPE* or T^2 statistics are calculated and plotted. The contribution of the i^{th} variable to the *SPE* is as follows:

$$SPE_i or \;\; Q_i = (x_i - \hat{x}_i\,)(x_i - \hat{x}_i)^T \quad\quad or \;\; e_i^2 \tag{3.11}$$

In chart form, the contribution of each variable is shown as a fraction of the total *SPE* given by $\mathrm{SPE_i/SPE}$, while the contribution of a variable to Hotelling'sT^2can be calculated using the following equation:

$$T_i^2 = x_i P_l \Sigma^{*-1/2} P_l^T \tag{3.12}$$

where$\mathrm{x_i}$denotes an i^{th} observation vector, $\mathrm{P_l}$ indicates PC/SPC loadings, and Σ^*represents a covariance matrix in PC/SPC scores. Again, the contribution of T^2 to each variable is shown as a fraction in the plot (Gajjar et al.,2018; Kourti & MacGregor.,1995; Tong et al.,2013; Joe.,2003; Jiang et al.,2013).

3.3. LASSO SPCA with FDR and FAR

In the context of fault detection, two important criteria are the fault detection rate (FDR) and false alarm rate (FAR). Also, SPCA is a preferred option in fault diagnosis because of its concise description of PCs allows for the precise diagnosis of the root cause of a fault. In the proposed SPCA algorithm, FDR and FAR criteria have been combined with the LASSO SPCA algorithm to determine the sparse loading matrix. Given a scaled normal (i.e., fault free) data set $X \in R^{n\times m}$, SVD is first applied to the data matrix to obtain the loading. Based on any of the selection criteria (e.g., SCREE plot, eignvalues), the significant number of PCs (l) and the associated loading vectors $P \in R^{m\times l}$are selected (Yin et al.,2012; Valle et al.,1999; Garcia et al.,2009; Imtiaz et al.,2007). Following the selection of the loading vectors, a corresponding indicator matrix $A \in R^{m\times l}$is created wherein any non-zero values of the loadings are designated by '1'and small values of the loadings are denoted by '0'. From the initial indicator matrix, many replicates of *A* matrix are created by randomly substituting '0s' in the indicator matrix. In each loading vector, there must be at least one non-zero value; therefore, the maximum number of '0s' in each column of the indicator vector will be (m-l). Using these permutation rules, there can be m^l sparse representations of the loading matrices and the corresponding indicator matrices. In the next stage, the loading vectors are adjusted for the assigned '0's. For each indicator matrix $A^{m\times l} = [\alpha_1\alpha_2 \ldots\ldots \alpha_l]$, the corresponding loading vector is calculated using Equation (3.3), also restated below:

$$(\hat{P}_j) = \underset{A,P}{arg\,min} \sum_{i=1}^{n} \|x_i - AP^T x_i||^2 + \lambda \sum_{j=1}^{l} ||P_j||^2 + \lambda_{1,j} \sum_{j=1}^{l} ||P_j||_1 \qquad (3.3)$$

For comparative purposes, the average FDR and FAR are calculated for each sparse loading set. The step-by-step implementation of the algorithm is shown in Figure 3.1. This will result in m^lsets of sparse loading matrices. From these large sets of loadings, the 'best' sparse set is selected using FDR and FAR criteria. If the calculated fault statistic is J and the fault threshold isJ_{th},then $f = 0$ denotes a no-fault condition and$f \neq 0$ denotes a fault condition. Therefore, the fault detection rate (FDR) and false alarm rate (FAR) can be respectfully defined as (Kourti & MacGregor.,1995; Valle et al.,1999; Garcia et al.,2009; Lee et al.,2006; Zhou et al.,2010):

$$FDR = \frac{(No.of\ samples\ (J > Jth\ |f \neq 0)}{Total\ samples\ (f \neq 0)} \times 100 \tag{3.13}$$

and

$$FAR = \frac{(No.of samples\ (J > Jth\ |f = 0)}{Totalsamples\ (f = 0)} \times 100 \tag{3.14}$$

Ideally, the sparse loading set that gives the maximum FDR and minimum FAR should be selected for the monitoring system. In order to implement the strategy, data with different fault signatures are collected from the system. Using each set of sparse loadings, the FDR and FAR for each fault is calculated for the T^2 and *SPE* statistics.

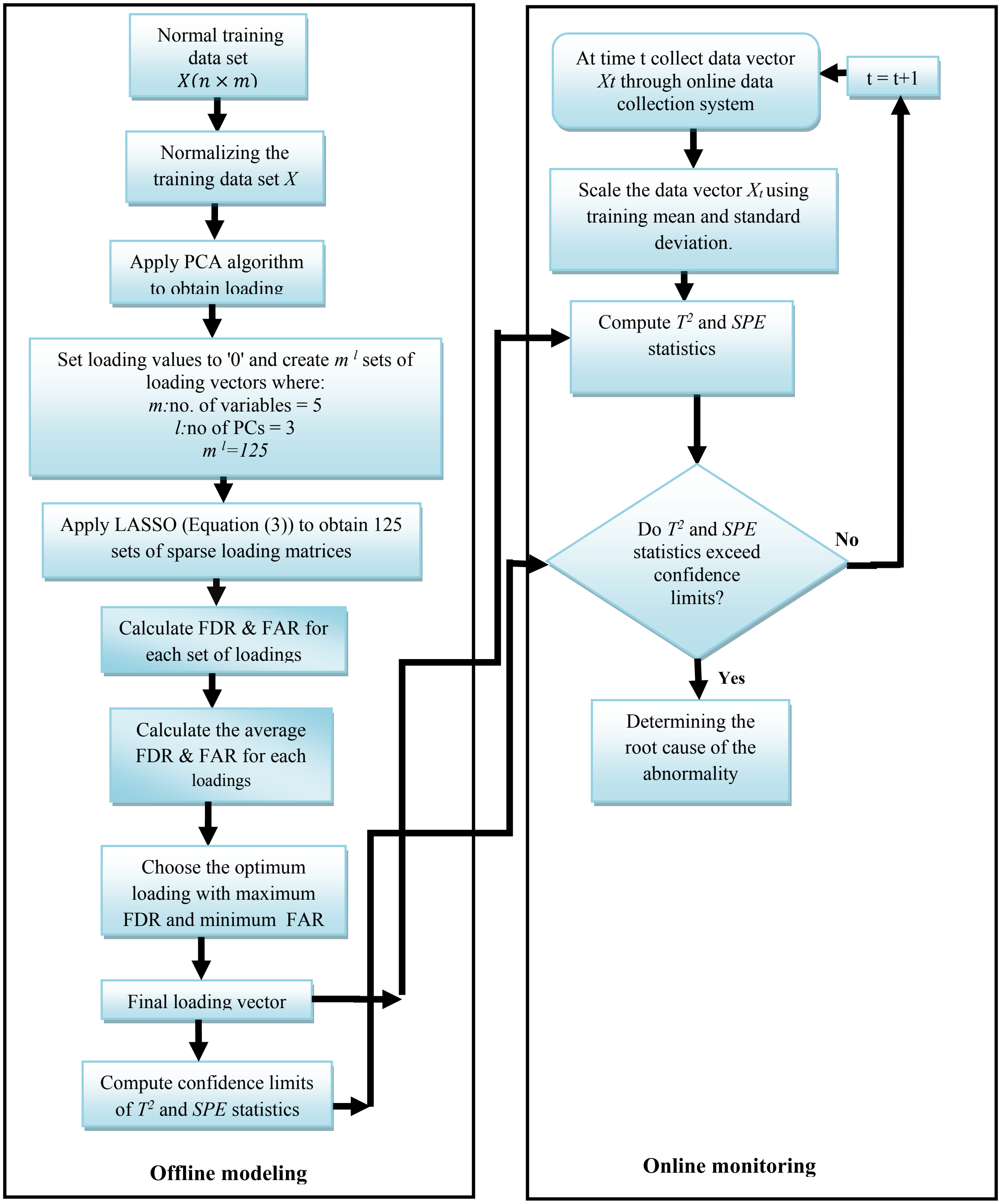


Figure 3. 1: Flow chart of the proposed process monitoring approach.

3.4. Case study: The continuous stirred tank heater (CSTH)

The CSTH system is a commonly used benchmark process for investigation the performance of monitoring techniques. As seen in Figure 3.2, the CSTH system has both a cold and hot water feed which are mixed in the tank. The water in the tank is also heated using a steam heater. A temperature controller maintains the tank temperature by manipulating the steam valve and the tank level is controlled by a level controller Cascaded to a flow controller manipulating the cold water valve.

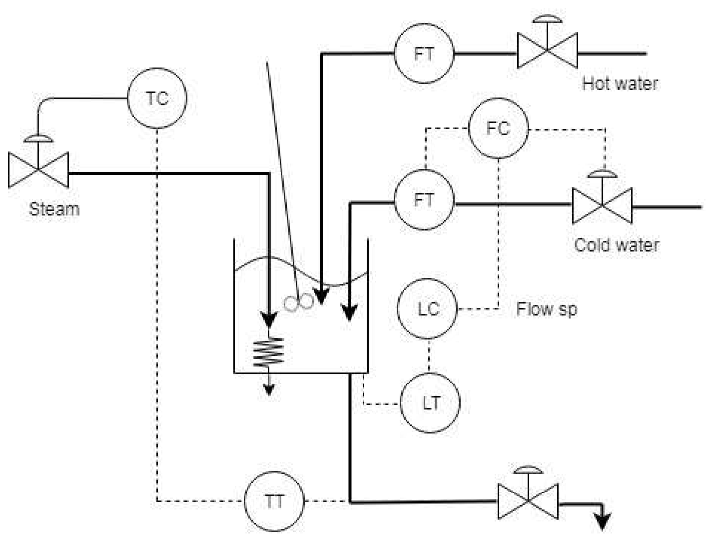


Figure 3. 2 : The continuous stirred tank heater (CSTH)

(Thornhill et al.,2008) developed a detailed Simulink model for the system. We used this benchmark CSTH model to evaluate the methodology proposed in the current study. The system was liberalized for the operating points as given in Table 3.1.

Table 3. 1: Operation conditions for the CSTH system

Variable Number	Name of the Variable	Nominal Operating Conditions	Unit
1	Cold water flow rate	3.823 x 10-5	m^3/sec
2	Hot water flow rate	5.215x10-5	m^3/sec
3	Steam flow rate	6.053	mA
4	Level	20.48	cm
5	Temperature	42.52	^oC

Through the simulations, the system started without fault to generate a normal data set containing 2500 samples. Then, five faults were introduced into the simulation to collect the faulty data sets to be evaluated using the proposed and other standard methods.

3.5. Results and discussion

3.5.1. Benchmark methods

From the classical version of PCA, three loading vectors were selected which cumulatively explained 85% of the total variance. As expected, the loading vectors are full; however, many small values that approached zero were present in the PCs. In order to develop the SPC, we used FDR and FAR-based criteria, which we call the FDR-FAR method. The proposed FDR-FAR is compared with three other existing algorithms, including the Index of Sparseness (IS), Adjusted Variance (AV), and Normalization (NL) methods. The first method creates all combinations of loading vectors by putting 'zeros' in the loading vectors and subsequently selecting the set of loading vectors that give the maximum IS using a genetic algorithm (Gajjar et al.,2017). The Adjusted Variance method focuses on the explained variances of the sparse loading. First, it creates multiple combinations of sparse loading vectors, then the explained variance of the sparse PCs is compared with the original non-zero PCs. The sparsest structure that also retains 90% of the variance of the original PC is selected (Gajjar et al.,2018). The normalization NL method can be used for creating absolute values on component loadings under a specific threshold. In order to interpret loadings, they first need to be normalized, after which a threshold is selected as a means to eliminate non-contributing values (Cadima & Jolliffe.,1995; Trendafilov.,2014). Finally, we used the proposed FDR-FAR method for selecting the sparse structure. As the name suggests, the focus of the algorithm is on fault detection and false alarm. Application details of the method for the CSTH system are described in Section 3.5.2.

3.5.2. SPCA model building using FDR and FAR

In order to develop the Sparse Principal Component Analysis (SPCA) using the FDR and FAR criteria, we first apply PCA to obtain the loading for the system. The CSTH system has five variables and 85% of the variance was explained by the first three PCs, which were selected for the PCA model. Next, different loading values in the original vector were set to '0'to obtain a sparse structure. For CSTH system, there are 5 variables and 3 loading vectors there will be 125 combinations (m=5,l=3,m^l=125) of sparse loading sets assuming that any of these loading values could be a “0” value. The fault detection performance of each set was evaluated using FDR and FAR criteria. The faults of the CSTH system are described in Table 3.2.

Table 3. 2: Process faults for the CSTH system

Fault Number	Fault Description	Fault Type
Fault 1	Step change in the hot water flow rate	Disturbance Fault
Fault 2	Cold water valve -fully open	Actuator Fault
Fault 3	Steam valve -fully open	Actuator Fault
Fault 4	Level sensor	Sensor Fault
Fault 5	Temperature sensor	Sensor Fault

For each fault, we calculated the FDR and FAR using theT^2 and *SPE* statistics. In order to compare different sparse set average, FDR and FAR were calculated for each sparse loading set. Table 3.3 reports the top four performing sets.

Table 3. 3: Fault Detection Rates and False Alarm Rates (%) of faults for model building

NNZL				*SPE*		T^2	
Fault no.	**Spc1**	**Spc2**	**Spc3**	**FDR**	**FAR**	**FDR**	**FAR**
1	1	2	1	91.9	5.9	50.5	2.5
2	1	2	1	69.9	6.2	91.6	2.7
3	1	2	1	96.1	7.2	No detection	
4	1	2	1	96.5	7.1	96.5	2.5
5	1	2	1	95.6	7.5	53.4	2.4
Average				**90.0**	**6.7**	**58.4**	**2.0**
Fault no.	**Spc1**	**Spc2**	**Spc3**	**FDR**	**FAR**	**FDR**	**FAR**
1	1	3	1	91.9	2.6	30.7	2.5
2	1	3	1	94.5	8.4	91.6	2.7
3	1	3	1	96.1	4.9	No detection	
4	1	3	1	96.5	3.3	96.4	2.5
5	1	3	1	95.6	3.0	56.8	2.5
Average				**94.9**	**4.4**	**55.1**	**2.0**
Fault no.	**Spc1**	**Spc2**	**Spc3**	**FDR**	**FAR**	**FDR**	**FAR**
1	1	3	2	91.6	4.4	97.2	10.3
2	1	3	2	No detection		91.5	11.8
3	1	3	2	96.1	6.3	No detection	
4	1	3	2	96.1	6.1	76.5	9.9
5	1	3	2	95.7	6.5	34.3	7.6
Average				**76**	**4.7**	**60**	**7.9**
Fault no.	**Spc1**	**Spc2**	**Spc3**	**FDR**	**FAR**	**FDR**	**FAR**
1	1	2	2	92.5	4.6	97.1	10.1
2	1	2	2	6.6	5	91.5	11.5
3	1	2	2	96.1	6.5	No detection	
4	1	2	2	96.2	6.3	77	9.8
5	1	2	2	95.6	6.6	34.7	7.4
Average				**77.4**	**5.8**	**60.1**	**7.8**

Note: The numbers in the SPC columns indicate the number of non-zeros in each SPC.

It appears that the *SPE* results are more consistent throughout this analysis (see Table 3.3). For the selection of the best loading set, we therefore focused on the *SPE* criteria.

Since FDR and FAR are interrelated, it is not always possible to obtain a set with high FDR and low FAR. As seen in Table 3, [1 3 1] has the highest FDR with marginally more FAR than the others. Therefore, we selected [1 3 1] as the optimal sparse structure for the monitoring model. The final structure of the SPCs are summarized in Table 3.4.

Table 3. 4: Summary of SPCA methods (number of NNZL in each PC)

Method	**NNZL**		
	SPC1	**SPC2**	**SPC3**
Index of Sparseness (IS)	3	2	1
Adjusted variance (AV)	3	2	3
Normalization (NL)	3	2	1
FDR-FAR	1	3	1

3.5.3. Monitoring faults using SPCA algorithms

Process abnormalities include sensor, actuator, and disturbance faults (MacGregor & Cinar.,2012). These different faults were introduced into the CSTH system and tested by PCA and the four different types of SPCA techniques mentioned above. The five faulty datasets are described in Table 3.2. The Classical PCA-based monitoring method was used for benchmarking purpose. In employing PCA and/or SPCA, Hotelling'sT^2 and *SPE* charts were applied during process monitoring. Table 3.5 summarizes the outcomes for the selected fault detection performance for all SPCA and PCA methods for the five faults.

As shown in Table 3.5, the FDR and FAR are computed for both the T^2 and *SPE* statistics for the conventional PCA and SPCA methods. The mean of FDR of the *SPE* statistic of the conventional PCA is less than that of the other SPCA methods. Although the mean

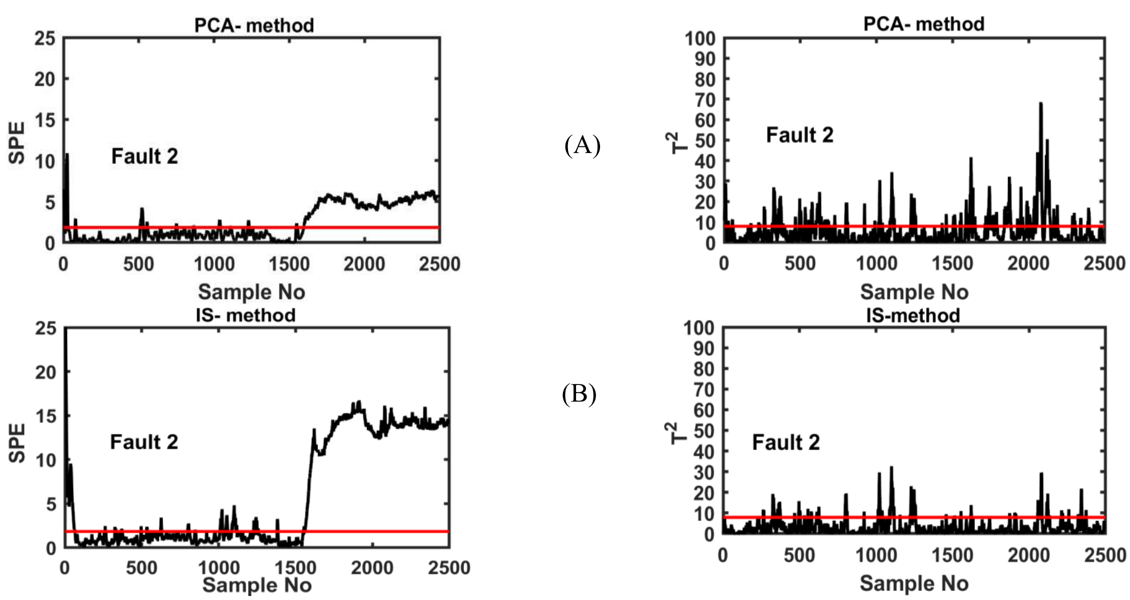
FDR of the T^2 statistic of the NL method is the highest at about 77.1%, the mean FAR of the *SPE* statistics is the highest (17.1%) with the lowest FDR performance. Both the IS and FDR-FAR SPCA approaches give the highest FDRs for the *SPE* statistic (93.4% and 93.8%, respectively), but the FAR of the IS method is quite high (10.2%) compared to that of the FDR-FAR method (4.4%). These results clearly show that on average the proposed FDR-FAR SPCA method has superior performance compared to other SPCA methods. Next, we investigate the result more closely for a specific fault.

Table 3. 5: Fault detection results of PCA and SPCA methods for faults

	Training				Validation			
	SPE		T^2		*SPE*		T^2	
PCA	**FDR**	**FAR**	**FDR**	**FAR**	**FDR**	**FAR**	**FDR**	**FAR**
Fault 1	47.8	4.0	97.8	7.0	42	6.1	99.0	11.8
Fault 2	90.4	4.2	33.1	12.6	91.7	9.4	32.6	17.2
Fault 3	96.1	5.8	No detection		95.5	10.6	18.9	16.4
Fault 4	No detection		No detection		No detection		21.5	16.3
Fault 5	95.7	5.8	No detection		94.8	11.2	33.7	16.5
Mean	**66**	**4.0**	**26.2**	**3.9**	**64.8**	**7.5**	**41.1**	**15.6**
IS method								
Fault 1	90.1	3.4	97.2	3.3	87.7	3.4	96.6	6.1
Fault 2	94.0	16.1	No detection		94.8	17.9	No detection	
Fault 3	96.1	9.2	7.9	26.1	95.5	18.5	21.3	23.7
Fault 4	96.5	13.4	16.3	35.5	94.2	19.5	22.3	23.5
Fault 5	95.6	10.7	10.2	30	94.8	19.1	21.3	23.5
Mean	**94.5**	**10.6**	**26.3**	**20.4**	**93.4**	**15.7**	**34.0**	**17.5**
AV method								
Fault 1	90.8	5.1	97.2	1.0	91.1	8.7	96.6	3.8
Fault 2	89.8	5.4	74.4	37.4	89.7	12.3	45.0	24.6
Fault 3	94.6	5.6	No detection		94.8	13.1	31.2	23.0
Fault 4	78.8	5.6	29.1	29.4	73.7	15.2	38.1	23.6
Fault 5	95.6	5.5	No detection		94.8	13.0	29.6	22.9
Mean	**89.9**	**5.4**	**44.0**	**22.6**	**88.8**	**12.5**	**48.1**	**19.6**
NL method								
Fault 1	37.5	6.4	94.4	2.0	46.6	8.1	92.6	2.4
Fault 2	91.5	10.8	90.1	2.0	89.9	9.8	91.5	3.2
Fault 3	41.7	27.8	31.5	0.9	33.7	28.1	95.9	38.6
Fault 4	96.5	9.2	96.4	1.1	94.2	11.0	94.1	1.3
Fault 5	95.6	29.7	No detection		95.4	28.9	11.6	40.3
Mean	**72.6**	**16.8**	**62.5**	**1.4**	**72.0**	**17.2**	**77.1**	**17.1**
FDR-FAR method								
Fault 1	91.9	2.6	30.8	2.5	91.6	3.5	35.1	2.3
Fault 2	94.5	8.4	91.6	2.6	93.0	10.2	91.9	3.4
Fault 3	96.1	4.9	No detection		95.6	5.3	No detection	
Fault 4	96.5	3.3	96.5	2.5	94.1	5.5	94.1	2.3
Fault 5	95.6	3.0	56.8	2.5	94.8	2.9	56.3	2.6
Mean	**94.9**	**4.4**	**55.3**	**2.5**	**93.8**	**5.5**	**55.5**	**2.6**

3.5.3.1. Case 1: Actuator fault (CW)

An actuator fault was introduced to the cold water (CW) valve. Both T^2 and *SPE* for the SPCA and PCA methods are shown in Figure 3.3. As can be seen in the figure, the *SPE* statistics for the standard PCA, IS, and AV approaches give nearly the same monitoring performance when compared for fault detection. The T^2 plot for the PCA, the IS, and AV SPCA approaches are insensitive to faults. On the other hand, for NL and FDR-FAR methods, the faults were detected both in in the SPE plot as well as in the T2 plot. As illustrated in Figure 3.3, the NL and FDR-FAR SPCA methods show better FDR performance with approximately the same FARs.



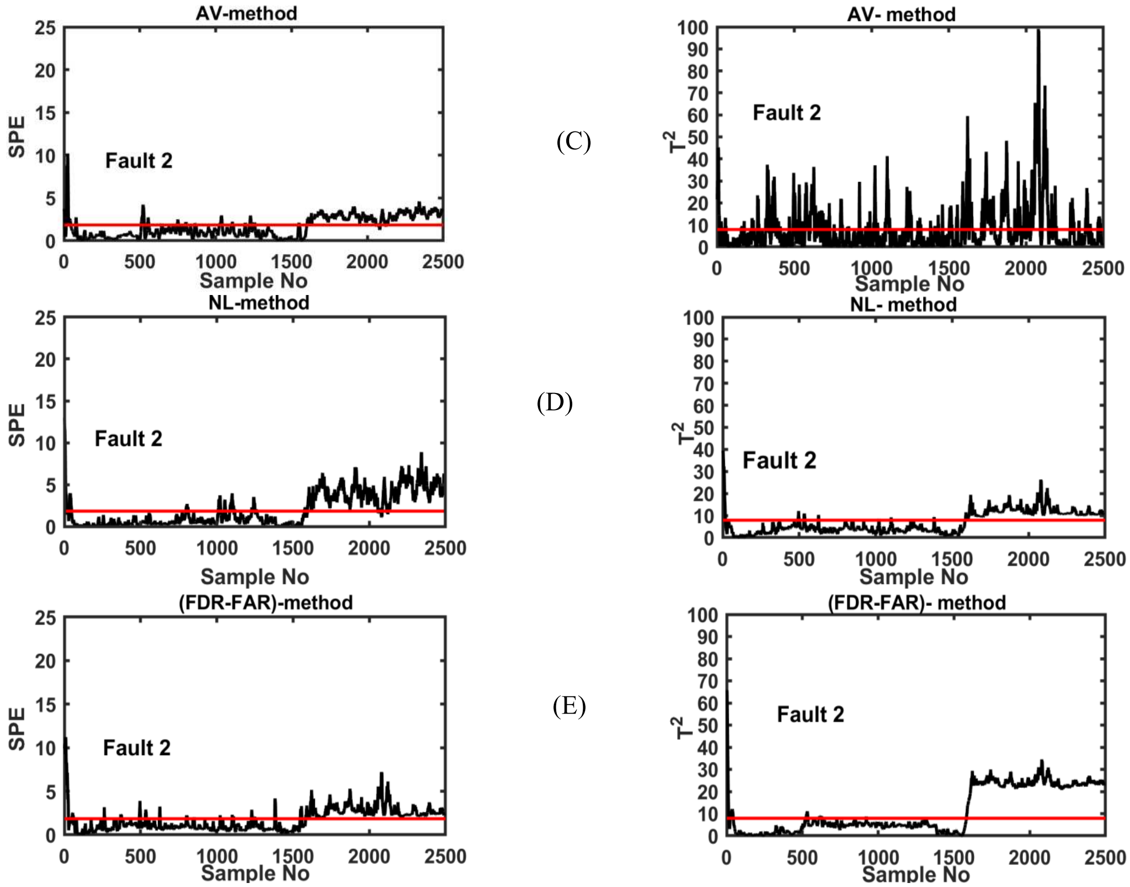


Figure 3. 3 : Monitoring the squared prediction error (SPE) (left) and T^2 (right) results of: A, principal component analysis (PCA); B, Index of Sparseness (IS); C, adjusted variance (AV); D, normalization (NL); and E, fault detection rate-false alarm rate (FDR-FAR) methods for detecting Fault 2.

3.5.2. Fault diagnosis

Fault diagnosis is mainly carried out by assessing the contribution of different variables to the *SPE* or to the relevant principal component (Jiang et al.,2013; MacGregor & Cinar.,2012). The diagnosis of faulty samples for the cold-water actuator fault simulated in the CSTH system using the FDR-FAR SPCA and four other methods (i.e., PCA, IS, AV, and NL) using each of these techniques is described below.

3.5.2.1. Fault diagnosis using contribution plots.

Contribution plots have been widely applied in the quest for fault diagnosis. Contribution plots can be developed from each process variable's contribution to T^2 and *SPE* statistics as soon as a fault is detected (Qin.,2012; Ge et al.,2013; MacGregor & Cinar.,2012). In Figure 3.4, variables 'contributions to T^2 and *SPE* with respect to faulty samples for the cold water actuator fault simulated in the CSTH system are presented. As can be seen in the *SPE* contributions plot for the PCA, IS, and NL methods, Variable 1 (CW flowrate) has the highest contribution and is diagnosed as the most likely reason for Fault 2. However, few other variables have contributions close to that of Variable 1 for these methods. The *SPE* statistics Variable 1 (CW flowrate) and Variable 4 (Level) in the AV method have almost equal contributions. Thus, the diagnosis is not very precise.

In comparison to these methods, fault diagnosis by FDR-FAR is more precise. The FDR-FAR method shows that Variable 1 is the only real faulty variable associated with Fault 2. Diagnosis of the FDR-FAR method based on the T^2 contribution plot (Figure 3.4) is also precise compared to other methods. Based on the T^2contribution of the FDR-FAR and the traditional PCA approaches, Variable 4 is directly associated with the root cause of the fault. However, the IS and AV methods provide that Variable 2 has the largest contribution, which is not exactly the actual fault variable. The NL method shows that Variables 1 (CW flowrate) and Variable 4 (Level) have approximately the same contributions, Variables 1 is identified to be the root cause of fault 2 while Variable 4 is directly related to Variable 1. From these outcomes, although the FDR-FAR SPCA and conventional PCA approaches deliver comparable detection based on the T^2 statistics, the

FDR-FAR method clearly offers superior fault diagnosis performance compared to other SPCA methods based on *SPE* statistics.

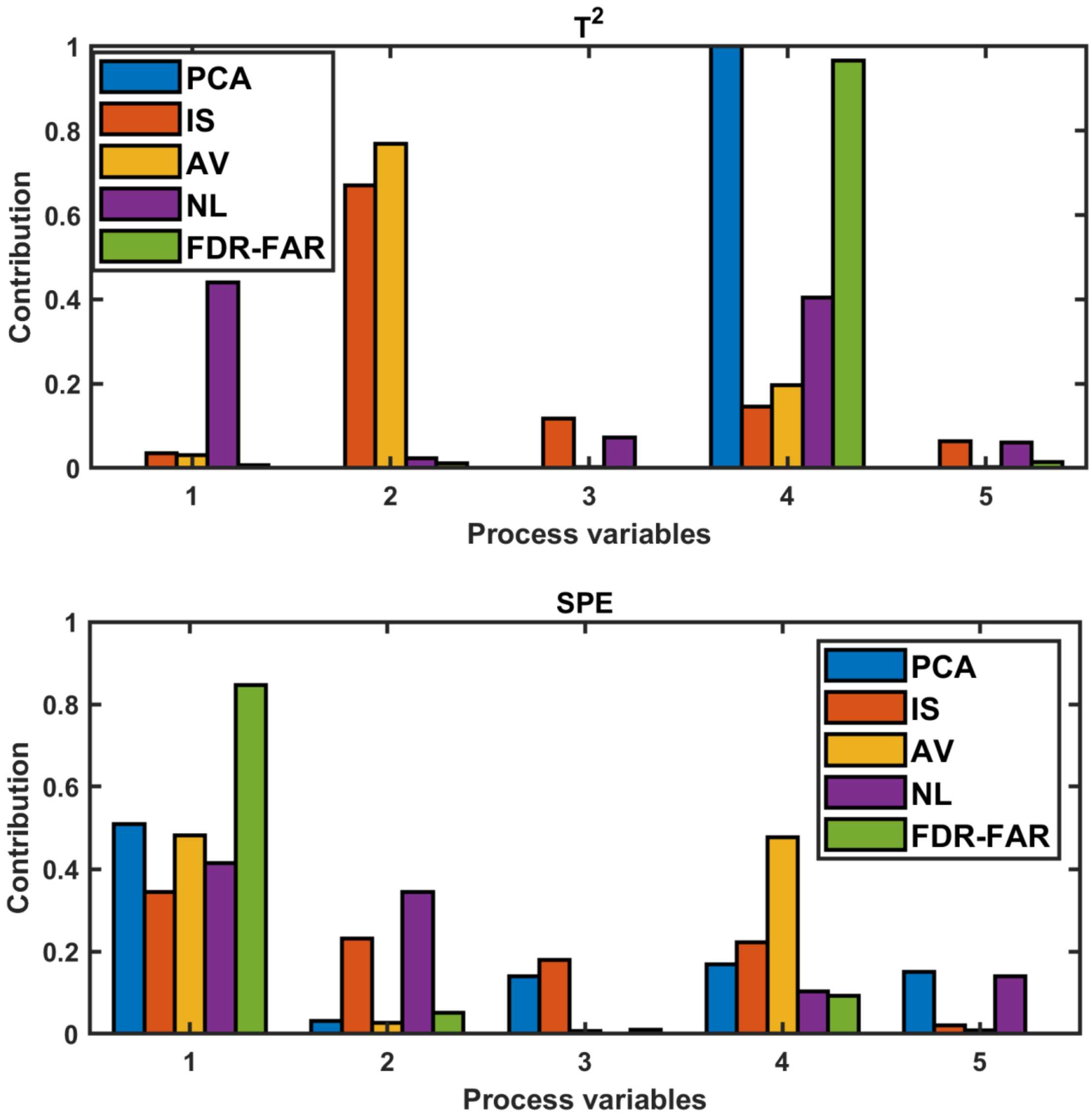
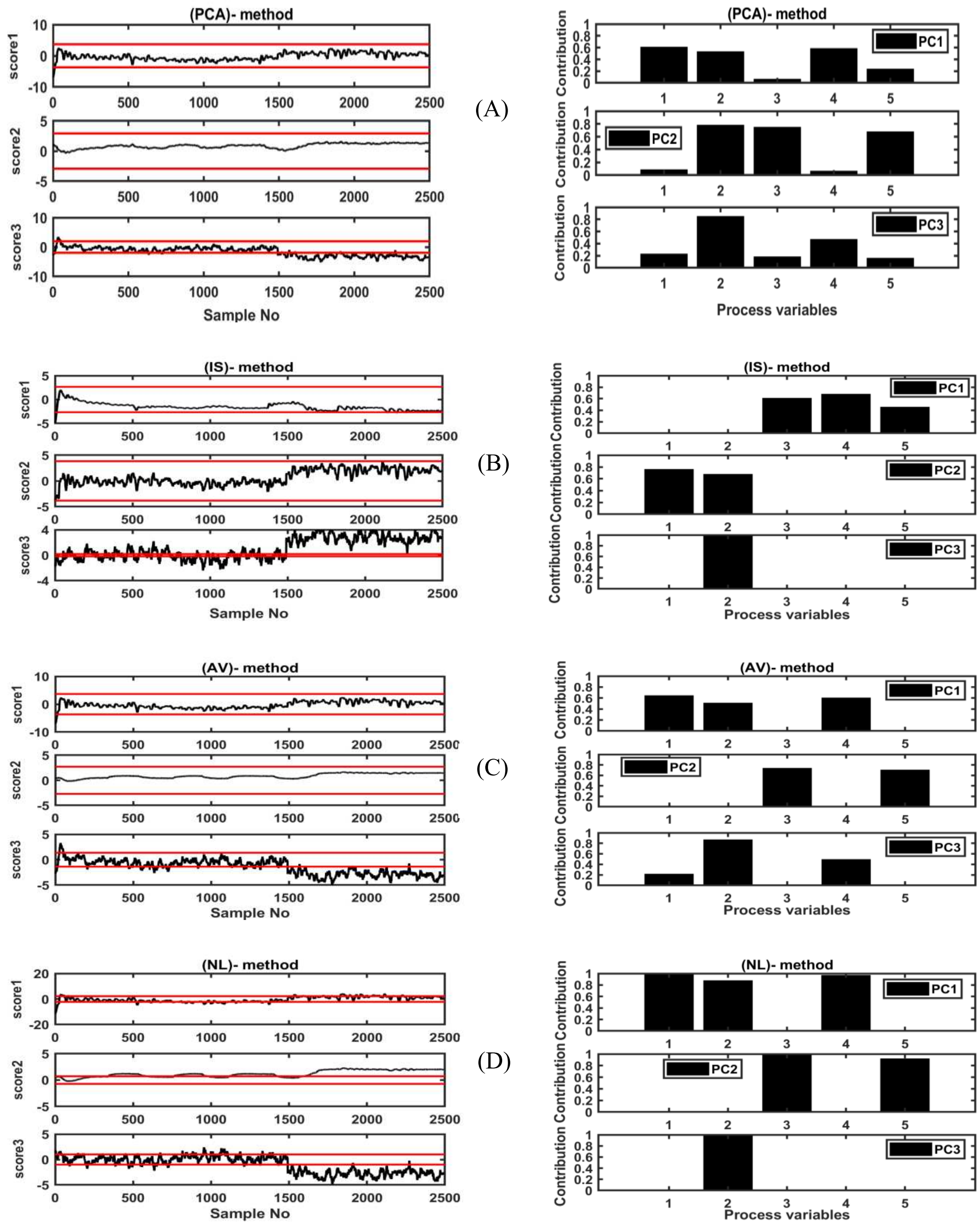


Figure 3. 4 : T^2 (top) and squared prediction error (*SPE*) (bottom) contribution plots for sparse principal component analysis (SPCA) and principal component analysis (PCA) for Fault 2

3.5.2.2. Fault diagnosis using PCs

In addition to contribution plots, faults can also be diagnosed by examining the contributions of individual variables to T^2 and *SPE*, or to the PCs (MacGregor & Cinar.,2012). SPCA has the advantage of diagnosing the faulty variable precisely due to the sparse structure of the loadings, especially when a principal component is used for detecting the fault. In this section, we investigate the diagnosis performance of the proposed SPCA algorithm in relation to other SPCA and PCA methods. We consider a step-type disturbance fault in the hot water flow line of the CSTH system.

Figure 5 depicts the PCs of the sparse and conventional PCA methods in relation to the fault. When scores breach the predetermined statistical limits (i. e., standard deviation), PCs can be applied to identify the reason for the abnormal operation. Figure 3.5A shows the third score PC exceeds the normal operational limits for PCA and the contribution plots for each variable reveal that Variable 2 (HW flowrate) has the maximum contribution to PC3. From this, it can be concluded that PCA accurately diagnoses the cause of the actuator fault. Figure 3.5B and 5C indicate that the third scores of both the AV and IS methods exceeded the normal operational limits. However, in the IS method, the detection of the fault is not very accurate, as can be seen from Figure 5B where the third score remains outside the threshold limits during normal operation.


(PCA)- method
score1
score2
score3
Sample No
Contribution
PC1
PC2
PC3
Process variables
(A)
(IS)- method
(B)
(AV)- method
(C)
(NL)- method
(D)

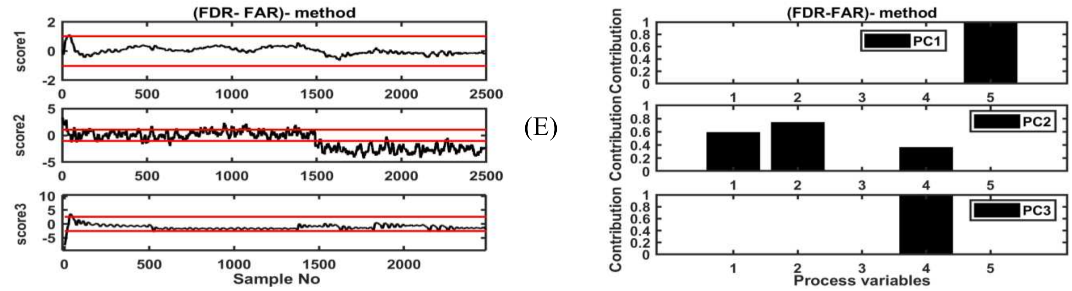


Figure 3. 5 : Principal component (PC) models (score) (left) and contribution plots (right) of Fault 1 assessed using: A, PC analysis (PCA); B, Index of Sparseness (IS); C, adjusted variance (AV); D, normalization (NL), and E, fault detection rate-false alarm rate (FDR-FAR) methods. Note hot water (HW) flow is denoted by Variable 2

In the NL method (Figure3.5D) both PC2 and PC3 detect the fault. The contribution of PC2 comes from Variable 3 (steam flowrate) and Variable 5 (temperature), whereas the contribution of PC3 comes solely from Variable 2. Thus, the diagnosis results are not very precise. Finally, Figure 3.5E shows an obvious deviation for the second score using FDR-FAR approach. Thus, the second score correctly detects the fault. Furthermore, Variable 2 has the highest contribution to the second score. Therefore, the diagnosis is also correct. However, in the second score, the contribution of Variable 1 is very close to that of Variable 2, which confounds the diagnosis to some extent.

3.6. Conclusion

Identifying the NNZL for SPCA is a challenging task. We propose a new criterion to choose NNZL for SPCA based on FDR and FAR performance indicators. The proposed criterion makes SPCA better suited for fault detection and diagnosis (FDD). A comparative study was performed to assess the proposed technique against three established SPCA methods. The FDD abilities of these different SPCA methods along with conventional PCA were compared. The benchmark continuous stirred tank heater

(CSTH) system was used as a case study to compare the methods. Overall, the results show that the proposed FDR-FAR SPCA method had a higher FDR and lower FAR relative to PCA and other SPCA approaches, and more accurately diagnosed faults compared to the other methods. However, the improved performance comes at the cost of more computation and requires faulty data set for calibration.

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Chapter 4
Sparse principal component analysis using bootstrap method

Abstract: Sparse principal component analysis (SPCA) gives a sparse description of the loading matrix. In order to determine the "0" values in the loading matrix, often artificial thresholds are set on the loading values. To resolve these issues, two methods are proposed to calculate the confidence intervals of the loading values. The first method is based on a resampling technique, while the second method estimates the error variance of data to calculate confidence intervals of the loadings. The position and number of non-zero loadings (NNZL) for the PCs are chosen based on a hypothesis test for "0". Both methods lead to sparse structures of PCs. The fault detection and diagnosis performance of the proposed SPCA techniques are compared with the traditional PCA and Adjusted Variance (AV-SPCA) methods for the benchmark continuous stirred tank heater (CSTH) process. The outcomes indicate that the proposed approaches perform better than the traditional PCA, Adjusted Variance (AV-SPCA), Index of Sparseness (IS), and Normalization (NL) and benchmark SPCA (i.e., AV) method in fault detection and diagnosis.

Keywords: principal component analysis (PCA), sparse principal component analysis (SPCA), confidence interval of loadings, iterative principal component analysis (IPCA)

4.1. Introduction

There are ever-increasing demands and regulations for process safety and production quality. In response, process monitoring, especially statistical process control has advanced in leaps and bounds in the last three decades. Several multivariate statistical process monitoring (MSPM) approaches are attracting interest due to their ease of implementation in complex industrial processes. Principal component analysis (PCA) is one of the most commonly used multivariate techniques for data dimension reduction and process fault detection, and it is achieving impressive success rates in real-life applications (Qin, 2012; Ge et al., 2013; Luo et al., 2014; Venkatasubramanian et al., 2003; Chiang et al., 2000). Although PCA is very successful for fault detection, diagnosis of a fault using PCA can be challenging. The difficulty arises because the loading vector elements being typically rated as nonzero, every principal component (PC) becomes a linear combination of most observed variables. These combinations indicate a relation among all variables, instead of just selected few. This wide-ranging relationship makes it challenging to interpret the physical meaning of any PC. PCA essentially gives little to no support in instances of fault isolation (Luo et al., 2016; Xie et al., 2013). As a remedy this issue, researchers have proposed some modifications to PCA (Ning et al., 2015; Tony et al., 2013; Liu et al., 2017; Adachi et al. 2016; d'Aspremont et al., 2008; Trendafilov, 2014; Sriperumbudur and David, 2011). Jolliffe (1995) described some normalization techniques for the rotation of PCs that are more useful for interpreting the components than regular PCs. In related research, Cadima and Jolliffe, (1995) introduced a thresholding method that resets PC loadings to zero in cases where the absolute values are smaller than a predesignated limit. Jolliffe and Uddin, (2000) presented the simplified component technique (SCoT) as a means to determine linear combinations. These combinations were intended to maximize criteria for balancing variances and other measures .The SCoT approach has resulted in better outcomes than rotated PCA when considering the varimax factor (Kaiser , 1958), but it still has difficulties for certain applications. For instance, the penalty function is applied in solutions that are problem-specific, i.e., solution from one application cannot be applied to another application (Jolliffe and Uddin, 2000; Jolliffe et al., 2002). Jolliffe et al. (2003) extended their work by introducing the least absolute shrinkage and selection operator (LASSO) and proposed SCoTLASSO. This method employs a LASSO penalty for PCA optimization problem loadings, which acts as a constraint on the SCoT. This constraint decreases a portion of components' loadings down to be zero. A few other strategies for gaining the necessary sparse loadings are proposed in the literature (Banerjee et al., 2008; Gajjar et al., 2016; Shen et al.; 2013). D'Aspremont et al., (2005) introduced a direct technique for sparse PCA called DSCPA, which is an algorithm that employs semi-definite programming (SDP) in order to achieve sparse PCA. In other studies, Zou et al., (2006) developed a sparse PCA algorithm by first framing PCA in a regression optimization format and then applying the lasso limitation to regression coefficients. Moghaddam et al., (2006) detailed a bi-directional greedy search algorithm called "greedy sparse PCA" (GSPCA). The result was a range of sparse loading vectors. Shen and Huang, (2008) showed how sparse structure in PCs can be achieved by using a normalized SVD approach. The researchers used normalization penalties as a means to aid sparsity in PC loadings and also highlighted cross-validation's relative usefulness as a systematic tuning method for sparsity levels. Witten et al., (2009) introduced a new technique that links ScoTLASS with SPCA to get the first PCs of ScoTLASS. Journée et al., (2010) investigated the GPower (generalized power) option for dealing with sparse PCA when specific constraints such as LASSO or cardinality are a factor in attaining optimal sparse loading vectors. Qi et al., (2013) proposed a new SPCA approach to replace the norm position of the conventional eigenvalue problem with a 'mixed-norm'. The iterative algorithm is used to obtain uncorrelated PCs (orthogonal loadings). Xie et al., (2013) presented shrinking principal component analysis (ShPCA) as a way to modify classical PCA to make all loadings attain near zero loss of information in PCs and for very simplified interpretation, both of which are achievable with this approach. In a similar work, Liu et al., (2015) developed an adaptive SPCA method that out-performed the traditional PCA strategy. Gajjar et al., (2017) applied genetic algorithms (GAs) to determine the correct non-zero loadings (NNZL) numbers for principal components. Specifically, the GAs formulated the NNZLs for every SPC, which maximized the Index of Sparseness (IS). Gajjar et al., (2018) introduced a technique that involved choosing several non-zero loadings for SPCA, with variances of more or less the same degree in corresponding PCs compared to traditional PCA. Moreover, as research has shown that SPCA has proven to be very easy to interpret when comparing with PCA, the application possibilities for SPCA are quite impressive, especially with regard to fault detection/diagnosis schemes. Although numerous algorithms are investigated and tested in the literature, they usually only look at degree of sparseness or level of variance in relation to PCs. While these factors can serve as excellent performance indicators for getting a sparse description, in an FDD context an algorithm's performance regarding fault detection and diagnosis also needs to be considered. Also, researchers have ignored the distribution of the loading elements and threshold on the loading elements were applied using ad hoc methods.

In this paper, we focus on finding the distribution of the loading elements and apply the threshold to the loading elements based on statistical significance tests. We propose two new SPCA algorithms that are based on bootstrap methods to calculate confidence intervals of the loadings. Bootstrap methods have been used to find the distribution of PCA parameters (Babamoradi et al., 2013). However, in the context of SPCA bootstrapping was not applied. In this study we combine bootstrapping with SPCA to find the distribution of the loading elements. Subsequently statistical tests were carried out on each element to determine if the value is effectively zero. This study also compares the two proposed SPCA methods with classical PCA and several SPCA methods (i.e., AV-SPCA, IS, and NL) in relation to fault detection/diagnosis for the continuous stirred tank heater (CSTH) benchmark process. The rest of the article is organized as follows: the preliminary section introduces PCA and SPCA concepts are introduced in section 4.2. The two proposed SPCA methods are presented in section 4.3. The benchmark process, the CSTH simulation case study, is introduced next in section 4.4. The complete results and discussions are presented in section 4.5. Finally, the conclusions of this study are summarized in section 4.6.

4.2. Methods Description:

4.2.1. Principal component analysis (PCA)

Principal component analysis (PCA) describes a dimensionality reduction strategy used for converting correlated variables set into uncorrelated variables set. The converted variables (i.e., PCs) feature nearly all the original data's variability. The main application of PCA in process industries is for detecting abnormalities in the processing. Consider n

observations in m measurement variables for the training data matrix $X \in R^{n\times m}$; the loading vectors $P_{m\times m} = [P_1 P_2 \ldots\ldots P_m]$ are obtained by applying singular value decomposition (SVD). In this case, the PCs$(T_{n\times m}) = [t_1\, t_2 \ldots\ldots t_m]$can be obtained as follows:

$$T = XP \tag{4.1}$$

The first few PCs capture the most variance of the data. The first l PCs $T_{n\times l=}[t_1\, t_2 \ldots\ldots t_l], (l < m)$ that represents the major variance information of the original data is retained and used for projecting the data set. The loading matrix, P is usually a full matrix. Each of these transformed variables (i.e., PCs) is a linear combination of all the original variables, which makes it difficult to interpret the PCs. From a fault detection and diagnosis perspective, if a PC exceeds the threshold this gives an indication a fault has occurred. However, because the loading matrix is full, a PC cannot clearly indicate which is the root cause for fault. The whole motivation of SPCA is to have a sparse description of the loading matrix; this will help in interpreting the PCs as well as the diagnosis of the fault (Choi et al., 2004; Gajjar and Ahmet,2016; Bakshi, 1998; Mallick et al.,2013; Imtiaz et al.,2007; Kourti and John,1995).

4.2.2. Sparse Principal Component Analysis (SPCA)

The SPCA algorithm proposed by Zou et al., (2006) is one of the most popular SPCA methods. The method utilizes LASSO (elastic net) constraints on the loadings (coefficients) of the PCA model to alter the PC loadings to sparse loadings. Assume that $\mathrm{A}^{m\times l} = [\alpha_1 \alpha_2 \ldots\ldots \alpha_l]$ is the indicator variable for the non-zero values of the loading matrix $\mathrm{P}_l^{m\times l} = [\mathrm{P}_1\ \mathrm{P}_2 \ldots\ldots \mathrm{P}_l]$.PCA is expressed as a regression problem as follows:

$$\left(\hat{A}, \hat{P}\right) = \underset{A, P}{arg\,min} \sum_{i=1}^{n} || \, x_i - AP^T x_i \left| P_j \right|^2 + \lambda \sum_{j=1}^{l} ||P_j \left| P_j \right|^2 \tag{4.2}$$

subject to $\mathrm{A^T A} = \mathrm{I}_{l \times l}$

Now, in order to derive sparse regression coefficients (i.e., loadings), the LASSO penalty is combined to Eq. (2) as:

$$\left(\hat{P}\right) = \underset{A, P}{arg\,min} \sum_{i=1}^{n} \|x_i - AP^T x_i||^2 + \lambda \sum_{j=1}^{l} ||P_j||^2 + \lambda_{1,j} \sum_{j=1}^{l} ||P_j||_1 \tag{4.3}$$

The same λ can refer to every l component (λ > 0) and $\lambda_{1,j}$ indicate LASSO penalties for managing loadings (variables) sparsity across differing PCs. Eq. (4.3) can also be referred to as a sparsity criterion. In the equation, the strategy can be reduced to PCA, if there are no penalties (Gajjar et.,2017).

4.3. Proposed SPCA methods

The main hypothesis that we propose in this work is that the spurious loading elements in a loading vector arise due to the uncertainty in data or the measurement noise in the data. Assume that the noisy data matrix X is comprised of noise-free underlying variables, and measurement noise ε is given as follows:

$$X = \tilde{X} + \varepsilon \tag{4.4}$$

$where\ \varepsilon \sim N(0, \sigma^2 I).$

If we have access to $\widetilde{X}$ and the loading vectors are obtained from these noise-free variables, the spurious values in the loading matrix will be exactly "0", resulting in a very sparse description of the PCs. Thus, if we calculate the loading matrix from many realizations of the data set, the distribution loading elements should encompass the "0", and clearly indicate the location of the "0" elements. In the present study, we propose two methods to evaluate the sparse PCs. Both of these methods create several different sets of data to find the distribution of the loading elements, and thus loosely belong to the bootstrap method. The first method uses bootstrap resampling to create several realizations of the data set and we call it "Bootstrap-SPCA". The second method adds different realizations of the noise to the noise-free data to create realizations of data. We used an algorithm called iterative principal component analysis (IPCA) to estimate the error covariance. Thus, we call the second method "Sparse-IPCA". These two methods are described in the following sections.

4.3.1. Bootstrap-SPCA

Bootstrapping is a resampling method proposed by Efron et al., (1979). In bootstrapping several realizations of the data set are created from the original data set by resampling with replacement. The resampled data set will have the same size as the original data set. However, because of the replacement in one data set a data point may be sampled several times while another data point may be completely omitted from the data set. Thus, each of the newly created realizations will be different. Parameters are estimated from each realization (Efron et al., 1979; Wehrens et al.,2000). The distribution of the parameters can be estimated from the realizations of the parameters. Consider the scaled dataset $X \in R^{n\times m}$, where n indicates the total number of observations and m denotes the total number of variables. From the data set, we create 100 realizations of the data set, $[X^{(1)}, X^{(2)},$

$X^{(3)}, , \dots\dots\dots\dots, X^{(100)}]$. Each realization will have the same dimension $n \times m$ as the original data set. SVD is applied to each realization; this gives 100 sets of loading matrices, $[P^{(1)}, P^{(2)}, \dots\dots\dots\dots, P^{(100)}]$ where superscript denotes the realization of the loading matrix. Each loading matrix has a dimension $P^{(k)} \in R^{m\times l}$, where l is the significant number of PCs selected using any suitable method (e.g., SCREE plot) (Valle et al.,1999; Jiang et al.,2013). These realizations of the loadings give the distribution information of the loading matrix. For example, consider an element of the loading matrix $p_{ij}^{(k)}$: there would be 100 realizations of the loading element $\left[p_{ij}^{(1)}, p_{ij}^{(2)}, p_{ij}^{(3)}, \dots\dots\dots, p_{ij}^{(100)}\right]$. Assuming that the loading elements follow a Gaussian distribution, $p_{ij} \sim N(\bar{p}_{ij}, \sigma_p^2)$ a hypothesis test is performed on each element to determine if the loading element is significant or not.

$$H_0: \quad p_{ij} = 0; \;\; if \;\; \bar{p}_{ij} - t_{N-1,\frac{\alpha}{2}}\, s \le 0 \le \bar{p}_{ij} + t_{N-1,\frac{\alpha}{2}}\, s$$

$$H_1: \quad p_{ij} \neq 0; \;\; otherwise$$

where N is the total number of samples, s is the calculated standard deviation and α is the significance level. If the hypothesis is accepted, the corresponding indicator, a_{ij} of the indicator matrix A is set to "0"; otherwise it will be "1". This process is repeated for all elements of the loading matrix giving the sparsity indicator matrix $A^{m\times l}$ for the loading matrix.

Keeping the indicator matrix A fixed, the corresponding sparse loading matrix can be calculated using Eq. (4.3) as below:

$$(\hat{P}) = \underset{A, P}{arg\,min} \sum_{i=1}^{n} \|x_i - AP^T x_i\|^2 + \lambda \sum_{j=1}^{l} ||P_j||^2 + \lambda_{1,j} \sum_{j=1}^{l} ||P_j||_1 \tag{4.3}$$

Following the estimation, the sparse loading set is used to detect and diagnose the faults of the CSTH system. The complete monitoring steps are shown in Figure 4.1.

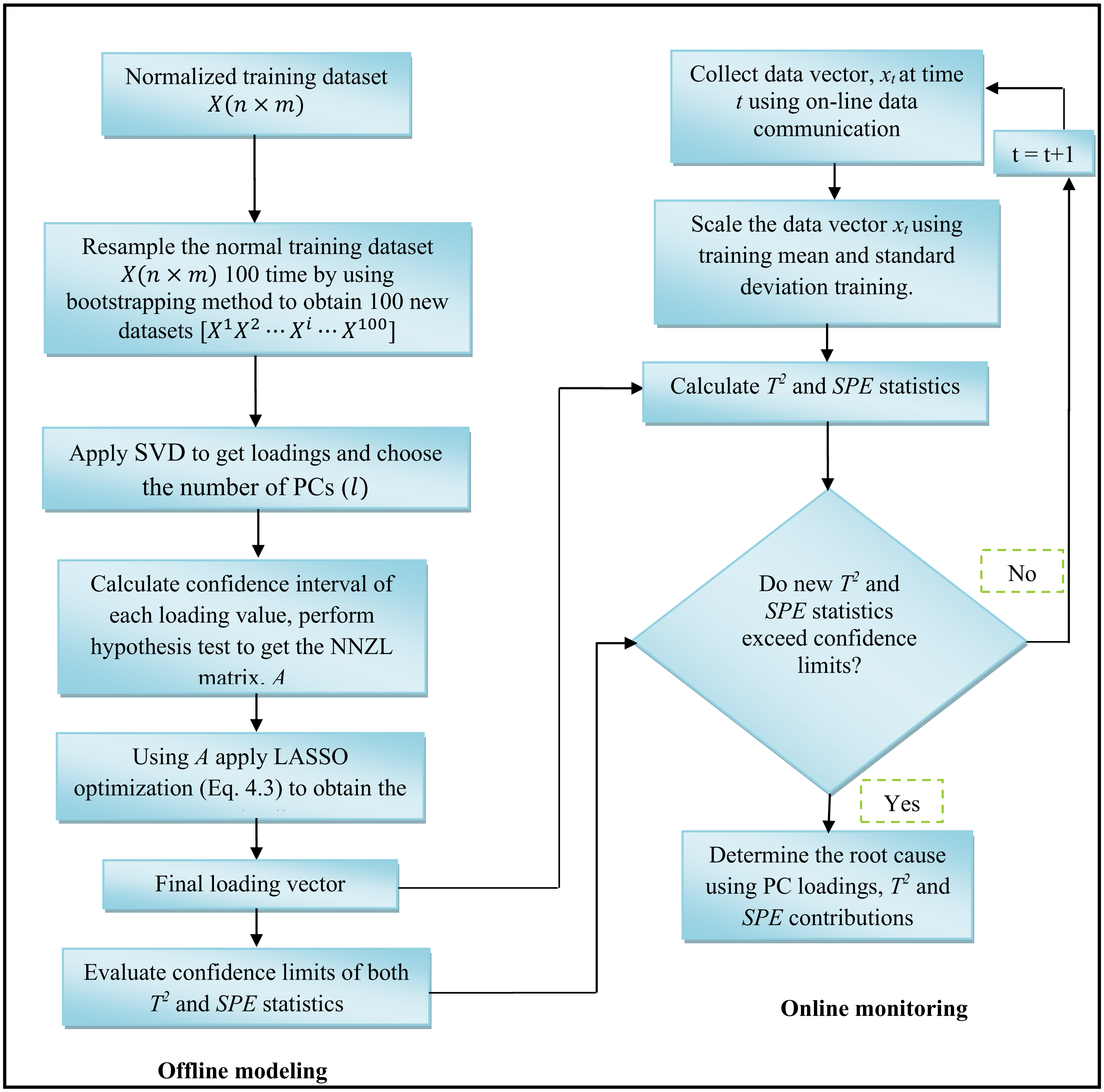


Figure 4. 1: Schematic Diagram Showing Bootstrap-SPCA method

4.3.2. Sparse - IPCA

The proposed method is based on the IPCA algorithm proposed by Narasimhan and Shah, (2008). IPCA is a special algorithm that uses error covariance to scale the data matrix. Consider a case where the noise-free data matrix $\tilde{X}$

$$X = \tilde{X} + \varepsilon$$

where $\varepsilon \sim N\ (0, \Sigma_{\varepsilon})$

The IPCA algorithm iteratively estimates the error covariance matrix by maximizing the likelihood function as in Equation (4.5)

$$\underbrace{min}_{\Sigma_{\varepsilon}}\ N\ log\left|\hat{P}_r \Sigma_{\varepsilon} \hat{P}_r^T\right| + \sum_{i=1}^{N} r_i \left(\hat{P}_r \Sigma_{\varepsilon} \hat{P}_r^T\right)^{-1} r_i \qquad (4.5)$$

where $\hat{P}_r$ comes from the loading matrix $P = \left[\overbrace{p_1\, p_2 \dots \dots\, p_l}^{\hat{P}_l} \mid \overbrace{p_{l+1}\ \dots \dots\ p_m}^{\hat{P}_r}\right]$; and $r_i = \hat{P}_r x_i$. Following the estimation of the error covariance matrix Σ_{ε}, the data is scaled using the standard deviation of the error, *L,* where $LL^T = \Sigma_{\varepsilon}$.

Since the initial estimate of $\hat{P}_r$ is not accurate as an arbitrary scaling or if/when no scaling has been applied, a new set of $\hat{P}_r$ is calculated from the scaled data matrix. These steps are repeated for better estimation of error covariance and the loading matrix. Since the estimation method requires iterations, the method is called Iterative PCA or IPCA (Narasimhan and Shah, 2008; Imtiaz et al.,2004).

IPCA provides the loading matrix, as well as the noise covariance matrix that can be used to reconstruct the noise-free data $\hat{\hat{X}}_s = P_l\, P_l^T X_s$, and $\hat{\hat{X}} = L\hat{\hat{X}}_s$. Using the estimated noise-free variables and noise covariance information, several realizations of the data can be created as follows:

$$X^{(i)} = \hat{\hat{X}} + L\nu_i \tag{4.6}$$

where $\nu_i \sim N(0, \Sigma_\varepsilon)$.

By changing ν_i we can create many realizations (i.e., 100 realizations) of the data matrix $\left[X^{(1)},\ X^{(2)},\ X^{(3)},, \dots \dots \dots \dots ., X^{(100)}\right]$. The rest of the steps are similar to the Bootstrap-SPCA method. Briefly, it involves SVD of each of the realizations, hypothesis testing on each of the elements of the loading matrix to determine if the value is significant or not. This includes the estimation of the sparseness indicator matrix, *A,* and finally, evaluation of the sparse loading matrix by minimizing the LASSO objective function given in Eq. (4.3). The overall methodology is shown in Figure 4.2.

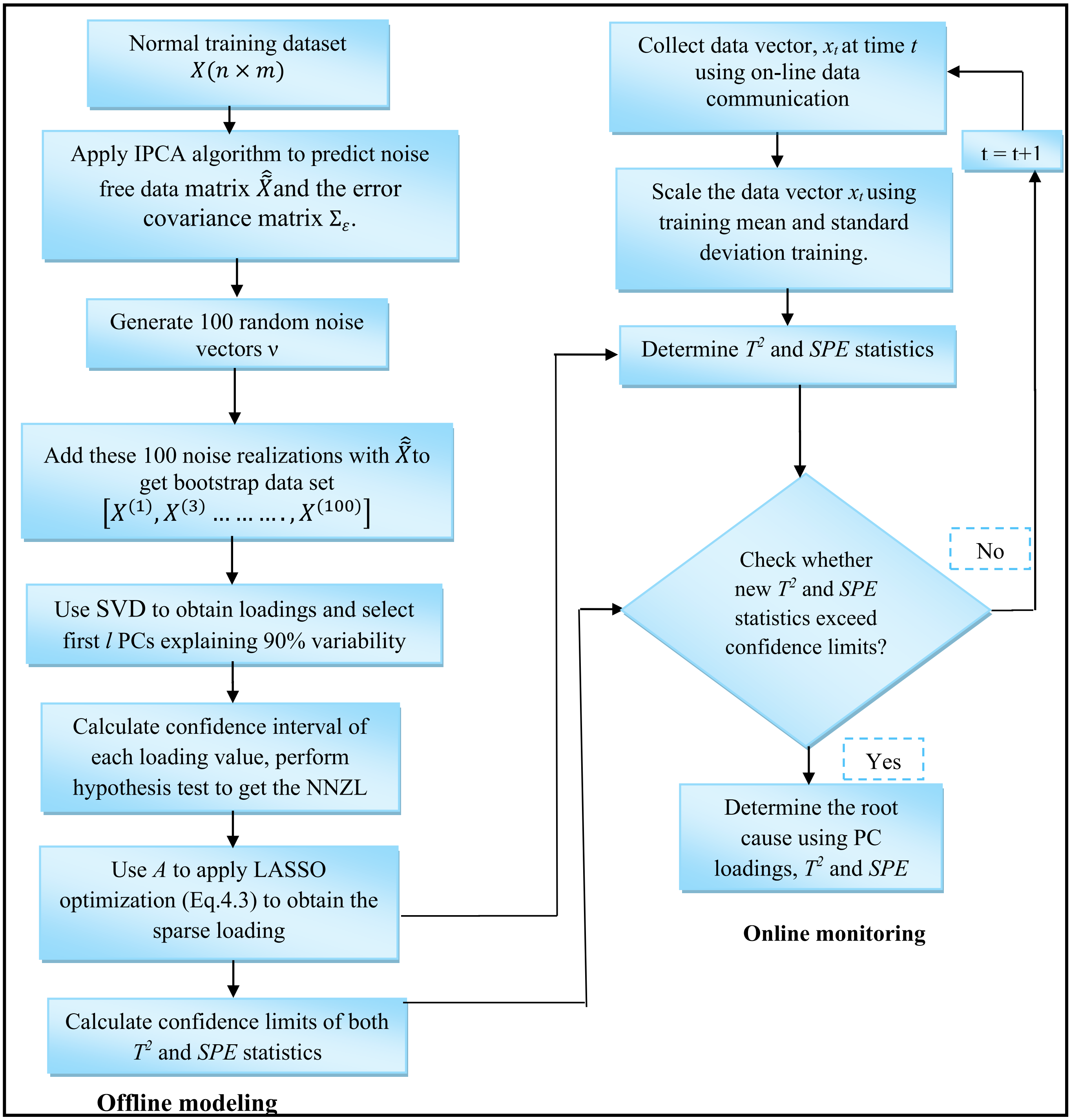


Figure 4. 2 : Schematic diagram showing Sparse- IPCA method

4.4. Case study: Continuous stirred tank heater (CSTH)

We tested the proposed method extensively on a simulated CSTH system described in Thornhill et al., (2008). This is a simulated system, built based on an experimental set up at the University of Alberta. The model is very realistic; it uses the system parameters and operating conditions, including the noise characteristic obtained from the sensors. The CSTH system is a heating tank that continuously mixes cold water with hot water. The steam heater is used to heat up the water in the tank. The tank temperature is controlled by manipulating the steam valve. Also, a level controller cascaded to a flow controller maintains the tank level by manipulating the cold water valve. Figure 4.3 illustrates the CSTH system.

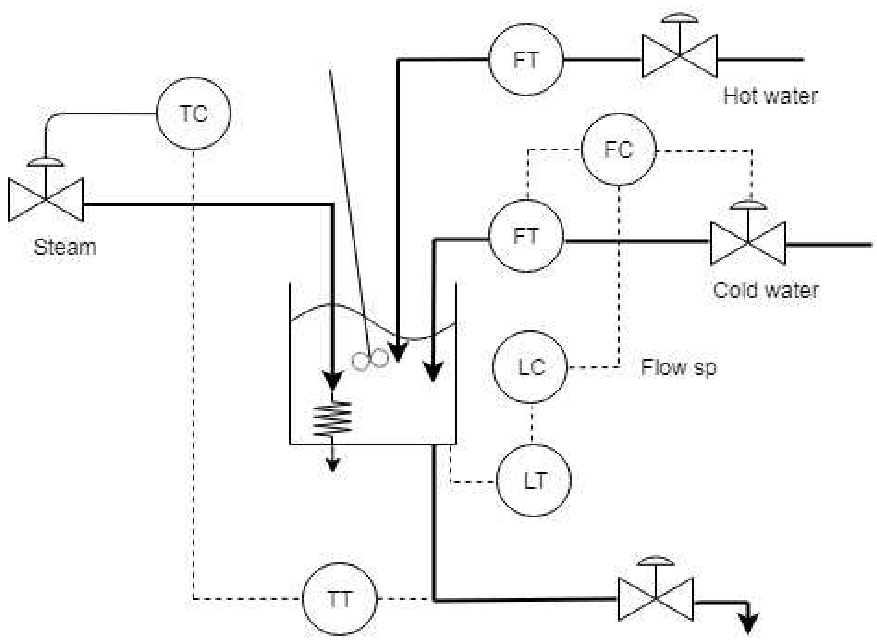


Figure 4. 3 : A schematic diagram of the continuous stirred tank heater (CSTH)

This benchmark CSTH system is used for the present study. The operating conditions for the system are given in Table 4.1.

Table 4. 1: Operation conditions for the CSTH system

Variable No.	Process Variable	Nominal Operating Conditions	Unit
1	Cold water flow rate	3.823 x 10-5	m^3/sec
2	Hot water flow rate	5.215x10-5	m^3/sec
3	Steam flow rate	6.053	mA
4	Level	20.48	cm
5	Temperature	42.52	^oC

4.5. Results and Discussion

4.5.1. Confidence intervals of loading elements:

As described in Section 4.3, we used two different methods: (i) Bootstrap-SPCA and (ii) Sparse - IPCA, to create the realizations of the data set. Subsequently, confidence intervals of the loading elements were calculated from the data sets.

4.5.1.1. Confidence Interval using bootstrap-SPCA method

Through sampling with replacement, 100 data sets were created. From these data sets the distributions of the loading elements were calculated following the procedure described in Section 4.3.1. The distributions of the loading elements are shown in Figure 4.4. The distributions clearly show that for the first two elements of PC1 "0" falls within $\pm 3\sigma$. As such, the value was set to "0". Similarly, in PC2, the third element, and in PC3, the first element is insignificant. This gives the sparseness indicator matrix, $A = [0\ 0\ 11\ 1; 1\ 1\ 0\ 1\ 1; 0\ 1\ 1\ 1\ 1]^T$. Keeping the A matrix fixed we calculated the loading matrix by minimizing the LASSO objective function (Eq. 4.3). Subsequently, keeping the loading matrix A fixed, we recalculated the loading matrix by minimizing the LASSO objective function. The loading matrix was used for fault detection and diagnosis.

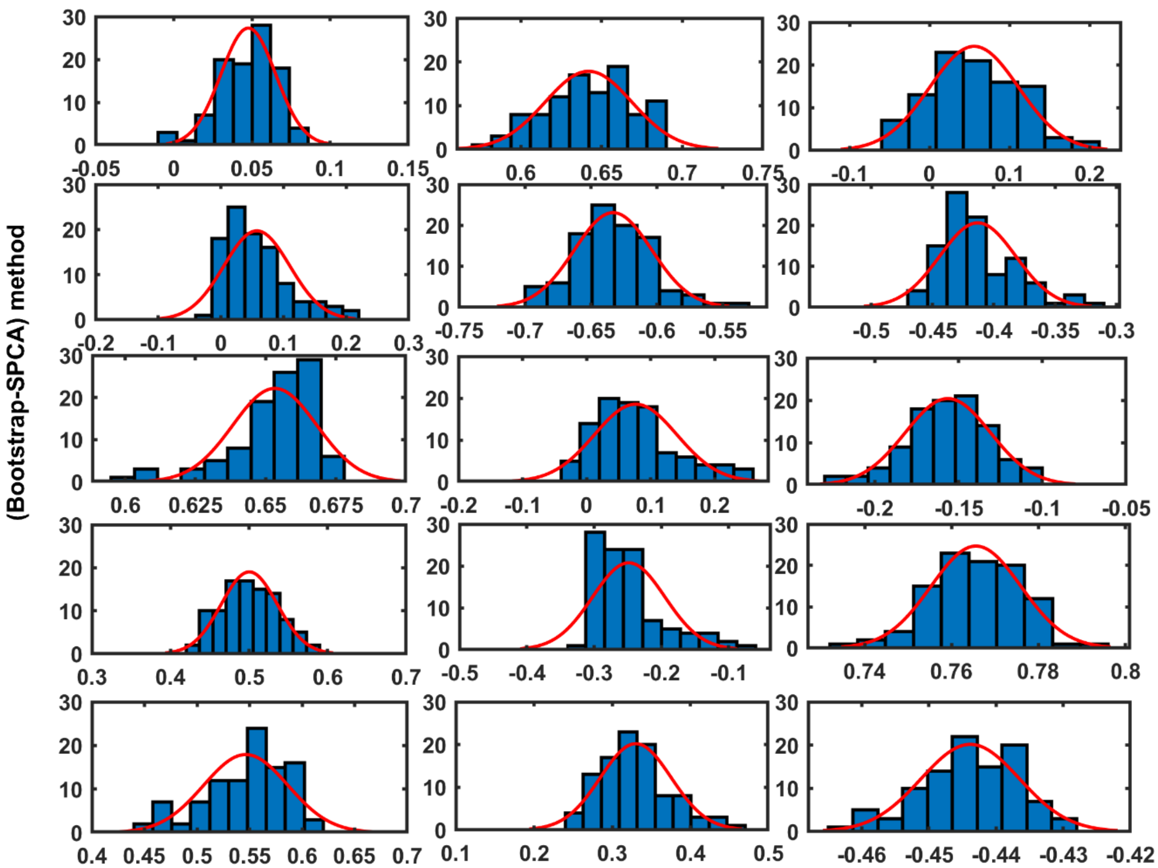


Figure 4. 4 : Distribution of loading elements using bootstrap-SPCA method

4.5.1.2. Confidence Interval using Sparse-IPCA method

The IPCA algorithm was used to calculate the error covariance of the measurement noise of data, and to estimate the noise-free variables. Next, measurement noise was added to the estimated noise-free variables. By randomly selecting the measurement noise, 100 realizations of the data set were created. From these 100 realizations, 100 sets of loadings were calculated. The distributions of the loading elements are shown in Figure 4.5.

Clearly, in PC1, the 1st and the 3rd elements are insignificant, in PC2 the 1st element, and in PC3 the 3rd, 4th, and 5th elements are insignificant. These elements were set to "0", which gave the sparseness matrix,

$A = [0\ 1\ 0\ 1\ 1; 0\ 1\ 1\ 1\ 1; 1\ 1\ 0\ 0\ 0]^T$. Subsequently, the loading matrix was calculated and used for fault detection and diagnosis.

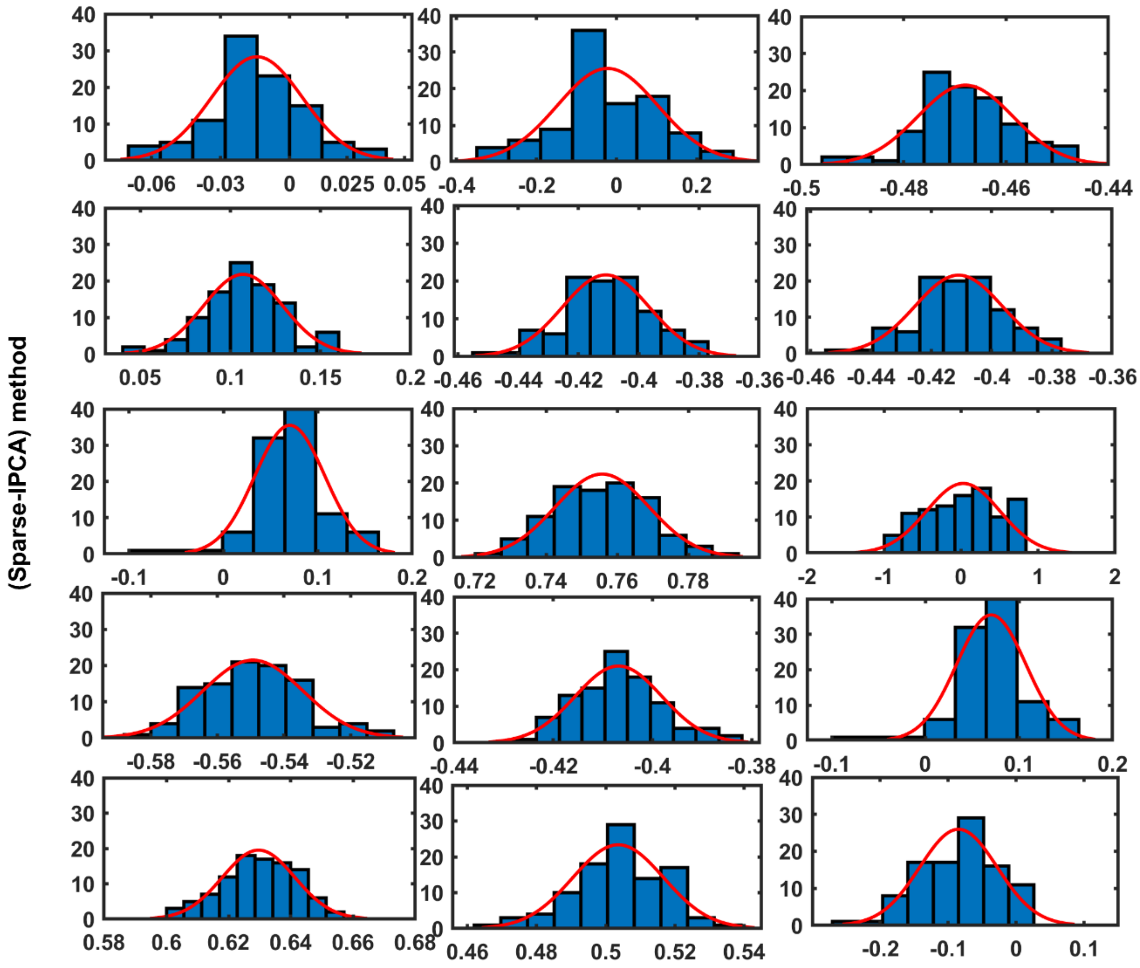


Figure 4. 5 : Distribution of the loading elements using the Sparse-IPCA method.

4.5.2. Monitoring results for PCA and SPCA algorithms

The fault detection performance is tested on five fault scenarios generated by the CSTH system. Two performance indices, FDR and FAR, are used to evaluate the fault detection performance of the proposed methods (Yin et al.,212; Luo et al.,2013). The results are compared with benchmark methods: traditional PCA, AV-SPCA, IS, and NL methods. The fault descriptions of the CSTH system are given in Table 4.2, and the comparison results are provided in Table 4.3.

Table 4. 2: Fault scenarios for the CSTH system

Fault No.	Fault Description	Type of Fault
Fault 1	Step change in the hot water flow rate	Disturbance Fault
Fault 2	Cold water fully open valve	Actuator Fault
Fault 3	Steam fully open valve	Actuator Fault
Fault 4	Level sensor	Sensor Fault
Fault 5	Temperature sensor	Sensor Fault

The FDR and FAR from T^2 and *SPE* statistics were calculated for each fault for the conventional PCA and SPCA methods using Equations 4.7 and 4.8 as shown below.

$$FDR = \frac{(No. of\ samples\ (J > Jth\ |f \neq 0)}{Total\ samples\ (f \neq 0)} \times 100 \tag{4.7}$$

And

$$FAR = \frac{(No. of samples\ (J > Jth\ |f = 0)}{Total\ samples\ (f = 0)} \times 100 \tag{4.8}$$

Where J is the calculated fault statistic and $\mathrm{f} \neq 0$ denotes a fault condition, while $\mathrm{J_{th}}$ is the fault threshold and $\mathrm{f} = 0$ denotes a no-fault condition.

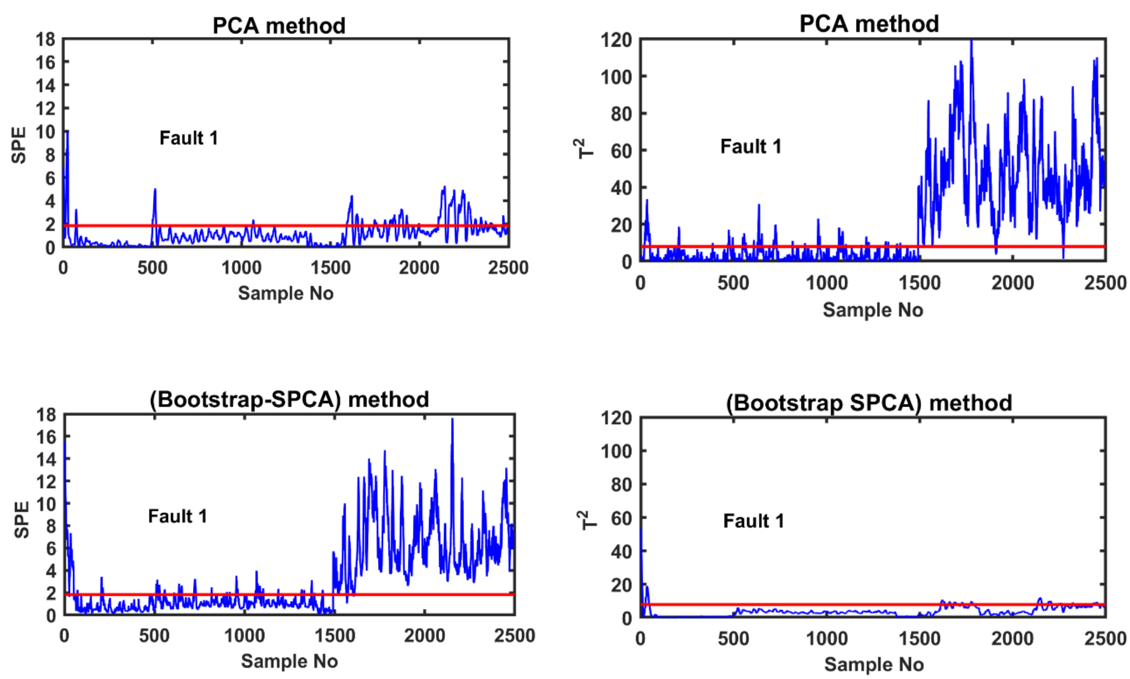
The *SPE* of the bootstrap-SPCA and Sparse-IPCA methods successfully detected the faults with over 90% FDR and the maximum FAR of 22%. Though the FAR was a little high for Fault 3 and Fault 4 for the proposed method, the FDR was also very high. Moreover, both the conventional PCA and AV- SPCA methods failed to detect Fault 4, whereas the proposed, IS, and NL methods detected the fault with over 90% FDR. The fault detection performance of the methods is further investigated in the T^2 and *SPE* plots in Figures 4.6 to 4.8.

Table 4. 3: Fault Detection Rates and False Alarm Rates (%) results for 5 faults of PCA and SPCA methods

	Training				Validation			
	SPE			T^2	SPE		T^2	
PCA	**FDR**	**FAR**	**FDR**	**FAR**	**FDR**	**FAR**	**FDR**	**FAR**
Fault 1	47.8	4	97.8	7	42	6.1	99	11.8
Fault 2	90.4	4.2	33.1	12.6	91.7	9.4	32.6	17.2
Fault 3	96.1	5.8	No Detection		95.5	10.6	18.9	16.4
Fault 4	No Detection		No Detection		No Detection		No Detection	
Fault 5	95.7	5.8	No Detection		94.8	11.2	33.7	16.5
(Bootstrap-SPCA) method								
Fault 1	97.9	6.8	No Detection		99.3	14.3	No Detection	
Fault 2	94.3	8.2	91.5	2.1	94.9	22.5	91.9	2.1
Fault 3	96.1	5.9	57	12.3	96.4	22.2	56.9	19.1
Fault 4	96.5	3.6	96.5	2.3	94.1	6.8	93.7	3.7
Fault 5	95.7	3.7	57.9	2.2	94.8	6.2	57	3.4
(Sparse- IPCA) method								
Fault 1	96.9	3.06	74.1	14.3	95.76	5.8	77.9	19.1
Fault 2	91.62	3.53	82.9	18.7	92.43	7.13	77.7	18.5
Fault 3	93.54	13.26	No Detection		86.9	21.4	No Detection	
Fault 4	96.5	5.66	58.63	19.73	94.15	6.4	44.3	22
Fault 5	95.7	4.2	90.72	16.13	94.85	7.1	88.2	24.4
(AV-SPCA) method								
Fault 1	90.8	5.1	97.2	1	91.1	8.7	96.6	3.8
Fault 2	89.8	5.4	74.4	37.4	89.7	12.3	45	24.6
Fault 3	94.6	5.6	No detection		94.8	13.1	31.2	23
Fault 4	78.8	5.6	No detection		73.7	15.2	38.1	23.6
Fault 5	95.6	5.5	No detection		94.8	13	29.6	22.9
IS method								
Fault 1	90.1	3.4	97.2	3.3	87.7	3.4	96.6	6.1
Fault 2	94.0	16.1	No detection		94.8	17.9	No detection	
Fault 3	96.1	9.2	7.9	26.1	95.5	18.5	21.3	23.7
Fault 4	96.5	13.4	16.3	35.5	94.2	19.5	22.3	23.5
Fault 5	95.6	10.7	10.2	30.0	94.8	19.1	21.3	23.5
NL method								
Fault 1	37.5	6.4	94.4		46.6	8.1	92.6	2.4
Fault 2	91.5	10.8	90.1		89.9	9.8	91.5	3.2
Fault 3	41.7	27.8	31.5		33.7	28.1	95.9	38.6
Fault 4	96.5	9.2	96.4		94.2	11.0	94.1	1.3
Fault 5	95.6	29.7	No detection		95.4	28.9	11.6	40.3

Fault 1: Disturbance Fault (hot water flow rate)

In Fault 1, a step type disturbance was introduced to the hot water flow rate. Figure 4.6 shows Hotelling's T^2 as well as *SPE* statistics charts. Figure 4.6 indicates T^2 statistic for PCA, AV-SPCA, IS, and NL techniques detected the fault immediately with a high FDR. However, the *SPE* chart of the bootstrap-SPCA method detected the fault. The Sparse-IPCA method detected the fault; however, the FAR was very high. Clearly, bootstrap-SPCA and Sparse-IPCA has detection performance at par with PCA and AV-SPCA methods.



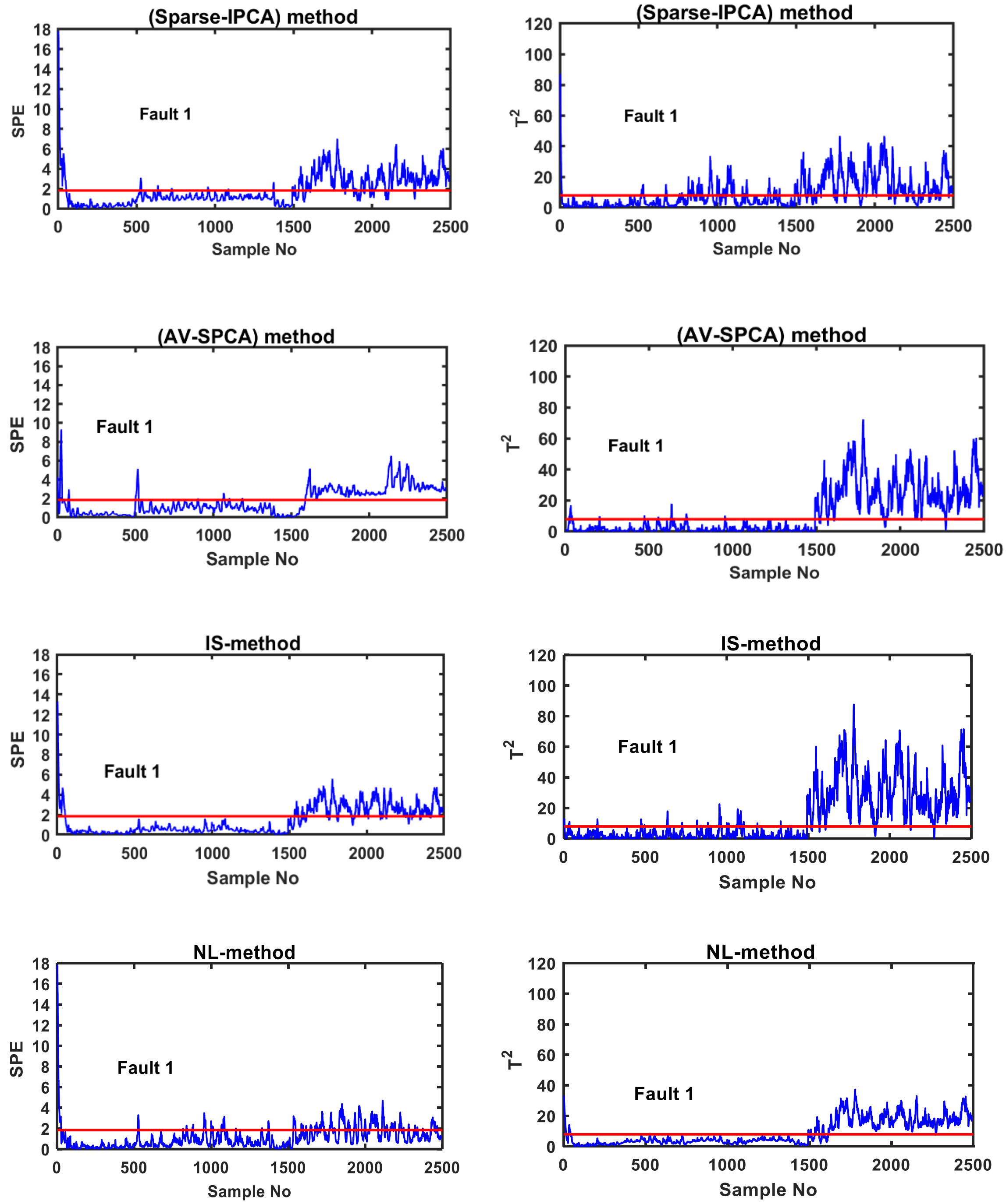
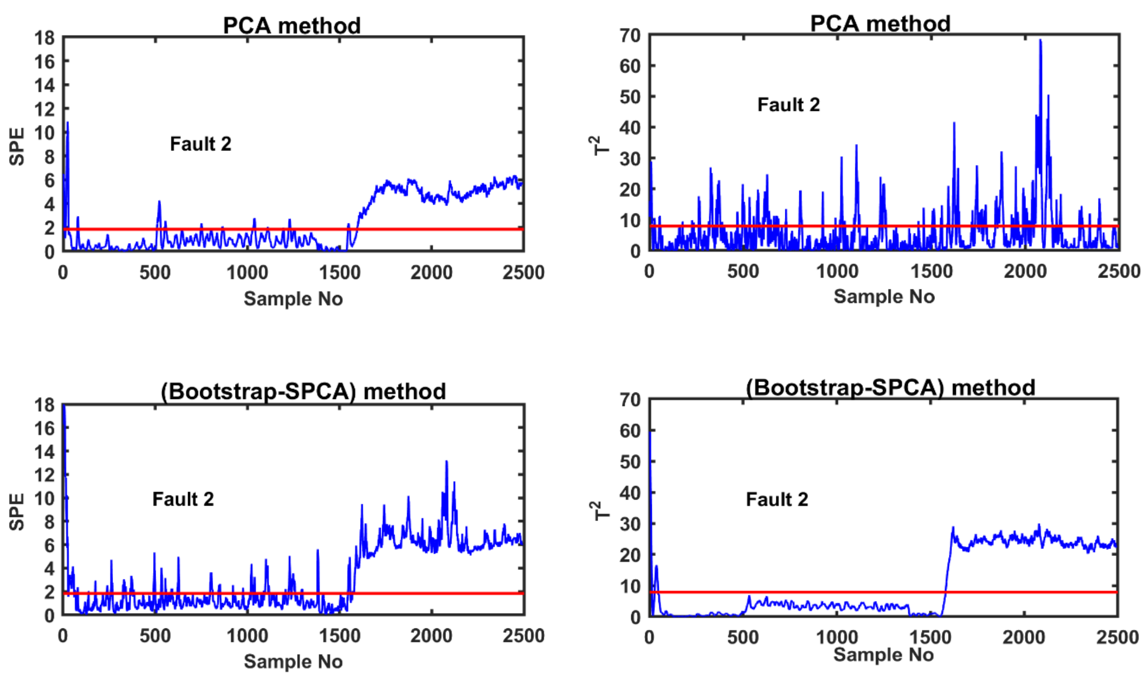


Figure 4. 6 : Monitoring the *SPE* (left) and T^2(right) results of PCA, Bootstrap-SPCA, Sparse-IPCA, AV-SPCA, IS, and NL methods for detecting Fault 1.

Fault 2: Actuator fault (cold water valve)

A cold water valve fault presents the second scenario for faulty behavior in CSTH process. Due to the cold water fault in the CSTH process, both T^2 and *SPE* for SPCA and PCA are shown in Figure 4.7. As seen in the figure, *SPE* statistics in the PCA, AV-SPCA, IS, and NL approaches detected the faults with a low false alarm. Both T^2 and *SPE* plots of the bootstrap-SPCA method detected the fault. The *SPE* plot of the Sparse-IPCA method detected the fault. Only the *SPE* plot of the Sparse-IPCA method detected the fault. Overall, the bootstrap-SPCA method showed the best performance in detecting the fault, and the T^2 plot showed especially clear detection of the fault.



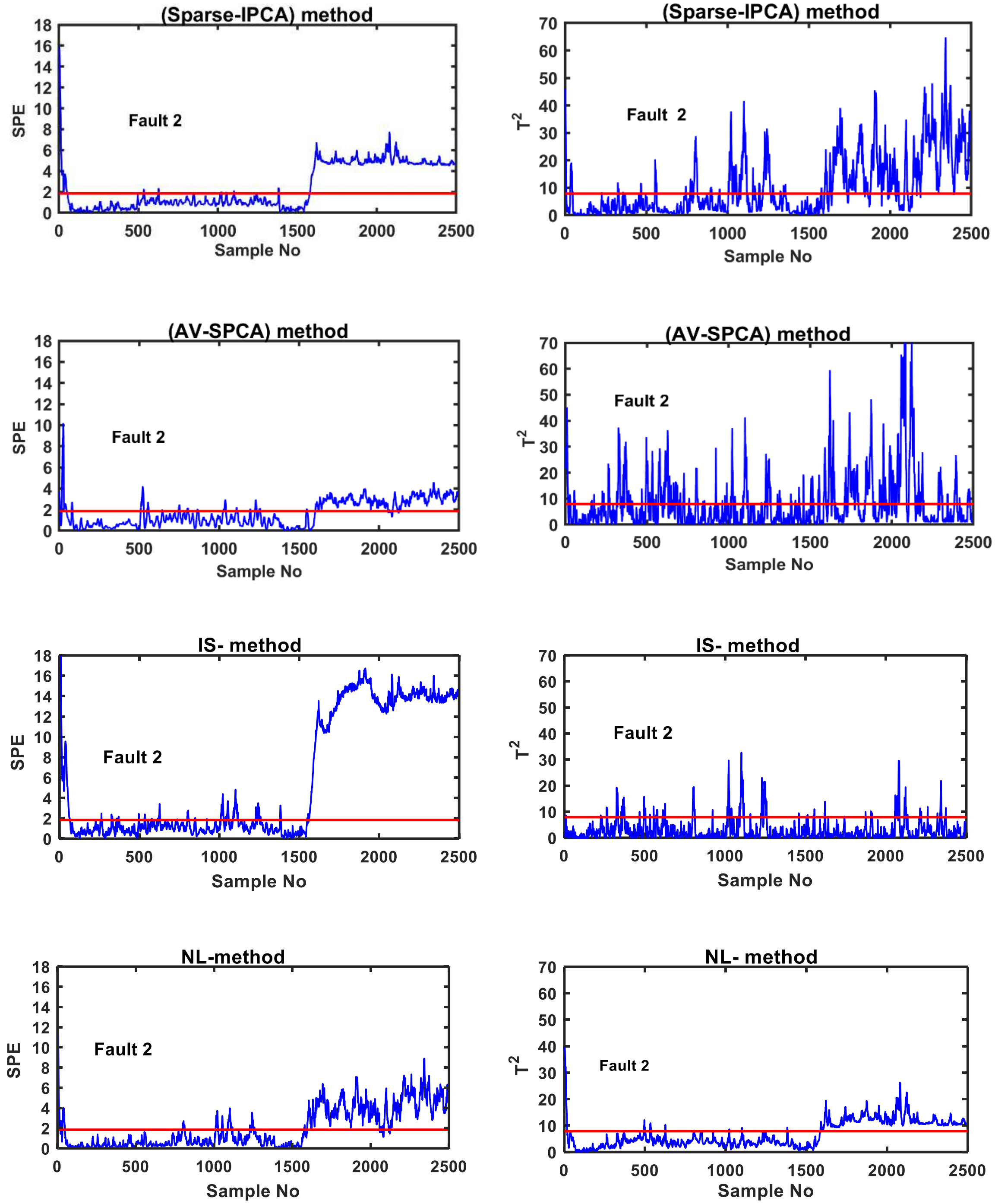
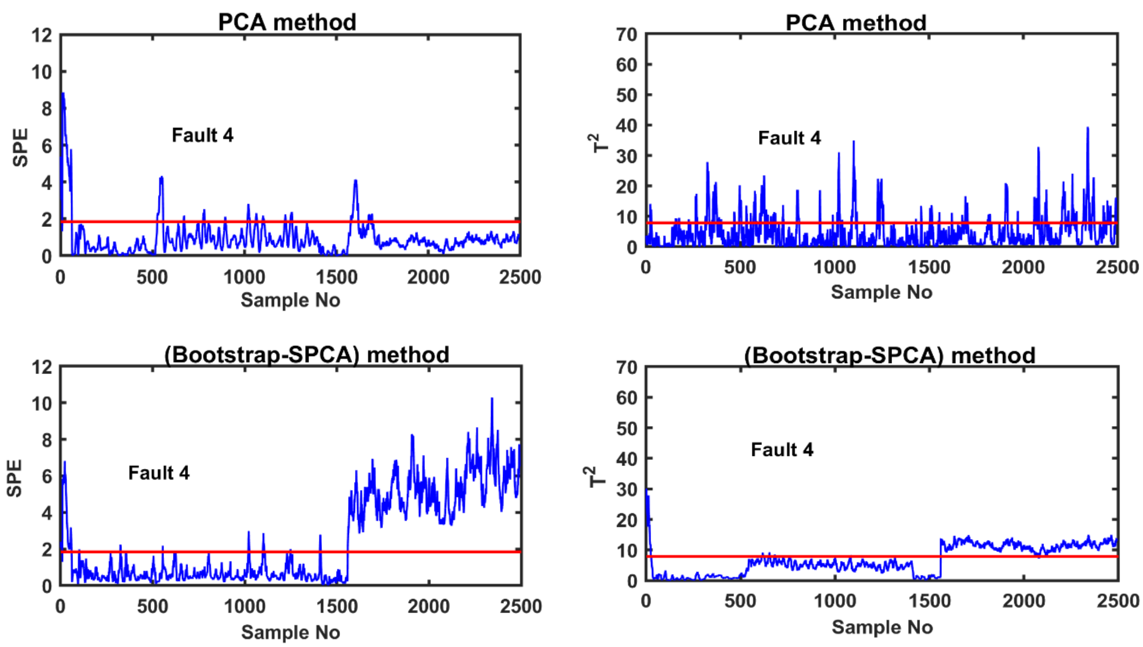


Figure 4. 7 : Monitoring the SPE (left) and T^2(right) results of PCA, Bootstrap-SPCA, Sparse-IPCA, AV-SPCA, IS, and NL methods for detecting Fault 2.

Fault 4: Sensor fault (level)

For the CSTH process, Fault 4 represents the level sensor fault. Figure 4.8 compares the $T^2$and *SPE* in the SPCA and PCA. As can be seen from the figure, Fault 4 has been easily detected by the SPCA methods. However, neither T^2 nor *SPE* statistics of the conventional PCA were able to detect the fault. Among the SPCA methods, the bootstrap-SPCA and NL methods are able to detect the fault using both T^2 and *SPE* with high FDR and low FAR. The results obtained by the *SPE* statistics show that bootstrap-SPCA, Sparse- IPCA, IS, and NL methods have over 94% FDR, compared to 79% with the AV-SPCA method.



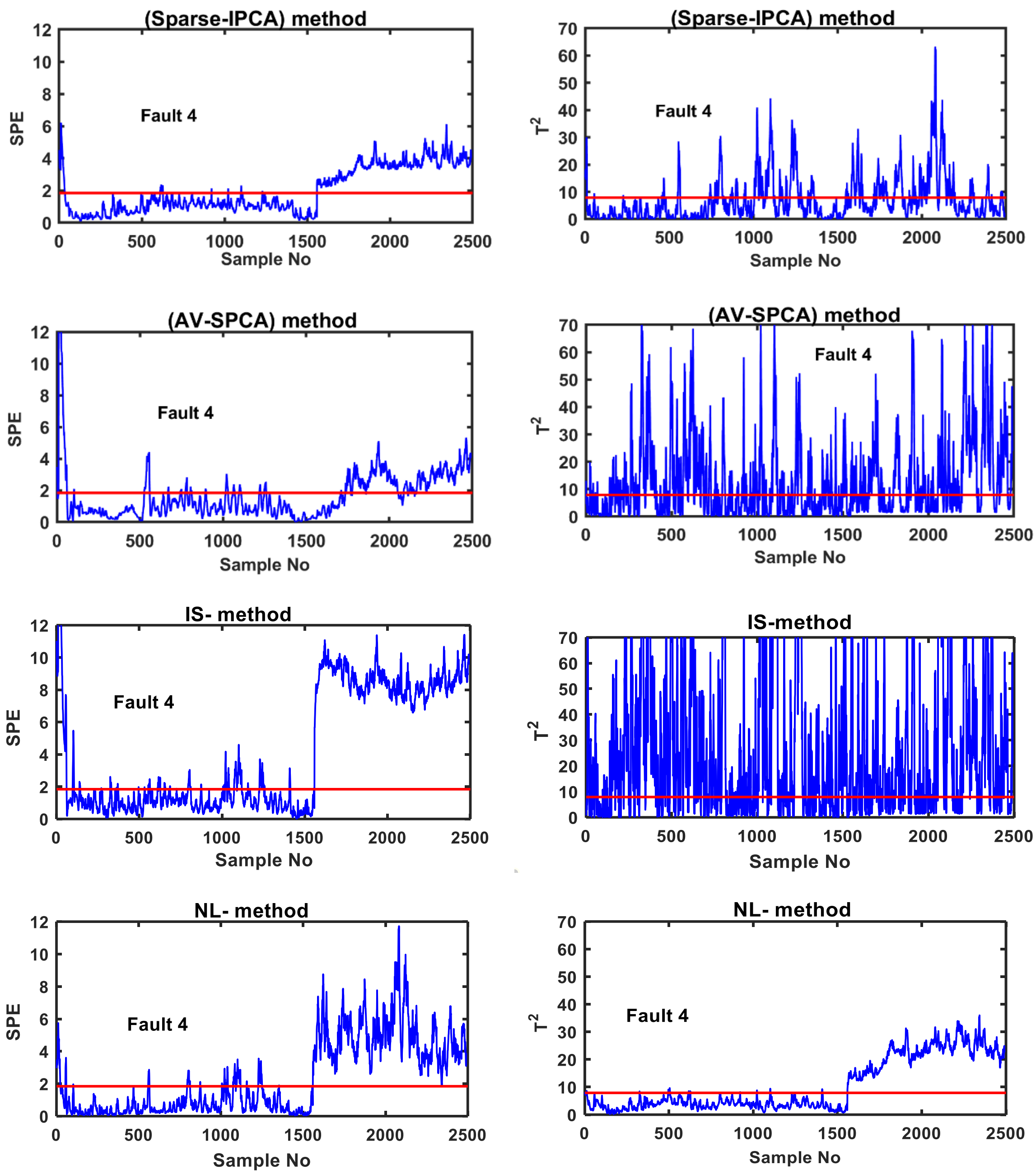


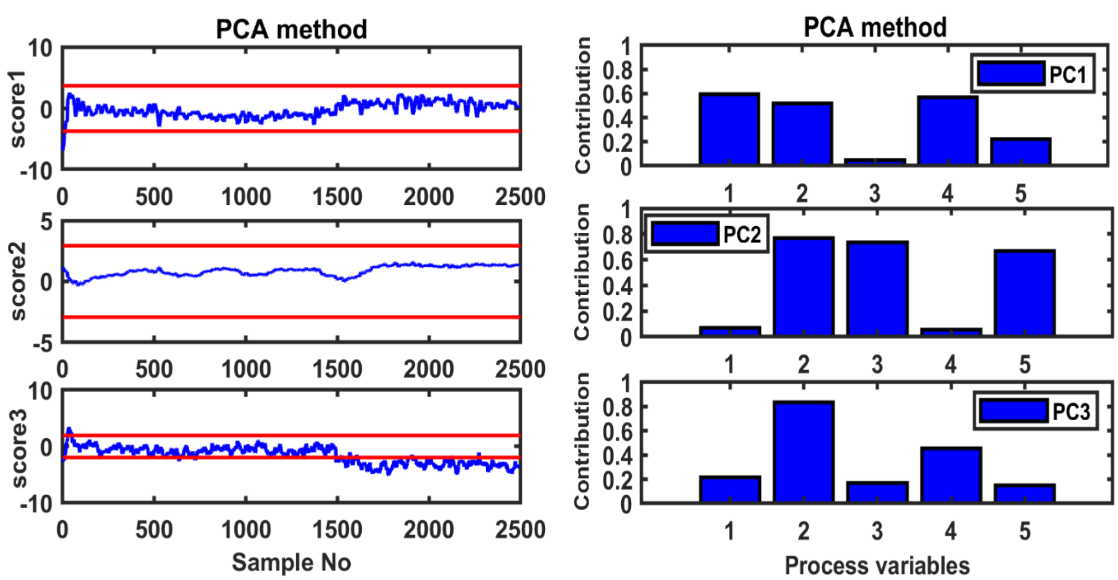
Figure 4. 8 : Monitoring the SPE (left) and T^2(right) results of PCA, Bootstrap-SPCA, Sparse-IPCA, AV-SPCA, IS, and NL methods for detecting Fault 4.

4.5.3. Fault diagnosis

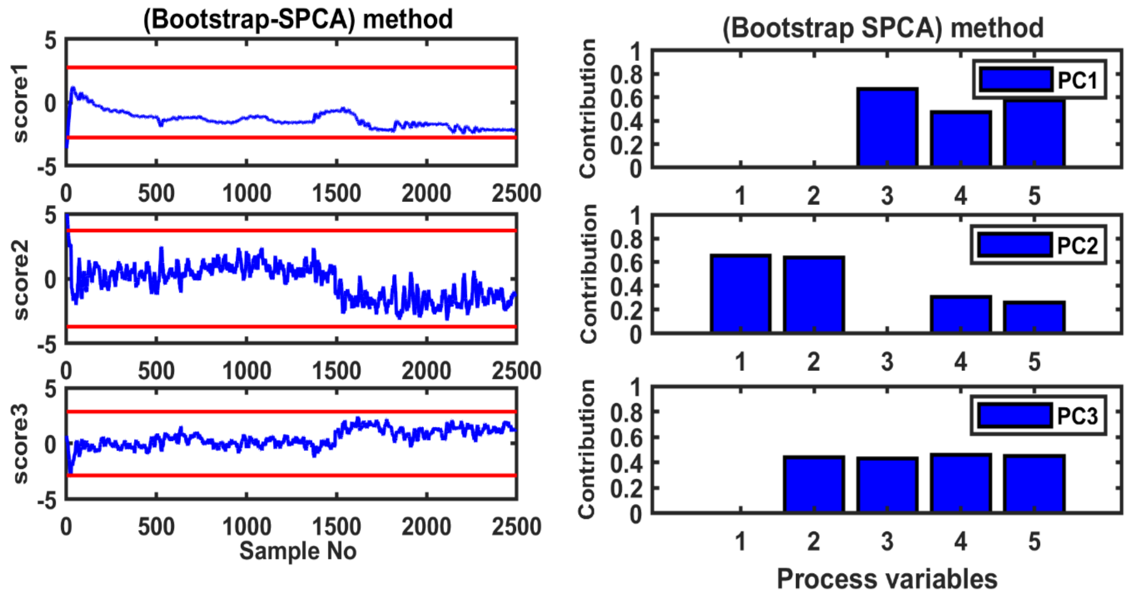
Although a broad range of diagnostic techniques can be applied to improve fault diagnosis performance, fault diagnosis using the limit violation of the PCs is the most relevant with respect to the SPCA method (Jiang et al.,2013). Below we discuss the fault diagnosis performance of the proposed methods using PCs and the *SPE* and T^2contribution plots.

4.5.3.1. Fault diagnosis with PCs

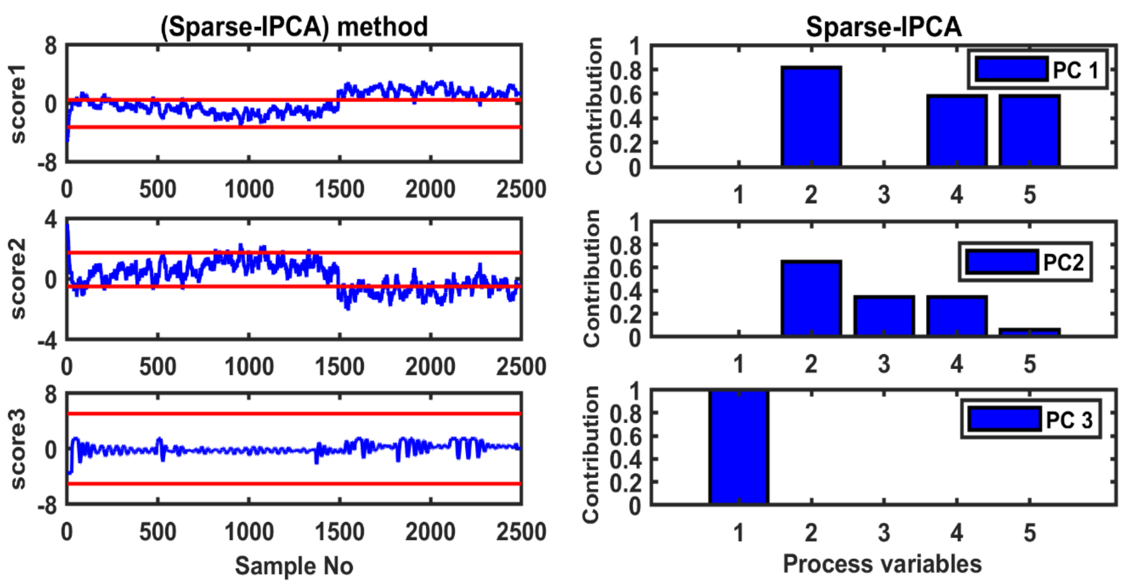
The diagnosis performances of fault 1 (hot water disturbance) for the different methods are compared in Figure 4.9. Hot water flow rate (variable 2) is the root cause of the fault; however, because of its close relation with temperature, we also expect to see deviation in Outlet temperature (variable 5).



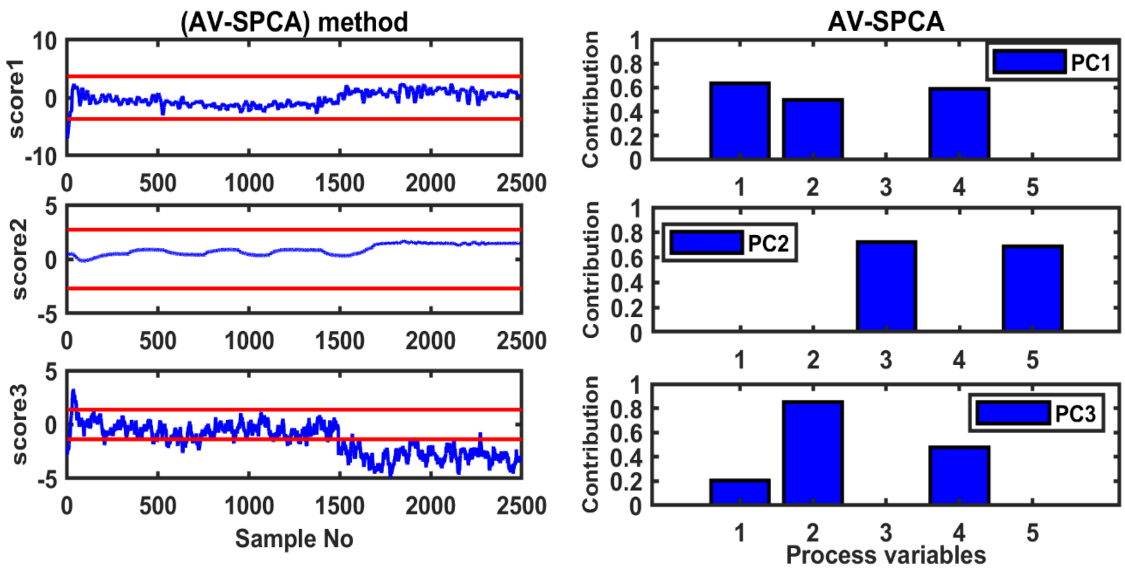
(a)


(Bootstrap-SPCA) method
score1
score2
score3
Sample No
(Bootstrap SPCA) method
PC1
PC2
PC3
Contribution
Process variables

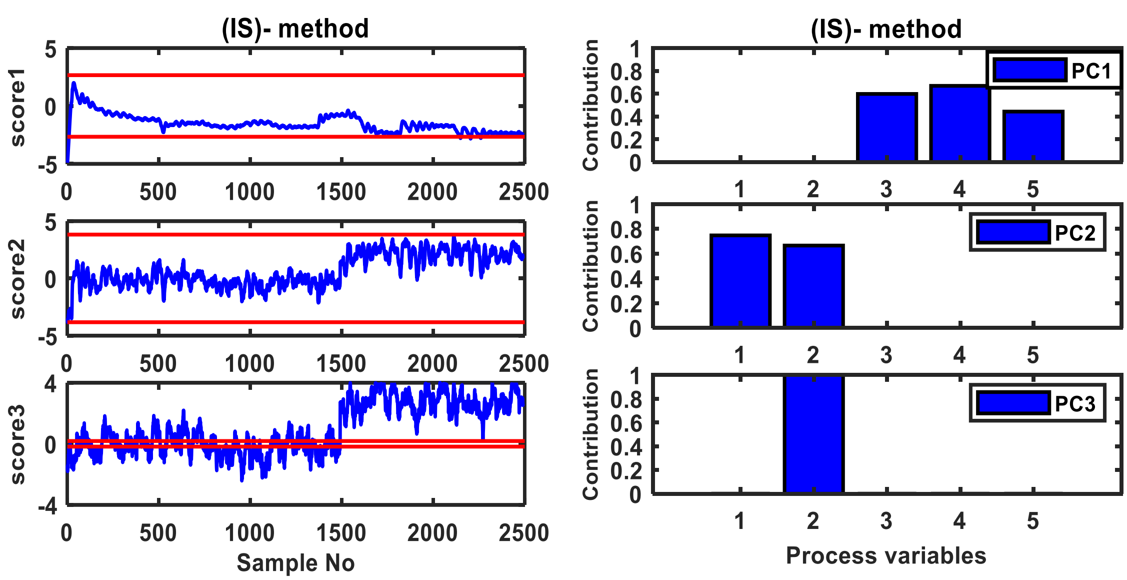
(b)


(Sparse-IPCA) method
score1
score2
score3
Sample No
Sparse-IPCA
PC 1
PC2
PC 3
Contribution
Process variables

(c)


(AV-SPCA) method
score1
score2
score3
Sample No
AV-SPCA
Contribution
PC1
PC2
PC3
Process variables

(d)


(IS)- method
score1
score2
score3
Sample No
(IS)- method
Contribution
PC1
PC2
PC3
Process variables

(e)

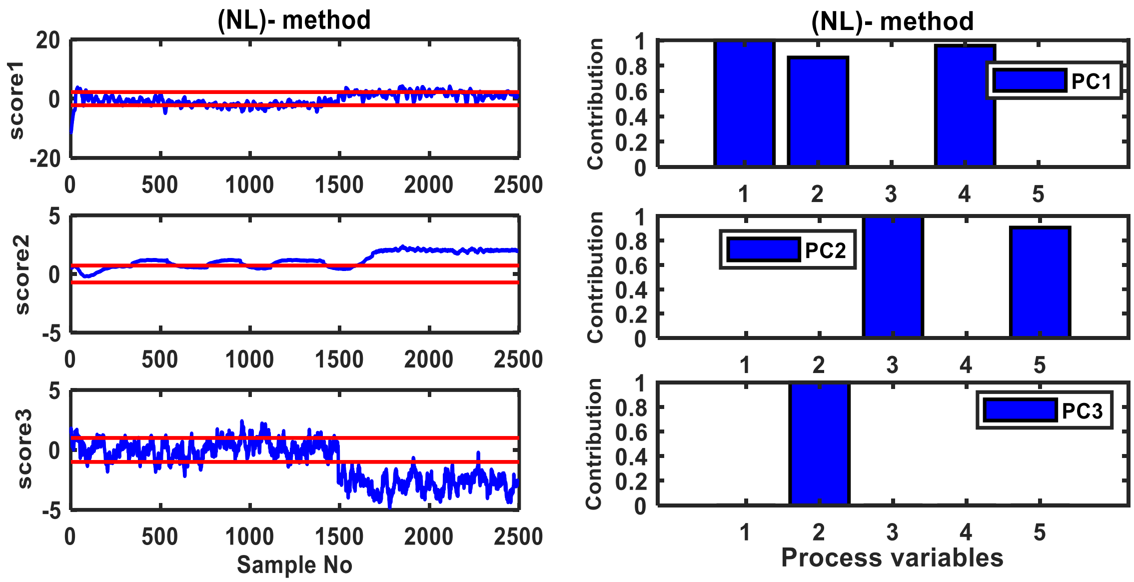


Figure 4. 9 : PC models (score) (left) and contribution plots (right) of Fault 1 assessed using (a) PCA, (b) Bootstrap-SPCA, (c) Sparse-IPCA, (d) AV-SPCA, (e) IS, and (f) NL methods. Note hot water flow rate is denoted by Variable 2.

Figure 4.9 (a) shows that the third PC score breaches the normal operational limits, variable 2 (hot water flow rate) has the maximum contribution in PC3. From this, PCA rightly diagnoses variable 2 (hot water flow rate) as the root cause for Fault 1. Additionally, Figure 4.9 (c) indicates that the first and second scores for the Sparse-IPCA method exceed the threshold, and variable 2 (hot water flow rate) makes the largest contribution in relation to the correct faulty variable. In the case of the AV-SPCA, the third score exceeds the normal limit and variable 2 shows the highest contribution. Additionally, Figure 4.9 (e) and 4.9 (f) depict that the third score of both the IS and NL methods breaching normal operational limits and variable 2 (hot water) shows the highest contribution. However, the IS method can clearly detect the fault, the PC3 styes outside the threshold limits during normal operation. Figure 4.9F shows that both PC2 and PC3 for the NL method detect the fault. To diagnosis the fault, Variable 3 (steam flow rate) and Variable 5 (temperature) have the maximum contribution related to PC2, whereas variable 2 (hot water) shows the maximum contribution in PC3. Therefore, the diagnosis outcomes are not very accurate. The figure also clearly shows the scores of the bootstrap-SPCA method have small deviations for all PCs. However, they do not exceed the threshold.

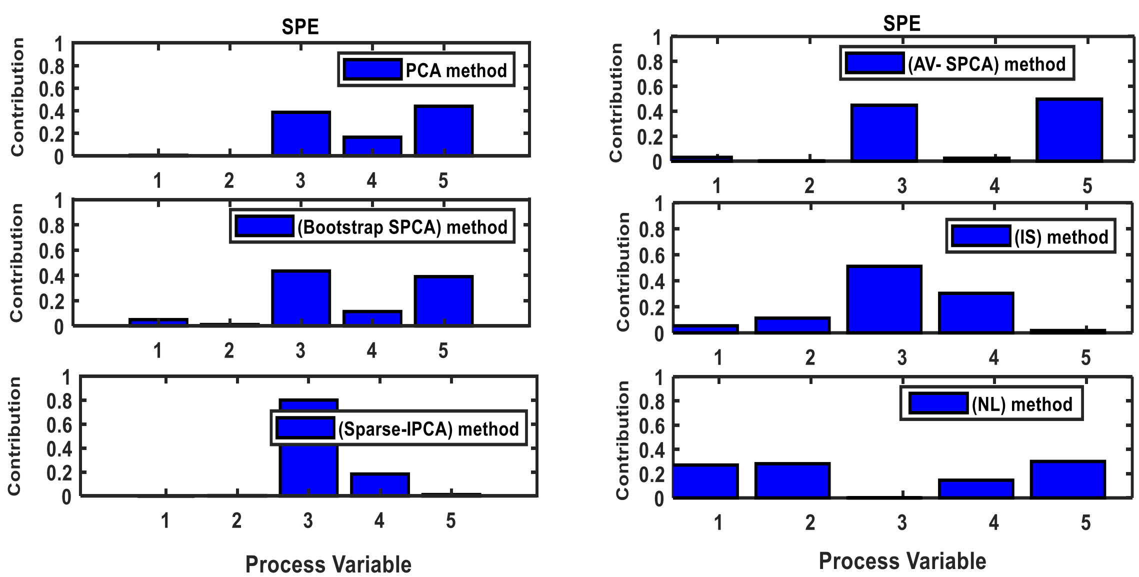
4.5.3.2 Fault diagnosis using contribution plots

In addition to the PCs, T^2 or *SPE* contribution charts are also widely used for fault diagnosis. Following the breach of the T^2 or *SPE* control limits, variable contributions are examined to isolate the variable (or variables) responsible for the deviation. In fact, these variables can offer important information to diagnose the potential root cause of the abnormal behavior. For fault diagnosis, the contribution plots are popular techniques. The contributions of each variable to T^2 and *SPE* statistics are plotted on a bar chart to diagnose the root cause of the fault (Joe,2003; MacGregor and Cinar ,2012; Raich and Cinar,1994).

<u>Fault 3: Steam actuator fault</u>

Figure 4.10 provides a comparative overview of the variables' contributions to T^2 and *SPE* in the PCA and various SPCA methods for faulty samples obtained from the steam actuator fault. The *SPE* contribution plots for the PCA and AV-SPCA methods point to variable 5 (outlet temperature) as the root cause for the fault, as the variable makes the greatest contribution. As can be seen in the figure, variable 2 (hot water flow rate) shows

maximum contributions for T^2 in the PCA and AV-SPCA, NL, and IS approaches. Given the close association of variable 3 (steam flow rate) with outlet temperature and hot water flow, it can be inferred that the steam valve is the root cause. Thus, the PCA and AV-SPCA methods only give an indication of the cause for the fault but do not give a direct diagnosis. For the bootstrap SPCA method, variable 5 (outlet temperature) and variable 3 (steam flow rate) have the most contribution to the SPE and T^2. Also, according to Fig 10, variable 5 (outlet temperature) and variable 3 (steam flow rate) make greatest contributions in T^2 for the NL method. Since between these two variables, steam valve is the cause and outlet temperature is the effect, it gives a more direct indication that variable 3 (steam flow rate) is the root cause. The Sparse-IPCA technique provides the most definitive diagnosis, and variable 3 (steam flow rate) has the most contribution on both T^2 and SPE, which clearly indicates that the steam flow rate is the root cause for Fault 3.



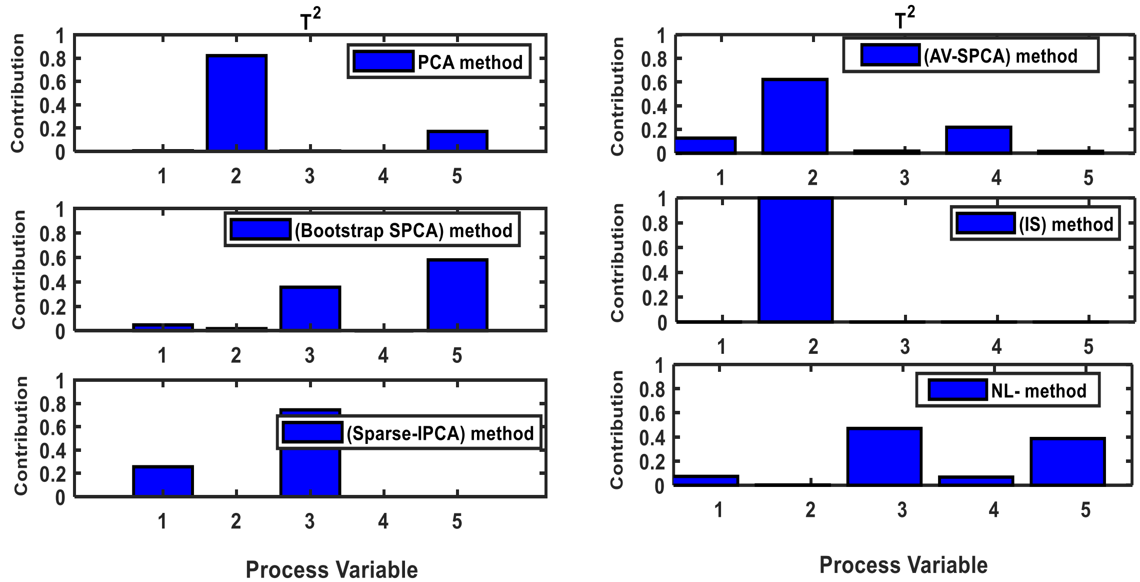


Figure 4. 10 : SPE (upper) and T^2 (lower) contribution plots for PCA, Bootstrap-SPCA, Sparse-IPCA, AV-SPCA, IS, and NL methods for Fault 3.

<u>Fault 4: Level sensor fault</u>

As shown in Figure 4.11, hot water flow rate (Variable 2) appears to make the greatest contribution to T^2 for the conventional PCA, AV-SPCA, and IS methods. The bootstrap-SPCA, Sparse-IPCA, and NL approaches point towards cold water flow rate (variable 1) as the most contributing variable. Combining this information with the *SPE* contribution plots of the bootstrap-SPCA and Spars-IPCA approaches clearly point towards variable 4 (level) as the root cause of the fault. These analyses indicate that the bootstrap-SPCA, Spars-IPCA, and NL strategies are more accurate in determining the underlying cause for Fault 4 than the traditional PCA and AV-SPCA approaches.

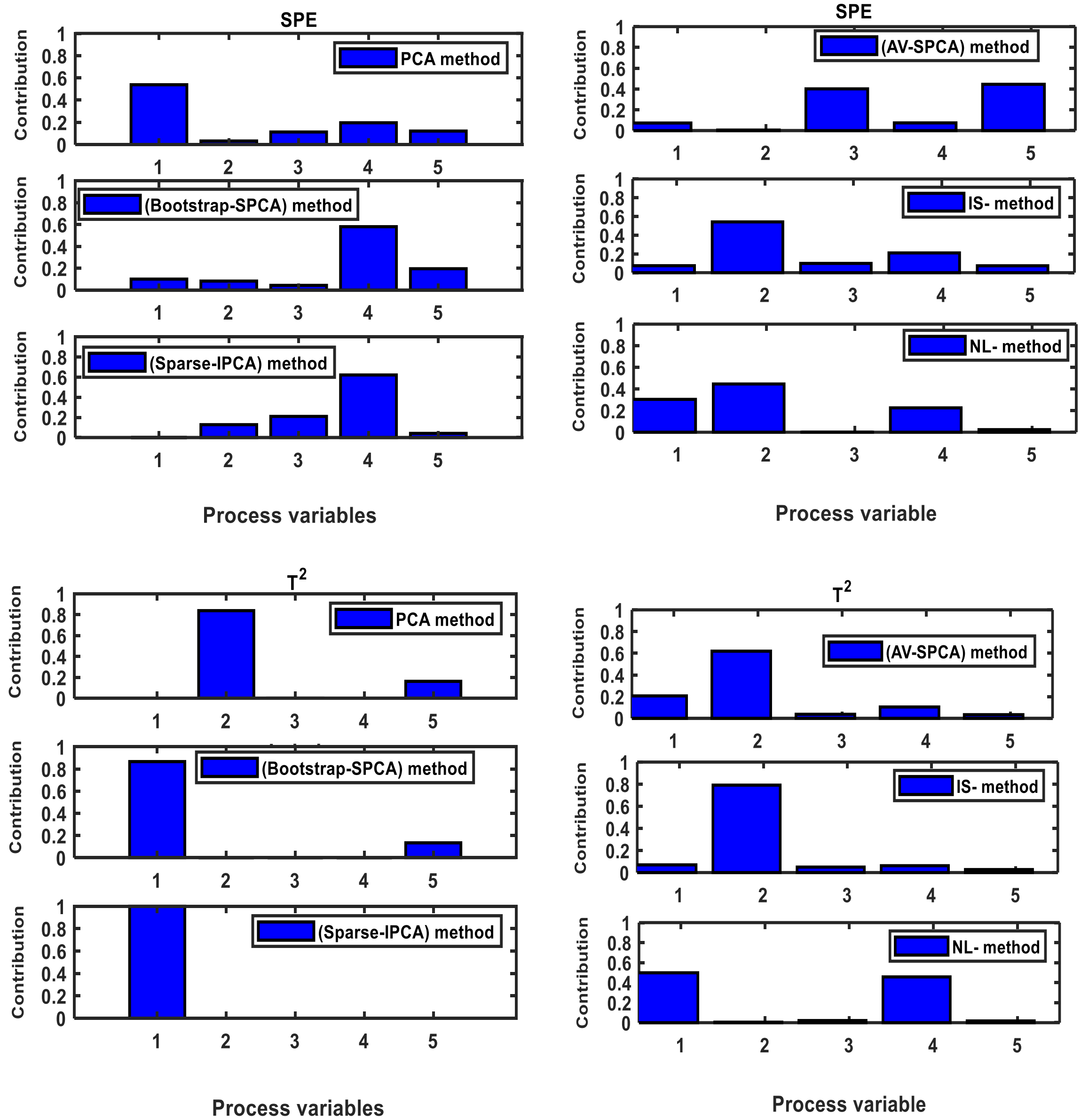


Figure 4. 11 : SPE (upper) and T^2 (lower) contribution plots for PCA, Bootstrap-SPCA, Sparse-IPCA, AV-SPCA, IS, and NL methods for Fault 4.

4.6. Conclusion

Two methods, namely, bootstrap-SPCA and Sparse-IPCA, have been proposed to produce PCs with sparse loadings. The proposed methods were implemented on a benchmark CSTH system. Performances of the proposed methods were compared with the traditional PCA, AV-SPCA, IS, and NL methods. The main contributions of the work are as follows:

- Using resampling and the measurement error covariance matrix, the distributions of the loading elements were obtained. The distributions of the loading elements give more complete information about the loadings, and clearly show the elements which should be set to “0”.
- The proposed methods showed better fault detection performance compared to the conventional PCA and AV-SPCA method. Both quantitative and qualitative results showed the proposed methods delivered better fault detection with a lower false alarm.
- The diagnostic performances of the proposed methods were similar or better when the T^2 and *SPE* contribution plots were used. The diagnosis performance of the Sparse-IPCA method was especially precise and pointed towards the root cause variable.
- The computational costs of the proposed methods were higher, especially for the Sparse-IPCA method, compared to PCA or other SPCA methods. However, these computations are done in an off-line manner; therefore, they do not limit the application of the proposed methods.

- In case of Sparse-IPCA, an inherent assumption is that the noise has a Gaussian distribution. On the other hand, the bootstrap method is a purely simulation based method, it does not require any such assumption. The Sparse-IPCA method uses the maximum likelihood estimation (MLE) to estimate the error covariance matrix. The log-likelihood function may become ill-conditioned especially for large data sets. There is possibility that the method may not converge if the size of the error covariance matrix (i.e., number of variables) is large.

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Chapter 5

Detection and diagnosis of process fault using unsupervised learning methods and unlabeled data

Abstract: Multivariate statistical analysis approaches are commonly applied for process fault detection and diagnosis. More recently, supervised learning methods are being used for process monitoring. Supervised learning methods require a labelled historical dataset for both normal and abnormal operations, which demands significant effort in data mining. To overcome this difficulty, we propose a methodology combining principal component analysis (PCA) with the k-means clustering algorithm. The k-means algorithm is used for fault detection and diagnosis by exploiting PCA for data mining. Based on the Euclidean distance between each dataset and cluster centroid of the training data, the k-means clustering algorithm is able to decide if the process is in a normal state or belongs to a particular faulty state. To illustrate the effectiveness of the methodology, the proposed method is applied to two industrial processes: (i) a separator unit from an offshore gas processing platform, and (ii) a distillation column of a crude refining unit. The results show that the proposed method is able to avoid the data labelling exercise and is effective in detecting and diagnosing large-scale industrial processes.

Key words: Principal Component Analysis (PCA), fault detection and diagnosis (FDD), k-means clustering algorithm.

5.1. Introduction

Chemical processes are increasing in scale and complexity, leading to a surge in data-driven applications for detection and diagnosis of process faults. In recent years, significant improvements have been made on the algorithm side that have vastly improved monitoring performance simply through exploring information contained within existing measurements. Advanced methods that use early detection features could signal issues as they emerge, thus preventing damage to the system (Bakdi & Kouadri, 2017). A key aspect in data-driven approaches is their ease of implementation across different applications, as the majority of these methods use historical data for deriving mapping relationships between fault modes and fault features. Nonetheless, in fault detection and diagnosis techniques, performance is mostly determined by the quality of the training data (Yin et al., 2012).

Among the data-driven methods, Fisher discriminant analysis (FDA), partial least squares (PLS), principal component analysis (PCA), and independent component analysis (ICA) are widely used in process industries (Huang & Yan, 2015; Chiang et al., 2000). (Pearson, 1901) proposed the PCA method, which (Hotelling, 1993) later developed as a linear optimal dimensionality reduction strategy. In industrial process monitoring, PCA is the most commonly applied FDD method (Kourti & McGregor, 1996). More recently artificial neural network (ANN), support vector machine (SVM), and other machine learning algorithms are being used for fault detection and diagnosis.

One of the primary limitations of these supervised methods, however, is that they require large training datasets containing both normal and abnormal data from various faulty conditions. Process data are large in size and usually unlabelled in the data historian, making it difficult to find suitable training datasets for supervised learning methods and thus ultimately limiting the utility of these methods. The main goal of the current study is to explore how unsupervised methods, especially clustering algorithms, can be used to overcome the data labelling problem and be applied to fault detection and diagnosis.

Cluster analysis (CA) is a data partitioning strategy that is commonly utilized in data mining. In CA, a data sample set is divided such that the samples in one group (cluster) share more similarities with each other in comparison with other groups (clusters) (Li & Hu, 2018). By using CA, the primary operating variables that directly impact a system may be grouped or classified. As mentioned previously, CA is a statistics-driven strategy for analyzing big complex data that include a wide range of interrelated variables. CA assigns variable sets or groups that share similar features as a cluster, thus enabling more accurate dataset behavior representation. After a data cluster featuring similar characteristics has been identified, multivariate analysis may be used to exploit the correlation between the variables for fault detection and diagnosis. (Sebzalli & Wang, 2001) used PCA for dimension reduction, discovering the operational zones of a fluid catalytic cracking (FCC) operation. Subsequently, they employed a fuzzy c-means algorithm to validate the clusters obtained from PCA and locate the cluster centers. In another study, PCA and clustering were used to classify dynamic system data into different states and modes of operations. The data dimension was first reduced using PCA, after which a clustering algorithm was applied to the scores to determine the states and modes. The operational state of the system (i.e., steady state vs transition state) was determined using a heuristic rule called dwelling time. According to this rule, if the system stays in a state longer than the dwelling time, the system is considered to be at steady state. After discerning between steady state and transition state, the system data were further segmented into different modes of operation. The method was validated using an FCC unit as well as Tennessee Eastman process simulations (Srinivasan et al., 2004).

(Imtiaz et al., 2006) used a clustering algorithm to discover the operational zones of datasets from a pulp and paper mill, which is characterized by multiple grades of products and frequent change- over between products. The clustering algorithm validated that a key operating parameter (i.e., basis weight) was a good indicator to classify the data into different operational zones. Subsequently, PCA models were developed for each cluster and the sub-PCAs were used for detection and diagnosis of sheet-break faults in the mill. A few years later, (Lam et al., 2008; 2009) used PCA and clustering to classify calendar days based on similarities in weather parameters. Regression models were then developed to predict chiller system power consumption from the climate data. In related work, (Li & Hu, 2018) presented a fault detection, diagnosis, and estimation (FDD&E) strategy that paired PCA with density-based clustering. Density-Based Spatial Clustering of Applications with Noise (DBSCAN) can automatically classify operation data into clusters and recognize the corresponding operation conditions. In the study, using sub-PCA models rather than a single PCA model to describe normal operational conditions enhanced both the reliability and sensitivity of the fault detection and diagnosis efforts. It also improved the accuracy of the sensor fault estimation. The researchers validated the novel approach by utilizing field operation data from a screw chiller plant applied to different sensor faults of various magnitudes. The outcome showed improved sensor FDD&E compared to conventional PCA-based sensor FDD&E with a single PCA model. (Du et al., 2017) conducted a test on a refrigeration compressor system by categorizing the test data as clusters and then developing PCA models for each cluster to enable sensor fault detection. Their test results showed significant increases in sensor fault detection in sub-PCA models. (Zanoli et al., 2010) proposed a fault detection and isolation strategy by using PCA and clustering methods along with pattern recognition analysis. The developed methodology was applied to data from an oil refinery's Integrated Gasification & Combined Cycle section to track the compression process.

More recently, the k-nearest neighbor (kNN) approach was successfully applied for fault detection. (He et al., 2010) proposed a PC-kNN method that charts the original data on a PC subspace, after which the kNN rule was added into the score matrix in building a fault detection model. This strategy resulted in a significant reduction in time and storage space.

(Guo et al., 2014) introduced a method for process-monitoring called the FS-kNN technique. FS-kNN works by projecting data samples into a feature space, after which principal components and squared prediction error (*SPE*) can be extracted as indicators from the space. These feature indicators are able to better capture information pertaining to raw data, making FS-kNN's detection accuracy greater than PC-kNN's performance.

The above literature review indicates that PCA and clustering algorithms have been combined mainly for data mining purposes in order to delineate the mode of operations.

More specifically, the actual online detection and diagnosis of faults was done by PCA, while clustering was used primarily for segmenting the data into different operational modes and improving the performance of the PCA model. However, we believe that a clustering algorithm has much more to offer and can in fact be used by itself as an online fault detection and diagnosis tool. Based on this assumption, we combine the k-means clustering algorithm with PCA in this study, using PCA to train the k-means clustering algorithm from unlabelled data. In this way, the k-means clustering algorithm can be effectively used for online fault detection and diagnosis.

5.2. Methodology

In the proposed method, we combine two unsupervised methods (PCA and k-means clustering) to build a robust method that is capable of precise diagnosis of faults. The combination of PCA with k-means overcomes the need for labelled data. In the following sections, the PCA and k-means methods are first reviewed, followed by a presentation of the proposed fault detection and diagnosis method.

5.2.1. Principal component analysis (PCA)

PCA is among the most popular methods for extracting information from raw measured data. It can handle high-dimensional data by projecting them onto a lower dimensional subspace that contains most of the variance of the original data. For this task, PCA searches for an optimal linear transformation of the original data matrix $X \in R^{n \times m}$, where *n* is the number of observations and *m* refers to a set of uncorrelated variables called principal components (PCs). The principal components are: $(\mathrm{T}_{\mathrm{n}\times\mathrm{m}}) = [\mathrm{t}_1\ \mathrm{t}_2 \ldots\ldots \mathrm{t}_\mathrm{m}]$

where

$$T = XP \tag{5.1}$$

The loading vectors $P_{m\times m} = [P_1 P_2 \ldots\ldots P_m]$ are then obtained by applying singular value decomposition (SVD) (Yin et al., 2012; Bakshi, 1998).

5.2.2. Clustering (K-means technique)

The main purpose for developing the data clustering algorithm is grouping datasets into clusters according to similarities (i.e., datasets in each cluster share a high degree of similarity). Here, a k-means clustering algorithm is used, with the centroid of the cluster being the mean value of each cluster's dataset. In this regard, the k-means algorithm reflects an iterative process, whereby datasets are designated as belonging to clusters that have the most similar centroid, as shown in Figure 1. This is determined by measuring the Euclidean distance between the datasets and their corresponding cluster centroids (Li & Ju, 2017; Sebzalli & Wang, 2001; Zhang et al., 2019).

The steps of the k-means algorithm are briefly summarized as:

- Identify the number of clusters (k).
- Choose random observations from the dataset as initial cluster centroids (CC).
- Designate each observation to their closest centroid based on the Euclidean distance measure, as shown in the following equation:

$$d(X, CC) = (X - CC)(X - CC)^T \tag{5.2}$$

Where CC is the cluster centroid

- Compute the new mean values of all the data points in the cluster to update the cluster centroid (CC) for each of the k clusters.
- Repeat steps 3 and 4 iteratively until the clusters created in the present iteration are similar to the past iteration.
- Obtain the column vector called $(idx)_{nx1}$ that has the same rows of $X \in R^{n\times m}$. Note that each element in $(idx)_{nx1}$ shows the cluster number.
- Keep the cluster centroid (CC) and the Euclidean distance ranges to calculate the distance between the testing dataset and the predefined cluster centroid (CC).
- Obtain the (*idx_ test*) vector that contains the cluster indices of each observation in new *X* for comparison purposes.

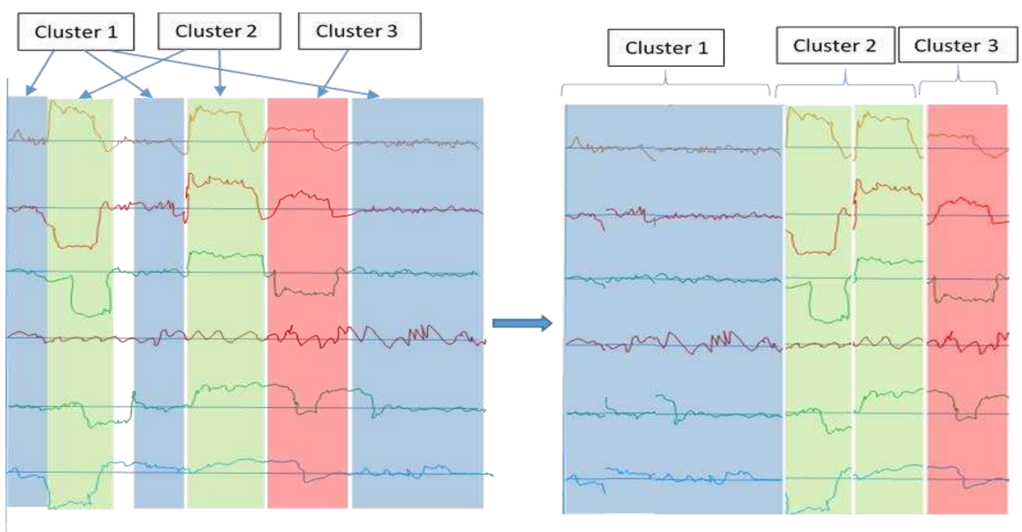


Figure 5. 1: Dataset classification for different clusters.

5.2.3. Fault detection based on clustering and PCA algorithm

The current study presents a novel fault detection and diagnosis method that uses PCA in combination with a k-means clustering algorithm. Although PCA is widely used for process monitoring, it often does not perform well in online scenarios diagnosing faults. In this algorithm, we combine the k-means clustering algorithm to improve the diagnostic ability of PCA. Figure 5.2 illustrates the proposed framework. As can be seen in the figure, the matrix $X\ (n \times m)$ indicates the training data matrix, showing n samples of m variables. The data matrix is obtained from a process data historian without any labelling. This data matrix will contain both normal data as well as faulty data arising from different types of faults. However, in any given process, a single fault may occur multiple times at different intervals in the system. Once the training dataset has been normalized, the k-means clustering algorithm can be used to categorize data samples as clusters (e.g., Cluster 1, Cluster 5). After clustering, the datasets belonging to the same cluster are concatenated to create a rich data repository. The calculation also provides the Euclidean distance of the datasets and their cluster centroids. The $(idx)_{nx1}$ implements k-means clustering to divide the observations of the matrix $X\ (n \times m)$ into k clusters. The $idx_{(nx1)}$ is a vector that includes cluster indices of each observation.

Parallel to the clustering exercise, the normalized data are used to train the PCA model. Singular value decomposition is applied to the dataset to determine the system's loading. Two fault detection metrics, e.g., squared prediction error (*SPE*) or Hotelling's T^2, are applied as aids to interpret operational conditions (i.e., normal or abnormal). In every *SPE* and T^2 group sample, datasets with larger values in relation to the corresponding control limit are deemed faulty, while those below the control limit are deemed fault-free. The normal datasets may then be used to build a PCA model.

In the following step, in each abnormal case that contains faulty data for both T2 and SPE, one or more cluster is related to the faulty data. To identify which cluster has the highest percentage in this specific faulty period, the faulty data sampling times of T2 and *SPE* need to be compared to the $(idx)_{nx1}$ vector. The datasets marked as faulty are further investigated using contribution plots to determine the cause of the fault and label it accordingly.

The centroids of clusters and the Euclidean distance ranges calculated from the training data are supplied to the online monitoring scheme for detecting and diagnosing the online faults. For the online monitoring process, the collected data are normalized in accordance with the initial step mentioned earlier. The test dataset is categorized by applying the distances between the CC point obtained from the training datasets and those in the monitoring dataset. These distances are used to determine the clusters to which the new data samples belong. Once the cluster identity has been determined, the offline mapping information (i.e., from the clusters to the faults and then to the root cause) is used to map and assign the root cause for the fault.

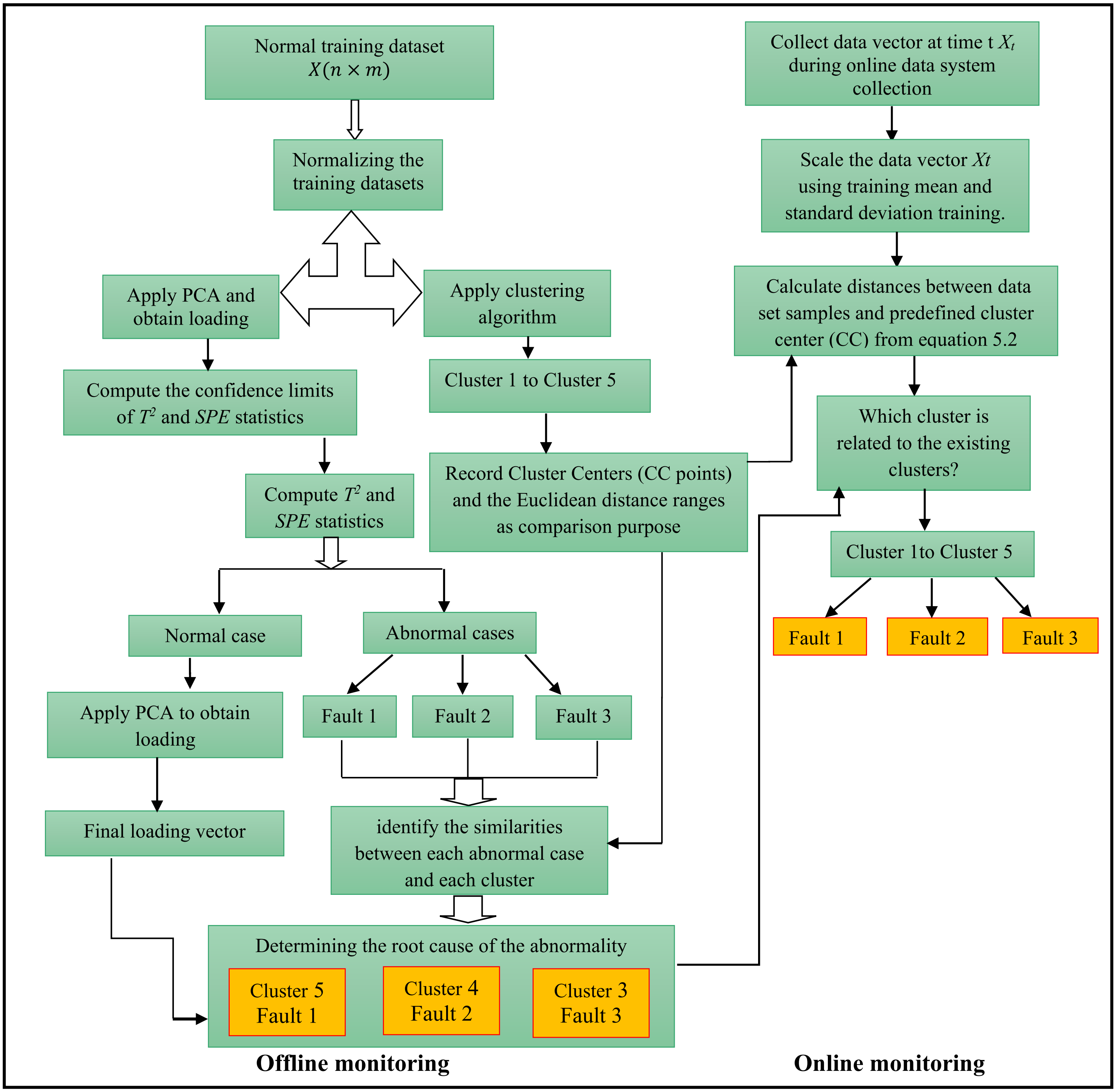


Figure 5. 2 : Flow chart of the proposed process-monitoring approach.

5.3. Case Studies

The proposed method was implemented on two case studies. The first one is a simulated separation unit of an offshore gas processing plant, and the second is an industrial case study. The methodology was tested on a dataset collected from a distillation unit of a petroleum refining operation.

5.3.1. Separator Unit of an Offshore Gas Processing Platform

A dynamic HYSYS model of a gas processing plant is available from Khaled et al. (2020). The model is based on the gas processing plant in the North Sea described in Voldsund et al.'s (2013) work. As shown in Figure 5.3, the process can be divided into the following eight main components: well section, separator unit, production manifold, export pump unit, fuel gas treatment, recompression unit, reinjection unit, and drainage system. The separation unit (Figure 5.4) features an electrostatic coalescer (V-102), along with a two-phase separator (V-114) and two three-phase separators (V-100, V-101). Gravitational separation is used to separate the water, oil and gas, with the pressure decreased at each separation stage in order to optimize production output. Specifically, the separated (oily) water that results from the first and second stages proceeds to the water treatment processing unit, but a portion of this fluid is recycled back to the second stage (three-phase separator). In this study, the simulation data generated by Khaled et al. (2020) is used for the FDD performance evaluation of the proposed method. The simulated model has 39 variables. Table 5.1 provides more details of the different types of faults (i.e., two disturbance faults and one actuator fault) that were investigated in the present study.

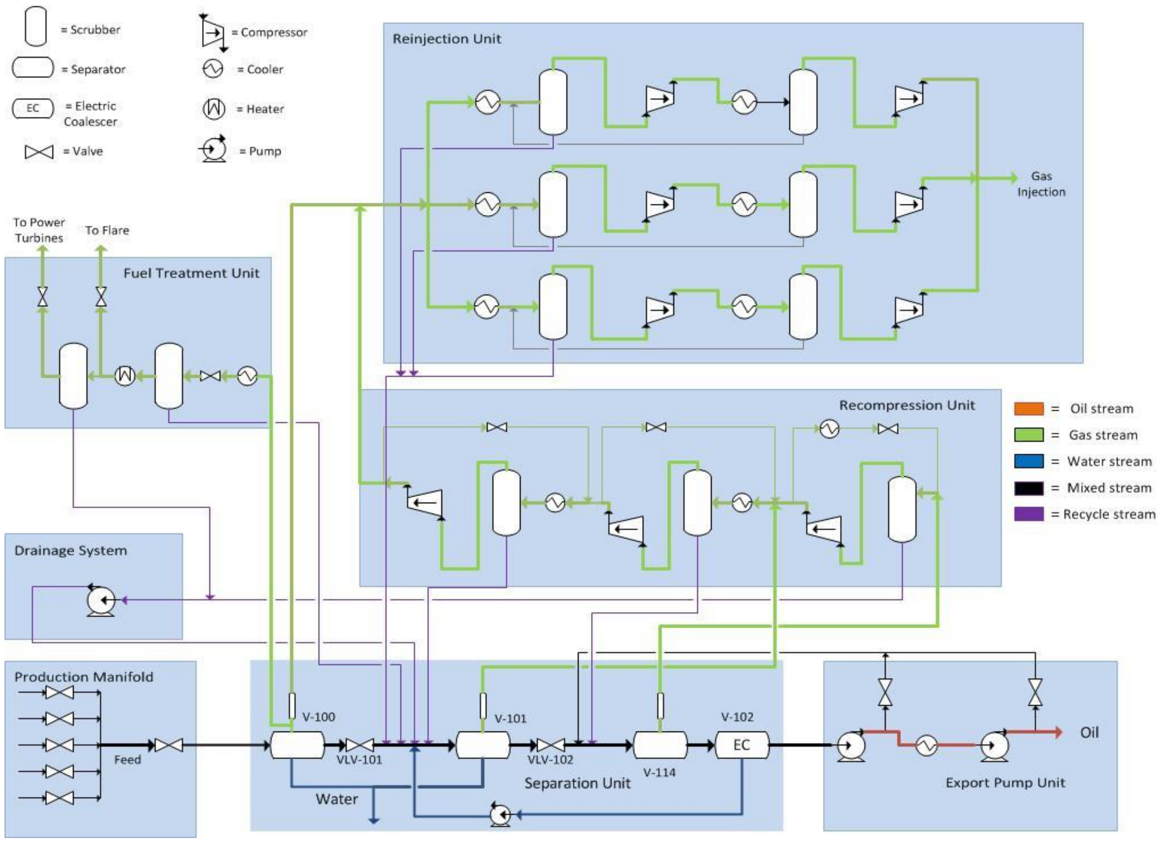


Figure 5. 3: Process flow diagram of Norwegian Sea oil and gas platform with modifications.

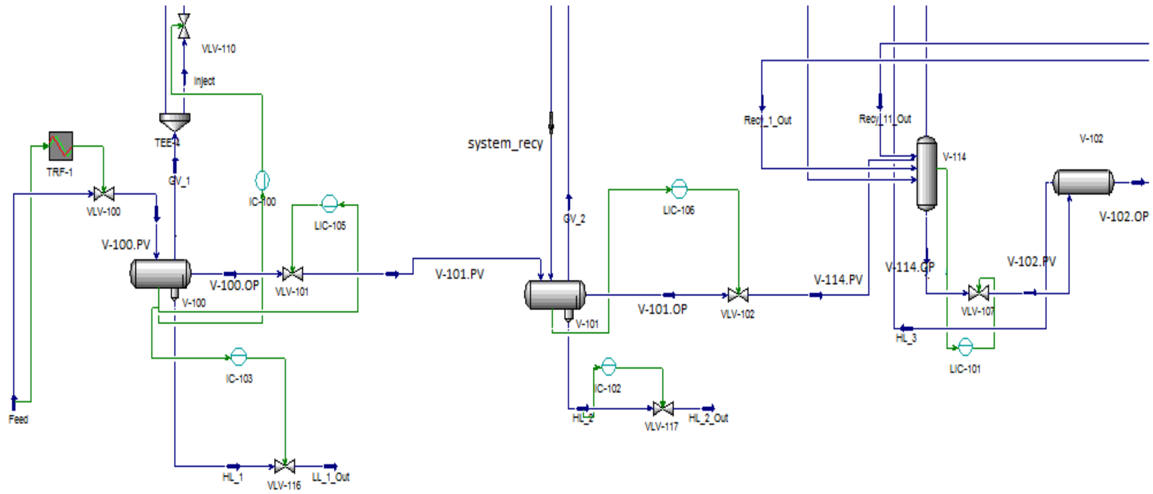


Figure 5. 4 : Separator unit of Norwegian Sea oil and gas platform

Table 5. 1**:** Summary of three different types of faults

Fault Number	Fault Type and Location	Fault Description
Fault 1	Disturbance Fault (High feed flow rate V-100.PV)	Feed flow emerging from five neighboring wells increases approximately 20% over the initial rated condition (2.45×10^5 Sm^3/h).
Fault 2	Disturbance Fault (High feed temperature T-100.PV)	Feed temperature rises approximately 3.6% over the initial rated temperature of 83 ˚C.
Fault 3	Actuator Fault (Fail hold VLV-102)	There is no reaction by a valve to either signal or power loss and the valve stays at the same position. The result is usually a fail hold condition.

5.3.2. Distillation column process

Removing lighter material from the reaction products is one of the main operations in the crude unit of a petroleum refinery. In this case study, eight months of operational data were collected from the distillation unit. Five months are selected as the training dataset, while the remaining three months are adopted as testing dataset.

In this study, 32 process variables are considered for the process-monitoring exercise. Due to confidentiality, we cannot provide the process flow diagram of the actual unit. The main components of the unit are the column, condenser, and reboiler. Additionally, a range of heat exchangers is used to recover heat from the feed and produce stream. A list of variables collected from the unit is provided in Table 5.2.

Table 5.2: Operating variables of distillation column Process

Variable No.	Variable Name	Description
1	XMEAS1	Overhead Liquid Flowrate
2	XMEAS2	Overhead Liquid to Light Ends
3	XMEAS3	Low Pressure Separator Level
4	XMEAS4	Distillation Overhead Temperature
5	XMEAS5	Low Pressure Separator Outlet Flow 1
6	XMEAS6	Low Pressure Separator Outlet Flow 2
7	XMEAS7	Distillation Overhead Receiver Level
8	XMEAS8	Distillation Waterboot level
9	XMEAS9	Fractionation Recycle Liquid Flow
10	XMEAS10	Circulation Kerosene Flow
11	XMEAS11	Circulation Diesel Flow
12	XMEAS12	Distillation Reflux Flow
13	XMEAS13	Distillation Tower Pressure
14	XMEAS14	Distillation Bottom Level
15	XMEAS15	Distillation Reboiler Cell 1 flow
16	XMEAS16	Reboiler Cell 1 flow Pass 1
17	XMEAS17	Reboiler Cell 1 flow Pass 2
18	XMEAS18	Reboiler Cell 1 flow Pass 3
19	XMEAS19	Reboiler Cell 1 flow Pass 4
20	XMEAS20	Fuel Oil Pressure to Reboiler Cell 1
21	XMEAS21	Reboiler Cell 1 Steam Pressure
22	XMEAS22	Reboiler Cell 1 Temperature
23	XMEAS23	Reboiler Average Temperature
24	XMEAS24	Fuel Gas Pressure to Reboiler Cell 1
25	XMEAS25	Fuel Gas Pressure to Reboiler Cell 2

26	XMEAS26	Reboiler Cell 2 Temperature
27	XMEAS27	Reboiler Cell 2 Steam Pressure
28	XMEAS28	Distillation Reboiler cell 2 flow
29	XMEAS29	Reboiler Cell 2 flow Pass 2
30	XMEAS30	Reboiler Cell 2 flow Pass 3
31	XMEAS31	Reboiler Cell 2 flow Pass 4
32	XMEAS32	Reboiler Cell 2 Fuel Oil Pressure

5.4. Results and Discussion

In this section we describe the performance of the developed FDD method on the two case studies described earlier. To evaluate the performance we mainly focus on the fault diagnosis ability of the proposed method. First we describe the results of the separator unit of the offshore gas process plant, next we demonstrate the efficacy of the method on a distillation column of a petroleum refining crude unit.

5.4.1. Separation Unit of Offshore Gas Processing Plant

5.4.1.1 Off-line Training of Model for Separation Unit

The gas processing plant has 39 variables measured throughout the separator unit. The simulation data includes normal condition and four different faulty conditions. A PCA model was built where the first six PCs cumulatively explained 85% of the total variance. Hotelling's T^2 and *SPE* charts were applied for fault detection.

Figure 5.5 depicts Hotelling's T^2 and *SPE* statistics. Assuming no prior knowledge of a fault, the T^2 statistics chart in Figure 5.5 is used to select different segments of faulty datasets. We mark these as Fault - a, Fault - b, and Fault - c.

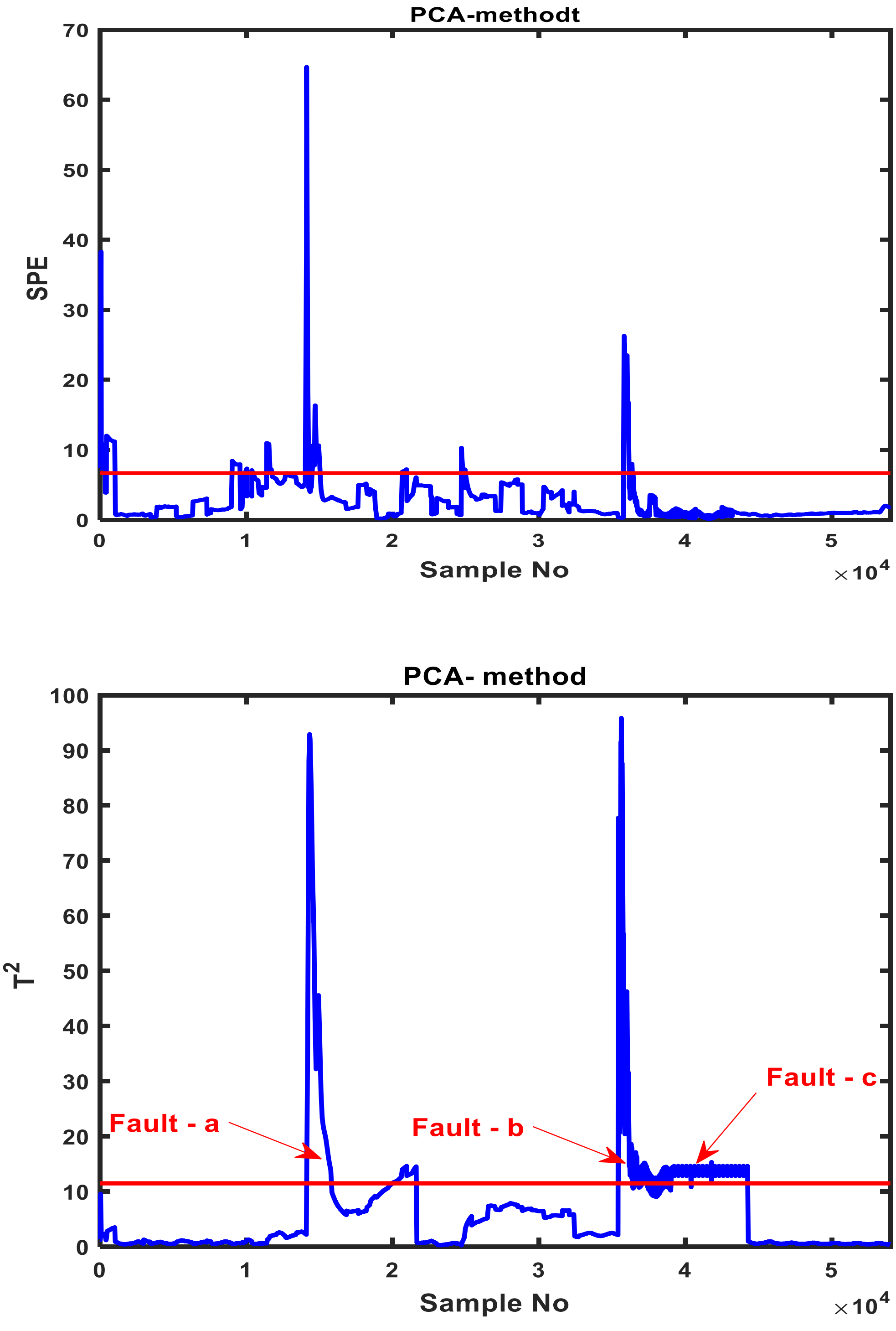


Figure 5. 5: Fault detection monitoring results of separator unit of offshore gas processing platform to PCA *SPE* (upper) and T^2(lower).

The same dataset is also run through the clustering algorithm. From the clustering analysis, five clusters were obtained, as illustrated in Figure 5.6.

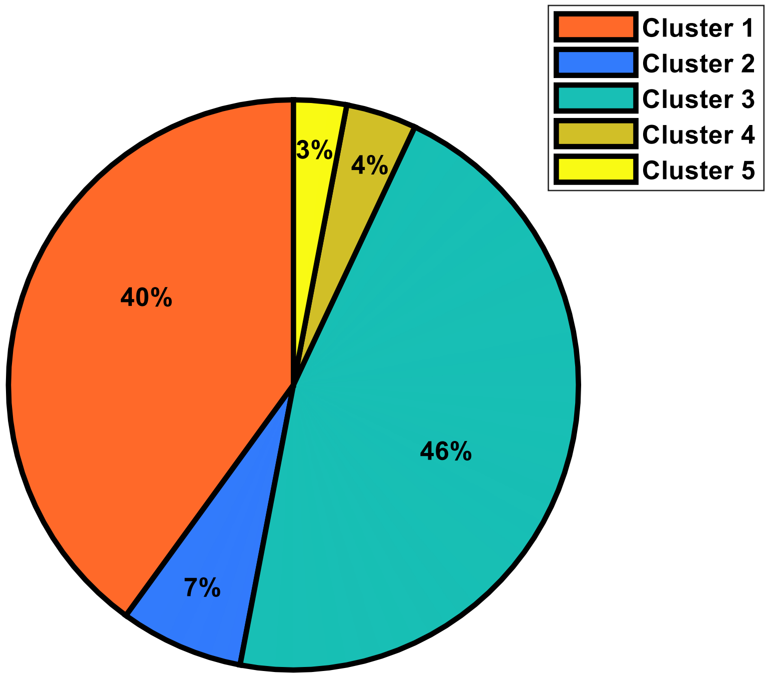


Figure 5. 6: Five clustering results of separator unit of offshore gas processing platform.

Cluster 3 has the maximum percentage of samples (46%), while 40% belongs to Cluster 1, 7% to Cluster 2, 4% to Cluster 4, and 3% to Cluster 5.

Mapping of separator data clusters to fault

In order to map the clusters to the fault conditions, the similarities between the faults and the clusters need to be calculated. In finding the similarity between each faulty dataset and the cluster, the $(idx)_{nx1}$ that contains cluster indices for each observation is used for each fault. Based on the *SPE* statistics in Figure 5.5, comparing the observation of each fault with the $(idx)_{nx1}$ is the main criteria. For example, Figure 5.7 shows the percentages of the clusters (i.e., Cluster 1 to Cluster 5) that matches with different faults (Fault - a, Fault - b, and Fault - c). As illustrated in Figure 5.7 (a), for Fault - a, Cluster 2 has the maximum similarity (80%), while 17% belongs to Cluster 4 and about 3% to Cluster 5. Thus, Cluster 2 is related to Fault - a.

Similarly, for Fault - b, Figure 5.7 (b) shows that Cluster 1 matches with 91 % of the samples, and that 9% of the samples belong to Cluster 3. In addition, Figure 5.7 (c) shows that most faulty samples are related to Cluster 3 (93%). It can therefore be concluded that Cluster 2, Cluster 1, and Cluster 3 represent three main faulty operation conditions as Fault - a, Fault - b, and Fault - c, respectively.

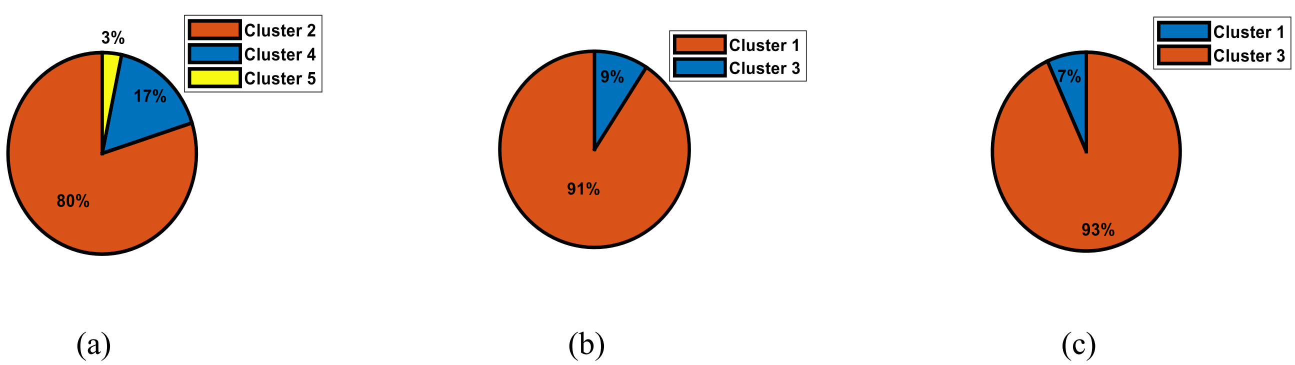


Figure 5. 7: Percentages of faulty samples for Fault - a, Fault - b, and fault - c for Cluster 1, Cluster 2, Cluster 3, Cluster 4, and Cluster 5.

Mapping of separator faults to root cause

After the clusters are mapped to the fault, the root cause of the faults is identified in the next stage. This will complete the mapping of the clusters to the root cause. Figure 5.8 shows the contributions of the variables to the *SPE* for Fault - a. The *SPE* contribution plots point to variables 3 and 39 (temperature) as being the variables that make the greatest contribution, thus identifying those variables as the root causes of Fault - a. In this case, the feed (TRF-1.PV) temperature (variable 3) is increased from 82 ˚C to 86 ˚C and the produced oil flow rate (variable 37) decreased. However, the temperature of the produced oil (V-102.OP) (variable 39) only slightly increased. The pressures (variables 2 and 38) for the above two sections are not affected by increasing the feed temperature.

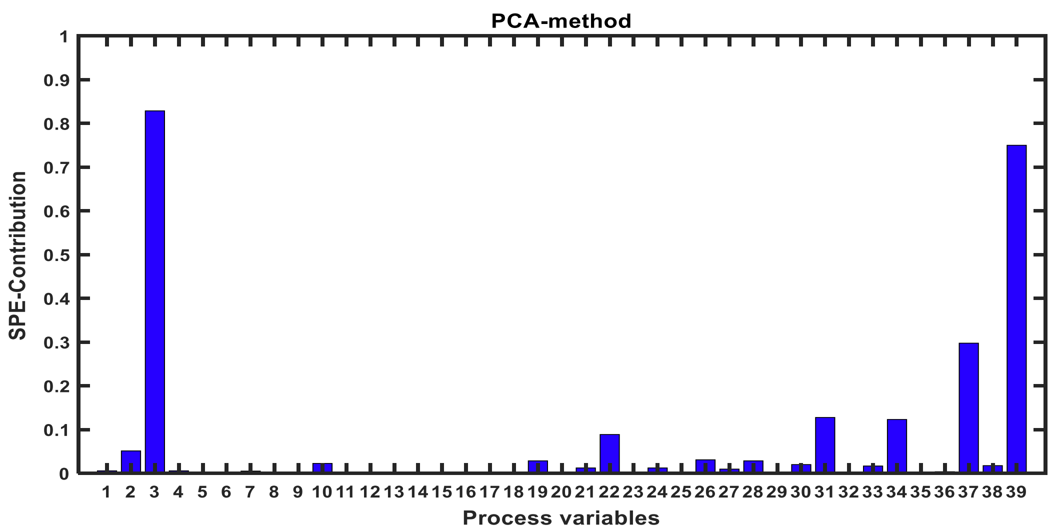


Figure 5. 8: Contribution plots of *SPE* for PCA for Fault - a.

Next, we investigate the root cause of Fault - b (Cluster 1). Figure 5.9 shows the variable contributions to *SPE* statistics. As can be seen in the figure, variables 18, 37, and 39 make the greatest contributions. The *SPE* contributions of the PCA model successfully points to the actuator fault.

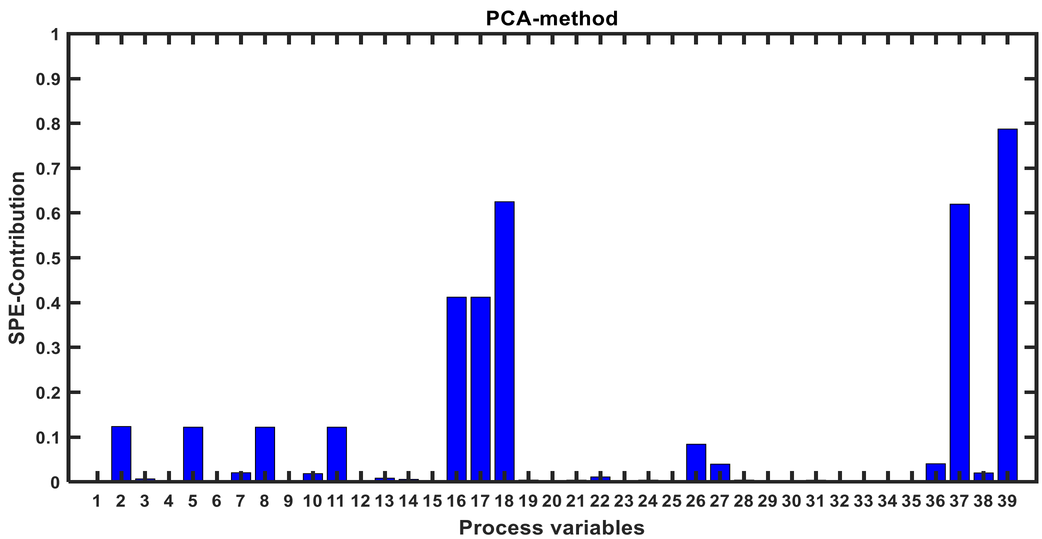


Figure 5. 9: Contribution plots of *SPE* for PCA for Fault - b.

In Figure 5.10, the *SPE* contributions for different variables calculated from the PCA model are presented for Fault - c (Cluster 3). As can be seen in the figure, variable 2 (pressure) has the highest contribution, while variable 39 (temperature) shows the second highest. Variable 2 (pressure) is directly related to the disturbance fault in variable 1 (feed flowrate).

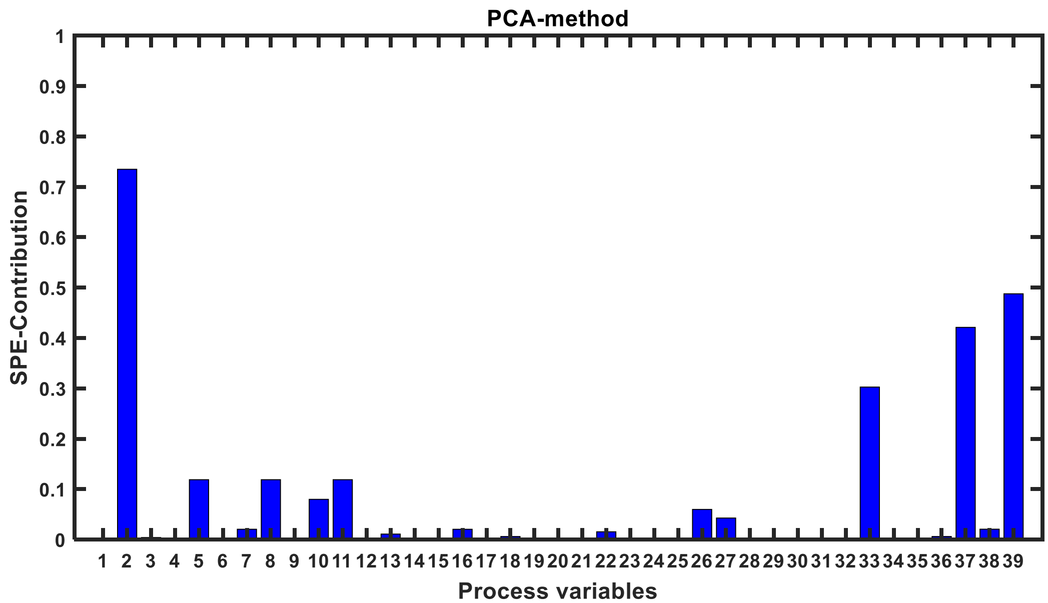


Figure 5. 10: Contribution plots of *SPE* for PCA for Fault - c.

5.4.1.2. On-line monitoring of separation unit

For the online monitoring process procedure, the new data are collected and then normalized based on the training mean and standard deviation. Next, the distance between the testing dataset and the five predefined CC points is calculated to identify the clusters to which the new data samples belong.

For classification and diagnosis purposes, the predefined fault cluster is the nearest to the new dataset. As well, the distance values between the new testing dataset and the CC point of any fault are associated with the Euclidean distance ranges. Therefore, the new fault cluster can be diagnosed based on the type of fault identified by the predefined fault clusters from offline monitoring. Figure 5.11 illustrates that both T^2 and *SPE* statistics charts can detect faults as well as cluster classifications.

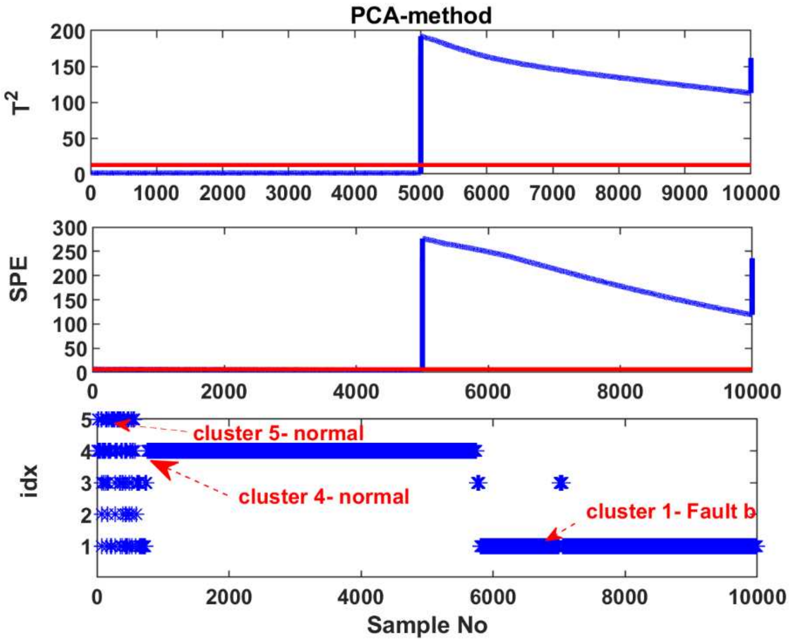


Figure 5.11: Online monitoring of T^2 (upper) and *SPE* (middle) results for PCA and classification of clusters (lower) in a separator unit of an offshore gas processing platform.

The final outcomes of the root cause of the faults are summarized in Table 5.3.

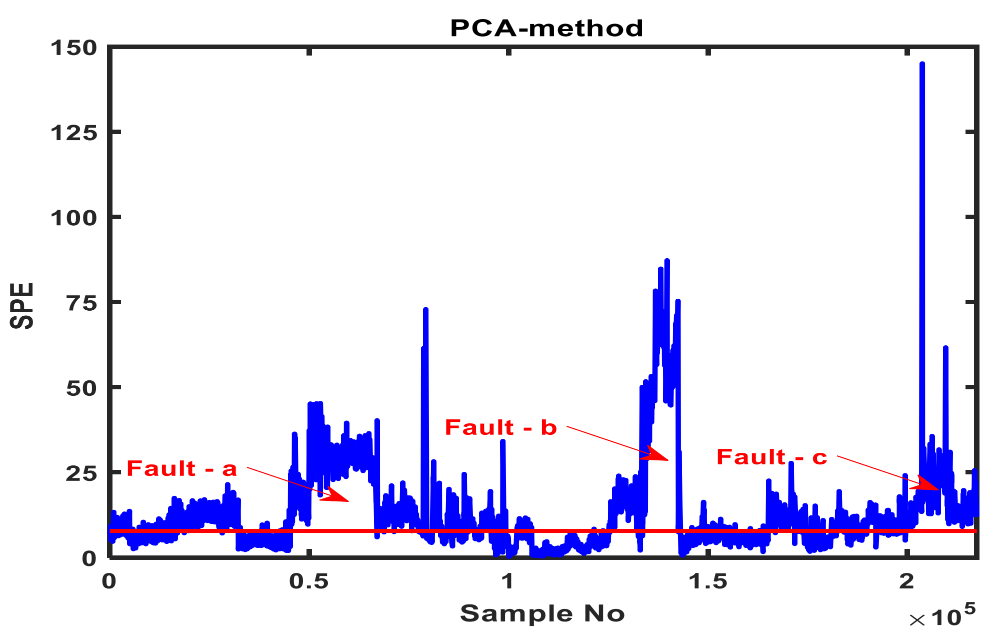
Table 5.3: Mapping of clusters to the root cause for the separator unit of offshore gas processing platform.

Cluster	**Fault**	**Root cause description**
Cluster 4,5	Normal	
Cluster 2	Fault - a	Feed temperature (Disturbance fault)
Cluster 1	Fault - b	Fail hold VLV-102 (Actuator fault)
Cluster 3	Fault - c	Feed flow rate (Disturbance fault)

5.4.2. Distillation column

5.4.2.1 Off-line training of distillation model

The distillation unit has 32 variables. Nearly 85% of the variance is explained by the first 15 PCs selected for the PCA model. The monitoring results obtained for *SPE* and T^2 are presented in Figure 5.12. As can be seen, the *SPE* and T^2-statistic used for fault detection show different behaviors. However, the T^2 is mostly within the limits (with some spurious points outside the limits), so the T^2 plot is not very useful in this case for fault detection. However, the *SPE* plot shows a clear violation of the limits for detecting faults on several occasions. It appears that the *SPE* results are more consistent throughout this analysis. For the selection of the faulty dataset from the distillation column, we therefore focus on the *SPE* criteria. Three faults are detected in the training data set by the *SPE*, as shown in Figure 5.12. Each fault is similar to one or more clusters.



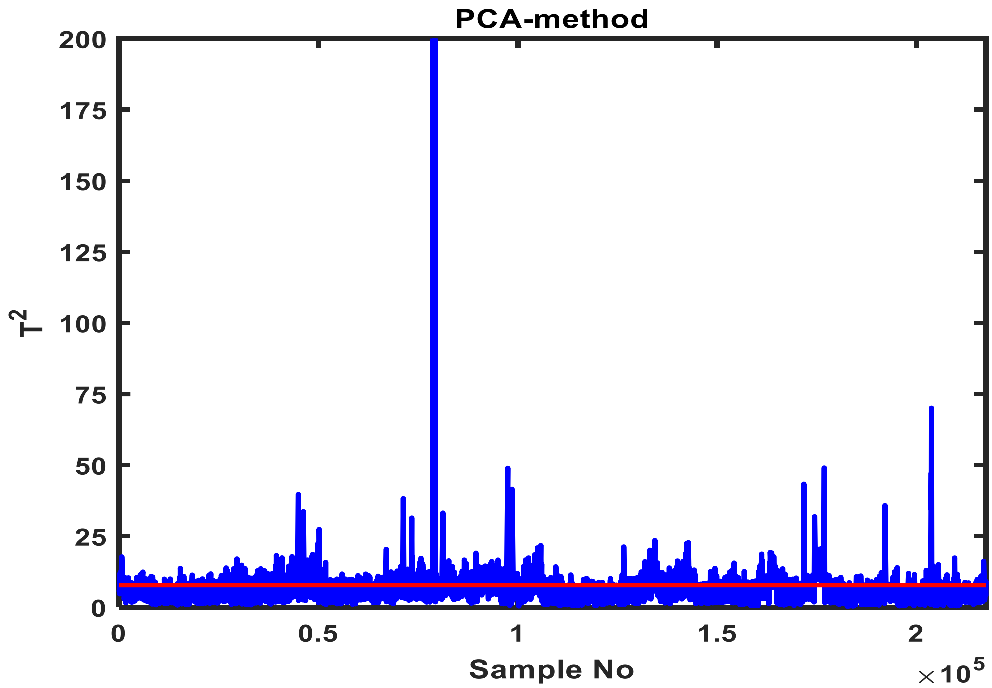


Figure 5.12: Monitoring results for PCA *SPE* (upper) and T^2 (lower) of the fault detection of the distillation column.

The training dataset of the distillation column process can be divided to five clusters, as shown in Figure 5.13.

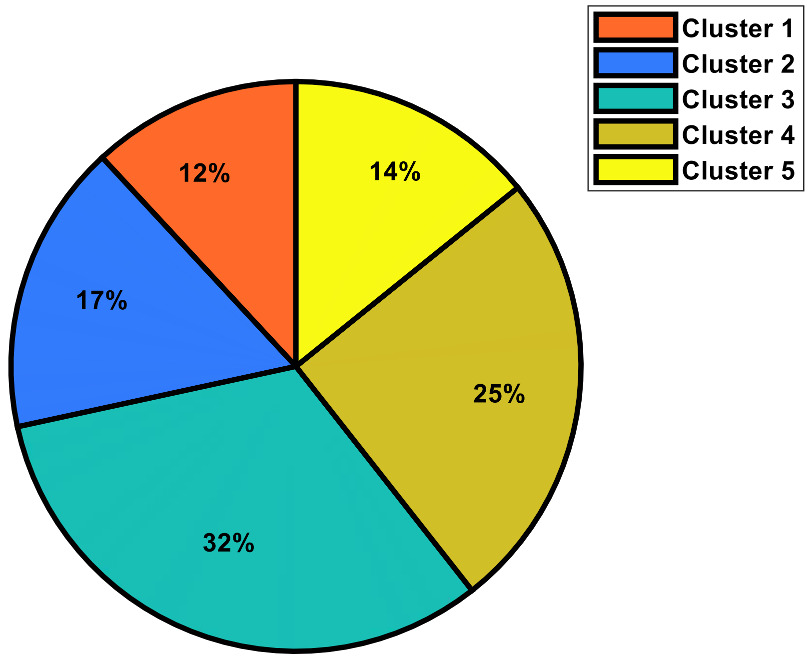
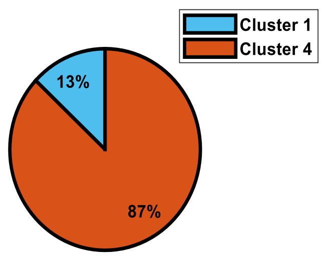


Figure 5. 13: Five clustering results of the distillation column process.

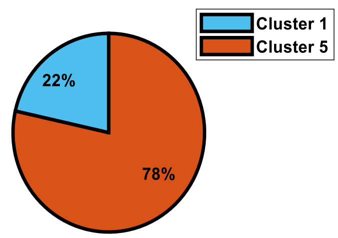
The frequencies of the five clusters obtained from the clustering are as follows: 32% of the training data set belongs to Cluster 3, 25% belongs to Cluster 4, 17% belongs to Cluster 2, 14% belongs to Cluster 5, and 12 % belongs to Cluster 1.

Mapping distillation Data Clusters to the Faults

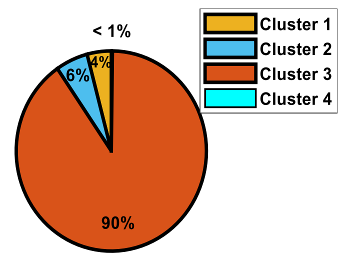
Following the clustering, the clusters were mapped to the different faulty datasets identified earlier from the *SPE* plots. The similarity between the clusters and the faults were evaluated using the similarity indexing function *"*$(idx)_{nx1}$*"* described above. Figure 5.14 shows the similarity results for Clusters 1 to 5 for Fault - a, Fault - b, and Fault - c. As illustrated in Figure 5.14 (a), Cluster 4 has the maximum similarity (~87 %) with the samples from Fault - a, but only a 13% similarity with Cluster 1. Clearly, the faulty dataset for Fault - a is related to Cluster 4. For Fault - b, Figure 5.14 (b) shows that Cluster 5 includes 78% of the fault samples and Cluster 1 includes 22%. In addition, Figure 5.14 (c) shows that Cluster 1 has less than 1%, Cluster 2 has about 6%, and Cluster 4 has 4%. Furthermore, the figure illustrates that the most faulty samples from Fault - c are related to Cluster 3 (90%). It can be concluded that Clusters 4, 5, and 3 represent three main faulty operation conditions as Faults - a, - b, and - c, respectively.



(a)



(b)



(c)

Figure 5. 14: Similarity in clusters of distillation data with (a) Fault - a, (b) Fault - b, and (c) Fault - c.

Mapping of distillation faults to the Root Cause

In this section, we use *SPE* contributions to diagnose the root cause of the faults. This will complete the cycle and connect the clusters to the root cause. Figure 5.15 shows the *SPE* contributions plot from the PCA method. As can be seen, variable 21 (XMEAS 21) has the highest contribution to *SPE* and is directly associated with the root cause of Fault - a.

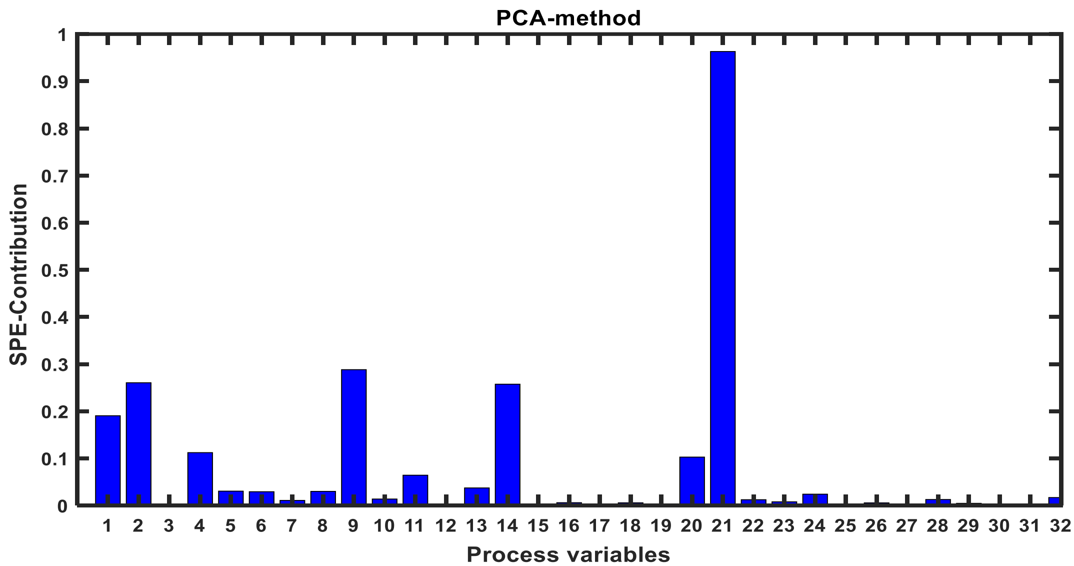


Figure 5. 15: Contribution plots *SPE* for PCA for Fault -a.

The diagnosis results for Fault - b from the PCA method are shown in Figure 5.16. The contributions of the variables to the *SPE* according to the PCA approach are also shown. As can be seen, variable 7 (XMEAS7) has the highest contribution and is therefore the root cause.

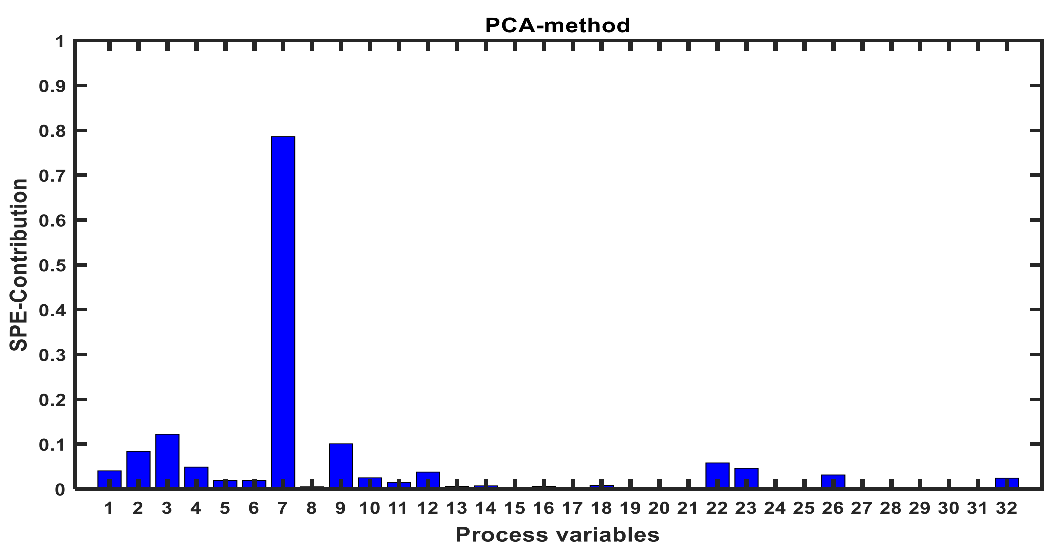


Figure 5. 16: Contribution plots of *SPE* for PCA for Fault – b.

In Figure 5.17, the *SPE* contributions of variables from PCA for Fault - c are presented. As can be seen in the figure, variable 17 (XMEAS17) contributes the most to the *SPE*.

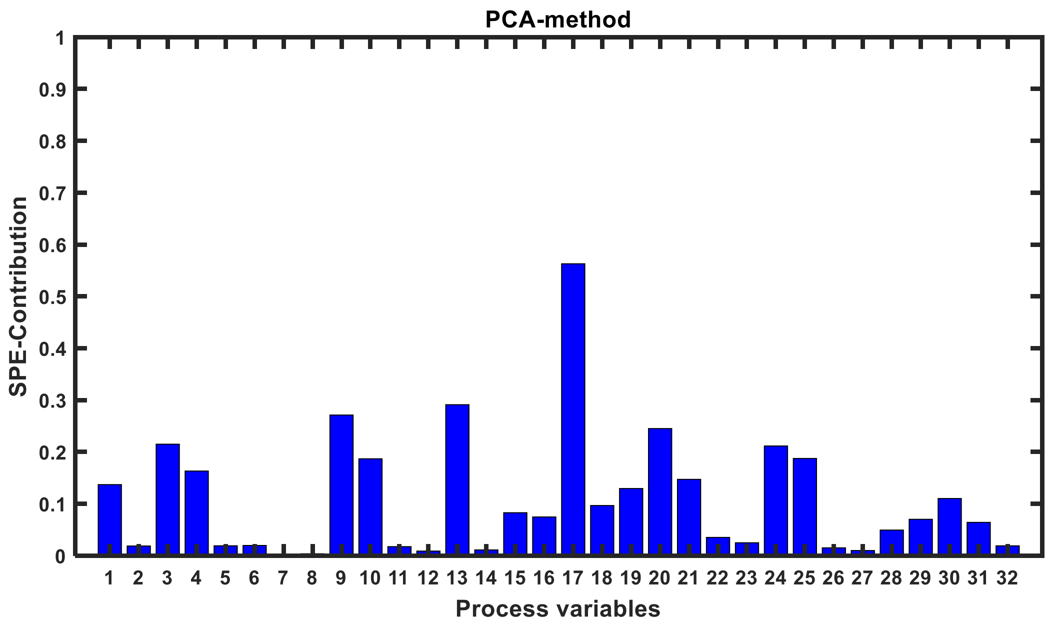


Figure 5. 17: Contribution plots of *SPE* for PCA for Fault - c.

5.4.2.2 On-line- monitoring of distillation column

For the distillation column process, both the T^2 and *SPE* for the PCA method are shown in Figure 5.18. As can be seen, the *SPE* statistics are sensitive to faults.

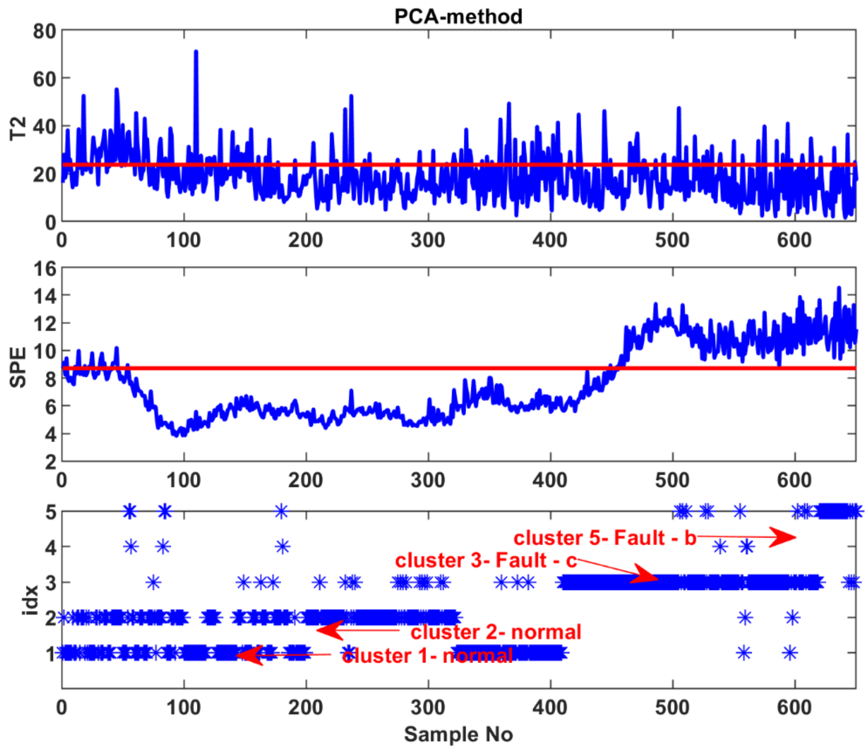


Figure 5.18: Online monitoring of T^2 (upper) and *SPE* (middle) results of PCA and the classification of the clusters (lower) of the distillation column.

Table 5.4 provides the root cause of the predefined fault clusters from offline monitoring to evaluate each type of fault (i.e., actuator, disturbance, or sensor).

Table 5. 4: Mapping of clusters to the root cause in distillation column

Cluster	**Fault**	**Root cause description**
Clusters 1 and 2	Normal	
Cluster 3	Fault - c	Reboiler (H1303) Cell 1 flow Pass 2 (XMEAS17); actuator fault
Cluster 4	Fault - a	(Reboiler Cell 1 Steam Pressure (XMEAS 21) faulty variable; Disturbance fault
Cluster 5	Fault - b	Low Pressure Separator Level (XMEAS7); Sensor fault

5.5. Conclusion

A new process-monitoring technique with root cause analysis using clustering algorithm (k-means) has been developed. The proposed method utilizes PCA as a data mining technique, with a clustering algorithm employed for online monitoring. The proposed method was implemented on two industrial processes: the distillation column of a crude unit, and the separator unit from an offshore gas processing platform. The proposed method shows that it can detect process faults earlier than PCA and eliminate some of the ambiguity of *SPE* contribution plots in fault diagnosis. Furthermore, the method can be applied to unlabelled historical process data without the need for labelling. Although the proposed method uses a k-means algorithm, the methodology is quite general and can be used in other unsupervised approaches.

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Chapter 6
Conclusion and Recommendations

6.1 Conclusion

As demonstrated earlier in this work, it can be very difficult to identify NNZL for SPCA. To overcome this barrier, this study proposed new criteria for choosing NNZL according to performance indicators of FAR and FDR. The mentioned criteria ultimately make SPCA more useful overall in fault detection and diagnosis (FDD). Following on the development of the proposed technique, three SPCA benchmark approaches were then compared using the novel strategy. Specifically, the FDD capabilities of the three SPCA approaches were compared by applying traditional PCA, and a case study with the continuous stirred tank heater (CSTH) system was highlighted for comparison purposes. The results of all these tests indicated that FDR-FAR SPCA showed lower FAR and higher FDR when compared with PCA or other SPCA methods; the proposed FDR-FAR SPCA was also able to diagnose faults more accurately.

This work also proposed the Sparse-IPCA and the bootstrap-SPCA methods to develop PCs that feature sparse loadings. The Sparse-IPCA and the bootstrap-SPCA techniques were then implemented on a CSTH system and their performance compared with that of the conventional PCA and AV-SPCA strategies.

Overall, the present work made the following contributions to the research area:

- Loading element distributions were obtained through the use of the measurement error covariance matrix and resampling. As demonstrated in the work, the loading element distributions provided better information on loadings and also clearly indicated which elements needed to be set at “0”.

- The novel approaches proposed in this study provided fault detection performance that was superior to traditional PCA and AV-SPCA. Results from both the qualitative and quantitative tests indicated improved fault detection along with fewer false alarms. The Sparse-IPCA and the bootstrap-SPCA methods have over 94% FDRs for the *SPE* statistics compared to 73.7% and ~ 0% with the AV-SPCA and PCA respectively for Sensor fault (level).
- When applying the T^2 and *SPE* contribution plots, the proposed methods' diagnostic performances were either similar or superior. The Sparse-IPCA diagnostic performance was particularly noteworthy for its precision and ability to indicate the root cause variable.
- Despite the above-cited advantages of the proposed methods, they did come at the cost of higher computation. The cost was particularly high for Sparse-IPCA in comparison with PCA and other SPCA strategies. However, because the computations can be performed off-line, the application of the proposed methods are not in any way limited by the enhanced computational requirements.

This work also addressed improvement to FDD using a novel approach based on PCA and k-means clustering. Applicability of the methods was demonstrated using industrial processes, namely, a distillation column and a separator unit in an offshore gas processing platform. This approach includes two parts: (1) the application of k-means clustering for categorizing the training sample set into various clusters; and (2) the application of the sum of squared prediction error (*SPE*) and the Hotelling T^2 statistic as a strategy for recognizing different faults. Every fault belongs to a cluster and can be used to find the reason(s) for the fault. The proposed method (PCA and k-means clustering) introduces greater sensitivity into the fault diagnosing process and can also monitor complicated processes at a much larger scale than the previous approaches.

4.2 Recommendations

The outcomes from this research may have an important role in developing regulations and requirements for product quality and process safety. The proposed SPCA methods are more sensitive for diagnosing process faults as well as powerful for monitoring large scale complex processes. The proposed methods can be further enhanced by considering the following:

- When process data adhere to multivariate Gaussian distribution, PCA may be the best strategy to use. For this purpose, KPCA can be applied as first-stage detection tool to obtain optimal detection in instances where the process data is non-linear and/or non-Gaussian.
- For second-stage detection, and to enhance fault diagnosis abilities, specific criteria may be applied when choosing NNZL for SPCA.
- A range of dimension-reducing strategies (e.g., FDA, PLS, etc.) could be applied for performance validation purposes.
- Different types of clustering algorithms can be combined with PCA or with a range of dimension-reducing strategies (e.g., FDA, PLS, etc.) to upgrade the FDD performance.