Fault Detection in Pressure Swing Adsorption Systems

By

Farshad Amiri

A Thesis Submitted to the Graduate Faculty of
Auburn University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

Auburn, Alabama
May 4, 2019

Keywords: Process Monitoring, Fault Detection, Principal Component Analysis,
Statistical Pattern Analysis, Cyclic Processes, Pressure Swing Adsorption

Approved by

Q. Peter He, Chair, Associate Professor of Chemical Engineering
Jin Wang, Co-chair, Walt and Virginia Woltosz Endowed Professor, Chemical Engineering
Mario Eden, Joe T. and Billie Carole McMillan Professor & Dept. Chair, Chemical Engineering

Abstract

Over the years, there has been a consistent increase in the amount of data collected by systems and processes in many different industries and fields. On the other hand, there is a growing push towards revealing and exploiting of the collected data. The chemical processes industry is one such field, with high volume and high-dimensional time series data. The massive amount of data can be used for better control and production. Because of the high level of complexity in chemical processes, mathematical modeling is mostly unachievable and impracticable. A number of model base on process data have been suggested and developed by researchers for batch and continuous processes. Compared to these type of processes, cyclic processes have not received enough attention in the literature and still, it is a relatively intact area for developers in fault detection and process monitoring. Moreover, because of the different nature of the batch and continuous, well-developed monitoring methods and frameworks in those processes cannot be employed to the periodic processes. Therefore, a new multivariate method based on combined Principal Component Analysis and Statistical Pattern Analysis framework is proposed to help to fill the existing gap in the monitoring of cyclic processes and to overcome fault detection issues.

Acknowledgments

I would first like to express my gratitude to my advisor Dr. Peter He, for the useful guidance, remarks, and engagement through the preparation of this master thesis. Furthermore, I would like to thank Dr. Jin Wang and Dr. Mario Eden for serving as my committee members and their beneficial advice and suggestions. I also appreciate the support from R&D group in Praxair Company, especially Dr. Jesus-Flores-Cerrillo, Associate R&D Director and Dr. Ankur Kumar, Process Systems Specialist. I like to thank my friends and fellow lab members who shared their precious time and ideas with me from the very first day of joining the group, I wish them all the best in their research work and future career. Most importantly, I would like to sincerely thank my inspiring wife, Marjan, for being a great supporter of me who without her love I could not finish the thesis.

Farshad Amiri

Auburn, Alabama

March 19th, 2019

Table of Contents

List of Figures

List of Tables

List of Abbreviations

PCA	Principal Component Analysis
SPA	Statistic Pattern Analysis
MAE	Mean Absolute Error
MAD	Mean Absolute Deviation
CV	Coefficient of Variation
SLL	Slope of Linear Regression Line
AFD	Average of First Derivative
PSA	Pressure Swing Adsorption
SPE	Squared Prediction Error
SPM	Statistical Pattern Monitoring
MSPM	Multivariate Statistical Process Monitoring
MQC	Multivariate Quality Control
PLS	Partial Least Squares
SPM	Statistical Pattern Monitoring
SPC	Statistical Process Control
RS	Residual Subspace
PCS	Principal Component Subspace
EWMA	Exponentially Weighted Moving Average
CUSUM	Cumulative Sum Control Chart

Chapter 1

Introduction

Process monitoring is one of the most important tasks in process system engineering to ensure plant safety, product quality, production profit, and environment sustainability. Due to the large number of process variables measured and recorded continuously in industrial plants, process monitoring has become a challenging task to not only detect abnormal process behavior as early as possible but also increase fault detection accuracy and mitigate false alarms. With the high-dimensional and correlated process data, multivariate statistical process monitoring (MSPM) methods have been developed to extract useful information from a large amount of process data and detect various types of process faults [1-6]. In this research, due to the lack of attention in literature compared to batch and continuous processes, fault detection in cyclic processes is considered. Also as a case study, a pressure swing adsorption plant is selected to have the benefit of using industrial data in proposing a new framework.

1.1 Introduction to Fault Detection

The development of new mechanisms and frameworks to better understand and analyze data collected in the course of routine process operations and, more importantly, during process upsets has become an important research field. A key direction in this area is monitoring process operations and, by extension, the identification and isolation of process faults. There has been significant progress made in the literature for the monitoring of multivariate processes. Available methods can be broadly classified into model-based and data-based methods. Model-based methods are reviewed by Venkatasubramanian et al. [2] perfectly. In the data-based method space, tools such as principal component analysis (PCA) and partial least squares (PLS) regression have been successfully used to detect and isolate faults pertaining to individual process variables and units. These ideas have been extended to account for process dynamics and nonlinearity via, e.g., dynamic PCA [7], kernel PCA [8] and multiway PCA [9]. Other approaches based on similar principles include independent component analysis [10] and statistical pattern analysis (SPA) [11]. Dimensionality reduction, a common result of many of the above-mentioned methods, has proven to be valuable, forming the basis for score and square prediction error (SPE) plots [12].

1.2 Periodic Processes

Periodic, cyclical operation has found several important applications in the chemical process industries. There are processes which, due to physical limitations, must be run in a cyclical fashion. Notable examples here include separation systems, such as pressure- and temperature-swing adsorption, whereby the limited capacity of the adsorbent is compensated for by operating multiple adsorbent-filled vessels (or beds) in parallel, with typically one bed being in contact with the process stream while the others undergo regeneration steps [13,14]. Chromatographic separations fall under the same category, the control and optimization of simulated moving beds, which involves the switching of inlet and outlet feeds periodically, has been a topic of exploration [15-18].

1.2.1 Existing Fault Detection Method in Cyclic Processes

The economic importance of periodic processes provides a strong incentive for ensuring their operational performance, with process monitoring and fault detection being a key enabler to this end. However, process monitoring techniques for periodic processes have received insufficient attention in the literature. It is important to note that the methods and tools used for monitoring continuous processes do not translate directly to the periodic realm, owing to the fact that a these processes are constantly in a transient regime- a periodic process is essentially never at a steady state in the sense utilized in continuous process operations. As an alternative method, Pan et al. proposed using a stochastic state space model to describe the statistical behavior of changes on a cycle-to-cycle basis and used a Kalman filter method for process monitoring on a waste water treatment system. They combined PCA with the subspace identification method to obtain a model that describes the period-to-period multivariate behavior of all the samples collected during each period [19]. On the other hand, tools used in batch process monitoring, such as Multiway Principal Component Analysis (MPCA), are to some extent applicable in periodic systems. For example, in Kim et. al. [20], MPCA was used to monitor periodic (daily as well as seasonal) air pollution in subway stations. Using MPCA, the authors were able to predict more accurately the air quality in subway stations compared to univariate monitoring methods, as well as to isolate characteristics of seasonal variations of different air pollutants. Nevertheless, there are important differences between batch and periodic systems: chemical batch processes follow a recipe with well-defined start point and desired end-point characteristics; the evolution of the process between these points may vary in duration and trajectory in the state space. On the other end, the start and end points for cyclical processes coincide, and a periodic steady-state is reached, whereby the state-space trajectory of one cycle differs minimally from the preceding and subsequent ones [18].

Some other types were proposed to address potential problems in production plants by adjusting process variables based on changes in measured process parameters. For example, United States Patent 8,016,914, Belanger et al., United States Patent 7,674,319, Lomax et al., and United States Patent 7,789,939, Boulin, teach various methods for measuring an impurity and adjusting a process variable, such as feed time, to control that impurity in a bed of a PSA system. Such single bed PSA control is widely used and has become an industry practice. Other production plant fault detection methods have been discovered and implemented. For example, as is described in the article, entitled, "Finding the Source of Nonlinearity in a Process With Plant-Wide Oscillation", Nina F. Thornhill, 2005, Thornhill proposes a non-linearity index that can be used to detect a root cause of oscillation for a dynamic system having a plurality of interacting control loops. This method can be used to detect oscillations caused by self-sustained limit cycles in a control loop. Such oscillations often originate in one loop but propagate to the other loops. With this current practice, the developed non-linearity metric produces high values for the source control loop and lower values for the secondary oscillations that allow a root cause analysis to be performed [21]. Arslan et al. in a US patent (US Patent 8,882,883) suggested an apparatus and methods which are disclosed that allow for the monitoring and analysis of production process data for a multi-step asynchronous cyclic production process (e.g.

pressure swing adsorption) in a steady state plant (such as a steam methane reforming plant). Data collected from cooperating sensors is processed applying a moving window Discrete Fourier Transform (DFT). The transformed data can be further analyzed in the broader steady-state plant environment to accurately detect any process anomalies and avoid false alarms [21].

Wang et al. presented a novel approach for monitoring and fault detection in periodic processes, based on a geometric representation of periodic process operating data. Specifically, they developed a time explicit multivariable representation of data collected from the process, which then provides a natural framework for defining "normal" operation and the corresponding confidence regions. The fault detection mechanism consists of two steps: first, intercycle detection is performed to identify a problematic operating cycle, followed by intracycle detection aimed at establishing the time of occurrence of a fault. In another study, they defined confidence ellipses for every sample across cycles of normal operation; this creates a cycle trajectory that corresponds to the dynamics of a normal operating cycle. By comparing the samples of a problematic cycle against the corresponding sample confidence ellipse, the moment when deviation begins to occur in the problematic cycle can be identified [12].

1.3 PSA Process Description

In this section for further understanding, a general overview for a poly-bed Pressure Swing Adsorption (PSA) unit for hydrogen purification is described. The purifier system uses a pressure swing adsorption to produce a high purity hydrogen product stream. The impurities in the feed are adsorbed at high pressure and desorbed at low pressure.

There are two basic steps for each cycle in the PSA process, Adsorption and Regeneration. The process temperature may change slightly due to the heat generated during the adsorption and desorption. During the adsorption step, the impurities are adsorbed in high pressure by the adsorbent in a vessel and at the end, the purified hydrogen product leaves the vessel. In the regeneration step, removing the impurities from the adsorbent, and makes the adsorbent ready for another adsorption step. Equalization steps are designed to maximize the hydrogen recovery which occurs between a depressurizing vessel and another vessel being repressurized. When repressurization steps are completed, the adsorption-regeneration cycle can be repeated.

1.3.1 Adsorption

The feed gas mixture enters the adsorber (vessel) from the bottom and the impurities are adsorbed by the adsorbent. The purified hydrogen product leaves from the top. Since several adsorbers are employed in the process, multiple vessels are normally on adsorption steps at any one time. But they are not brought online or taken offline simultaneously. In other words, the beginning time for adsorption step is staggered so that at any one time only one vessel is switched to the adsorption step.

1.3.2 Regeneration

After the adsorption step, the adsorber is relatively loaded with adsorbed impurities. A large part of the impurities are adsorbed in early stages in the adsorber therefore, the concentration of impurities is high at the bottom of the adsorber. Recovering hydrogen from the top of the adsorber using a series of co-current depressurizations steps helps to obtain better hydrogen recovery. The pure hydrogen remaining in the bed is used to provide the gas for the Equalization and Provide Purge Steps, for other vessels. In equalization steps, a vessel at high pressure equalizes with another vessel at low pressure by forwarding the trapped high-pressure hydrogen in the high-pressure vessel to the vessel at low-pressure state. When the co-current depressurization steps are performed, the concentration of the impurities will be increased at the top stages of the vessel and a downflow is needed to sweep them from the vessel. In these steps, the adsorber is depressurized countercurrently to the lowest pressure in the system and the impurities are desorbed from adsorbents and expelled to the tail gas system. Purging the adsorber countercurrently with pure hydrogen gas from another depressurizing adsorber continues the Regeneration process. The remaining impurities are removed from the Adsorbent by another countercurrent step which is named purge which makes the vessel ready for repressurization steps.

1.3.3 Repressurization

After the vessel has been purged and cleansed of the trapped impurities, it is repressurized to adsorption pressure in order to be brought back online to purify hydrogen. Thus, using the high-pressure flow supplied by other vessels in high-pressure state, the pressure continues to rise during the repressurization steps. A repressurized vessel (to adsorption step's pressure) is being ready for another adsorption step or another cycle.

Chapter 2

General Review on Fault Detection Methods

2.1 Process Monitoring

Process monitoring and diagnosis are essential for detecting unusual operating conditions, process abnormalities, equipment malfunctions and failures, and other faults in industrial plants. Thousands of process variables are measured and recorded continuously in industrial plants so the process monitoring and data analysis become a challenge for researchers and scientists. On the other hand, the huge amounts of process data can be employed to build various kinds of models for better process control and monitoring. Traditionally, univariate statistical process control (SPC) techniques have been used for monitoring industrial processes. Nevertheless, the highly correlated process measurements in industrial plants often result in the failure of univariate methods [22].

2.2 Multivariate Process Monitoring

Process monitoring techniques are not only key in determining equipment malfunctions and instrument failures, but also are fundamental in ensuring process safety, product quality, and process efficiency. As large amounts of variables are measured and stored automatically by governing control systems, multivariate statistical monitoring methods have become increasingly common in process industry. Multivariate process monitoring techniques are based in different mathematical algorithms. In addition, the way to detect and diagnose faults vary from one approach to the other [23]. This chapter reviews process monitoring technique using PCA with a brief review of dynamic PCA and nonlinear monitoring techniques such as Kernel PCA (KPCA) and Independent Component Analysis (ICA). The complete consideration of these process monitoring methods is out of the scope of this thesis.

2.3 Multivariate Statistical Process Monitoring

Multivariate statistical process monitoring (MSPM) techniques like principal component analysis (PCA) and partial least squares (PLS) have been widely employed for fault detection and fault diagnosis in industrial data [24]. These kinds of methods first project the multivariate and collinear data onto a lower dimensional subspace. Then the test statistics like T^2 and SPE are developed to monitor the multivariate data. The effectiveness of these conventional methods requires that the process data approximately follow multivariate Gaussian distributions for the derivation of control limits. However, industrial data often obeys non-Gaussian distribution so that the PCA/PLS based monitoring techniques become ill-suited. On the other hand, ICA is adopted to decompose multivariate data into linear combinations of statistically independent components (IC). ICA imposes independency on latent variables beyond second-order statistics and thus can extract the non-Gaussian features of process data [25]. Moreover, ICA based monitoring statistics like I^2 and SPE have been developed to describe the variability within the independent component and residual subspaces [22, 26].

Moreover, unsupervised pattern matching techniques are proposed to identify similar patterns between multivariate time-series data sets. Various PCA based pattern matching methods compare PC subspaces using similarity factors, which are developed from the geometric angles between principal components [27]. Alternately, eigenvalue decomposition of the covariance matrices is used to determine the dissimilarity factor between two data sets [28]. The dissimilarity method is extended to ICA for comparing two data sets using independent components [22, 29].

2.3.1 Principal Component Analysis

The central idea of principal component analysis (PCA) is to reduce the dimensionality of a data set consisting of a large number of interrelated variables, while retaining as much as possible of the variation present in the data set. This is achieved by transforming to a new set of variables, the principal components (PCs), which are uncorrelated, and which are ordered so that the first few retain most of the variation present in all of the original variables [30].

2.3.1.1 Geometric Explanation of PCA

Consider the data, collected in a matrix X, contains rows that represent an object of some sort which is called observation. The observations in X could be a collection of measurements from a chemical process at a particular point in time, various properties of a final product, or properties from a sample of raw material. The columns in X are the values recorded for each observation which are called variables. Consider a K-dimensional space when referring to the data in X. For looking into geometric interpretation of PCA, let's say X has 3 columns, in other words a 3-dimensional space, using measurements: [x_1, x_2, x_3].

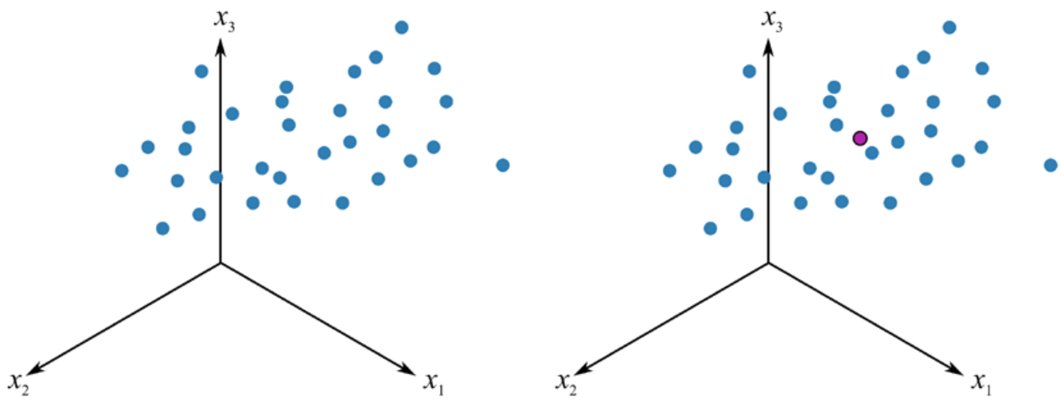

Figure 2.1 The raw data in the cloud swarm [31]

In figure 2.1 the raw data in the cloud swarm shows how the 3 variables move together. The first step in PCA is to move the data to the center of the coordinate system. This is called mean-centering and removes the arbitrary bias from measurements that we don't wish to model. Researchers also scale the data, usually to unit-variance. This removes the fact that the variables are in different units of measurement. After centering and scaling we have moved our raw data to the center of the coordinate system and each variable has equal scaling. In figure 2.2 the best-fit line is drawn through the swarm of points. The more correlated the original data, the better this line will explain the actual values of the observed measurements. This best-fit line will best explain all the observations with minimum residual error. Another, but equivalent, way of expressing this is that the line goes in the direction of maximum variance of the projections onto the line. When the direction of the best-fit line is found we can mark the location of each observation along the line.

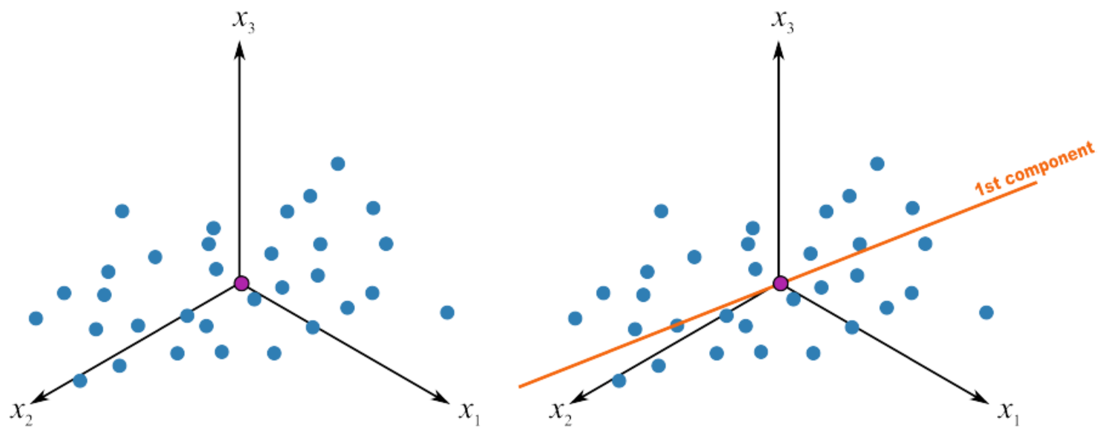

Figure 2.2 Data after centering and scaling and the best-fit line [31]

Figure 2.3 shows the 90 degree projection of each observation is found onto the line. The distance from the origin to this projected point along the line is called the score. Each observation gets its own score value. The best-fit line is in the direction of maximum variance that the variance of these scores will be maximal. (There is one score for each observation, so there are N score values; the variance of these N values is at a maximum). Notice that some score values will be positive and others negative. After the best-fit line has been added to the data, the first principal component will be calculated, also called the first latent variable.

Hence, the first principal component is fixed and now the second component needs to be added to the system. The second component should be perpendicular to the first component's direction. Notice that this vector also starts at the origin, and can point in any direction as long as it remains perpendicular to the first component. The direction gives the greatest variance in the score values when projected on this new direction vector.

A principal component model is one type of latent variable model. A PCA model is computed in such a way that the latent variables are oriented in the direction that gives greatest variance of the scores. There are other latent variable models, but they are computed with different objectives [31]. Further details about PCA in [30, 31].

2.3.1.2 Fault Detection Using PCA

Once the PCA model has been determined based on the historical data, new multivariate observations in a sample vector x can be referenced against the model. This is achieved by projecting these observations onto the plane defined by the PCA loading vectors to obtain their scores and residuals [32]. Traditionally, the projections or scores are plotted to reveal the relationships of the variables forming a new multivariate observation x. In addition, to reveal data patterns, to identify clusters, and to determine the influence of different multivariate observations, two-dimensional plots of the most significant scores related to the dominant directions of variability (e.g. dominant eigenvectors) are used. Furthermore, an evaluation of the magnitudes of the loadings can serve as an indication of the relationships between the process variables contained in X. For fault detection, Hotelling's T^2 [33] and SPE charts [34] are commonly used. The SPE index measures variability that breaks the normal process correlation [35], in other words, measures the variation in the residual subspace (RS) [23].

The SPE statistic provides a way to test if the process data are outside the normal operating region. The SPE statistic is normally complemented by the use of the Hotelling's T^2 [33] statistic. The T^2 index measures the distance to the origin in the principal component subspace (PCS), i.e., provides an indication of abnormal variability in the space defined by the PCS.

2.3.2 Multi-way Principal Component Analysis

Multi-way PCA (MPCA) is considered a data-driven technique in monitoring of batch processes. Data in continuous processes are projected into matrixes with two dimensions, whereas in the batch processes the data are projected into a three-dimensional matrix because the batch number constitutes a dimension. The MPCA method covers this extra dimension. Ideally, online measurements of process variables can be fed into MPCA to develop real-time monitoring. It is capable of hand ling highly correlated data including batch process variables because it reduces dimension of data by using principal components methodology. The dimensions of batch data are batch number, process variables, and sampling time of each process variable. In order to apply PCA to data obtained from a batch process, data arrays should be re-organized from three-dimensions to two dimensions through a procedure called unfolding [36]. Several multidimensional techniques have been proposed for re-organizing batch data arrays into the sum of a fewer vectors and matrixes, and to summarize the variation of the data in the reduced dimension of these spaces. Two different techniques for data unfolding are discussed by Nomikos et al. [1] and Wold et al. [37]. MPCA has proved to be a very effective and easy to understand method for analyzing batch data because of its simplicity and well defined properties. Figure 2.3 describes the unfolding of a matrix batch data for a data set consisting of 36 batches with 10 variables and 228 time units in the two different unfolding methods [36].

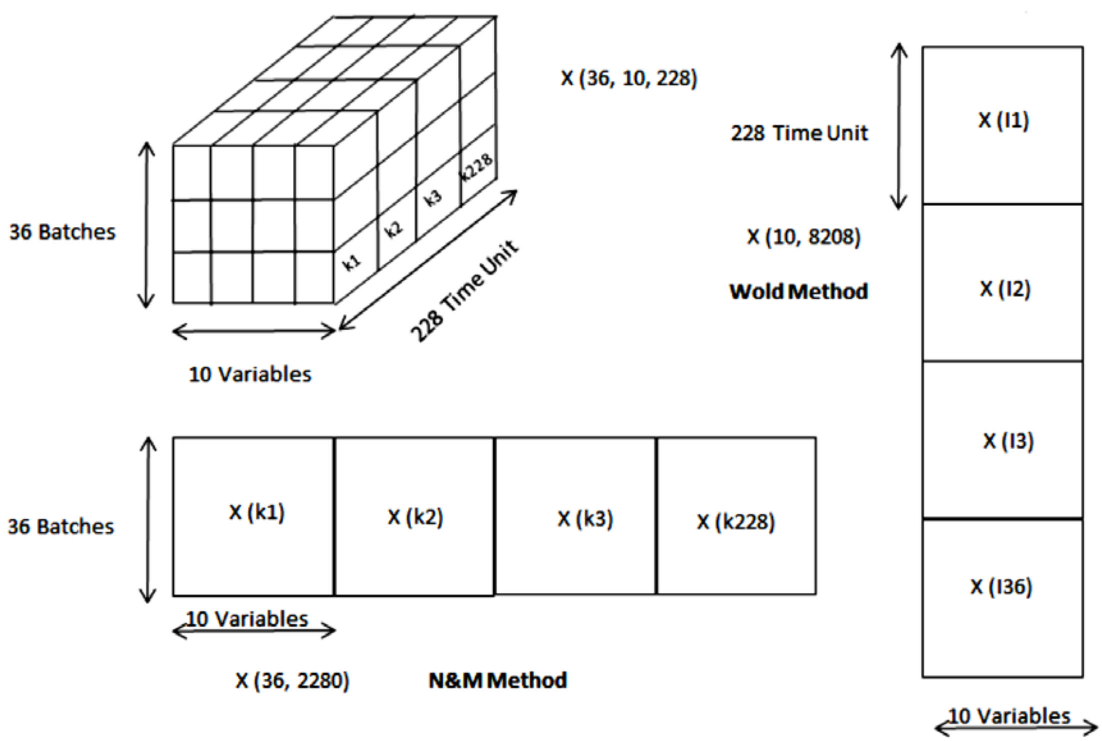

Figure 2.3 Unfolding batch data from 3D to 2D [36]

2.3.3 Kernel Principal Component Analysis

PCA-based monitoring methods have been extremely successful in many applications. However, as PCA only considers the mean and the variance-covariance of variables to characterize the process, and it assumes a linear relationship among the process variables, it lacks the capability to provide higher order representations for non-Gaussian data. Complex chemical and biological processes are nonlinear in nature. As a consequence, the process data inherits a nonlinear behavior. The nonlinearity present in the process variables causes PCA to perform poorly [38]. Kernel PCA (KPCA) has emerged as a solution to address this problem [23, 39]. In KPCA the input data is first mapped into a higher-dimensional space via a nonlinear function. After the higher-dimensional nonlinear mapping, the variables in the feature space are more likely to vary linearly [40]. Similar to PCA, for fault detection, the T^2 and SPE statistics are utilized and the confidence limits of the monitoring indexes can be determined theoretically via F-distribution [41] and x^2 distribution [32], respectively, or empirically using validation data [23].

2.3.4 Independent Component Analysis

The presence of unmeasured disturbances, correlations and noise hides the valuable factors that govern industrial processes. Revealing these hidden factors can be used to better characterize a process. In PCA, this is achieved by projecting the input data onto a lower-dimensional space that captures most of the variance and accounts for correlations among variables. Since the objective of PCA is to decorrelate the scores (e.g. projections) and only consider up to second-order statistics to characterize a process, it lacks the capability of represent processes where nonlinearities are prevalent (e.g. non-Gaussian distribution of input variables). Independent component analysis (ICA) is a recently developed technique [23, 42] that by satisfying formal statistical independence and implicitly using higher-order statistics, it decomposes the process data into linear combinations of statistically independent components (ICs) that contain the main governing characteristics of the process. Applications of ICA have been reported in several fields of engineering, some examples are signal processing, machine vibration analysis, radio communication, infrared optical source separation etc. [23, 43].

It should be expressed that, there is still much information in detail about the mentioned methods in literature for those who want to learn more.

Chapter 3

The Proposed Framework

3.1 Challenges in Process Monitoring

Big data analytics is arguably a major focus in cybermanufacturing, and could become a key basis of competitiveness, productivity growth, and innovation [44, 45]. In this section, some challenges process monitoring could face in addressing the 4 V's of big data generated in cybermanufacturing: volume, variety, velocity and veracity are discussed. Moreover, the potential of SPA to address the challenges is described.

• **Volume**: Cybermanufacturing will generate a massive amount of data, both due to increased sensoring (more variables) and increased sampling (more observations). Therefore, the massive amount of collected data and the way of extracting useful information from the "big data" presents significant challenges for process monitoring and should be dealt with attentively. In addition, process nonlinearity and process data non normality will become more dominant or even become norm instead of exception for cybermanufacturing. Generally speaking, more observations do not pose a problem to existing multivariate statistical process monitoring (MSPM) methods or SPA. In fact, more observations are beneficial for SPA because they allow better estimation of statistics. However, significantly increased variables in cybermanufacturing is more difficult to handle than just large number of observations, particularly when different variables are sampled at different frequencies. Since SPA uses a window approach to compute different statistics, it can naturally handle the different sampling frequency by using all samples available within the window to compute the statistics. One concern associated with window approach is that detection delay. However, it is shown that the detection delay associated with SPA is similar or even shorter than that of PCA [11, 46]. Consequently, effective variable (statistics) selection will play a key role to improve SPA's performance, and will help address the challenge of large number of variables to certain extent.

• **Variety**: By monitoring different parts of a system, measuring different phases of a process, which can be sampled at very different frequencies, different forms of data is generated. Current MSPM approaches (e.g., PCA) usually make use of one type of data at a time because the data have to form a matrix or matrices. In this aspect, SPA has the potential to integrate different data types relatively easily, because the statistics of different data types (such as machine data and metrology data) are much easier to integrate than the original data. Note that different statistics from different data forms or different parts of the process are simply augmented together for process monitoring; there is no restriction on the number of the selected statistics. If PCA is applied to monitor the statistics (i.e., SP), the same sampling frequency of statistics are required. This can be easily satisfied by using all samples available for a given variable within a fixed window to calculate the desired statistics. In addition, it has been shown that the information contained in the raw data would be altered more or less during data pre-processing, which may negatively impact the monitoring performance [11, 46]. Therefore, minimizing required data pre-processing would be desirable for cybermanufacturing systems.

• **Velocity**: For process monitoring and control, streaming or online models is expected to be employed (e.g., diagnostics and prognostics). To address large volume of streaming data for real-time statistical analysis and online monitoring, SPM methods that do not require data pre-processing such as SPA, or methods that require minimum and automated data preprocessing, will have advantage in handling steaming data [46].

• **Veracity**: For modern process monitoring, it is expected that the veracity of the data (e.g., data quality or cleanness such as missing data, outliers, noises, delays and data asynchronism) will be significant. While the traditional MSPM methods emphasize the cleanness of the data to prevent potential misleading conclusions, it is expected that the future MSPM methods should consider data errors or messiness as unavoidable, and are robust to the imperfections in the data [45]. Because missing data, outliers, or data uncertainty has much less impact on various statistics than variable themselves, SPA offers advantages in this aspect. For example, the mean of a variable will not be affected significantly by the noise or infrequent missing data or outliers [46].

3.2 Introduction to Statistical Process Monitoring

Process Chemometrics (which is the application of multivariate statistical methods to industrial process data characterized by a large number of correlated process measurements) applies multivariate analysis techniques to process data analysis and process improvements. An important area of tremendous success in process Chemometrics is statistical process monitoring (SPM), which has become one of the most active research areas in process control over the last decade. Using methods from multivariate statistical analysis, SPM has found wide applications in different industrial processes, including chemicals, polymers, micro electronics manufacturing and pharmaceutical processes. The tasks involved in SPM typically include: fault detection, fault identification and diagnosis, fault estimation, which assesses the fault magnitude, and fault reconstruction, which estimates the fault-free values to keep control and monitoring on-going even if some faults have occurred. Owing to the data-based nature of SPM, it is relatively easy to apply to real processes of rather large scale, in comparison with other methods based on systems theory or rigorous process models. While the process control community began to investigate the use of multivariate statistics for SPM in the late 1980s, the use of multivariate statistics for abnormal situation detection has been studied intensively in the area of multivariate quality control (MQC) [47]. Typically, the Hotelling's T^2 statistic and the Q statistic, which is also known as the squared prediction error (SPE), are used for the detection of an out-of-control situation. These two statistics, typically calculated based on a model from principal component analysis (PCA) or partial least squares (PLS), give superior performance to the univariate quality control methods which monitor one variable at a time. The MQC literature, however, mainly focuses on the monitoring of quality variables and the detection of a quality problem, with few methods available for identifying root causes [35].

Statistical process monitoring relies on the use of normal process data to build process models. These models include PCA, PLS, and their variants. PCA models are predominantly used to extract variable correlation from data [35].

3.3 Motivation

Pressure swing adsorption (PSA) is a well-established gas separation technique in air separation, gas drying, and hydrogen purification separation. Recently, PSA technology has been applied in other areas like methane purification from natural and biogas and has a tremendous potential to expand its utilization. It is known that the adsorbent material employed in a PSA process is extremely important in defining its properties, but it has also been demonstrated that process engineering can improve the performance of PSA units significantly [48].

In many chemical industries pressure swing adsorbers are important process unit which are used for separating desired products from impurities. For obtaining desired product yield in PSA plants which are classified as complex processes, it is required to maintain normal operation condition. To minimize production loss and equipment damage due to different abnormal conditions, immediate fault detection seems necessary. Constant manual monitoring of PSA plants leads some practical limitations, therefore, implementation of an automatic fault detection method is essential. Compared to continuous and batch processes just a few methods were suggested by researchers in the literature. The important reason behind that is the cyclic and unsteady nature of the process. On the other hand, highly automated control systems in industrial sites are able to collect thousands of process measurements every day. The data captures the governing phenomena occurring in the process. However, the m variables that are selected to represent any given process are normally highly correlated and noisy. In addition, the number of variables that adequately represent a process can be very large. These factors can make the analysis of process data very difficult. The central idea of PCA is reducing the dimensionality of the original correlated process data while retaining as much as possible the variation present originally. This is achieved by projecting the process data into a lower-dimensional space, where a new set of uncorrelated variables, the principal components, contain most of the variation of the original variables in the first few principal components [23, 30].

Therefore, it can easily handle high dimensional, noisy, and highly correlated data generated from chemical processes, and provide superior performance compared to univariate statistical monitoring methods such as Shewhart, CUSUM, and EWMA charts. In addition, the PCA-based process monitoring methods are attractive because they only require a good historical data set of normal operation, which are easily available for the computer-controlled industrial processes [49]. The stored process data corresponds to different measurement instruments can be utilized to address several aspects. These include monitoring the process over time in order to detect special events (e.g. faults) and assign causes for them [23].

Motivated by all mentioned above, a novel approach for monitoring and fault detection is presented in this chapter to address the challenges associated with fault detection in cyclic processes and the capability of SPA is studied for real industrial PSAs operating in hydrogen manufacturing plants. As it will be demonstrated in chapter four, it provides superior fault detection performance with employing some statistical features. Industrial data from historical PSA failures are used to compare the performances.

3.4 Statistical Features

In order to monitor the process (pressure data in the PSA case), a set of statistics which will be called statistical features (or just features) is needed. These features together make a matrix for each segment in the process which will be considered as the data that explains the characteristics of the corresponding section of the process. With all statistics calculated for the whole cycle (period) the final training matrix is obtained by stacking all features together to build a master matrix. This matrix, which represent normal status of the process since various calculated features obtain different characteristics of the process. Therefore the matrix contains the information of the whole system for a certain amount of time and will be used as training matrix (input matrix for principal component analysis). The features are selected in the way to reveal different type of fault which may be occurred in the system. In other words, one of the statistics may be good enough to capture a certain type of fault. For this work, 11 different statistics are considered. In the following paragraphs all the employed features are presented.

3.4.1 Mean

One of the most useful and simple statistics which is employed as a feature in this study is arithmetic mean. The average of all the points in each step will be the first statistics in the set of features.

3.4.2 Standard Deviation

Standard deviation (SD) is a measurement of variation or dispersion of a dataset and it is the square root of variance. A low standard deviation indicates that the data points tend to be close to the mean of the set, while a high standard deviation indicates that the data points are spread out over a wider range of values [50].

3.4.3. Coefficient of Variation

In probability theory and statistics, the coefficient of variation (CV), also known as relative standard deviation (RSD), is a standardized measure of dispersion of a probability distribution or frequency distribution. It is often expressed as a percentage, and is defined as the ratio of the standard deviation to the mean of a series of data. In other words, it shows the extent of variability in relation to the mean of the population. [51].

3.4.4 Slope

The slope or gradient of a line is a number that describes both the direction and the steepness of the line. Slope is considered as one of our statistics and may be very helpful for detecting fault in the depressurization and repressurization steps because it monitors the rate of change of pressure in each step.

3.4.5 Slope of Linear Regression Line

Slope of linear regression line (SLL) is another type of feature which provides information about the shape of the pressure versus time plot in each certain time interval (step). It is the slope of the best-fit line (linear regression) which is plotted through all the points for each step.

3.4.6 Average of First Derivative in an Interval

Although slope is employed to measure the slope of the curve in each step, average of first derivative (AFD) considers all the points between start and end point of each step. Actually, it is the average of the slope between the first point and all other points in the same step.

3.4.7 Interquartile Range

The interquartile range (IQR), also called the midspread or middle 50%, is a measure of statistical dispersion, being equal to the difference between 75th and 25th percentiles, or between upper and lower quartiles. The IQR is a measure of variability, based on dividing a data set into quartiles. Quartiles divide a rank-ordered data set into four equal parts. The values that separate parts are called the first, second, and third quartiles; and they are denoted by Q_1, Q_2, and Q_3 respectively [52].

3.4.8 Mean Absolute Deviation

The mean absolute deviation (MAD), also referred to as the "mean deviation" or sometimes "average absolute deviation", is the mean of the data's absolute deviations around the data's mean: the average (absolute) distance from the mean. It is a summary statistic of statistical dispersion or variability. The mean absolute deviation of a set $\{x_1, x_2, \ldots, x_n\}$ is [53]:

$$MAD = \frac{1}{n}\sum_{i=1}^{n} |x_i - m(x)|$$

3.4.9 Median Absolute Deviation

In statistics, the median absolute deviation (MAD) is a robust measure of the variability of a univariate sample of quantitative data. For a univariate data set $\{x_1, x_2, ..., x_n\}$, the MAD is defined as the median of the absolute deviations from the data's median [54]:

$$Median\ AD = median(|x_i - \widehat{x}|)$$

3.4.10 Mean Absolute Error

In statistics, mean absolute error (MAE) is a measure of difference between two continuous variables. Assume X and Y are variables of paired observations that express the same phenomenon. The Mean Absolute Error is given by [55]:

$$MAE = \frac{\sum_{i=1}^{n} |y_i - x_i|}{\mathrm{n}} = \frac{\sum_{i=1}^{n} |e_i|}{\mathrm{n}}$$

3.4.11 S_n

It is an estimator alternative to the median absolute deviation which was presented by Rousseeuw and Croux. It was offered because of the fact that median absolute deviation is aimed at symmetric distribution and its low (%37) Gaussian efficiency. As it is reported in the paper authors, the Gaussian efficiency of Sn is %58. It is defined as [56]:

$$S_n = 1.1926\, med_i(med_j(|x_i - x_j|))$$

3.5 Statistics Usefulness

In the proposed SPA framework for fault detection in PSA processes 11 statistical features were introduced. Now it is needed to clarify the reason for selecting the set of statistics. In other words, for a certain type of fault in the system, the degree of contribution of features are not the same and some features are more important than the others. Thus, by dividing all the features into four subsets, the reasons for choosing them are discussed. It is necessary to keep all of them in the set of features to detect different abnormal conditions in the system.

- **Mean related statistics**: Most of the deviations from the normal condition have a detectable effect on mean related statistics like Mean, Mean absolute deviation, Mean absolute error, and Coefficient of variation. If only one point has been changed significantly or several points have been changed abnormally as it is shown in figure 3.1, using mean related statistics would be advantageous. One exception here is oscillation similar to sinusoidal oscillation which cannot be captured by the mean but MAE and CV may still be helpful.

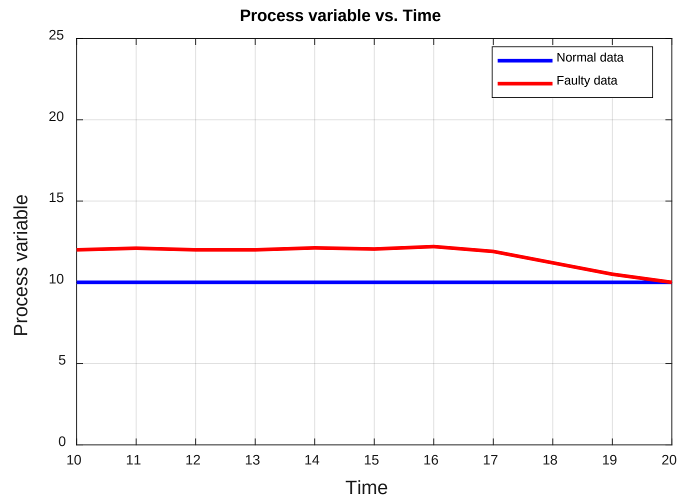

Figure 3.1 Type of an abnormal situation can be captured by mean related statistics

- **Slope related statistics:** These type of statistics are selected for unsteady part of the process. Since the pressure in PSA processes is swing and there are some steps in which the pressure trend is upward or downward slope related statistics like Slope, Slope of linear regression line and Average of the first derivative would disclose any probable deviation from normal pressure trace. For instance, consider a situation in which pressure decreasing in one of the depressurization steps takes more time than usual as demonstrated in figure 3.2. That is an obvious fault in valves and has a notable effect on the slope of pressure trace in the corresponding step. Moreover, in steps with steady pressure, if leakage in valves happens, the pressure will decrease and slope related statistics can detect the fault.

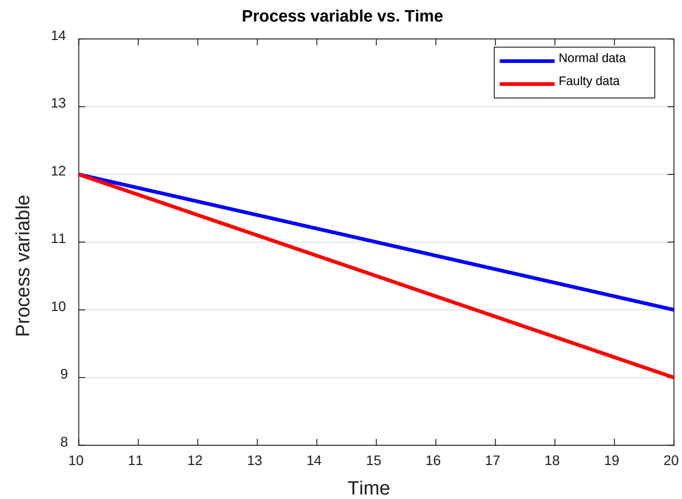

Figure 3.2 Type of an abnormal situation can be captured by slope related statistics

- **Median related statistics:** Median absolute deviation and Sn are useful when a system oscillates or fluctuates around the normal condition of the process. This type of fault in such systems shifts most of the points from their normal situations as it is represented in figure 3.3. Therefore, the median of the dataset would be shifted and the mentioned related features may reveal the fault.

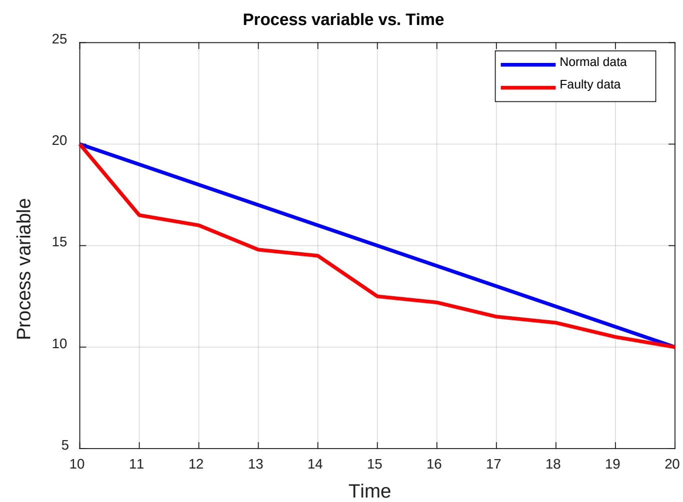

Figure 3.3 Type of an abnormal situation can be captured by median related statistics

- **Standard deviation related statistics:** Standard deviation and mean are the most important and the most employed statistics in statistical analysis. It is used to measure the amount of dispersion or variation in a dataset. For example in one type of fault which is called sinusoidal oscillation and is shown in figure 3.4, mean is not able to detect the fault. But the deviation can be revealed by standard deviation easily.

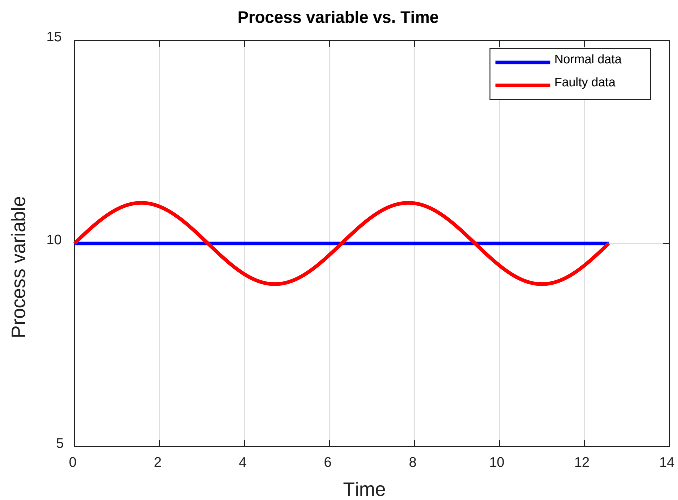

Figure 3.4 Type of an abnormal situation can be captured by standard deviation related statistics

3.6 Proposed Framework

Statistical pattern analysis is a framework for process monitoring which was developed by He and Wang for batch processes [11]. In the framework, statistics of the process variables are used for monitoring rather process variables themselves to perform fault detection. SPA framework provides many advantages in continues and batch processes which have been presented by the mentioned authors [49].

The basic idea of the SPA-based process monitoring is that the process statistics under abnormal conditions would show some deviation from the distribution of the process statistics under normal operation. Therefore, in the SPA framework, the process behavior is characterized by different statistics of the process variables, instead of by the process variables themselves. In other words, the SPA-based fault detection method monitors the variance-covariance structure of the process statistics, instead of the variance-covariance structure of the process variables.

In the last part, all of the statistical features have been introduced. For developing the SPA framework, the whole cycle of the process (for each vessel) is divided into several meaningful segments which are called steps. The proposed framework is employed the mentioned features for each step and build a matrix by putting the eleven features for all of the steps together. For example, for 9 steps (a whole cycle in PSA), the matrix is going to have 99 statistic features. This SPA-based method does not use the raw pressure data but the all the data points (pressure data) are involved in calculating the features and finally build the model. It has been considered a promising framework by author to monitor the state of the PSA process and to address the challenge of fault detection in periodic processes.

3.7 SPA Approach

The major difference between the traditional PCA-based and the proposed SPA-based fault detection methods is that PCA monitors the process variables while SPA monitors various statistics of the process variables. In other words, in PCA singular value decomposition (SVD) is applied to the original process variables to build the model for normal operation, and the new measurements of the process variables are projected onto the PCA model to perform fault detection; while in SPA, SVD is applied to various statistics of the process variables to build the model, and the statistics calculated using the new measurements are projected onto the model to perform fault detection. In this way, different statistics that capture the different characteristics of the process can be selected to build the model for normal process operation [49].

As described in literature repeatedly, variable selection plays an important role in traditional PCA method. Similar to that, variable selection is a key step in the detection performance of the SPA-based methods. Obviously, to select the best set of statistics, some well-defined rules and regulations are needed. So, in order to avoid defining rules and guidelines, which can be a time consuming procedure and it is out of the scope of this study, a set of statistics (features) is employed for different segments of each cycle.

Due to the calculation of different statistics compared to traditional PCA method, the computation load of SPA-based methods is higher, but the calculation of mentioned statistics is not computationally intensive. Therefore, the increase in computation load should not be an issue [49].

In this study, two major steps are involved in the SPA-based monitoring: statistics pattern generation and dissimilarity quantification. For cyclic processes, a statistics pattern is a collection of various statistics calculated for each segment of the process cycle. These segments are defined based on the process characteristics and properties. These statistics capture the characteristics of each individual segment, the interactions among different variables (such as correlation), as well as process dynamics (such as autocorrelation and cross-correlation) [49, 57].

After computing all of the statistics from the training data, the dissimilarities among the training statistics are quantified to determine an upper control limit for defining the normal operating zone. Then, PCA is employed to quantify the dissimilarities between training statistics and test statistics using two detection indices T^2 and SPE. In the PSA case study, just one of the indices is helpful and the reason behind that will be explained in the next chapter.

3.8 Modeling Based on the Proposed Method

In previous paragraphs, the advantages and disadvantages of PCA-based model were discussed. In this study, statistical pattern analysis is employed to address the disadvantages of using PCA and challenges of process monitoring in periodic (cyclic) processes. This fault detection methodology consists of two major stages. The first stage is preparing a master matrix contains features for all of the defined segments of the process which is based on the proposed SPA framework. The other one is making a model based on the training master matrix which will be used to define the normal operating zone and dissimilarity quantification. After detecting dissimilarities, contribution plots will be employed to find the abnormal part of the process. Figure 3.1 demonstrates the schematic of the step by step procedure for fault detection in periodic processes.

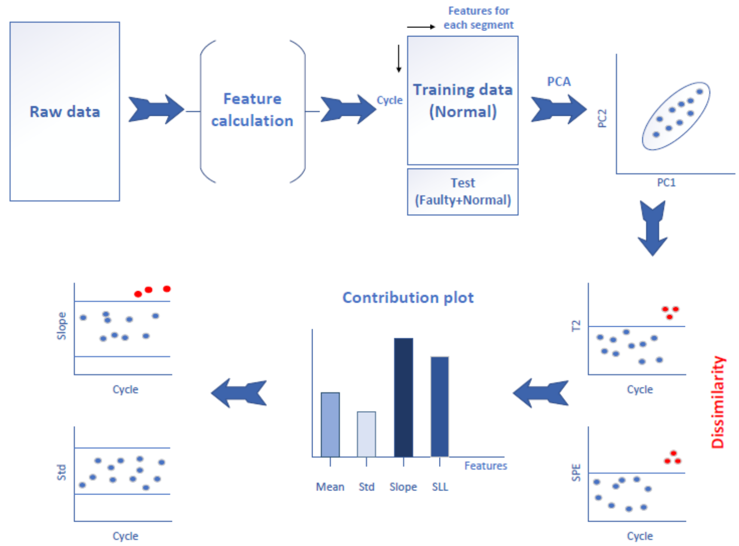

Figure 3.5 Schematic of the step by step procedure for fault detection in periodic processes

Chapter 4

Case Study

In chapter 3, the proposed method was discussed. To show the potential of the methodology, a pressure swing adsorption plant is chosen as a case study to perform fault detection. Using real industrial data, provided by the industrial partner, brings a great opportunity to exhibit the superb performance of the proposed method. Although in this work the application of the method in the offline analysis is accomplished, it can be definitely applied for online analysis and monitoring with taking some considerations which are out of the scope of the present study. In this case study, monitoring is based on pressure data which is collected every second for 12 vessels in a PSA plant. It should be noted that the data for about two days are used to calculate the mentioned features and build a model.

4.1 PSA Fault Detection Pipeline

Step by step procedure of the proposed approach is presented in PSA fault detection pipeline in figure 4.1. It begins with data preprocessing which is mainly auto-scaling. So, all the data is subtracted by mean of the data and after that divided by the standard deviation of the operation data. In this way, the operation data will have zero mean and unit variance. The next step is feature extraction. All the statistics are calculated in this stage for every segment. Hence, at this point, all the segments in each cycle should have been defined. Then, the master matrix of the training set is built by stacking statistics of a certain number of cycles in the matrix. The feature matrix for the testing set is built in the same way as the training set using a combination of normal and faulty operation data.

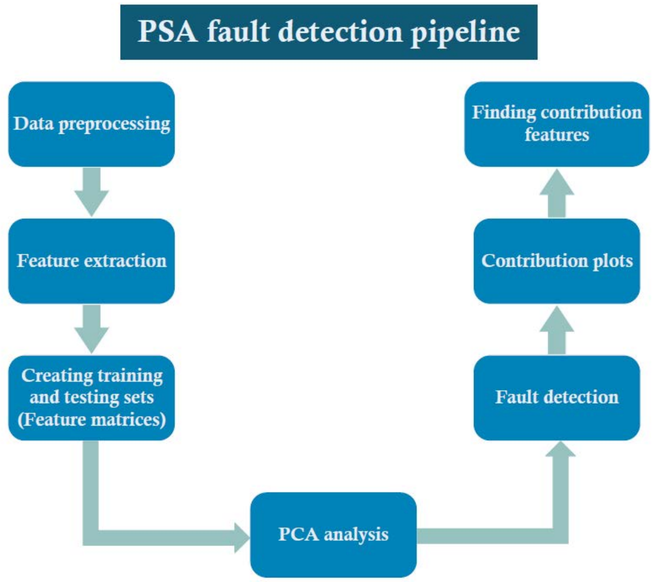

Figure 4.1 PSA fault detection pipeline

Now, everything is ready for performing PCA and finding dissimilarities. As a result of PCA, T^2 or SPE plots will disclose fault in the dataset by revealing discrepancies between normal and abnormal (faulty) data. Then, by generating contribution plots the exact faulty segment of each abnormal cycle of the process will be revealed.

4.2 Different Types of Fault

Since this work is a collaboration with industry, it was a great opportunity to work with real industrial data and real problems which usually happen in a PSA plant. Therefore, the faults will be presenting in the next paragraphs are real faults which operators are dealing with, in abnormal situations. Provided faults are simulated and tried to be as analogous to real ones.

- **Adsorption pressure drifting**: It happens in adsorption step (first segment of a cycle) and it is related to the pressure of a vessel in adsorption step. In this type of fault, a vessel may be working under or above of a reference pressure. The reference pressure is defined as the average pressure of all other vessels in the plant in the adsorption step. Figure 4.2 represents the abnormal situation for several cycles. It should be noted that due to the industrial partner's policy the pressure and time data is omitted intentionally in all of the Pressure-Time plots.

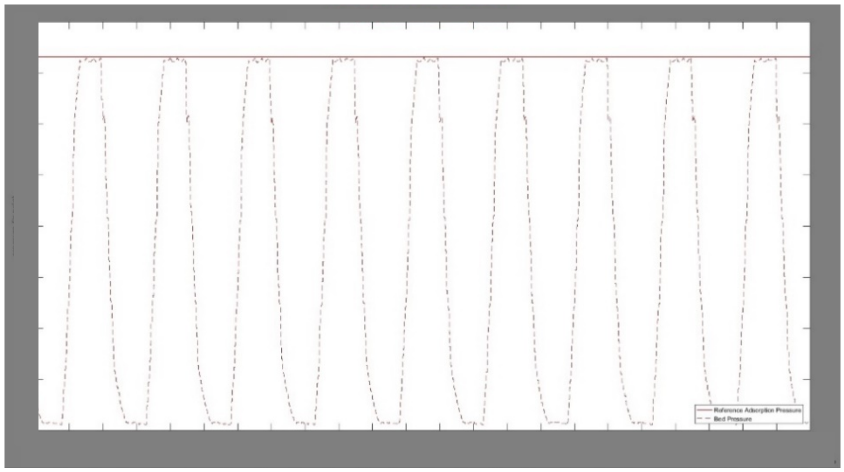

Figure 4.2 Adsorption pressure drifting

- **Pressure profile mismatch**: This abnormal situation occurs in unsteady segments when the pressure is being changed either increasing or decreasing. If the pressure profile is not matched with the reference profile in pressurization or depressurization segments, a very clear discrepancy will be distinguished. The mismatch in pressure profile is shown in figure 4.3 for one pressurization section.

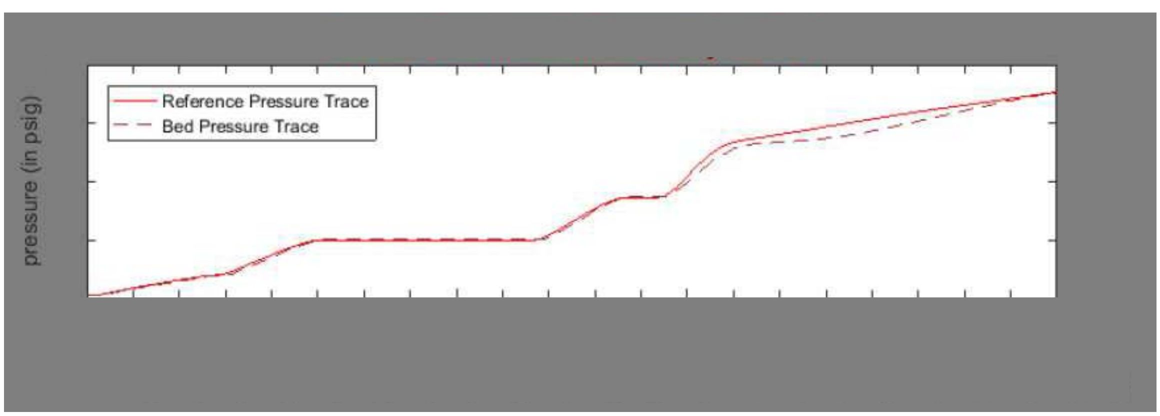

Figure 4.3 Pressure profile mismatch

• **Pressure fluctuation**: This is another type of fault which takes place during the adsorption step or purge step. As it was presented before, the pressure in the steady steps is supposed to stay constant, but as it is clear in figure 4.4 the pressure fluctuates around the actual pressure for one adsorption step. These unusual oscillations can be considered as a fault.

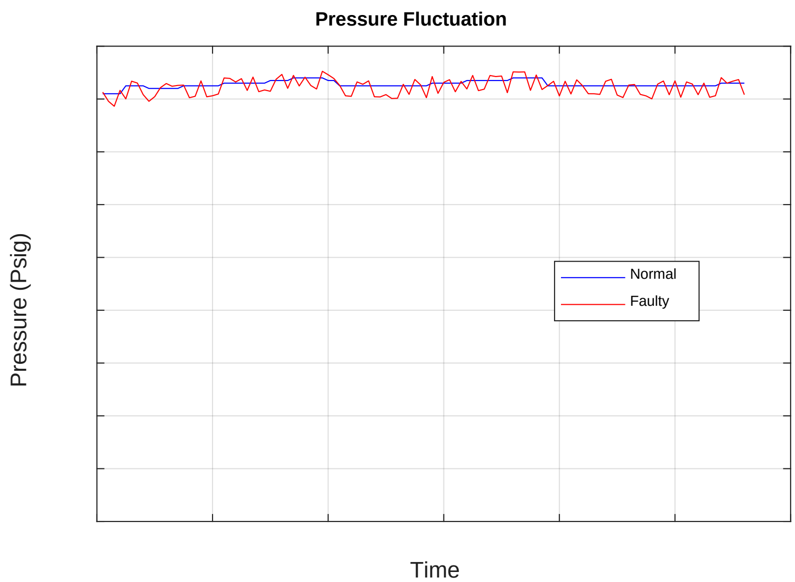

Figure 4.4 Pressure fluctuation

• **Sudden pressure drop**: If during repressurization or depressurization of a vessel some harsh and sudden increase or decrease in pressure happens, there must be an issue with equalization valves and it is considered as a fault. Figure 4.5 illustrates the fault (in a depressurization part of a cycle) which is called sudden pressure drop.

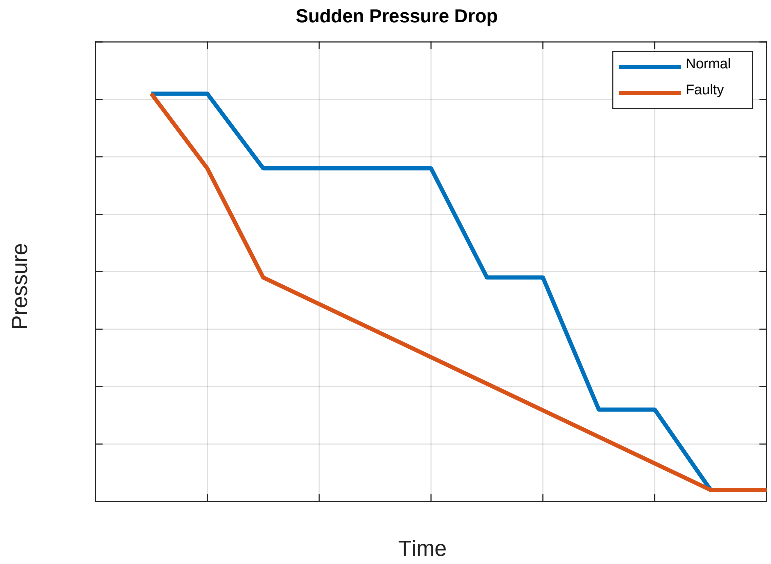

Figure 4.5 Sudden pressure drop

4.3 Fault Visualization

Fault visualization is performed to make a good picture of simulated faults beside normal data. The aim of visualization is not performing fault diagnosis as it is used by process engineers. These are the main issues in abnormal situations that operators deal with them in the PSA process. Most of the reasons of mentioned problems are valve malfunction (e.g. leakage in the valve, late closing, etc.) in the process. In figures 4.6 to 4.8 mentioned simulated faults are plotted along normal situation to demonstrate the discrepancies between normal and abnormal status of the PSA process. It should be noted that except pressure fluctuation, there are two types for other faults. One is related to the situation that a vessel is working above the normal pressure and the other one below the normal pressure as can be realized.

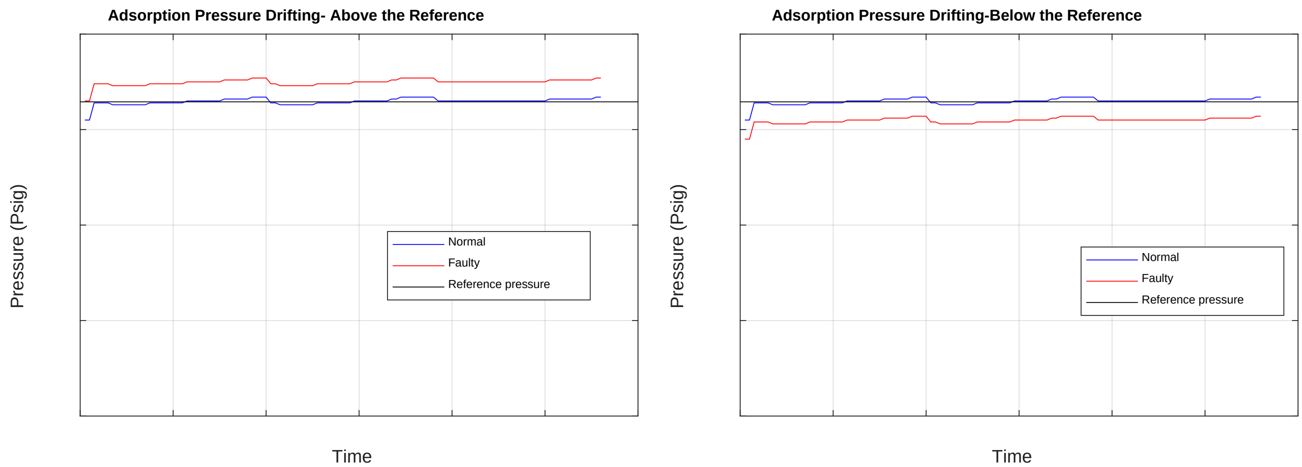

Figure 4.6 Adsorption pressure drifting-above and below the reference

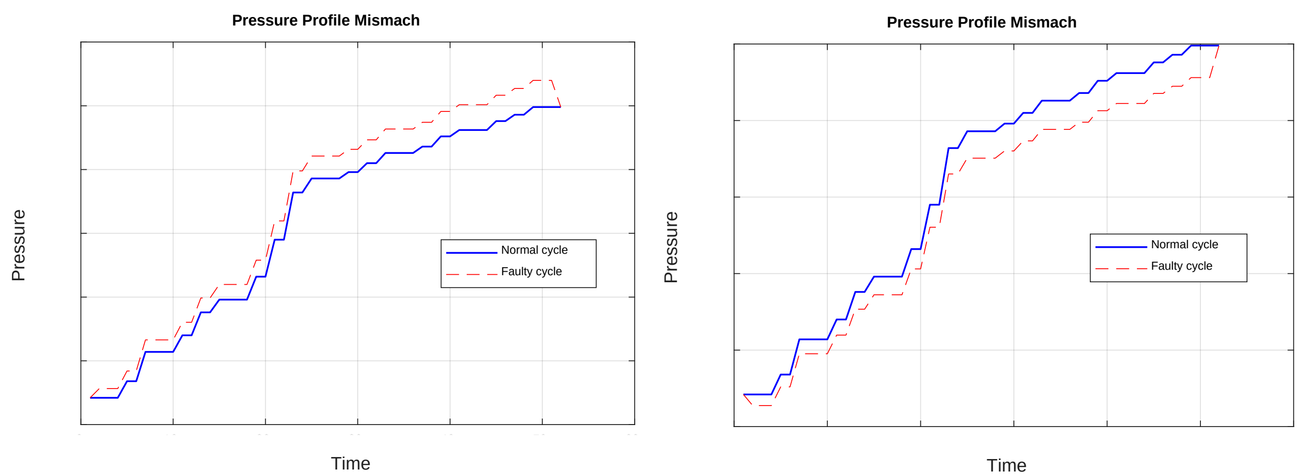

Figure 4.7 Pressure profile mismatch-above and below the normal condition

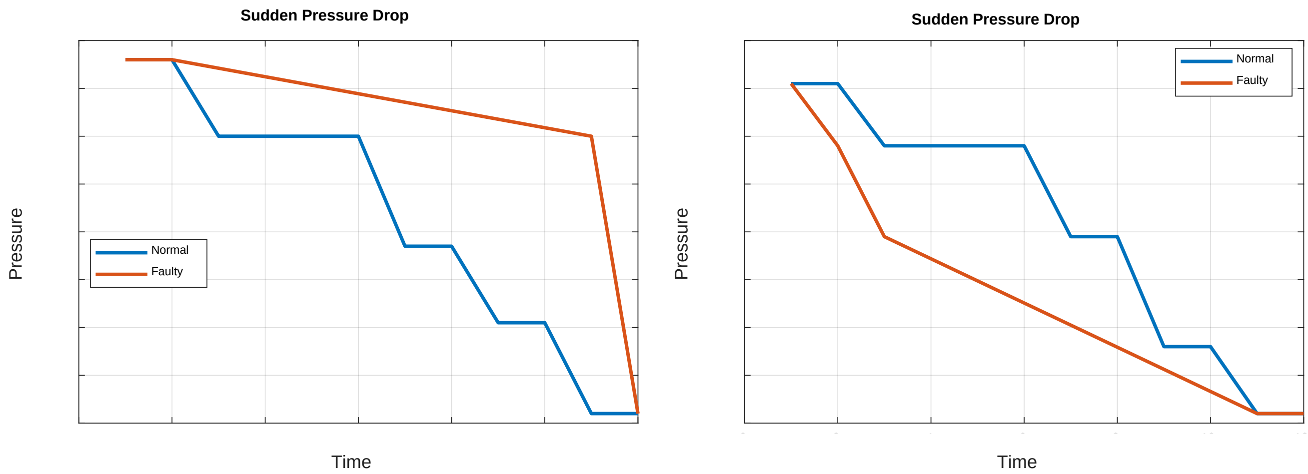

Figure 4.8 Sudden pressure drop-above and below normal condition

4.4 An Overview of a Normal Cycle

Before presenting fault detection results and exhibiting the performance of SPA based approach, it would be a great idea to picture an overview of a repetitive cycle of the PSA process. In figure 4.9 all different steps (segments) of a single cycle are tagged. All of the mentioned faults are intentionally introduced into these steps for detection and diagnosis purposes.

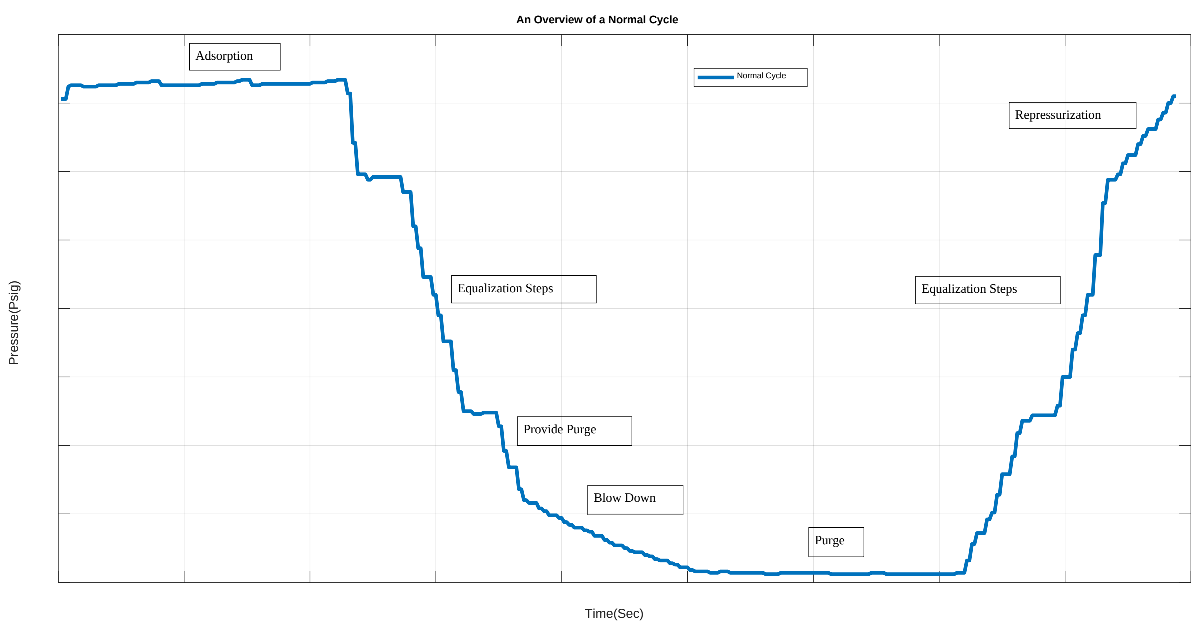

Figure 4.9 An overview of a normal cycle

4.5 Threshold Lines and False Alarm Rates

As mentioned before, for capturing abnormal situation, T^2 and SPE indices are employed separately as detecting indices which are calculated on the model of PCA. So, it is needed to define a normal region for them to capture discrepancies. If an observation violates the defined control limit (threshold line) and locates far off the model plane then it is inconsistent with the model, indicating an issue with the process, and can be recognized as a fault.

After calculation of statistical features from the training data, the dissimilarities among the training features are quantified to determine an upper control limit of the detection indices [49]. The way of defining the threshold line for T^2 and SPE indices has a great impact on the false alarm rate. Similar to any other process monitoring and fault detection approach, it is desired to reduce the rate of false alarms to a certain low level. For this study, the threshold lines for monitoring are determined using the empirical method by the normal validation data as suggested in the literature [58, 59]. The confidence level is set to 99% which enables the approach to reach not more than 1% false alarm which is great in the industrial scale.

4.6 Training and Testing Sets

As mentioned earlier, for performing the principal component analyses two sets of data is required, training and testing sets. After statistical features are computed from the process variable dataset (in this case pressure of the PSA vessels) and lumped into a master matrix, the input matrix for PCA is ready. A model is built based on training set for performing the quantification of dissimilarities between training and testing sets. Then the model for normal process operation is able to indicate any probable dissimilarity by comparing feature in testing and training datasets. Testing set usually consists of normal and faulty data. In the next paragraphs, the performance of the proposed approach in capturing the simulated faults is demonstrated. For crafting the model by PCA, a training set of 260 cycles of normal data is employed. Moreover, a combination of 20 normal cycles followed by 20 faulty cycles create the testing set (extracted from the same vessel).

4.7 Dissimilarity Quantification

After all the statistical features are computed and the training and testing master matrix are obtained, a modeling phase is followed. This model prepared by PCA (using training set) is utilized to quantify the dissimilarities of training and testing datasets. Quantification of dissimilarities in PCA is being performed by distance-based metrics like SPE and T^2 separately. The major difference between the traditional PCA-based methods and the proposed approach is that PCA observes the process variables, while the SPA based approach tracks different type of statistical features of the process variables. As noted earlier, these statistics gain the characteristics of the normal process condition and therefore, various features are being involved in creating the model. Consequently, any deviation from normal status of the process (which is in the testing set) will be revealed by dissimilarity indices.

4.8 Fault Detection Step

As pointed out earlier, for performing the principal component analyses two sets of data is required, training and testing sets. After statistical features are computed from training data (which consists of normal data) and lumped into a master matrix, the input matrix for PCA is ready. A model is built based on training set for performing the quantification of dissimilarities between training and testing sets. Then the model for normal process operation is able to indicate any probable dissimilarity by comparing features in testing and training datasets. Testing set usually consists of normal and faulty data. In the next paragraphs, the performance of the proposed approach in capturing the simulated faults is demonstrated.

4.9 Fault Diagnosis Using Contribution Plots

It is desired to know which statistical feature in the testing set, is most related to the deviation off the model. Thus, it is significantly important to generate contribution plots when PCA is used for dissimilarity quantification [31]. It should be noted that for each case (type of fault) a plot of detection index and a corresponding contribution plot will be presented. Hotelling's T^2 and SPE can detect an out of control situation precisely, but they are not able to reveal which feature deviates from normal condition. Therefore, the importance of using contribution plots for fault diagnosis purposes is indisputable. In literature these plots are well known and beneficial for fault diagnosis based on PCA [60, 61, 35], since they break down the SPE and Hotelling's T^2 into each element (individual terms) related to the contribution from of each statistics in this work.

Contribution plots are very easy to generate with no prior process knowledge. Contribution plots show the contribution of each process variable to the observed statistic, that is, SPE or T^2. It is assumed that the process variable with the high contribution is likely the root cause of the fault. However, the contribution plots may not explicitly identify the cause of an abnormal condition [61], and sometimes may lead to incorrect conclusions [59]. Therefore, some new fault diagnosis methods like a method using fault directions in Fisher Discriminant Analysis (FDA) have been suggested in the literature [59]. It needs to be mentioned that despite some of the shortcoming of using the contribution plots, the results of employing them for diagnosing faults show that they are precise and helpful in this study.

4.10 Detection and Diagnosis the Results in Simulated Faults

In this sections, the results of the analysis and detecting the mentioned simulated faults based on the proposed approach are presented. Then for better understanding the effect of simulated faults on the statistical features and more importantly fault diagnosis,, the result of contribution plots of detection indices are discussed.

4.10.1 Detecting Pressure Drifting in Adsorption Step

According to section 4.2, if a vessel in the adsorption step works above or below the reference pressure, it can be considered as a fault. For the two types of the fault, 3.5 Psig pressure deviation from the reference pressure is considered to introduce the fault as it was presented in figure 4.6. In figure 4.10 and figure 4.11 the detection performance of the proposed approach using SPE or Hotelling's T^2 indices for training and testing sets are presented respectively. In these plots, all 300 samples (cycles) are lumped together to make a better pictorial understanding in the way that first 260 cycles are normal cycles in training set and first 20 cycles after dashed line are normal cycles in the testing set. Obviously, the rest of them (last 20 cycles) are cycles with simulated pressure drifting fault.

As it can be deduced from plots of detection indices, SPE index can easily detect the fault since the threshold line is violated by all of the faulty cycles. But, Hotelling's T^2 is not able to reveal the fault as the fault is introduced to the last 20 cycles intentionally.

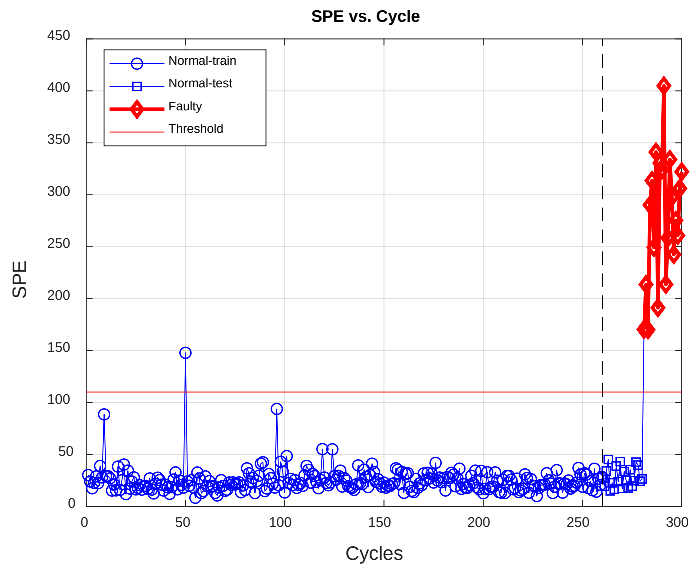

Figure 4.10 SPE index for adsorption pressure drifting (above)

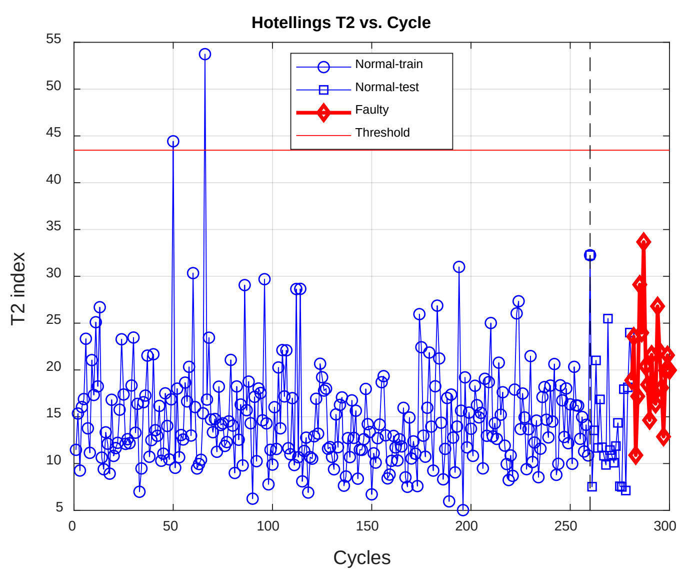

Figure 4.11 Hotelling's T^2 index for adsorption pressure drifting (above)

Figure 4.12 and figure 4.13 demonstrate contribution plots to detection indices respectively. In these plots, each step is separated by a dashed line from the next step. Higher bars have greater contributions in the corresponding index. For example, in figure 4.12 MAE for the adsorption step has the greatest contribution in SPE index. Since the contribution to Hotelling's T^2 index is very low compared to contribution to SPE and most of the bars are relatively in the same range, nothing meaningful can be inferred from the contribution to Hotelling's T^2. In other words, based on the magnitude of the contribution of features to T^2 index, which are close to zero, the results of contribution to T^2 index is meaningless and uninterpretable. Consequently, Hotelling's T^2 index is less informative for detecting pressure drifting in adsorption step.

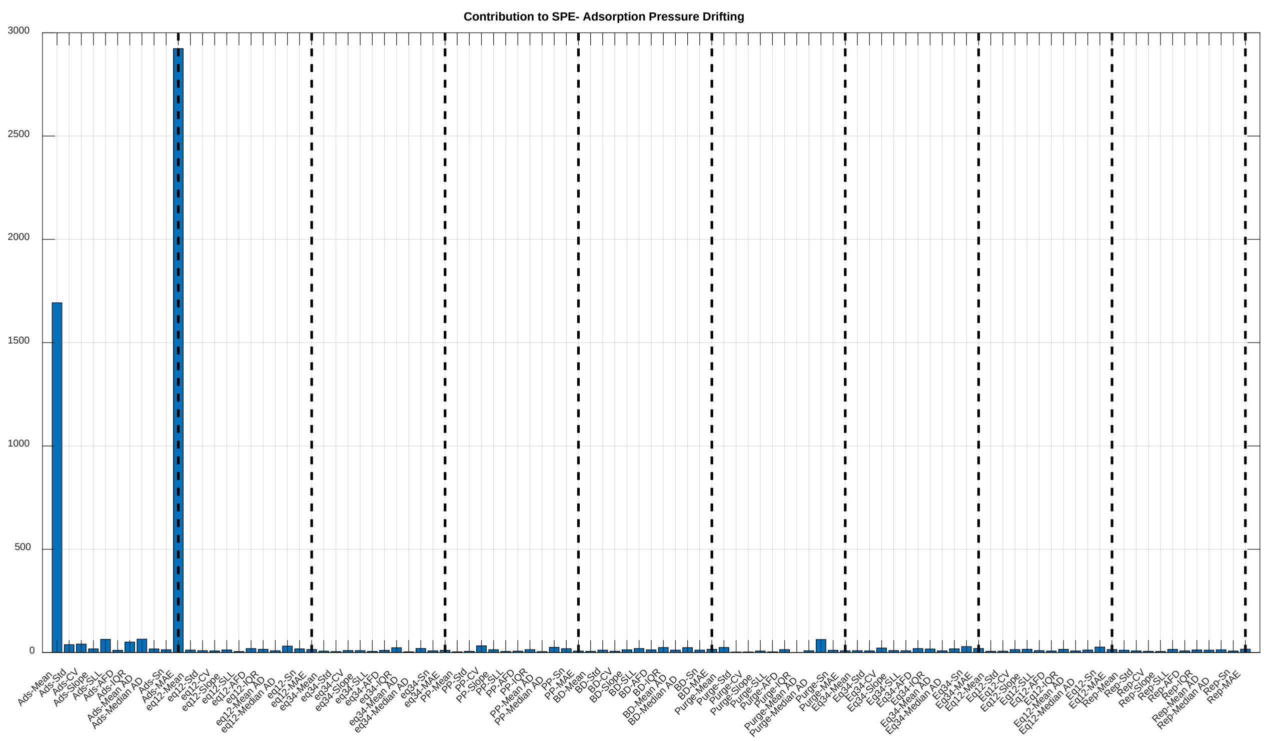

Figure 4.12 Contribution to SPE for adsorption pressure drifting (above)

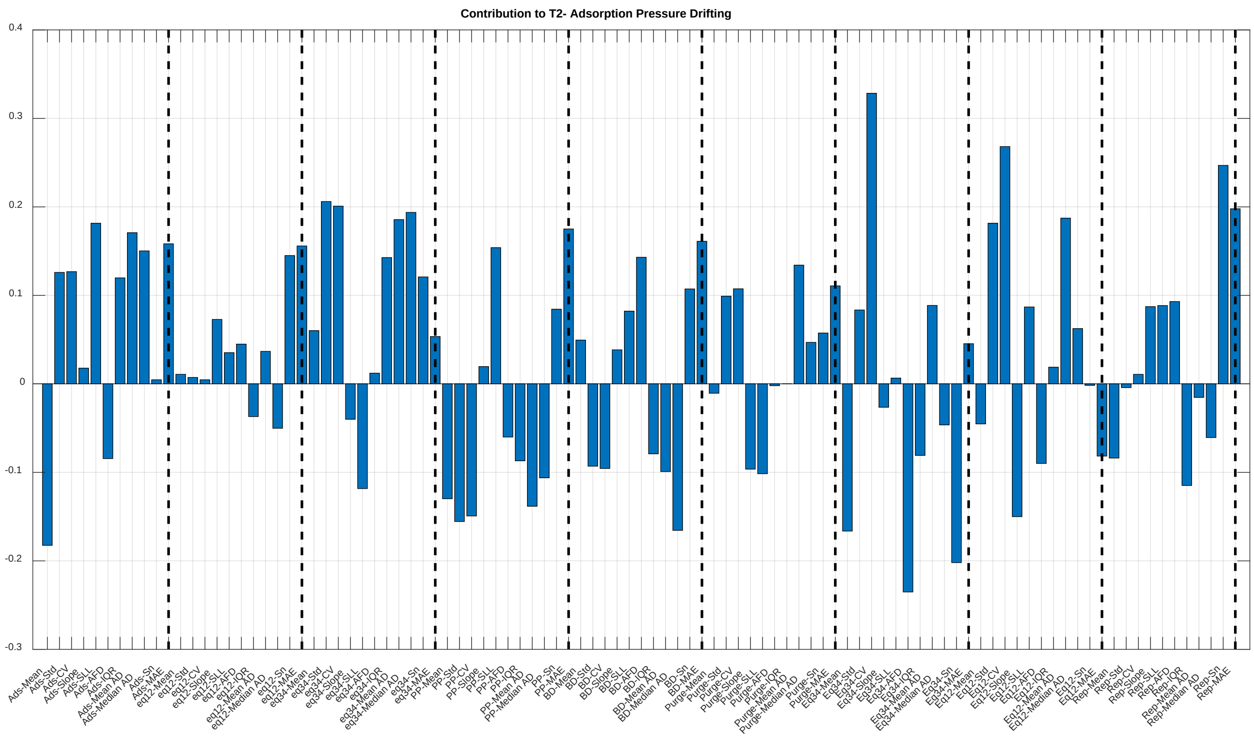

Figure 4.13 Contribution to T^2 for adsorption pressure drifting (above)

Figure 4.14 shows the step-wise contribution of features to SPE index. As it is demonstrated in section 4.4 a normal cycle consists of 9 different steps. In the step-wise contribution plots, the contribution of each step to SPE or Hotelling's T^2 indices is assessed. The height of each bar in the step-wise is the summation of all 11 features of the corresponding step. In the first case (adsorption pressure drifting), adsorption is the highest bar since the fault is simulated into the adsorption step. Hence, the proposed approach is helpful to capture this type of fault.

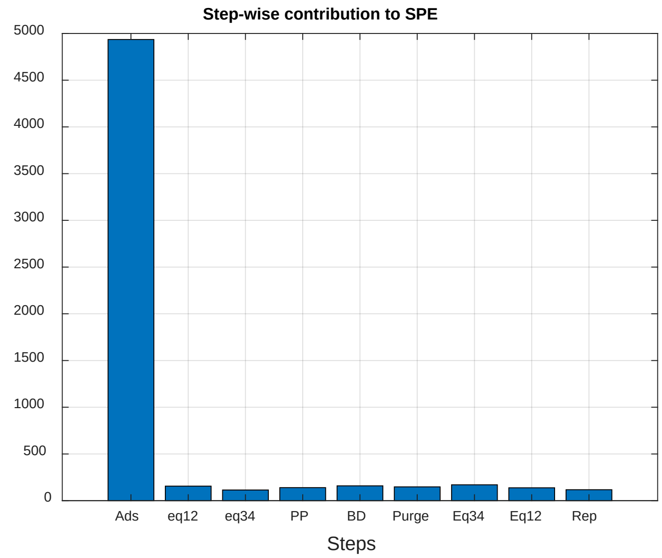

Figure 4.14 Step-wise contribution to SPE for adsorption pressure drifting (above)

Figure 4.15. indicates the degree of association of features in adsorption step with the deviation off the model. As it can be seen, MAE and Mean have higher contribution to SPE index among all of the employed statistics.

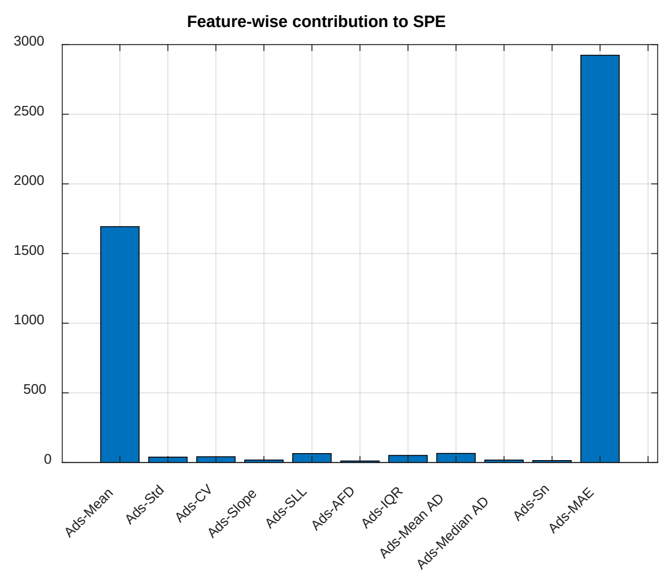

Figure 4.15 Feature-wise contribution to SPE in adsorption step

4.10.2 Detecting Pressure Profile Mismatch in Repressurization Step

As it was shown in figure 4.3, if the pressure profile, whether in pressurization or in depressurization, deviates from the reference pressure profile, the PSA system can be experiencing a common type of fault. The detection analysis of this type of fault, which is introduced into repressurization step, is reported in figure 4.16 and figure 4.17 by using SPE and Hotelling's T^2 indices respectively. In these plots, all 300 samples (cycles) are lumped together to make a better pictorial understanding in the way that first 260 cycles are normal cycles in training set and first 20 cycles after dashed line are normal cycles in the testing set. Obviously, the rest of them (last 20 cycles) are cycles with the simulated pressure profile mismatch fault.

As it can be inferred from plots of detection indices, SPE index perfectly detects the fault since the upper control limit line is violated by all of the faulty cycles. But, Hotelling's T^2 is not able to reveal the fault as the fault is introduced to the last 20 cycles intentionally.

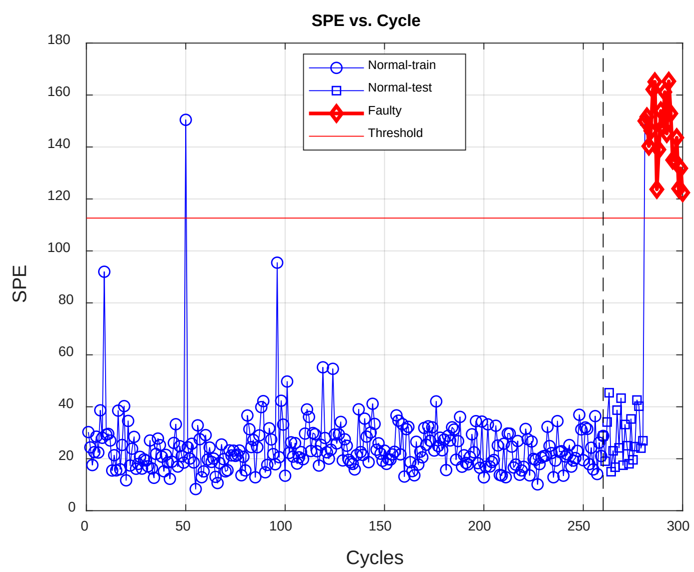

Figure 4.16 SPE index for pressure profile mismatch

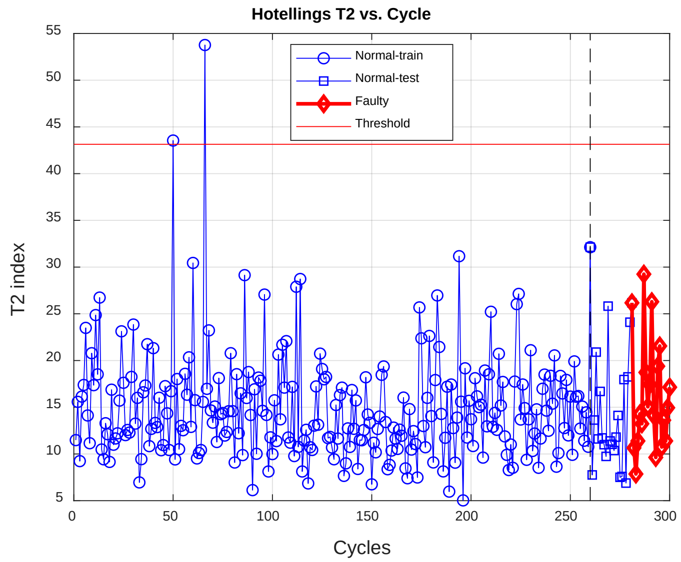

Figure 4.17 Hotelling's T^2 index for pressure profile mismatch

Contribution plots to detection indices are presented in figure 4.18 and figure 4.19 respectively. In these plots, each step is separated by a dashed line from the next step. In the last segment, which is related to the repressurization step, Mean has the highest bar; it means Mean has the greatest contribution in the SPE index. Since the contribution to Hotelling's T^2 index is very low compared to contribution to SPE and most of the bars are relatively in the same range, nothing meaningful can be inferred from the contribution to Hotelling's T^2.

Based on the results of Hotelling's T^2 index in section 4.10.1 for adsorption pressure drifting and outcomes of figure 4.17 and figure 4.19, it seems that Hotelling's T^2 index is not as effective as SPE index for fault detection in the PSA process. As it is mentioned before, based on the magnitude of the contribution of features to T^2 index the results of contribution to T^2 index is meaningless and uninterpretable. The reason behind that will be discussed later. Accordingly, for the rest of the faults, the performance of the SPE index will be considered.

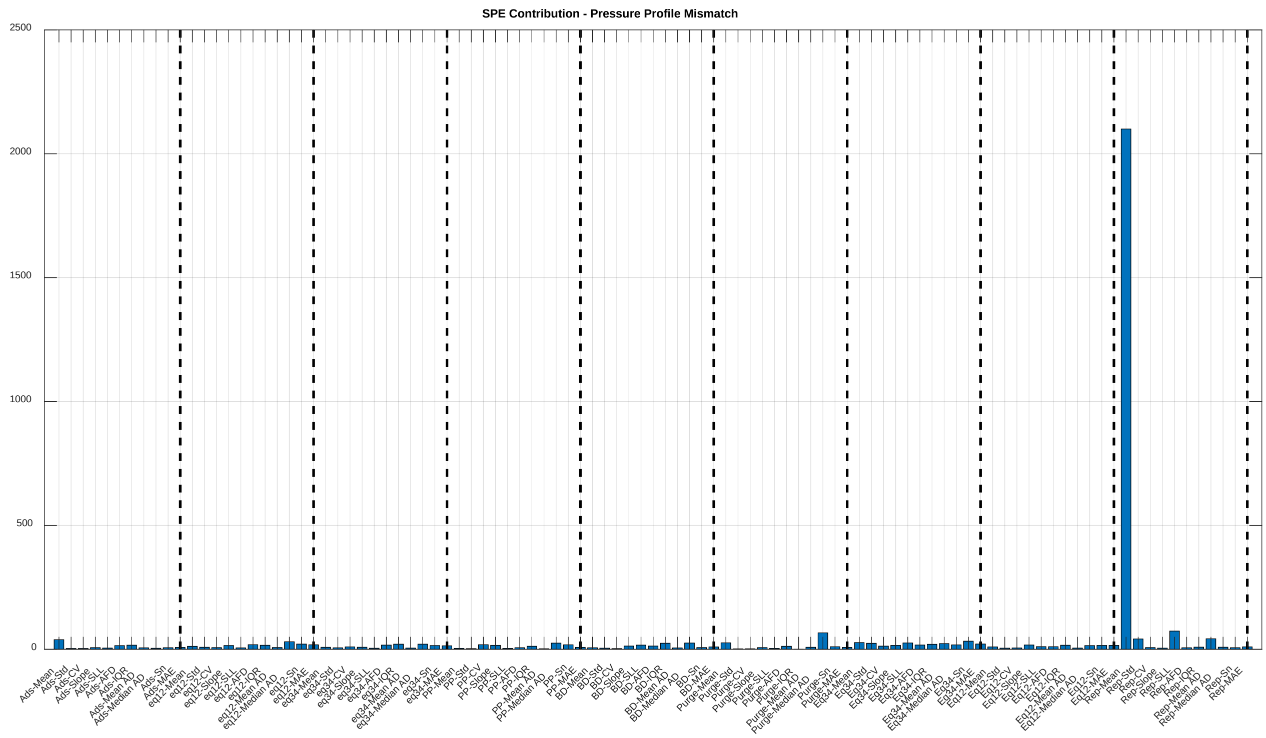

Figure 4.18 Contribution to SPE for pressure profile mismatch (below)

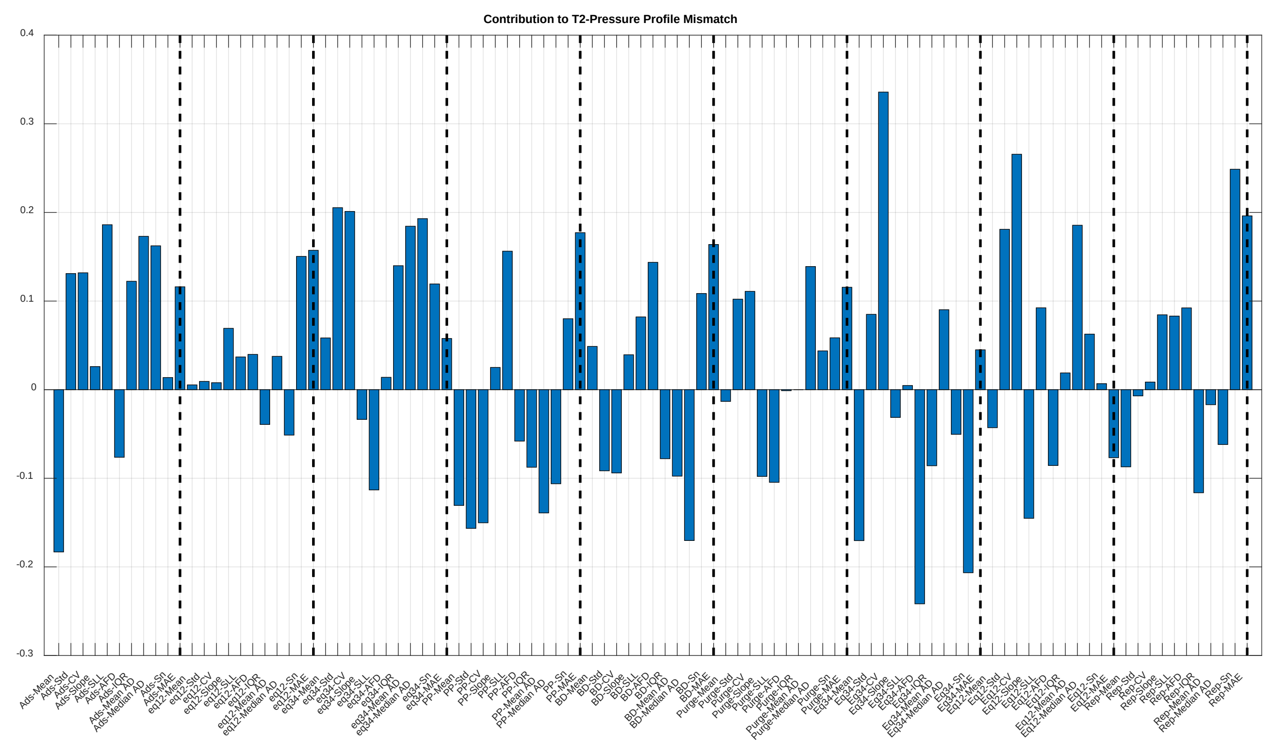

Figure 4.19 Contribution to T^2 for pressure profile mismatch (below)

Step-wise contribution to SPE index is presented in figure 4.20. As the fault is introduced to the last step of the cycle, repressurization step, it is expected to have higher bars in this graph for the corresponding step. The result in figure 4.20 is in a good agreement with what has been simulated as fault.

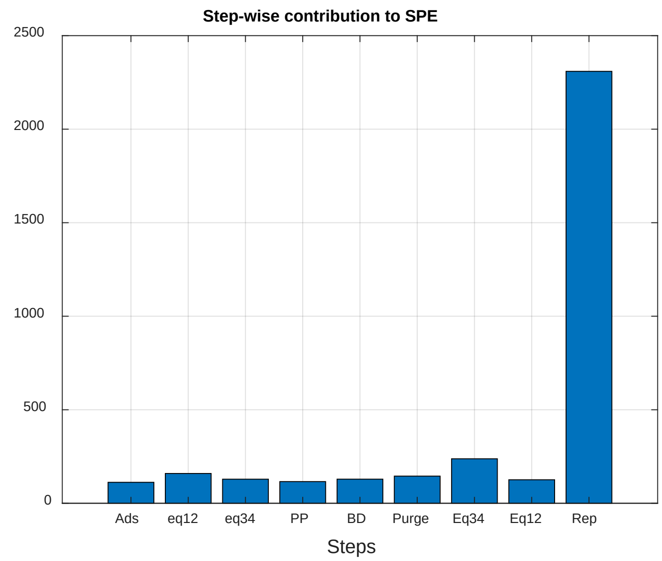

Figure 4.20 Step-wise contribution to SPE for pressure profile mismatch (below)

Figure 4.21. shows the degree of contribution of each feature in reppressurization step with the deviation off the model. As it can be seen, Mean has the highest contribution to SPE index among all of the employed statistics.

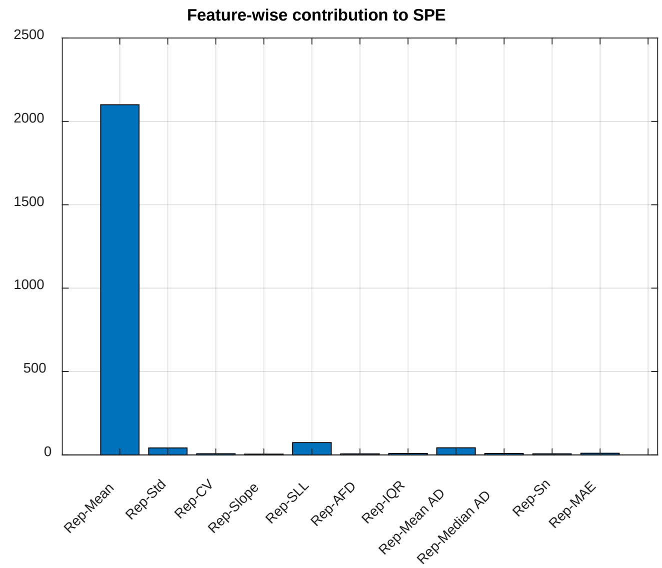

Figure 4.21 Feature-wise contribution to SPE for pressure profile mismatch (below)

4.10.3 Detecting Pressure Fluctuation in Adsorption Step

According to section 4.2, in the steady steps like adsorption and purge steps, the pressure is supposed to be constant. Any probable pressure fluctuation in these steps, due to valve malfunction, has an adverse effect on product quality and can be considered as a fault. In figure 4.22 the detection performance of the SPA based approach using SPE index is presented. Combination of training and testing sets are the same as what is used for the analysis of pressure drifting described in section 4.10.1.

As it can be concluded from plots of SPE detection index, SPE correctly detects the fault since threshold line is violated by all of the faulty cycles.

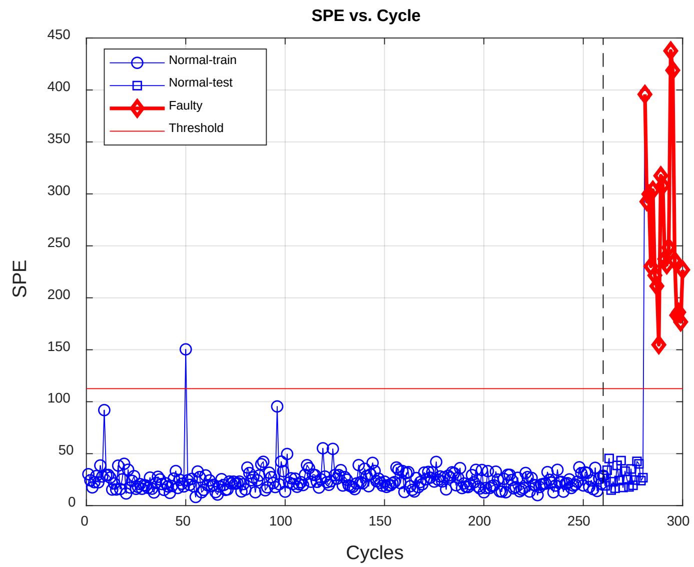

Figure 4.22 SPE index for adsorption pressure fluctuation

Figure 4.23 illustrates contribution plot to SPE detection index. As it mentioned before, each step is separated by a dashed line from the next step. Higher bars have greater contributions in the corresponding index. For example, in figure 4.23 MAE for the adsorption step has the greatest contribution in SPE index.

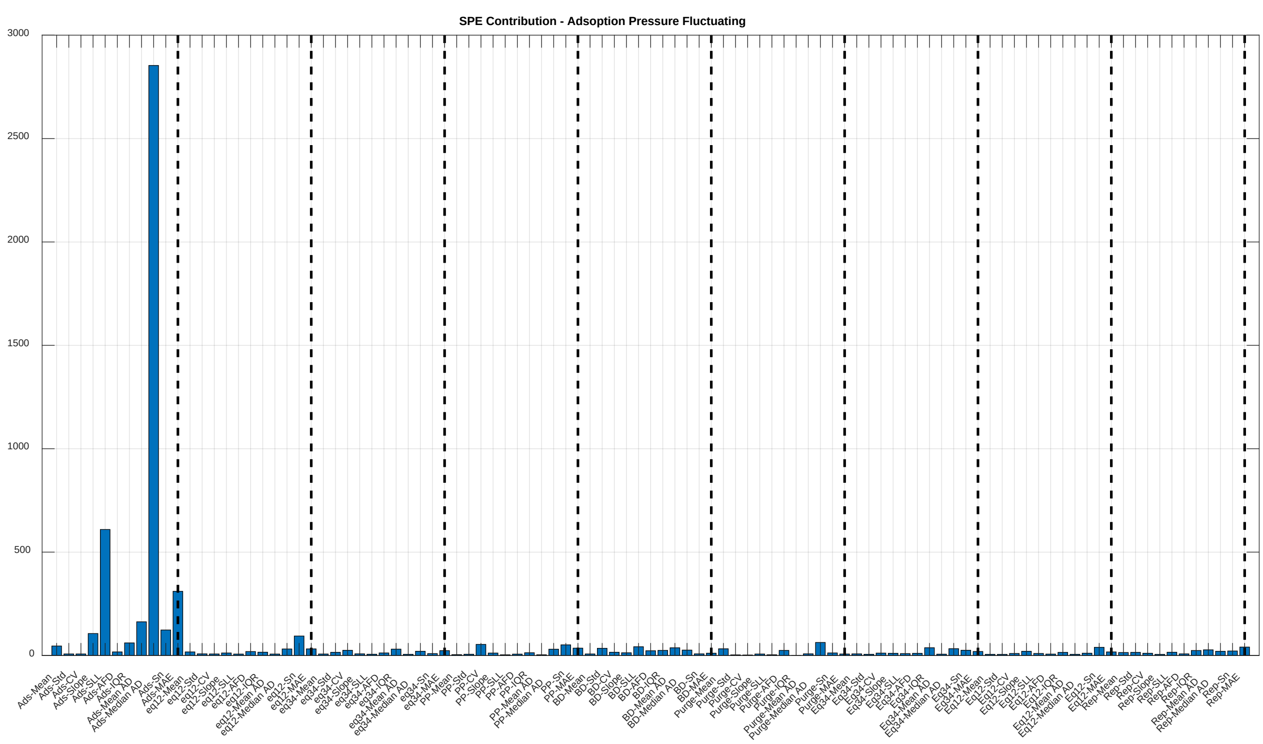

Figure 4.23 Contribution to SPE for pressure fluctuating

Figure 4.24 and figure 4.25 show the step-wise and feature-wise contribution to SPE index respectively. As it can be found out from the step-wise contribution plot, adsorption step has the greatest contribution to SPE index since the pressure fluctuation has been introduced into that step. According to the feature-wise plot, Median AD has the greatest contribution to capture the simulated fault.

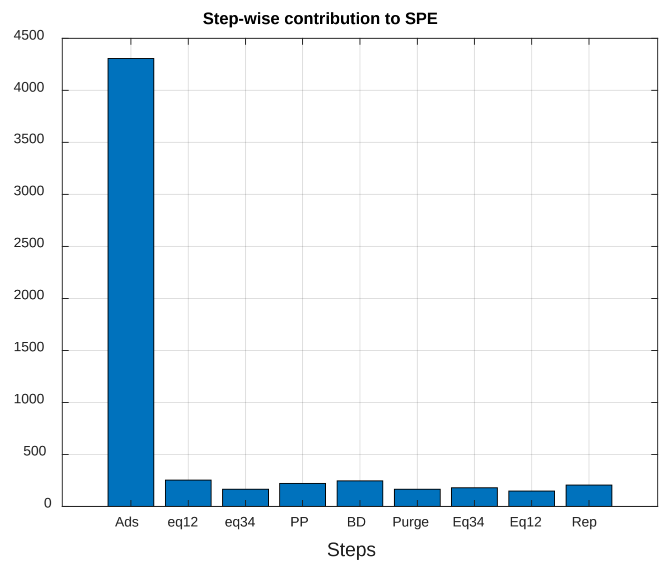

Figure 4.24 Step-wise contribution to SPE for pressure fluctuation

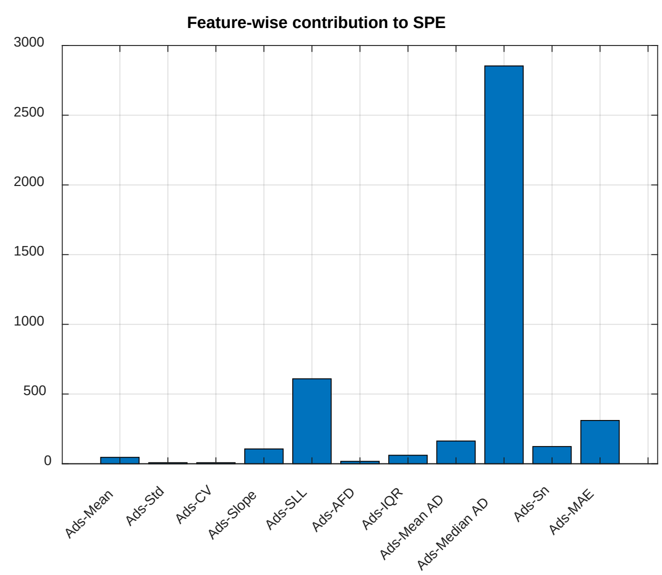

Figure 4.25 Feature-wise contribution to SPE for pressure fluctuation

4.10.4 Detecting Sudden Pressure Drop in Blowdown Step

As it was shown in figure 4.5, any sudden pressure decrease in depressurization steps in the PSA system can be called a sudden pressure drop which is a fault due to valve malfunction. The detection analysis of this type of fault using SPE index is reported in figure 4.26. Combination of training and testing sets are the same as what is used for the analysis of pressure drifting described in section 4.10.1. Again for this type of fault, SPE index exhibit a great performance since all the faulty cycles violate the upper control limit line in figure 4.26. It should be mentioned that number of principal components for all faults are considered 15 PCs which provides variance total captured around 75-80%. Using scree plot in figure 4.27, variance captured by the first 15 PCs is almost 75% and by increasing that to 20 PCs variance captured would be around 80%. In terms of accuracy in fault detection and diagnosis, which is the center of interest in this work, 15 PCs seems sufficient in order to capture the variability in the dataset.

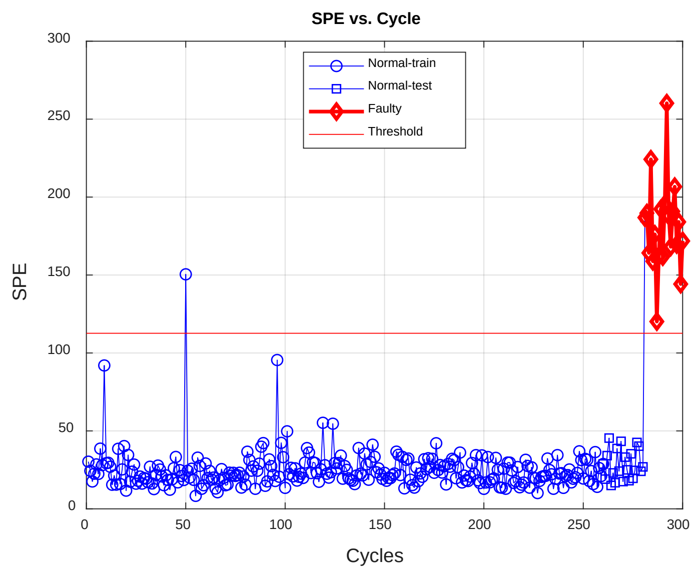

Figure 4.26 SPE index for sudden pressure drop (below)

Contribution plot to SPE index is presented in figure 4.28. Right in the middle of the plot, which is related to the blowdown step, higher bars compared to other steps can be observed that indicates which features are associated with the deviation off the model the most.

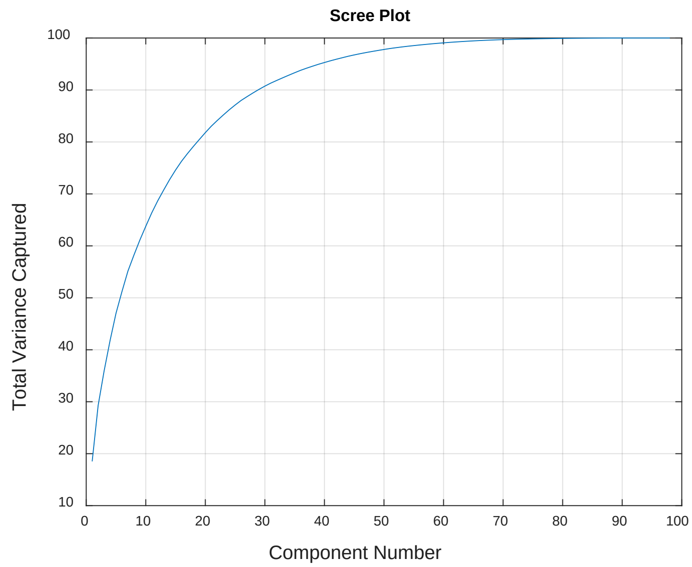

Figure 4.27 Scree plot

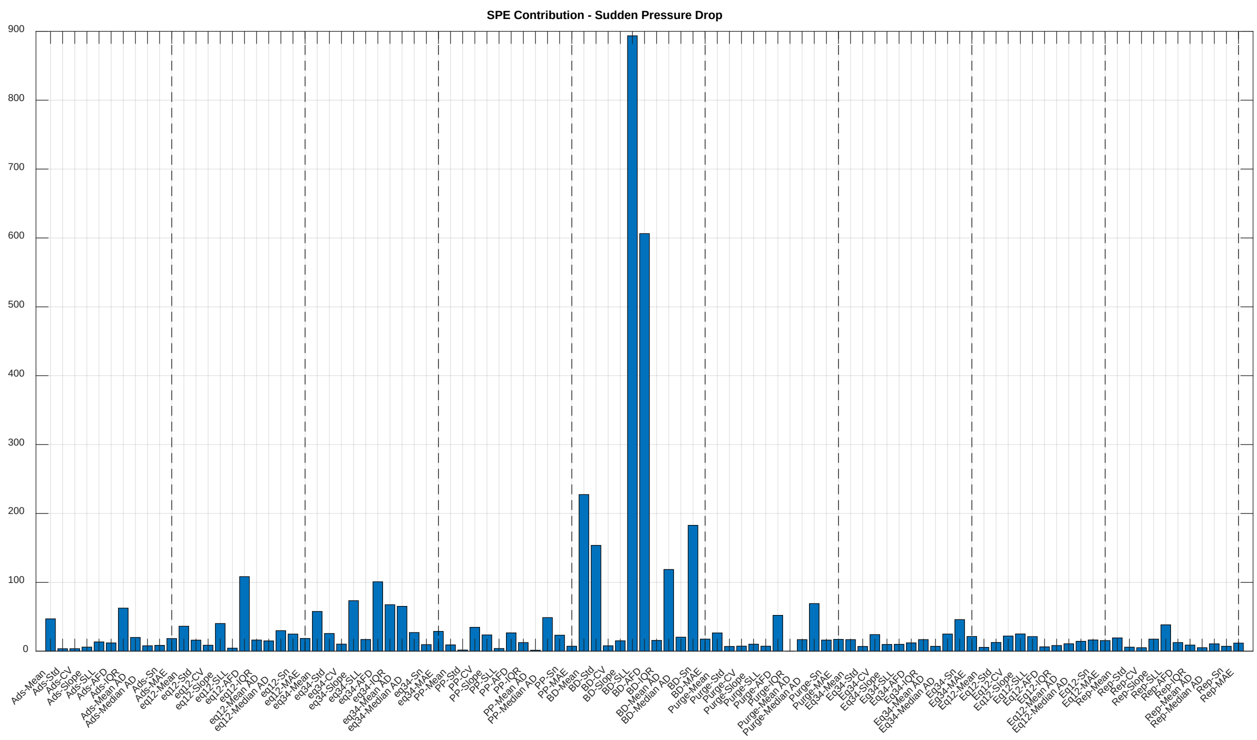

Figure 4.28 Contribution to SPE for sudden pressure drop (below)

Step-wise contribution to SPE index is reported in figure 4.29. As the fault is introduced to the blowdown step in depressurization part of the cycle, it is expected to see higher bars in this graph for the blowdown step compared to other steps that are in normal condition.

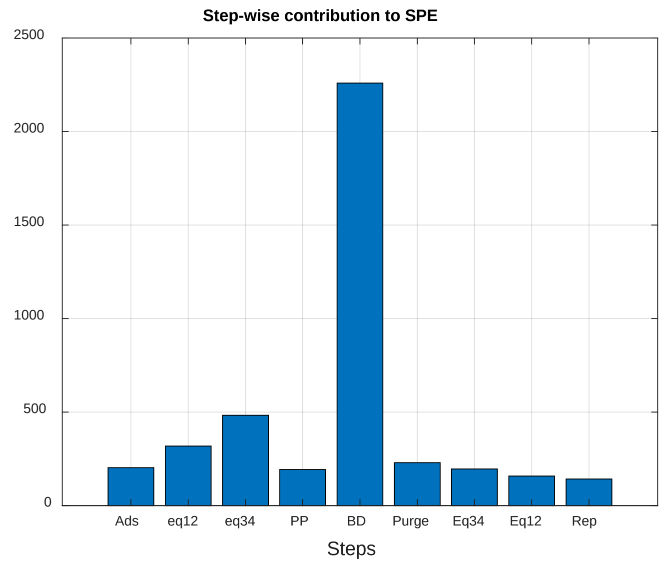

Figure 4.29 Step-wise contribution to SPE for sudden pressure drop (below)

Figure 4.30. shows the degree of contribution of each feature of blowdown step with the from the normal behavior. As it can be seen, slope of linear regression line and average of first derivative have the highest contribution to SPE index among all of the employed statistics.

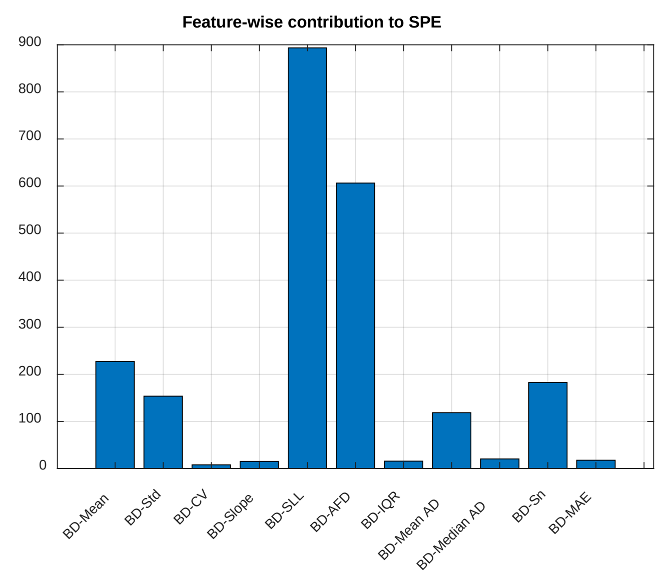

Figure 4.30 Feature-wise contribution to SPE for sudden pressure drop (below)

4.11 Advantage of SPE over Hotelling's T^2

Although SPE and T^2 indices are used in conjunction for process monitoring, as noted in [35], the normal region defined by the T^2 statistic is usually much larger than the one defined by the SPE. The SPE statistic defines a tighter region of normal operation, and a sample that breaks the correlation structure defined in the model can easily exceed the SPE control limit. Thus giving a more reliable indication of the presence of a fault. The T^2 index measures the distance to the origin in the principal component subspace. Since the principal component subspace typically contains normal process variations with large variance that represent signals, and the residual subspace contains mainly noise, the normal region defined by the control limit for T^2 is usually much larger than that of SPE. Therefore it usually takes a much larger fault magnitude to exceed the T^2 control limit. The normal region defined by the SPE control limit includes residual components that are mainly noise. Therefore faults with small to moderate magnitudes can easily exceed the SPE control limit. This causes the SPE index to have lower chances of false alarms and missed detection rates compared to the T^2 [23, 35].

4.12 Analysis of Fault Detection in Simulated Faults

As stated in section 4.10 repeatedly, SPE index has an undeniable and key role in fault detection in the PSA plant. It works perfectly and captures 100% of the various simulated fault into the system. For the fault which has to do with a mean shift like pressure drifting or somehow pressure profile mismatch, Mean and MAE are very helpful to capture the fault which is rational. Because a considerable change in mean is obvious and also a notable change in slope cannot be seen.

For pressure fluctuation fault, median related features plays a significant role since by definition it is a robust measure of the variability. For sudden pressure drop, slope related features like Slope of Linear Regression Line and Average of First Derivative are very important. Due to an abrupt change in pressure, the slope of the pressure profile in the corresponding segment is being under influence of the fault. The most useful features in detecting the presented faults are summarized in table 4.1.

Table 4.1 The most useful features in fault detection

Type of fault	Useful features in fault detection
Pressure Drifting	MAE and Mean
Pressure Profile Mismatch	Mean
Pressure Fluctuation	Median Absolute Deviation
Sudden Pressure Drop	SLL and AFD

4.13 Detecting Real Fault

After simulating the common faults into the dataset and obtaining satisfactory detection results, examining the proposed approach by a real type of fault seems necessary. Using real plant operating data would be very helpful to show the excellent performance of the proposed approach. In other words, the results of fault detection for a real failure can draw a more realistic picture of the strength of the proposed approach in dealing with real out-of-control situations in PSA systems or even in other cyclic processes.

Thus, in this section, it is desired to consider the same procedure for fault detection with a small change in defining training and testing sets. Since the faulty dataset is not from the same plant as the available normal dataset and due to the difference in cycle time between the mentioned datasets, a bed-to-bed modeling approach is proposed to address this limitation. It should be noted that in the faulty dataset, there are 12 vessels and the pressure profile mismatch was found in one of them. Figure 4.31 demonstrates a comparison of the repressurization part between vessel 1 and vessel 2 for one of the cycles.

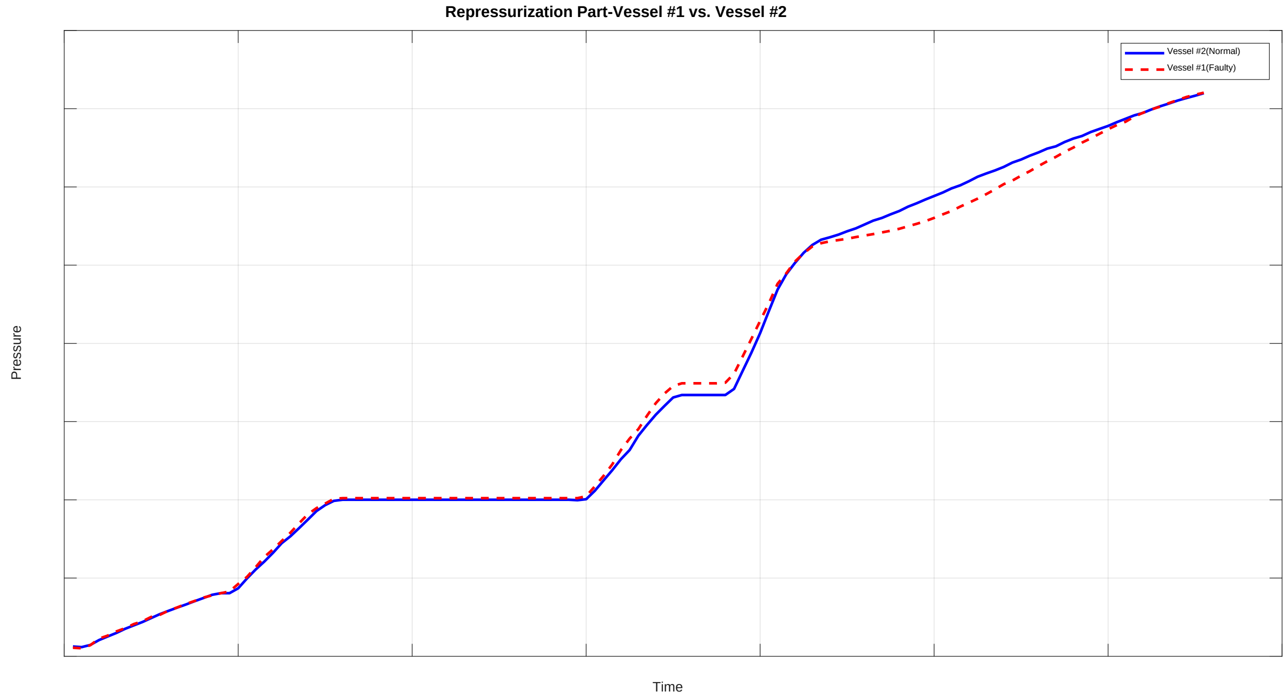

Figure 4.31 A comparison between a normal and faulty vessels in the repressurization step-one cycle

A clear deviation in vessel 1 compared to a normal vessel (vessel 2) can be noticed in figure 4.31. Based on previous explanations about the different type of fault, a clear pressure profile mismatch in the repressurization step has occurred. Therefore, due to the current limitation with the normal data, 171 cycles from 9 vessels (2 to 8, 10, and 11), 19 cycles each, are used to calculate the statistic features and build the training matrix. To create the testing set, 19 cycles from vessel 12 are combined with 19 cycles of vessel 1 which is the faulty one. The rest of the process is the same as presented previously.

Figure 4.32 shows only 4 cycles out of 19 cycles of vessel 1 violates the threshold line which is in a good agreement with figure 4.33 which demonstrates all of the cycles of vessel 2 in solid line and vessel in dashed line. Only 4 cycles of the vessel 1 deviate enough from normal cycles of vessel 2 and SPE index captured them perfectly. It seems that the rest of the cycles in vessel 2 are in normal operating zone.

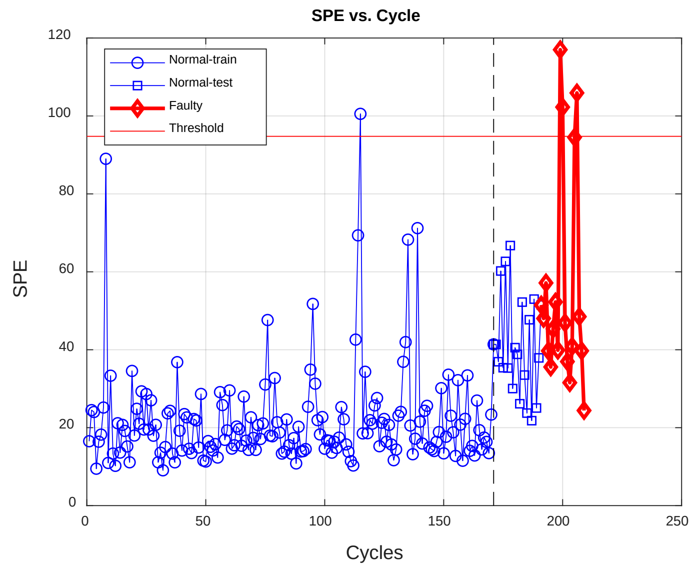

Figure 4.32 SPE index for the real fault

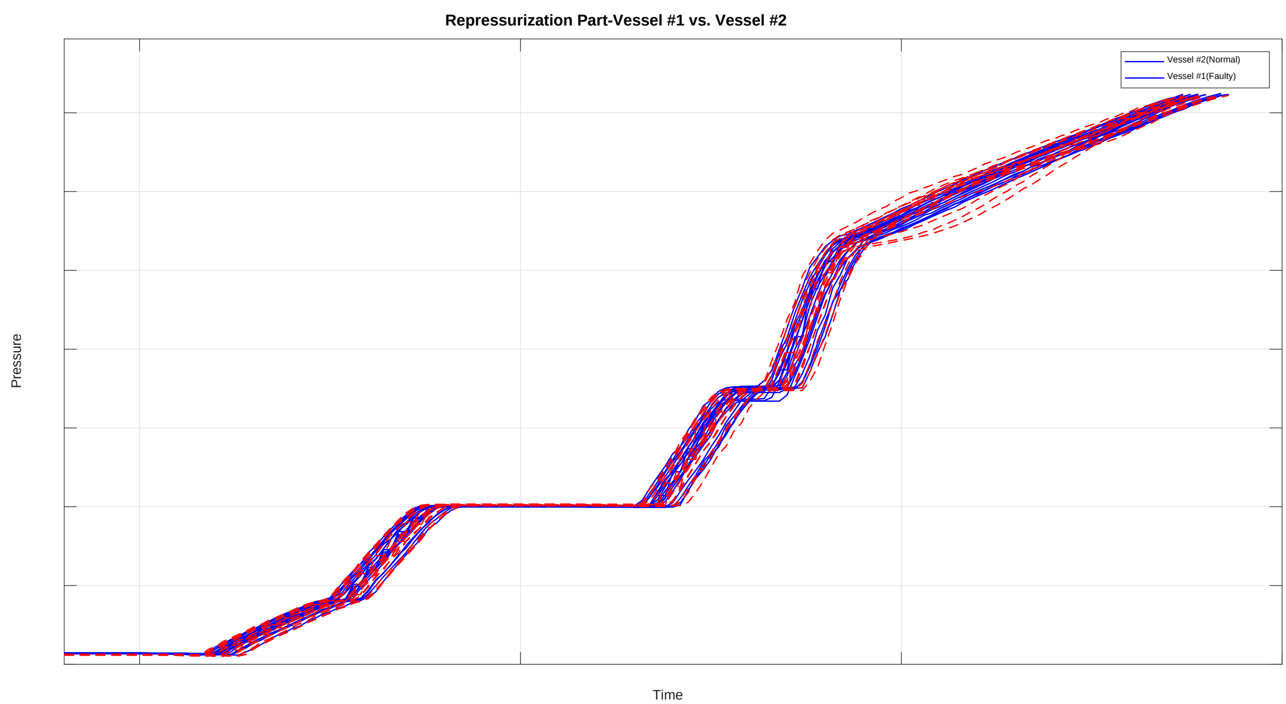

Figure 4.33 A comparison between a normal and faulty vessels in the repressurization step-all cycles

Contribution plot to SPE index is presented in figure 4.34. Based on the information from figure 4.31 and 4.33, it is expected to see the higher bars in the repressurization step, but it seems EQ34 step has the most contribution to SPE index. But no deviation from normal cycles can be seen in figure 4.31 and 4.33.

The reason behind the inconsistency is that the way of defining training and testing sets is different for bed-to-bed modeling. Previously, for defining these sets for simulated faults in section 4.10, statistic features were calculated based on the pressure data of just one vessel. Although all of the vessels are in the same size and shape, they do not work identically because of the operating conditions. Thus, making the model based on the data from different vessels may lower the sensitivity of the model and makes the model less efficient in fault detection.

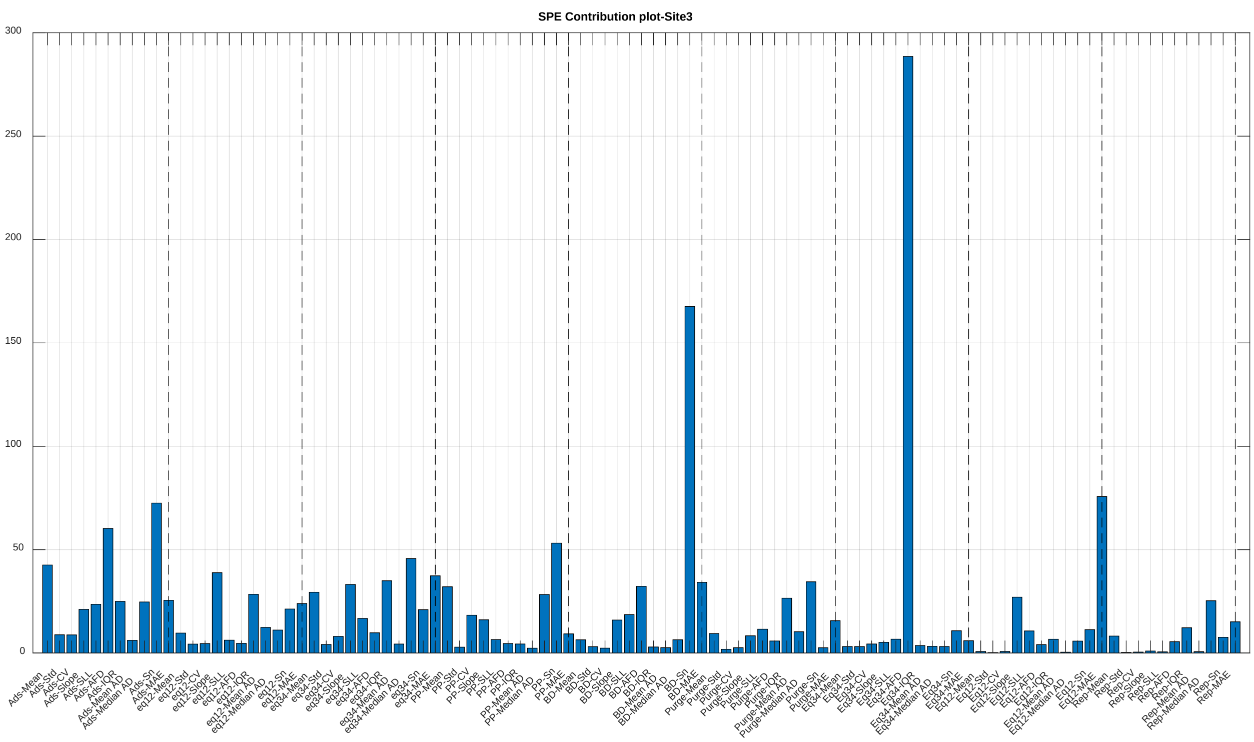

Figure 4.34 Contribution to SPE for the real fault

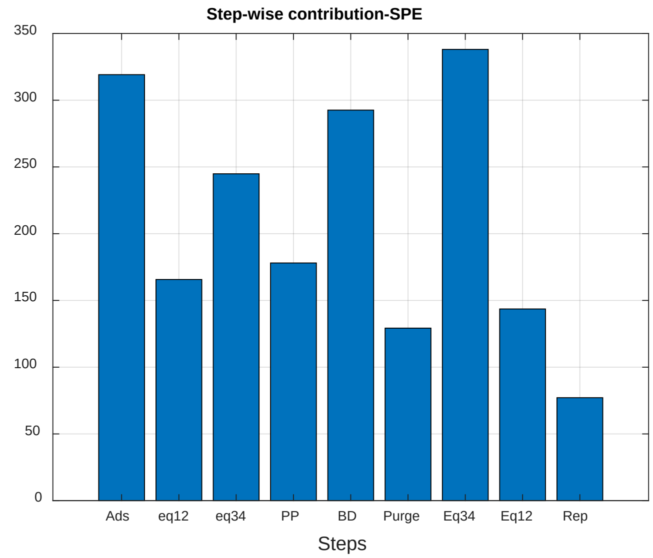

Figure 4.35 Step-wise contribution to SPE for the real fault

Step-wise contribution to SPE index is given in figure 4.35. It can be seen that contribution to SPE for all steps are in the same range. Comparing figure 4.35 with 4.20, as they are plotted for the same type of fault and for the same step, reveals that even without simulating fault for adsorption step through EQ12 step, level of contribution to SPE index for different steps are around 200 to 300. Therefore, based on the result of figure 4.35, it cannot be sure that the fault has occurred in that step. Moreover, considering the visualization of the faulty and normal cycles in vessel 1 and 2, no deviation can be seen in the EQ34 step.

Chapter 5

Conclusion and Proposed Future Work

5.1 Conclusion

Fault detection and diagnosis are essential for revealing unusual operating conditions, abnormal status, and equipment failure in industrial processes. Immediate detection leads to gain higher efficiency and product quality and also it can increase the safety level in the plant. In this study, a new SPA based approach for fault detection in PSA systems, which have the cyclic nature, is proposed. PCA is used for quantifying the dissimilarities in the data. The employed statistic pattern analysis framework is beneficial to avoid utilizing process variables that brings many advantages and improves detection performance and the false alarm rate.

Fault detection is performed using industrial data and some important faults which are very common in the PSA process, are introduced to the system. After simulating the faults, excellent performance of the proposed approach is presented using the fault detection index, SPE rather than Hotelling's T^2. Then, by generating contribution plots the exact faulty segment of each abnormal cycle of the process is revealed. Hotelling's T^2 index is meaningless compared to SPE index for fault detection in the PSA process. It is shown that the proposed framework yields promising results of fault detection in the PSA processes. The set of statistics used in this study are very useful for different segments of the PSA process.

5.2 Future Work

Further investigation can be performed around the proposed approach as follows. As discussed in chapter 4, one of the main requirements of the proposed approach is data availability. Generally, big datasets can help to make stronger and more efficient models.

Apart from that, industrial data with real fault inside can be very helpful to find any hidden probable weakness of the proposed approach. By carrying out further studies on different type and amount of fault, a good library of helpful features can be built. It will be very advantageous to recognize the type of fault by just knowing which set of statistical feature contributes more to detecting an unknown fault. The other type of dataset which is available for this study is valve opening. A robust fault diagnosis using the valve dataset will complete the fault diagnosis part of the project and can reveal the root cause of each fault for immediate actions. After this stage, developing a real-time application of the proposed approach would be very beneficial not only for PSA systems but also for other cyclic processes. To do so, a method for updating the training and testing set is required. The model itself and the calculation part are very simple which make the model attractive enough for different industries. Bed-to-bed modeling can be considered as a very good start point to develop an industry-scale model.

Bibliography

[1] Nomikos, P. and MacGregor, J.F., 1994. Monitoring batch processes using multiway principal component analysis. AIChE Journal, 40(8), pp.1361-1375.

[2] Venkatasubramanian, V., Rengaswamy, R., Yin, K. and Kavuri, S.N., 2003. A review of process fault detection and diagnosis: Part I: Quantitative model-based methods. Computers & chemical engineering, 27(3), pp.293-311.

[3] Miletic, I., Quinn, S., Dudzic, M., Vaculik, V. and Champagne, M., 2004. An industrial perspective on implementing on-line applications of multivariate statistics. Journal of Process Control, 14(8), pp.821-836.

[4] Qin, S.J. and Yu, J., 2007. Recent developments in multivariable controller performance monitoring. Journal of Process Control, 17(3), pp.221-227.

[5] AlGhazzawi, A. and Lennox, B., 2008. Monitoring a complex refining process using multivariate statistics. Control Engineering Practice, 16(3), pp.294-307.

[6] Chen, J. and Yu, J., 2013. Independent component analysis mixture model based dissimilarity method for performance monitoring of Non-Gaussian dynamic processes with shifting operating conditions. Industrial & Engineering Chemistry Research, 53(13), pp.5055-5066.

[7] Russell, E.L., Chiang, L.H. and Braatz, R.D., 2000. Fault detection in industrial processes using canonical variate analysis and dynamic principal component analysis. Chemometrics and intelligent laboratory systems, 51(1), pp.81-93.

[8] Lee, J.M., Yoo, C. and Lee, I.B., 2004. Fault detection of batch processes using multiway kernel principal component analysis. Computers & chemical engineering, 28(9), pp.1837-1847.

[9] Lee, J.M., Yoo, C.K. and Lee, I.B., 2004. Enhanced process monitoring of fed-batch penicillin cultivation using time-varying and multivariate statistical analysis. Journal of Biotechnology, 110(2), pp.119-136.

[10] Lee, J.M., Yoo, C. and Lee, I.B., 2004. Statistical process monitoring with independent component analysis. Journal of Process Control, 14(5), pp.467-485.

[11] He, Q.P. and Wang, J., 2011. Statistics pattern analysis: A new process monitoring framework and its application to semiconductor batch processes. AIChE journal, 57(1), pp.107-121.

[12] Wang, R., Baldea, M. and Edgar, T., 2017. Data Visualization and Visualization-Based Fault Detection for Chemical Processes. Processes, 5(3), p.45.

[13] Hedin, N., Andersson, L., Bergström, L. and Yan, J., 2013. Adsorbents for the post-combustion capture of CO_2 using rapid temperature swing or vacuum swing adsorption. Applied Energy, 104, pp.418-433.

[14] Ko, D., Siriwardane, R. and Biegler, L.T., 2003. Optimization of a pressure-swing adsorption process using zeolite 13X for CO2 sequestration. Industrial & engineering chemistry research, 42(2), pp.339-348.

[15] Kawajiri, Y. and Biegler, L.T., 2006. Optimization strategies for simulated moving bed and Power Feed processes. AIChE Journal, 52(4), pp.1343-1350.

[16] Grossmann, C., Amanullah, M., Erdem, G., Mazzotti, M., Morbidelli, M. and Morari, M., 2008. 'Cycle to cycle optimizing control of simulated moving beds. AIChE journal, 54(1), pp.194-208.

[17] Abel, S., Erdem, G., Mazzotti, M., Morari, M. and Morbidelli, M., 2004. Optimizing control of simulated moving beds—linear isotherm. Journal of Chromatography A, 1033(2), pp.229-239.

[18] Wang, R.C., 2017. Geometric fault detection using 3D Kiviat plots and their applications (Doctoral dissertation).

[19] Pan, Y., Yoo, C., Lee, J.H. and Lee, I.B., 2004. Process monitoring for continuous process with periodic characteristics. Journal of Chemometrics: A Journal of the Chemometrics Society, 18(2), pp.69-75.

[20] Kim, Y., Kim, M., Lim, J., Kim, J.T. and Yoo, C., 2010. Predictive monitoring and diagnosis of periodic air pollution in a subway station. Journal of hazardous materials, 183(1-3), pp.448-459.

[21] Arslan, E., Neogi, D., Li, X.J. and Misra, P., Air Products and Chemicals Inc, 2014. Apparatus And Methods To Monitor And Control Cyclic Process Units In A Steady Plant Environment. U.S. Patent Application 13/737,323.

[22] Chen, J., 2014. Statistical Methods for Process Monitoring and Control (Doctoral dissertation).

[23] Galicia Escobar, H.J., 2012. Advanced monitoring and soft sensor development with application to industrial processes (Doctoral dissertation).

[24] Rashid, M.M. and Yu, J., 2012. A new dissimilarity method integrating multidimensional mutual information and independent component analysis for non-Gaussian dynamic process monitoring. Chemometrics and Intelligent Laboratory Systems, 115, pp.44-58.

[25] Albazzaz, H. and Wang, X.Z., 2004. Statistical process control charts for batch operations based on independent component analysis. Industrial & engineering chemistry research, 43(21), pp.6731-6741.

[26] Lee, J.M., Yoo, C. and Lee, I.B., 2004. Statistical process monitoring with independent component analysis. Journal of Process Control, 14(5), pp.467-485.

[27] Singhal, A. and Seborg, D.E., 2006. Evaluation of a pattern matching method for the Tennessee Eastman challenge process. Journal of Process Control, 16(6), pp.601-613.

[28] Kano, M., Hasebe, S., Hashimoto, I. and Ohno, H., 2002. Statistical process monitoring based on dissimilarity of process data. AIChE Journal, 48(6), pp.1231-1240.

[29] Ge, Z. and Song, Z., 2007. Process monitoring based on independent component analysis− principal component analysis (ICA− PCA) and similarity factors. Industrial & Engineering Chemistry Research, 46(7), pp.2054-2063.

[30] Jolliffe, I., 2011. Principal component analysis (pp. 1094-1096). Springer Berlin Heidelberg.

[31] Dunn, K., 2011. Process Improvement Using Data. No fixed edition. Available online at http://learnche.org/pid.

[32] MacGregor, J.F. and Kourti, T., 1995. Statistical process control of multivariate processes. Control Engineering Practice, 3(3), pp.403-414.

[33] Hotelling, H., 1992. The generalization of Student's ratio. In Breakthroughs in statistics (pp. 54-65). Springer, New York, NY.

[34] Jackson, J.E. and Mudholkar, G.S., 1979. Control procedures for residuals associated with principal component analysis. Technometrics, 21(3), pp.341-349.

[35] Joe Qin, S., 2003. Statistical process monitoring: basics and beyond. Journal of Chemometrics: A Journal of the Chemometrics Society, 17(8-9), pp.480-502.

[36] Khorami, H. 2013. Multivariate Modeling in Chemical Toner Manufacturing Process (Master Thesis).

[37] Wold, S., Kettaneh, N., Fridén, H. and Holmberg, A., 1998. Modelling and diagnostics of batch processes and analogous kinetic experiments. Chemometrics and intelligent laboratory systems, 44(1-2), pp.331-340.

[38] Dong, D. and McAvoy, T.J., 1996. Nonlinear principal component analysis—based on principal curves and neural networks. Computers & Chemical Engineering, 20(1), pp.65-78.

[39] Ge, Z., Yang, C. and Song, Z., 2009. Improved kernel PCA-based monitoring approach for nonlinear processes. Chemical Engineering Science, 64(9), pp.2245-2255.

[40] Haykin, S., 1994. Neural networks (Vol. 2). New York: Prentice hall.

[41] Tracy, N.D., Young, J.C. and Mason, R.L., 1992. Multivariate control charts for individual observations. Journal of quality technology, 24(2), pp.88-95.

[42] Jutten, C. and Herault, J., 1991. Blind separation of sources, part I: An adaptive algorithm based on neuromimetic architecture. Signal processing, 24(1), pp.1-10.

[43] Kano, M., Tanaka, S., Hasebe, S., Hashimoto, I. and Ohno, H., 2003. Monitoring independent components for fault detection. AIChE Journal, 49(4), pp.969-976.

[44] Manyika, J., Chui, M., Brown, B., Bughin, J., Dobbs, R., Roxburgh, C. and Byers, A.H., 2011. Big data: The next frontier for innovation, competition, and productivity.

[45] Qin, S.J., 2014. Process data analytics in the era of big data. AIChE Journal, 60(9), pp.3092-3100.

[46] He, Q.P., Wang, J., Shah, D. and Vahdat, N., 2017. Statistical process monitoring for IoT-Enabled cybermanufacturing: opportunities and challenges. IFAC-PapersOnLine, 50(1), pp.14946-14951.

[47] Jackson JE., 1991. A User's Guide to Principal Components. Wiley- Interscience: New York.

[48] Grande, C.A., 2012. Advances in pressure swing adsorption for gas separation. ISRN Chemical Engineering, 2012.

[49] Wang, J. and He, Q.P., 2010. Multivariate statistical process monitoring based on statistics pattern analysis. Industrial & Engineering Chemistry Research, 49(17), pp.7858-7869.

[50] https://en.wikipedia.org/wiki/Standard_deviation- Feb15.

[51] https://en.wikipedia.org/wiki/Coefficient_of_variation-Feb15.

[52] https://en.wikipedia.org/wiki/Interquartile_range-Feb15.

[53] https://en.wikipedia.org/wiki/Average_absolute_deviation-Feb15.

[54] https://en.wikipedia.org/wiki/Median_absolute_deviation-Feb15.

[55] https://en.wikipedia.org/wiki/Mean_absolute_error -Feb15.

[56] Rousseeuw, P.J. and Croux, C., 1993. Alternatives to the median absolute deviation. Journal of the American Statistical association, 88(424), pp.1273-1283.

[57] Galicia, H.J., He, Q.P. and Wang, J., 2012. A comprehensive evaluation of Statistics Pattern Analysis based process monitoring. IFAC Proceedings Volumes, 45(15), pp.39-44.

[58] Chiang, L.H., Russell, E.L. and Braatz, R.D., 2000. Fault detection and diagnosis in industrial systems. Springer Science & Business Media.

[59] He, Q.P., Qin, S.J. and Wang, J., 2005. A new fault diagnosis method using fault directions in Fisher discriminant analysis. AIChE journal, 51(2), pp.555-571.

[60] Miller, P., Swanson, R.E. and Heckler, C.E., 1998. Contribution plots: A missing link in multivariate quality control. Applied mathematics and computer science, 8(4), pp.775-792.

[61] Kourti, T. and MacGregor, J.F., 1994. Multivariate SPC methods for monitoring and diagnosing of process performance. In Proceedings of PSE (pp. 739-746).