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FAULT DETECTION AND DIAGNOSIS FRAMEWORK USING WAVELET BASED KERNEL PRINCIPAL COMPONENT ANALYSIS FOR CHEMICAL PROCESS SYSTEMS

By

MUHAMMAD NAWAZ

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19/8/2022

FAULT DETECTION AND DIAGNOSIS FRAMEWORK USING WAVELET BASED KERNEL PRINCIPAL COMPONENT ANALYSIS FOR CHEMICAL PROCESS SYSTEMS

by

MUHAMMAD NAWAZ

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hereby declare that the thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at UTP or other institutions.

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DEDICATION



The road to success comes through hard work, determination, sacrifice and guidance of elders, especially those very close to the heart.

My humble effort I dedicate to my sweet and loving

Parents, Wife and Daughter,

whose affection, love, encouragement and prayers day and night enable me to achieve much success and honour.

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ABSTRACT

Process monitoring is essential for ensuring that the chemical process system functions smoothly and consistently. Multivariate statistical process monitoring (MSPM) plays a significant role in assuring the safe and efficient operation of industrial and chemical processes. Existing techniques are incapable of dealing with real-time nonlinear process data, resulting in inaccurate process fault interpretation. The objective of this study is to develop multiscale fault detection and diagnosis framework capable of detecting faults in real-time nonlinear process systems as well as identifying the underlying cause of faulty variables. In the proposed framework, wavelet transform (WT) is combined with kernel principal component analysis (KPCA). WT was initially used to extract the dynamics of process data at various scales. A moving window technique was introduced in WT, which aided data extraction for real-time process data. The wavelet coefficients from the analysis were reconstructed and then put into the KPCA for dimensionality reduction. Finally, T^2 and squared prediction error (SPE) statistics are utilized to locate faults, and the reconstruction-based contribution (RBC) model is used to identify fault variables. The proposed fault detection and diagnosis framework was tested using two different chemical processes: the continuous stirred tank reactor (CSTR) system and Tennessee Eastman (TE) process. The average fault detection rate for the CSTR system's faults is found to be 69.67% and 81.20% for T^2 and SPE monitoring charts. Whereas for the TE process, the average fault detection rate for all faults is found to be 45.85% and 82.51% for T² and SPE monitoring charts. The diagnosis investigation is carried out by using SPE based RBC model and the results showed that the proposed framework successfully identifies the faulty variables. Furthermore, it is observed that the proposed framework provides better fault detection compared to principal component analysis (PCA) and KPCA methods. The proposed framework in this research work could be used for early and accurate fault detection as well as successfully identifies the root cause of the faulty variables.

ABSTRAK

Pemantauan proses adalah penting untuk memastikan sistem proses kimia berfungsi secara lancar dan konsisten. Pemantauan proses statistik multivariate (MSPM) memainkan peranan penting dalam memastikan operasi yang selamat dan cekap dalam proses industri dan kimia. Teknik sedia ada tidak berupaya menangani data proses tidak linear masa nyata, mengakibatkan tafsiran kesalahan proses yang tidak tepat. Objektif kajian ini adalah untuk membangunkan rangka kerja pengesanan dan diagnosis kerosakan berbilang skala yang mampu mengesan kerosakan dalam sistem proses tidak linear masa nyata serta mengenal pasti punca asas pembolehubah rosak. Dalam rangka kerja yang dicadangkan, transformasi wavelet (WT) digabungkan dengan analisis komponen utama kernel (KPCA). WT pada mulanya digunakan untuk mengekstrak dinamik data proses pada pelbagai skala. Teknik tetingkap bergerak telah diperkenalkan dalam WT, yang membantu pengekstrakan data untuk data proses masa nyata. Pekali wavelet daripada analisis telah dibina semula dan kemudian dimasukkan ke dalam KPCA untuk pengurangan dimensi. Akhir sekali, statistik T² dan ralat ramalan kuasa dua (SPE) digunakan untuk mencari kerosakan, dan model sumbangan berasaskan pembinaan semula (RBC) digunakan untuk mengenal pasti pembolehubah kerosakan. Rangka kerja pengesanan dan diagnosis kerosakan yang dicadangkan telah diuji menggunakan dua proses kimia yang berbeza: sistem reaktor tangki kacau berterusan (CSTR) dan proses Tennessee Eastman (TE). Purata pengesanan kerosakan untuk senario kerosakan sistem CSTR didapati 69.67% dan 81.20% untuk carta pemantauan T^2 dan SPE. Manakala untuk proses TE, pengesanan kerosakan purata bagi semua senario kerosakan didapati 45.85% dan 82.51% untuk carta pemantauan T² dan SPE. Penyiasatan diagnosis dijalankan dengan menggunakan model RBC berasaskan SPE dan keputusan menunjukkan rangka kerja yang dicadangkan berjaya mengenal pasti pembolehubah yang rosak. Tambahan pula, adalah diperhatikan bahawa rangka kerja yang dicadangkan menyediakan pengesanan kerosakan yang lebih baik berbanding kaedah analisis komponen utama (PCA) dan KPCA. Rangka kerja yang dicadangkan dalam kerja penyelidikan ini boleh digunakan untuk pengesanan kerosakan awal dan tepat serta berjaya mengenal pasti punca pembolehubah yang rosak.

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LIST OF ABBREVIATIONS

ANFIS	Adaptive Neuro-Fuzzy Interface System
AHWR	advanced heavy water reactor
ANN	artificial neural network
BPA	backpropagation
BN	Bayesian networks
BF	bearing fault
BAFP	biological anaerobic filter process
BWWTP	biological wastewater treatment plant
BG	Bond Graph
CSM	cad system in E. coli model
CS	chiller system
CAP	continuous annealing process
CSTR	Continuous stirred tank reactor
CFT	cracking furnace tube
CUSUM	cumulative sum
DC	distillation column
DKPCA	dynamic KPCA
DPCA	dynamic PCA
EFMF	electro fused magnesium furnace
EMD	empirical mode decomposition
EEMD	ensemble empirical mode decomposition

ECF	ethylene cracking furnace
EWMA	exponentially weighted moving average
FAR	false alarm rate
FDI	fault detection and identification
FDA	Fisher Discriminant Analysis
FCCU	fluidized catalytic cracker unit
FFE	furnace feed event
FMF	fused magnesium furnace
GMM	Gaussian Mixture Model
GRNN	general regression networks
GLRT	Generalized Likelihood Ratio Test
HHS	home heating system
ICA	Independent component analysis
IBD	industrial boiler data
IPPPP	industrial polypropylene production process
ISD	industrial spray dryer
ITRS	industrial tubular reactor system
IT-NN	input-training neural network
IMF	intrinsic mode functions
KF	Kalman Filter
KFDA	kernel FDA
KGMM	kernel GMM
KICA	kernel ICA
KPCA	kernel PCA

KPLS	kernel PLS
LSBTS	laboratory slewing bearing test stand
LLNF	local linear Neuro-fuzzy
LSBTT	low speed bearing test stand
MLP	multilayer perceptron
MSNLPCA	multiscale NLPCA
MSPLS	Multiscale PLS
MSPCA	Multiscale principal component analysis
MCUSUM	Multivariate CUSUM
MEWMA	multivariate EWMA
MSPM	Multivariate statistical process monitoring
MGMM	multi-way GMM
MKICA	multiway KICA
МКРСА	multiway KPCA
NC	ne concentrations
NLIP	nonlinear industrial process
NLKGMM	nonlinear kernel GMM
NLPCA	nonlinear PCA
NE	numerical example
PMP	paper mill plant
PLS	Partial least squares
PFP	penicillin fermentation process
PSP	pilot scale plant
PP	polymerization process

PCA	principle component analysis
PNN	probabilistic neural networks
QTP	quadruple tank process
RN	recurrent networks
SM	sensor malfunction
SBRS	sequencing batch reactor system
STP	sewage treatment process
SBG	signed bond graph
SDS	simulated datasets
SS	simulated system
SSA	singular spectrum analysis
SPC	Statistical process control
SFSS	steel-frame scale structure
SVM	support vector machines
SD	synthetic data
TE process	Tennessee Eastman process
TTS	Three tank process
WWTP	wastewater treatment processes
WT	Wavelet transforms

LIST OF SYMBOLS

Α	Cross-section area of the reactor, (m ²)
С	Concentration of reactant A in the reactor, (mol L^{-1})
C_i	Initial concentration of reactant A in feed stream, (mol L ⁻¹)
C_p	Heat capacity of reactant A, (J K ⁻¹ kg ⁻¹)
C_{pc}	Heat capacity of cooling liquid, (J K ⁻¹ kg ⁻¹)
E_A/R	Activation energy, (K)
F	Flowrate of outlet stream, (L min ⁻¹)
F_c	Flowrate of cooling liquid, (L min ⁻¹)
F_i	Flowrate of feed stream, (L min ⁻¹)
Н	Liquid level in the reactor, (m)
k_o	Pre-exponential factor, (min ⁻¹)
Т	Temperature in the reactor, (K)
T_c	Cooling liquid temperature in cooling jacket, (K)
T_{ci}	cooling liquid temperature, (K)
T_i	Temperature of feed stream, (K)
$U\!A_c$	Heat transfer coefficient, (J min ⁻¹ K ⁻¹)
V_c	Volume of the cooling jacket, (L)
- <i>Д</i> Н	Heat of reaction, (J mol ⁻¹)
Р	Density of the reactant A, (kg L ⁻¹)
$ ho_c$	Density of the cooling liquid, (kg L ⁻¹)
Σ	Covariance matrix of the combined dataset

μ	Mean
L	Number of PCs retained for model
Λ	Diagonal matrix representing eigenvalues
A	Eigenvector of covariance matrix
Λ	Eigenvalues
Σ	Standard deviation
Ф(.)	Non-linear mapping function

CHAPTER 1

INTRODUCTION

1.1 Chapter overview

This chapter aims to introduce process monitoring in the process industries. This contains a brief background, an overview of process monitoring methods, and recent developments, primarily multiscale fault detection and diagnosis in process industries. Following that, there is a discussion of the research problem statement, relevant research objectives, and the scope of the study. The chapter concludes with an outline of the whole complete thesis.

1.2 Research background

The increasing complexity of industrial processes raises concerns about plant safety, product quality, efficiency, and energy consumption. These industrial processes handle hazardous materials and operate at very high pressures and temperatures [1]. Failure of any component in the process could lead to abnormal events. An abnormal event might occur in any process component due to the observed variable deviating from the allowed range. A malfunction of the coolant pump or a controller might cause a process anomaly, such as high temperature in the reactor or poor product quality, resulting in an abnormal event. Other sources of process abnormalities include changes in process parameters, significant disturbances, actuator problems, and sensor problems. All process industries have benefited substantially from the widespread use of sensor networks, sophisticated data collecting technologies, and the broad usage of distributed control systems [2,3]. However, many essential control tasks are still manual and performed by human operators. Developing and implementing intelligent

technologies to assist human operators in abnormal events, particularly in fault isolation, is a significant problem in the process industry.

Although process industries have benefited from improvements in control systems, some terrible chemical plant accidents have occurred in recent times. For instance, thousands of people have been killed in an accident at the Union Carbide pesticide plant in Bhopal, India, due to the leakage of highly toxic gas (methyl isocyanate) [4]. This accident is considered as the worst industrial disaster in history. The 1988 Piper Alpha disaster remains one of the worst safety-related accidents of its kind in the Oil & Gas sector [5]. In June 2000, an explosion at Kuwait Petrochemical's Mina Al-Ahmedi refinery caused about \$100 million in damage [4]. As per industrial statistics, there are minor incidents every day, particularly in the chemical and process industries, that not only cause injuries but also cost billions of dollars annually due to unsafe and abnormal event management [6].

Abnormal event management is critical to maintaining safe and efficient process industry operations. It aids in the identification and diagnosis of faults in order to maintain a safe, controllable working environment and reduce production losses caused by abnormal conditions [7]. In general, fault detection is the identification of the occurrence of a fault. Fault identification is the determination of the observation variables most pertinent to the fault, whereas fault diagnosis is the determination of the fault's source and location. After a fault has been identified and diagnosed, the process is restarted to complete the loop, as shown in Figure 1.1. [1]. The fault can lead to critical failure if it remains undetected. A tolerable fault can seriously affect the overall process by breaking down the system component and function. Fault detection and diagnosis has been used to evaluate various industrial processes, including the Tennessee Eastman (TE) process, the reactor system, the distillation column, bearing failures, and industrial gas turbines.



Figure 1.1: Process monitoring loop [1].

Fault detection and diagnosis has been an active study field throughout the previous decades. They may typically be grouped into three categories: analytical model-based, knowledge-based, and data-driven techniques. The model-based techniques are based on the first principle to develop the system's mathematical model. These methods incorporate the system's physical understanding of the fault detection and diagnosis process [8,9]. The quality of model-based approaches depends on model accuracy. However, developing an accurate model for large-scale and complex systems can be difficult and sometimes impossible [8]. Besides this, the knowledge-based approaches are rule-based expert systems [10]. These methods are based on the plant operator's expert knowledge and experience. It takes time and effort to build a comprehensive knowledge base, especially for large-scale processes [11]. The mathematical model and related expert knowledge are not required in data-driven approaches. These approaches have been increasingly popular in recent years, particularly for complicated processes requiring complex models and expert knowledge. Multivariate statistical process monitoring (MSPM) approaches are the most prominent data-driven techniques that have shown their potential and are being progressively used to monitor chemical processes [9-11].

The key idea of the MSPM methods consists of process features that may have been extracted via a particular multivariate analysis process. Thus, the highly dimensioned information is projected to a less dimensional space, followed by the evaluation of the statistics. Principal component analysis (PCA) [12-15] and partial least squares (PLS) [16,17] are the leading MSPM techniques and are frequently applied for the monitoring of chemical processes. Such traditional MSPM methods can easily handle the simpler processes; however, their performance weakens in a plant-wide process [18-20]. PCA has limitations for fault detection and identification in chemical processes with strong

nonlinearity and dynamics, despite its capability to effectively analyse high dimensional, noisy, and highly correlated data [21]. As a result, MSPM methods for nonlinear large-scale dynamic process monitoring have been extensively researched over the past decade. Several enhancements were developed to address the original limitations and are expected to cater to intricately complex process features in large-scale process industries [22,23].

The development of process monitoring strategies for large-scale process systems is a challenge due to the complexity and nonlinear behaviour, a strong correlation between the measured variables, and the presence of multiple sensors that have to be critically observed [24]. In recent years, nonlinear process monitoring has become an attractive research feature. For handling nonlinear processes, McClure et al. [25] proposed a supervised locally linear embedding for projection-based nonlinear process monitoring technique. A new online process monitoring technique for multimode and nonlinear processes was proposed by Ruomu et al. [26]. A recently developed kernel learning method for nonlinear process monitoring has been combined with specific conventional MSPM methods [27-29]. A kernel function improved the performance by preventing nonlinear mapping and inner product computation. Additionally, the kernel-based techniques could simultaneously handle both nonlinear and non-Gaussian data [11].

MSPM approaches and extensions have been used successfully; however, their application is limited as they only examine single-scale events [30]. Contrarily, chemical processes have to be operated at different scales [31]. The majority of available methods depend on the data collected on a fixed scale. In contrast, the multiscale approach has the potential to depict information through wavelet transform in different scales. Wavelet transforms (WT) is the most effective multiresolution analysis tool, categorizing input signals into several different resolution levels [32]. In this way, the process signals with distinct physical patterns or decomposed disruptions are viewed as a combination of several signals at different resolution scales. To address the multiscale nature in process monitoring, multiscale process monitoring frameworks have been proposed by various researchers [31, 33, 34].

The fault detection and diagnosis is a tough job in real processes owing to complex interconnections between faults and symptoms, a strong correlation between the measured variable, and the nonlinear behaviour of the plant. As a result, an fault detection and diagnosis framework must be developed to identify and diagnose faults in nonlinear systems properly. Hence, this study focuses on developing and evaluating fault detection and diagnosis techniques using data-driven techniques to detect and diagnose multiple simultaneous faults.

1.3 Research problem

The increasing complexity of industrial processes, as well as their associated performance requirements, has led to development of new approaches to their monitoring. MSPM methods are the most widely utilized data-based process monitoring techniques for monitoring industrial processes [35,36]. However, it should be noted that traditional MSPM methods, such as PCA and PLS, have several inherent limitations. These techniques assume that the process date is Gaussian-distributed, that the process variables are linearly correlated, and that the process operates under a single stationary condition [11]. Therefore, various improvements to the traditional MSPM methods, multiscale fault detection and diagnosis have been commonly used in the process industry [31,33]. However, most of the processes are inherently nonlinear, and it is expected that fault detection and diagnosis methods should be based on nonlinear dynamic methods. Numerous works have been done using the simulated CSTR and TE process data and reported in the literature [37-39].

Real-time process monitoring is one of the most crucial and challenging tasks for efficient control of the final product and process optimization. However, in existing multiscale nonlinear methods, conventional wavelet decomposition of process data is restricted to offline use. The process monitoring was performed for the real-time signals and modified by offline processing, restricting real-time application requirements. This introduced a time delay in the computation. The contribution plots are the most common method for identification of faulty variables. Fault information is not required for diagnosis by fault identification, but process knowledge is needed to interpret contribution patterns [40,41]. Many authors have adopted the contribution plot approach in multiscale process monitoring methods to determine the root cause [31,34]. However, it has been reported that the contributions plots have a smearing effect, resulting in the highlighting of the non-faulty variables, and obscured faulty variables during the contribution analysis [42]. This smearing effect quickly results in ambiguity in diagnosing complex process faults. Based on these gaps, there is a need to develop a fault detection framework capable of detecting faults in real-time nonlinear chemical process systems. In addition, the approach should be capable to accurately diagnose process faults and determining their root cause.

1.4 Objective of the study

This research aims to develop multiscale fault detection and diagnosis framework for real-time nonlinear chemical processes that can detect and diagnose various faults. Specifically, the objectives are:

- 1. To develop a wavelet-based multiscale fault detection framework for real-time monitoring of nonlinear processes.
- 2. To develop a wavelet-based fault diagnosis framework that can correctly diagnose the detected faults in real-time nonlinear processes.
- 3. To evaluate the performance of the proposed wavelet-based multiscale fault detection and diagnosis framework using an appropriate case study.

1.5 Scope of the current study

The study focuses on developing multiscale fault detection and diagnosis framework for nonlinear chemical process systems. Therefore, the scope of the present research work is as follows:

a) The case study for this research is a continuous stirred tank reactor (CSTR) system, for which a simulated model has been developed using Simulink

MATLAB 2018a. The data is generated using CSTR simulation model. For process monitoring research purposes, six different faults are simulated, including input disturbances, sensor bias, and complex faults (change activation energy and heat transfer coefficient).

- b) For the fault detection framework, a wavelet-based multiscale fault detection framework is proposed to detect the fault in the CSTR system. A moving window is introduced into the wavelet transform, satisfying the real-time application requirement. After the wavelet decomposition and reconstruction of data using wavelet transform, the kernel principal component analysis method detects faults. The proposed fault detection framework is compared with other methods such as PCA and KPCA.
- c) For the fault diagnosis framework, the reconstruction-based contribution (RBC) method is proposed. The RBC method is used after detecting faults, and its performance is compared with the contribution plots.
- d) The second case study is the TE process, which is a realistic simulation of a chemical process that has been widely used in process control studies.

1.6 Thesis layout

This thesis is organized as follows:

Chapter 1 is an introductory chapter that briefly discusses fault detection and diagnosis in the process industries. Besides, the problem statement, the research objectives, and the scope of this study are also outlined in this chapter.

Chapter 2 describes the relevant knowledge and clarification of related concepts to understand the study. It provides desirable characteristics of the fault diagnostic system. It also reviews the most common model-based and data-based fault detection and diagnosis methods along with the comparison. A detailed review of previous studies of wavelet-based multiscale fault detection and diagnosis in the chemical processes has been presented. The literature based on multiscale fault detection and diagnosis is classified under various issues and presented in this chapter.

Chapter 3 illustrates the development of wavelet-based multiscale fault detection and diagnosis framework for real-time processes. The development of the proposed framework requires two steps, i.e., decomposition and reconstruction of process data and detection and diagnosis of fault presented in the process data. The development and formulation related to both proposed frameworks are presented in this chapter.

In this chapter, two case studies, i.e. CSTR system and TE process are presented and selected to evaluate the performance of the proposed fault detection and diagnosis framework. The description of various faults has been discussed in this chapter.

Chapter 4 documents the results obtained in the current study and critical discussions on these results comprehensively. The results and discussion analysis are segregated into two main parts: (1) fault detection in the CSTR system and TE process, and (2) fault diagnosis in CSTR and TE process.

Chapter 5 outlines the general conclusions drawn from the present work. Future recommendations and suggestions are also presented.

CHAPTER 2

LITERATURE REVIEW

2.1 Chapter overview

The chapter is arranged in such a manner to identify the emphasis of fault detection and diagnosis in process industries, followed by the description of desired features of a fault diagnostic system. The chapter further explores the detailed overview of the fault detection and diagnosis approaches, including model-based and data-based approaches in section 2.4. Furthermore, the comparison of the diagnostic methods has been discussed in section 2.5. A comprehensive review of statistical monitoring methods and their developments is presented in section 2.6. Multiscale process monitoring methods are discussed, and the discussion is focused on the concept applied, issues involved in the methods, and the limitations of the present multiscale fault detection and diagnosis methods.

2.2 Need for fault detection and diagnosis

The emergence of widespread sensor networks and distributed control systems have complicated modern chemical processes' dynamics. Chemical processes need to operate at a minimal level of risk to ensure plant safety and lives of the workers. Chemical plants must handle a variety of feedstocks effectively and maintain a high level of product quality.

As a result of these challenges, there is necessary to develop a fault detection and diagnostic approach. In a chemical plant, this approach will aid in maintaining the process under optimum operating conditions and minimizing the risk level. This method should identify and diagnose any faults in the process. This will enable plant operators to take a necessity action in the case of an unexpected event.

2.3 Desirable characteristics of a fault diagnostic system

The performance of various fault detection and diagnosis approaches involves the knowledge of the desirable characteristics of the diagnostic system. These methods are assessed based on this set of standards. A single diagnostic system cannot possess these characteristics and are useful for various benchmarks. These characteristics include prior knowledge of computational efficiency and reliability. It is better to have a complete concept of these characteristics before proceeding with any diagnostic classifier [6]. The desirable characteristics of any diagnostic system are illustrated in Figure 2.1.



Figure 2.1: Desirable characteristics of a diagnostic system [43]

2.3.1 Quick detection and diagnosis

Quick fault detection and diagnosis is essential characteristic of a diagnostic system. Every diagnostic system should respond early in detecting process malfunctions. The quick response of failure in diagnosis and tolerable performance during normal operation are two different approaches. A few systems are designed to detect a failure quickly, and they are sensitive to the influence of high frequencies. This makes the system sensitive to noise and can lead to frequent false alarms, even during normal operations.

2.3.2 Isolability

The ability to design isolable classifiers depends on the process characteristics. An efficient diagnostic system should have the ability to distinguish between different kinds of faults. The diagnostic system must be free of noise and uncertainties of modelling. Therefore, it is said that the diagnostic classifier must be able to develop those outputs which are orthogonal to faults that have not occurred. Most of the classifiers have a limited degree of freedom for design purposes due to unnecessary information. Therefore, the classifiers with a high degree of isolability are usually given unsatisfactory performance in refusing the uncertainties of the modelling job.

2.3.3 Robustness

The diagnostic system should be robust to noise and modeling uncertainties. It will aid in the diagnostic approach's reliability and robustness. It is also preferable that the diagnostic system's performance deteriorate gradually rather than abruptly. Disturbance, noise, and model uncertainty are unavoidable in an actual system. As a result, all effects must be considered while designing any fault detection and diagnostic system.

2.3.4 Novelty identifiability

Any diagnostic system must be capable of adjusting to different process conditions. Most processes have enough data to predict the behaviour in distinct regions. The diagnostic system must be able to distinguish between normal and abnormal processes. In the case of an abnormality, it can predict whether the fault is known to malfunction, unknown, or any novel malfunction. This is known as novelty identification.

In certain instances, historical data may be unavailable to model an aberrant or faulty condition of the process. However, only a few data trends are available for the abnormal region, and they only cover a few portions of the process in their entirety. As a result of this situation, it is possible that the abnormal region was not adequately modelled. As a result, it will give severe contests to achieve novel identification. Under these conditions, a diagnostic system should identify the fault occurrence and not misclassify it with other known abnormalities as a normal operation.

2.3.5 Adaptability

Processes generally change and evolve due to changes in external inputs or structural modifications due to retrofitting. Variations in production quantities, changes in raw material quality, and environmental conditions may affect the process operating conditions. As a result, the diagnostic system should be flexible enough to accommodate changes. It should be possible to progressively expand the system's scope when new cases and issues arise as more information becomes available.

2.3.6 Explanation facility

A diagnostic system should indicate how the fault originated and spread to the present condition and identify the cause of failure. This is an important consideration while developing online decision support systems. This necessitates the ability to reason about cause-and-effect relationships in a process. A diagnostic system must justify its recommendations so that the operator may evaluate and respond appropriately
based on their expertise. One would hope that the diagnostic method would explain why some hypotheses were proposed while others were rejected.

2.3.7 Storage and computational requirements

The modelling process is critical in the creation of a diagnostic system. It is recommended that modelling efforts be kept to a minimum to build a rapid and accurate diagnostic classifier. Early and real-time fault detection often necessitates a less complex computational technique. However, it may require a significant amount of storage space. When designing a diagnostic system, it is recommended to have balanced features related to modelling, storage, and computational requirements.

2.3.8 Multiple fault identifiability

As a result of the correlation between the parameters in most processes, it is difficult to detect multiple faults simultaneously. However, it is an essential and demanding characteristic that the diagnostic system identifies multiple faults. Individual fault patterns are insufficient to represent the combined effects of the fault in nonlinear systems since the interaction between the variables is typically interdependent. As a result, the diagnostic system should be adequately built for multiple fault combinations for large processes.

2.4 Fault detection and diagnosis approaches

Process safety and product quality are two significant problems for modern industrial processes. Process monitoring also termed fault detection and diagnosis, is a key technology in process engineering and control. Hence it can be used for quality products and safety enhancement. Various fault detection and diagnosis methods have been proposed and studied in the literature and classified in different ways [6,43,44]. These methods are classified into analytical model-based, knowledge-based, and data-driven strategies, as shown in Figure 2.2 [45,46]. The model-based approaches are

based on the first principle to construct the system's mathematical model. These approaches integrate the physical understanding of the system into the fault detection and diagnosis process. Model-based approaches rely on model accuracy. However, it can be difficult and sometimes impossible to build an accurate model for large-scale and complex systems [8,9]. Besides this, the knowledge-based approaches are rule-based expert systems that rely on plant operators' expertise and experience. However, developing a comprehensive knowledge base is time-consuming and difficult, particularly in large-scale processes [10,11]. Data-driven approaches do not require the mathematical model and associated expert knowledge. These methods have become most common in recent years, particularly for complex processes that have difficulty building models and expert knowledge [8].



Figure 2.2: Classification of fault detection and diagnosis methods [45,46]

2.4.1 Model-based approaches

The model-based approaches are reliable when there is an unavailability of data. However, an analytical model is available. These models are developed using physical laws and first principle equations. The residual is generated at each step, indicating the difference between the measured process and the process estimates. The residuals are processed further to define the fault signature when a fault occurs in the system. The residual generation can be done by various methods such as parameter estimation, parity relations diagnostic observers, and bond graph.

2.4.1.1 Observers

The system state determines its behaviour by using the system's output, and all the parameters of the process are known. Using an observer, the process output can be estimated by the residuals generated by reconstructing the unknown intern states of the system. The residuals should be robust and may not be affected by the input disturbances of the system. Various fault detection and diagnosis observers are proposed, such as for better fault discrimination, the H ∞ based observer 1, the Kalman filter in a stochastic setting [47], and the Luenberger in a deterministic setting [48]. Patton and Chen [49] proposed an observer to deal with robust fault detection and isolation, which decoupled the effects of a fault from the input disturbances. The diagnostic for the nonlinear systems have also been proposed in the literature by Frank [50].

The robustness of observer-based approaches has improved in the presence of model uncertainty, but it has also reduced fault sensitivity. Bastin and Gevers [51] developed adaptive observers to overcome this limitation, which is suitable for both linear and nonlinear systems [52]. For the residual generation, the linear observer theory was extended to the nonlinear system using H- and H ∞ formulation [53] and fuzzy logic [54]. An extended kalman filter approach is proposed, which addresses the robust fault detection and diagnosis by reducing the measurement noises; however, this approach

only deals with the sensor fault [55]. A new strategy was also proposed by combining internal analysis and statistical behaviour of the noise based on improved internal Kalman filter [56]. A comparison between a statistical decision and an interval-based approach can be found in [57].

2.4.1.2 Parity space

Parity space was developed initially for static systems [58], one of the residual generation based approaches extended to dynamic systems [59]. Parity space is based on the transformation of the state-space model of the plant to obtain the parity relations by observing the system on a finite horizon [60]. The model-based residual generator can be represented in the form of parity relations. The author demonstrated the complete equivalence of diagnostic observers and parity relations and the complete equivalence of diagnostic observers and parity relationships. Many studies have explored the issue of fault isolation, robustness to noise, disturbances, and model errors [61-63]. Ding et al. [62] have shown that an increase in order of the parity equations will increase the system's robustness. However, this approach usually does not include significant model uncertainties, unmodeled disturbances, or multiplicative faults.

It is worth noting that a balance between performance and computational costs is defined in designing the relation-based residual generation [64]. A low-level Waveletbased parity vector is proposed to achieve a useful performance index with low computational costs, but this method presents a misdetection problem [65]. This method is then extended to improve the performance index by introducing an infinite impulse response filter. However, the introduction of the filter leads to a slow response when faults occur [66]. A stationary wavelet transform is used to resolve this problem with a low detection rate, a satisfactory response rate to faults, and a good performance index [67].

2.4.1.3 Parameter estimation

The parameter drifts are not measurable directly; therefore, the diagnosis requires an online estimation for the parameter. The parameter estimation method can be used to detect the faults which occur as time-dependent parameter drifts. This approach can be utilized when the process faults are linked to the parameter changes in the process model [44, 68]. Various parameter estimation techniques were presented [68,69]. These include estimation via discrete time models, least square methods.

Generally, the process models can be developed using input/output data, a reduced order model, and a nonlinear first principle model. It is very reliable when the process model is developed from the first principles, where each model parameter has the physical meaning of the process. These methods are computationally intensive for large-scale processes and require an accurate dynamic model of the process. Therefore, the complexity has marked a significant drawback of using this approach for fault diagnosis. However, the real-time optimization problem is still a significant issue using this approach. It is also required to address the robustness issue accurately. The estimation algorithms based on measured data are Kalman filter [70] and the extented Kalman filter [71]. For fault detection, a comparison between the nominal parameter determined in normal operation and the online estimated values, a fault is detected. [72].

2.4.1.4 Bond Graph

The Bond Graph (BG) is an integrated graphical representation of a domain independent and energy-based method for dynamic modelling the physical system using a different domain. The BG can generate residuals generically and systematically among all graphical approaches. The BG framework includes various information due to its structural feature that can help to generate fault signatures. They generate a robust threshold for evaluating residuals, and the BG has been merged with parameter uncertainties. The residuals are obtained by covering casual paths [73] by applying software [74,75].

Using parameter uncertainties, a new BG modelling approach was proposed for the linear fractional transformation configuration [76]. However, this approach cannot address the measurements uncertainties. Therefore, Chatti et al. [77] proposed a new method based on the signed bond graph (SBG) to handle the issue of uncertain measurements. This method generates quantitative as well as qualitative diagnoses. The quantitative and qualitative structural properties allow generating multiple predictions. The various filtering and parameter estimation methods based on statistical hypothesis testing have been developed in recent years [78].

2.4.2 Data based approaches

Since developing an accurate model for large-scale industrial processes is difficult, most applications are based on data-based approaches. Data-based methods do not require any prior information related to the process. However, it is presumed that historical data is available, and it is comprised of various measurement features for the development of fault detection and diagnosis. The process data are obtained from the normal and abnormal behaviour of the process plant. Since these techniques are based on data-based techniques, the efficiency of these methods is dependent on the quantity and quality of the process data. A large amount of data has been achieved in the process industry due to the wide use of distributed control systems. This data contains useful information for monitoring and control purposes. Hence, most researchers adapted because of the wide usage of a distributed control system in most industrial processes. A detailed discussion of these fault detection and diagnosis approaches for process monitoring methods is presented.

2.4.2.1 Bayesian networks

Bayesian networks (BN) have been widely used in several areas for the diagnosis of various diseases [79], clinical applications [80], and the field of cancer modelling and prognosis [81], as well as fault detection and diagnosis [82-84]. The BN is a probabilistic modelling approach that can be used to represent a relationship between the variable using the acyclic graph. The networks can be used to see the probabilistic

dependency within the group. Pear introduced the BN in the 1980s [85,86]. It has also attracted much interest in industrial applications such as aircraft engine applications [87], power plants [88], the manufacturing of semiconductors [89], and sensor faults [90]. It can also be used for incomplete, complex, and uncertain systems [91].

Moreover, it can help to complete the lack of data by using expert knowledge and historical data. Murphy addressed another problem in modelling sequential relationships between the variable in 2002 [92]. It was solved using a Dynamic BN to combine the static network with sequential information. It has been used to detect transient faults, diagnose fault propagation patterns, determine root cause variables, and improve the problem of online services [93,94]. The control charts are other statistical control techniques that BN classifiers can also model for detecting and isolating faults [95]. This technique is viable and performs well; however, it requires numerous assumptions about the process and a large amount of data for the network's training. On the other hand, the artificial neural network had proven itself an excellent alternate modelling technique because its adjustment to the data deprived of any extra specification related to the distribution of input data [96].

2.4.2.2 Artificial neural networks

The neural network can be used to map between input and output variables in several ways. This machine learning technique is diverse and originated from the mimicking of a human brain. McCulloch-Pitts models in the 1940s [97] developed the first artificial neural network (ANN). This model comprised all the necessary elements to execute logic operations, but its implementation was not feasible. It was not technically solved by Hebb in 1949 [98] when he proposed a learning scheme. These ideas build the foundation of the first neuro-computer that can automatically adapt the connection, which Minsky developed in 1945. Finally, in the 1980s, the neural network gained a lot of advancement and momentum by different researchers such as those Amari [99,100], Anderson et al. [101], Grossberg and Carpenter [102,103], Hopfield [104,105], Rumelhart and McClelland [106]. In general, the neural network is a computational structure that consists of a large number of processing units connected

parallel to each other. Due to the collective behaviour of these nodes, the neural network can be used to represent complex relationships and data structures.

The neural network has been used in different applications such as credit scoring [109], transportation forecasting [107], medical treatment and diagnosis [108], image processing, and classification [109]. In recent years, significant interest has been seen the application of neural networks for fault detection and diagnosis. It has gained consideration for its capacity to learn complex and nonlinear processes [110,111]. ANN has been successfully utilized in the various applications of pattern recognition to extract useful information from the data and handle incomplete noisy data. It has also been used for classification and function approximation problems [96]. Neural network developments can be classified into two distinct categories:

- a) the architecture of the network such as radial basis, sigmoidal, linear function, etc.
- b) the learning strategy used for the training of data such as supervised or unsupervised learning.

Currently, ANN has set a broad application in chemical engineering to develop fault detection and diagnosis methods to meet the demand from the industry regarding product quality, safety, and efficiency [112-114]. The real-time process monitoring and control system for the polymerization process was developed by Gonzaga et al. [115] using ANN as a process monitoring tool. A generalized neural network with wavelet transforms for the estimation of fault location in transmission lines was proposed by Jamil et al. [116]. Liu and Jolley [117] developed a tool for condition monitoring. Xu and Liu [118] proposed a dynamic fuzzy neural network to predict melt indices. A combination of resilient backpropagation and least square support vector regression to monitor the grinding process online was developed by Pani and Mohanta [119].

MLP with BP network applied by Hwang et al. [120] for fault detection and diagnosis of a pressurized reactor in the nuclear plant. Nagpal and Brar [121] presented a comparative study based on the performance evaluation of various neural networks for fault classification on power transformers. Nozari et al. [111] developed and tested

a robust fault detection and diagnosis approach for industrial gas turbines based on the MLP neural network and local linear Neuro-fuzzy.

2.4.2.3 Control charts

The conventional representation of online process monitoring using statistical process control was control charts. Control charts are ubiquitous in the field of fault detection. In 1931, Shewhart [122] introduced the control charts, and it was further developed as cumulative control charts by Page [123] in 1954. These charts have had more comprehensive applications in process industries for decades. To maintain process reliability and improve product quality, SPC charts have been growing extensively. These charts are applicable to provide diagnostic information and real-time process monitoring source. In general, there are upsets in process plants that bring the process away from the normal regime. However, control charts are beneficial for loss prevention and failure prognosis [124].

The basic theory behind the development of control charts assumes that every process, regardless of its design and maintenance, can face a certain amount of variability in the process over time. This will ensure the proper monitoring of the process over time for the early detection of any abnormal event. This early detection will lead to the diagnosis to correct the problem and bring the process to its normal operation. Parameter monitoring can be done either by univariate control or multivariate control plots [125]. There can be misleading information from the univariate control charts because they cannot handle correlation, and the parameters are independent [43]. The multivariate control charts can handle many variables, which helps to show the correlation between the variables. The identification of correlation helps to control the false alarm rate.

2.4.2.4 Principal component analysis and Partial least squares

Multivariate statistical techniques are used in statistical process control to find and fix problems. These methods, such as principal component analysis (PCA) and partial

least squares (PLS), have been used in a wide range of situations in the literature because they can compress and reduce the processing data without losing any important information. It can also help to analyze a lot of data, deal with noise, get the most out of your data, and get accurate information quickly. The process makes it easier to analyze the data than the original data. The main goal is to turn a large set of related data into a smaller set of unrelated data [43]. First, Pearson came up with the idea for PCA in 1901. Hotelling made it work for him in 1947 [126]. PCA has been used for long-term, real-time processes [127-129]. Most chemical processes do not work linearly, so PCA is not very good at modelling them. Various studies have been done to develop nonlinear PCA (NLPCA) to solve this problem [130]. Kramer [131] came up with NLPCA in 1992, and it was based on an auto-associative neural network.

Multiscale principal component analysis (MSPCA) [31] is another tool that could be useful for fault detection and diagnosis applications. It combines PCA and wavelets analysis [33]. There are two parts of PCA: The PCA part removes the correlation between a set of variables, and the wavelet part extracts the features from the data. Using MSPCA and the Adaptive Neuro-Fuzzy Interface System (ANFIS), a framework was built to help find faults in the distillation column while it is still running. By giving each classifier a single fault, the multiple ANFIS classifier can be used. It can reduce the amount of time it takes to run and improve the new fault identification by expanding the framework [132]. In order to keep track of things that change over time, the recursive algorithm has been used. This includes KPCA [30], multi-block and multiscale PCA [133], and the moving window KPCA [27].

In MSPM methods, the PLS model focuses more on quality-related faults. PLS can capture the relationships between a large number of highly correlated process variables and a few quality variables [134]. Numerous studies have been done in the field of fault detection, diagnostics, and process analysis, as well as PCA and PLS [135]. The multiway and multi-block PLS [136] were made for fault detection. Similar to PCA, PLS is also a statistical tool that can be used to project massive data. However, the resultant variable has all the information from the original data.

2.5 Comparison of model-based and data-based approaches

Numerous published studies show that the data-based approaches require a considerable amount of data and output measurement variables to develop a diagnostic system. The data-based methods are simple and easy to apply. They can deal with highly correlated parameters of the process [6]. Thus, they are reliable for large-scale and complex process plants. Since they do not require any model development [45], they can also minimize time and cost. The data-based approaches require an extra pre-processing step to extract useful information from the data. The data is then used to train the model; hence the model performance depends on the training data. The performance can be reduced if the system gets unknown data or with the occurrence of unknown faults. The performance of data-based techniques such as classifiers or patterns towards isolability requirements and the robustness to noise is high compared to model-based approaches. Despite numerous studies published in the literature, no single approach is adapted to all the requirements for a diagnostic system.

Conversely, the model-based approaches used the first principle model to develop and identify various estimation techniques. As the complexity of the process plant increases, the estimation becomes challenging and sometimes impossible. These approaches require a small amount of data along with a mathematical model. These approaches can only deal with linear system and some classes of nonlinear systems. These approaches are only suitable for small-scale systems and depend on the developed model's accuracy [8]. Since these models are based on various approximations and assumptions, the validation step is essential [137].

2.6 Industrial applications of process monitoring approaches

To improve many necessary outcomes in industrial processes, a variety of extensive process monitoring approaches has been developed as a common process supervision instrument for many industrial systems engineering, including semiconductors, the automobile industry, nanotechnology, and others [68,138,139]. Isermann [68] provided a brief overview of fundamental fault detection techniques, including parameter estimation methods for continuous-time functions such as an electrically powered centrifugal pump

with a water vascular system. Furthermore, basic issues and methods of process supervision, including fault detection and diagnosis in specific technological processes. In this study, the authors proposed a knowledge-based technique and several different fault detection methods that extract crucial details from data and make use of models of processes and signals. They developed analytic symptomatic and interpretative symptoms, which were frequently caused by human operators, as an additional source of information for comparing process features. They also suggested classification methods, approximation reasoning, and fuzzy approaches based on if-then logic [138].

Furthermore, fault detection and diagnosis in chemical processes is recognized as a critical component of the abnormal event management system, which includes the three crucial functions of prompt fault detection, fault diagnosis, and remedial action for faults in a process [6]. In the chemical industry, fault detection and diagnosis is a useful process monitoring tool for assuring process safety and efficiency. As a result, for effective and sustainable operations, the advanced chemical industry requires fault detection and diagnostic strategies that can more efficiently identify and diagnose process faults. [140]. The majority of datasets obtained from online chemical processes contain multiscale characteristics. This data has a variety of time-varying and frequency-varying properties as well as noise, and certain key components are often masked since the measured data may be contaminated with potential adverse effects [141]. However, in the fault detection and diagnosis implementations, many research findings focus on resolving several practical problems in fundamental chemical processes, such as how to control data characteristics such as nonlinearity, non-stationarity, autocorrelation, cross-correlation, and non-Gaussian distribution. This study reviewed the uses of advanced analytics and artificial intelligence technologies to tackle common difficulties in actual chemical processes [142]. PCA-based techniques have been widely employed for fault detection and diagnosis in a variety of chemical processes [143-145]. Chiang et al. [8] established an information criterion for deciding the order of feature reduction for Fisher's discriminant analysis (FDA) and discriminant PLS to improve fault diagnosis ability. They gave an ideal declaration of feature reduction of fault diagnosis by leveraging the features of FDA and DPLS approaches. Using a simulation model TE process example, they demonstrated that FDA and DPLS are superior dimension reduction methods for identifying faults than PCA.

Zhou et al. [146] investigated fault diagnosis techniques for two distinct chemical processes. This study examined the prediction error of neural network models for sensing or components fault detection and then used an RBF neural classification strategy for fault isolation. They used two different chemical processes to assess the effectiveness of the neural network models. Wang et al. [147] proposed a subspace technique for developing a fault detection, isolation, and identification system. They presented four distinct methods in this work to create residuals. Through simulated research of the vehicle horizontal complex system, they demonstrated that each of the suggested algorithms is resistant to inputs while sensitive to sensing and actuation faults. Wang et al. [148] introduced a new collaborative process monitoring technique based on multiset canonical correlation analysis for chemical processes. In this study, they used this technique to draw standard inherited features in the overall processes, predicted the measurement results in an independent operations division into the subspaces of shared and individual characteristics, and derived statistical data from investigating the variability in the subspaces of shared and unique features at the same time.

The semiconductor industries demand greater process and quality management approaches and automation technologies to enhance production effectiveness. The most pressing challenge is developing and implementing effective fault detection and classification systems for semiconductor manufacturing operations [149]. Fault detection and classification in semiconductor technology have been acknowledged as one of the essential components of the advanced process control framework for improving overall production efficiency and decreasing process variability [150-152]. Several fault detection and classification methods have been established and deployed in the semiconductor industry to detect faults in processes and find the relevant root causes. However, due to the significantly higher complexity of silicon wafer computation and the different natures of information recorded by semiconductor processes such as nonlinearity and multimodality [152]. Most conventional fault detection and diagnosis strategies may be insufficient to explain faults presented in both procedures and semiconductor wafers. In semiconductor production, for example, the photoresist is a very intricate nonlinear process that significantly influences wafer quality. Thus, numerous effective fault detection and diagnosis strategies for semiconductor manufacturing processes have been researched during the last three decades [153-155]. To solve the limitations of traditional PCA-based fault detection and diagnosis approaches, He and Wang [150] proposed FDkNN, a fault detection methodology based on k-NN, for semiconductor production processes that typically contain nonlinearity and multimodal trajectory attributes. Fan et al. [156] proposed using random forests to determine critical status parameters, processing periods, and stages in semiconductor production processes. They used k-NNs and naive Bayes classifications in the prediction models and the t-distributed stochastic neighbour embedding approach to show the critical fault detection and classification parameters in this work.

Process condition monitoring is a critical responsibility in wind farms, one of the most popular renewable energy sources. As a result, adequate supervision and management of wind turbines are required to save operating and maintenance expenses. Laouti et al. [157] investigated a fault detection and diagnosis issue in wind turbines. They used a support vector machine (SVM)-based FDI technique to diagnose defects in a horizontal-axis wind turbine with fixed blades and a total converter. They used RBF as the kernel in SVM and then looked at actuators, sensors, and processes problems. Dong and Verhaegen [158] examined data-driven design strategies for FDI on a nonlinear wind turbine issue with unpredictable wind disruptions. They designed a bank of resilient fault detection filters and applied them in a simulation model to demonstrate its performance. Kusiak and Li [159] developed a three-level fault prediction technique for wind turbines, including identifying faults, categorizing problems based on severity, and predicting a specific defect utilizing data from SCADA systems and fault files.

Many faults occur inside solar arrays in photovoltaic power generating systems due to changing external temperature conditions [160,161]. However, due to the inherent nonlinearity of photovoltaic applications, fault detection in solar arrays is highly challenging. Zhao et al. [161] present a semi-supervised learning approach based on graph theory using a few normalized labelled data for training to identify and categorize hidden flaws in solar arrays. Pei and Hao [160] demonstrated a data-driven technique for identifying typical PV array flaws. They first identified several significant fault features and then established solar system voltage and current indicators to create the fault detection technique. They found the fault detection thresholds and evaluated the hands to the appropriate values using the defined indicators that carry fault parameters. They demonstrated the detection accuracy of the suggested technique using numerical simulations.

The robotic fault detection and diagnosis task in rolling elements is critical for testing in rotating machines because faults in roller bearings primarily cause machine collapse. Kankar et al. [162] developed a new fault detection method for rolling elements in rotating machinery. This study proposed fault detection algorithms based on two machine learning algorithms, ANN and SVM. They demonstrated the effectiveness of the recommended approaches through comparative experimental research. A data mining technique has also been developed for detecting faults in wind turbine generator components. Improvements in various neural network models have been made in this technique to establish a correlation between several inputs and temperature in generator bearings and to construct malfunction predictions models utilizing historical wind turbine data. They validated the neural network models by running them through two different turbine scenarios [159].

Liu et al. [163] introduced a systematic fault diagnostic technique for identifying defective blocks and finding complex variables in a continuous annealing process line. This work developed new frame contribution and variable contribution methodologies based on a reconstruction methodology for determining complex variables and diagnosing faulty blocks

An adaptive technique has been developed to deal with false alarms that may occur during a real-time operation. For fault isolation and identification, PCA-based approach was employed in conjunction with the generalized likelihood ratio test and the SVD method [164].

2.7 Statistical process monitoring

In the process industry, statistical process monitoring has become a popular method for monitoring performance. There are two types of statistical process monitoring methods: univariate and multivariate statistical process monitoring methods.

2.7.1 Univariate statistical process monitoring methods

These methods are also known as statistical process control (SPC) methods, in which each variable is evaluated individually [165]. Walter Shewhart introduced the first SPC chart in 1924, one of the earliest charts used for process monitoring without applying any filter. This chart identifies typically large faults. SPC charts also employ linear filters to identify minor faults, such as cumulative sum (CUSUM) or exponentially weighted moving average (EWMA). Such approaches remain dominant in the process industry, but their performance deteriorates with highly correlated variables [166]. They often cause alarm flooding, which becomes a significant challenge to many process systems [167]. Such shortcomings in the SPC charts have led to multivariate extensions of Shewhart control charts to monitor different variables simultaneously [126]. Extensions of the Shewhart control charts are used when the process parameters of the underlying process are known or unknown. These charts are called multivariate Shewhart charts. Multivariate CUSUM (MCUSUM) and multivariate EWMA (MEWMA) have been developed for the detection of small changes [168], and they provided unsatisfactory results for highly correlated process variables [169].

2.7.2 Multivariate statistical process monitoring methods

Highly correlated and high-dimensional process data can be analyzed using multivariate statistical process monitoring methods (MSPM). The main concept of MSPM methods is process features that can be obtained through a particular analysis process. Thus, the higher dimensional information is projected into a less dimensional space, followed by an evaluation of the statistics [170]. Figure 2.3 demonstrates the classification of well-known MSPM methods.



Figure 2.3: Classification of multivariate statistical process monitoring [171].

The most extensively used MSPM approaches are PCA and PLS. One dataset is used to input data and output results with the PCA model. PLS splits variables into input and output categories before identifying the principal components that optimize their covariance [172]. Gaussian distribution is assumed in both techniques. Non-Gaussian issues may be solved using independent component analysis (ICA), which enforces separate components and high-order statistics. More relevant information may be found in non-Gaussian data with its help [173]. It is possible to deal with non-Gaussian data using the Gaussian Mixture Model (GMM), which treats a complicated process as a linear mixture of many Gaussian models [174].

2.7.3 Recent developments in MSPM methods

Even while traditional MSPM systems have greatly improved monitoring performance compared to SPC approaches, they still have limitations. These approaches' monitoring statistics and control limits are developed based on the assumption that process data is Gaussian-distributed. A linear connection between process variables is also required. However, most of these assumptions may be readily broken due to the following features of process data from sophisticated processes: multimodal distribution, dynamics, nonlinear interactions between variables, non-Gaussian, and time-varying. Consequently, some improvements have been made to standard MSPM methodologies and other data-based solutions for process monitoring in recent years.

The most frequent approach to dealing with nonlinearity is to use linear approximation with a kernel function. Nonlinear issues may be thought of as a mixture of a number of local linear models, but it is difficult to establish how many models there are. Methods that use kernels to translate nonlinear variables into higher-dimensional spaces with linear variables are preferable to linear approximations. KPCA [175] and kernel PLS (KPLS) [176], kernel ICA (KICA) [177], and nonlinear kernel GMM [178].

The dynamic data from industrial chemical processes always have problems with the process and noises in the data. A dynamic PCA (DPCA) model was used to keep disturbances out of the industrial process [179]. Adding several time-lagged samples of each variable to the model dataset is the initial stage in this approach. The process data's autocorrelation may be recovered by developing the PCA model on this enhanced data matrix. PLS [180], ICA [181], and GMM [178] have all been improved using similar dynamic approaches by supplementing time-lagged data.

In batch processing, the data has a certain three-way structure that distinguishes dynamic processes. Traditional multivariate statistical techniques may be used to solve a two-dimensional matrix that has been unwrapped from the three-way structure of the process data by Nomikos and MacGregor [182,183]. More than one characteristic is always present in the data from complicated chemical processes: non-Gaussianity, nonlinearity, numerous modes. Consequently, hybrid techniques like MGMM, MKPCA, MKICA, DKPCA, or integrated approaches using statistical methods and other methodologies have been presented in recent years [21,184-186].

The process data collected from chemical processes usually involve high noise levels and autocorrelation and may also vary from normality and, consequently, impact MSPM process monitoring methods [187]. Such techniques are also based on a singlescale representation of measurements and cannot capture the information from multiscale representations of measurements [188]. Wavelet-based multiscale process monitoring methods have been developed to address these problems. Process monitoring models have been developed in these techniques by using wavelet coefficients at each scale [33,188,189]. Multiscale process monitoring methods are being effectively used to analyze chemical processes from the last two decades. Various multiscale process monitoring techniques have been applied based on the process data obtained from different chemical processes.

2.8 Multiscale process monitoring methods

The demand for operation safety and product quality are critical issues in modern industrial processes. Although, the widespread use of sensor networks, advanced data acquisition technology, and the broad use of distributed control systems have added considerable benefits to all process industries [2,169]. They are becoming increasingly integrated, automatic, more complex, and intelligent operations. These developments in modern industrial processes increase process monitoring systems [190]. Conventional MSPM techniques and their extension concentrate on the analyses of onescale phenomena, typically the sampling frequency. Therefore, the applications of these techniques are restricted to only a single scale and cannot derive the amount of information from process data showing multiscale phenomena [38]. The multiscale approach can get information through different decomposition techniques in different scales.

WT is the most effective multiresolution analysis technique for breaking down the original process measurements into their multiscale components based on the time and frequency characteristics of the input data set [32]. The process signals, which have unique physical patterns or disturbances, are dissected and seen as a collection of signals with various resolution scales. To deconstruct a signal, WT convolves it with a preset mother wavelet, the choice of which is generally determined by the kind of data.

Figure 2.4 illustrates the multiresolution analysis principle utilizing WT. First, the original signal is decomposed into approximation and detail coefficients. The approximation function is a low-frequency signal, which contains the essential underlying deterministic features. The detail function includes the high-frequency component, which is mainly noises. The approximation function is further decomposed into even coarser approximation until the average signal has been approximated. This

reconstruction perfectly composes the original signal if all wavelet coefficients are used.



Figure 2.4: The basic idea of multiresolution analysis using wavelet transform [191].

The major issues identified based on the careful study of the research articles related to multiscale process monitoring are presented in Figure 2.5. The figure shows the percentage of papers that addressed each of them. Although some of these issues are not unique to multiscale process monitoring methods alone, we review them within the context of multiscale process monitoring. The research articles based on multiscale process monitoring are dedicated to discussing these issues. A list of all the reviewed research articles is given in Table 2.1. The table also shows the decomposition technique they used, the method they used, the case studies they used, and, more importantly, the issues they addressed. The purpose of this table is to help the reader choose a specific issue of interest and peruse down the column for papers that address it. The statistical analysis based on the used methods, name of case study and the type of case study is presented in Appendix A.



Figure 2.5: Issues discussed in multiscale fault detection and diagnosis methods.

Sr.	Decomposition Monitoring Year					Issu	ie ado	dress	ed			Application	Types of o	case study	Reference
No		Technique	method	A *	A	В	C	D	E	F	G	area	Simulated	Real-time	
1	1998	WT	PCA	~								NE, FCCU	\checkmark		Bakshi [33]
2	1999	WT	NLPCA	~					~			ISD		~	Shao et al. [192]
3	1999	WT	PCA	~			1					NE	~		Haitao et al. [193]
4	1999	WT	PCA	~				~				DC, CSTR	~		Luo et al. [194]
5	2000	WT	NLPCA	~		~						NLIP		~	Fourie & de Vaal [195]
6	2000	WT	PCA, MPCA, DISSIM	~								TE process	✓		Kano et al. [196]
7	2000	WT	PLS	~	1							WWTP		\checkmark	Teppola & Minkkinen [191]
8	2001	WT	PCA	~								WWTP		~	Rosen & Lennox [197]
9	2002	WT	PCA	~					~			IBD, ITRS	~	~	Misra et al. [31]
10	2002	WT	PCA, MPCA, DISSIM	~				~				NE, TE process	~		Kano et al. [198]
11	2002	WT	DPCA	~			1					WWTP	~	~	Yoo et al. [199]

Table 2.1: Comprehensive overview of multiscale fault detection and diagnosis methods.

12	2002	WT	PCA	√			~		WWTP		✓	Lennox & Rosen [200]
13	2003	WT	PCA	~			*		TE process, TTS	1		Lu et al. [128]
14	2004	WT	РСА	~			~		NE, CFT	√	√	Zhiqiang & Qunxiong [201]
15	2004	WT	РСА	~			~		CSTR	~		Yoon & MacGregor [189]
16	2005	WT	PCA	~					PSP		~	Wang & Romagnoli [202]
17	2005	WT	MPCA	~				~	SBRS		1	Lee et al. [133]
18	2005	WT	NLPCA	~	~				ECF		✓	Geng & Zhu [130]
19	2005	WT	NLPCA	✓	~				CSTR	~		Maulud et al. [203]
20	2005	WT	GDM	~		~			TE process	~		Alabi et al. [204]
21	2006	WT	PCA	~					SS	~		Reis & Saraiva [205]
22	2006	WT	NLPCA	✓	~				CSTR	~		Maulud et al. [37]
23	2006	WT	PCA	✓					NE	~		Zhang & Wang [206]
24	2006	WT	KPCA	~	~				CSTR	~		Deng and Tian [207]
25	2006	WT	PCA	\checkmark					NE, CSTR	\checkmark		Reis & Saraiva [208]
26	2007	WT	MPCA	\checkmark			~	~	PFP	~		Alawi & Morris [209]

27	2007	WT	PCA	✓						BWWTP	~		Borowa et al. [210]
28	2008	WT	PCA	~						SM, FFE		~	Reis et al. [211]
29	2008	WT	PCA	~				~		CS		~	Xu et al. [212]
30	2008	WT	КРСА	~		~				TE process	~		Tian & Deng [213]
31	2008	WT	PCA, KPCA	~		~		~		CSTR	\checkmark		Choi et al. [214]
32	2008	WT	ICA	✓					~	TE process	\checkmark		Salahshoor & Kiasi [215]
33	2009	WT	PLS	√	1					SDS, BAFP	~	~	Lee et al. [216]
34	2010	WT	PCA	~						PMP	~		Xia and Pan [217]
35	2010	WT	PCA, KFDA	~		~		*		IPPP, TE process, CSTR	~	~	Liu et al. [218]
36	2010	EEMD	PCA	✓			~			LSBTS	~		Zvokelj et al. [219]
37	2011	EEMD	КРСА	~		~	~			NE, BF, LSBTS	V	~	Zvokelj et al. [220]
38	2011	WT	KPCA, KPLS	~		~		~		FMF, CAP	√		Zhang & Ma [34]
39	2011	WT	PCA	 ✓ 				~		HHS	√		Giantomassi et al. [221]

40	2011	WT	PCA	~				✓		PMP		~	Ferracuti et al. [222]
41	2011	WT	KPLS	~	~	~		~		NE, PFP, EFMF	✓	1	Zhang & Hu [223]
42	2011	WT	PLS	~	~					TE process	\checkmark		Roodbali & Shahbazian [224]
43	2012	WT	КРСА	~		~				NE, EFMF, TE process	√		Zhang et al. [38]
44	2013	WT	РСА	~						NC		√	Harrou et al. [225]
45	2013	WT	PCA	~		~				NE, TE process	~		Shi et al. [226]
46	2013	WT	РСА	~				✓		TE process	\checkmark		Lau et al. [132]
47	2013	EEMD	KPCA, SKC	~		~				CSTR	\checkmark		Deng & Tian [227]
48	2014	WT	PCA	~						STP		~	Mirin & Wahab [228]
49	2015	EEMD	KPLS	~	~	~				NE, PFP	~		Liu & Zhang [229]
50	2015	WT	KFDA	~		~				TE process	~		Nor et al. [230]
51	2016	WT	GMM, KFDA	~				~		TE process	\checkmark		Nor et al. [231]
52	2016	EEMD	ICA	~				~	√	LSBTS	~	~	Zvokelj et al. [232]

53	2016	WT	PLS	~	✓						DC	~	Madakyaru et al. [233]
54	2017	WT	PCA	~							SD, TE process	~	Sheriff et al. [32]
55	2017	WT	EWMA, KPLS	~	~	~					CSM	V	Mansouri et al. [234]
56	2017	WT	GMM, KFDA	~		~			1		TE process	~	Nor et al. [24]
57	2017	WT	PLS	~	1						DC	\checkmark	Madakyaru et al. [235]
58	2017	WT	КРСА	~		~					CSTR	\checkmark	Sheriff et al. [39]
59	2017	WT	PLS	~	~						TE process, CSTR	✓	Botre et al. [236]
60	2017	WT	РСА	~					~		TE process	\checkmark	Zhang et al. [237]
61	2018	WT	PLS	~	1						SFSS	\checkmark	Chaabane et al. [238]
62	2018	EEMD	PCA, CUSUM	~				~			TE process	\checkmark	Du & Du [239]
63	2018	EEMD	PCA, CUSUM	~				~	~		TE process	\checkmark	Du & Du [240]
64	2019	WT	PCA	~							AHWR	\checkmark	Yellapu et al. [241]
65	2019	WT	DPCA	√			~				TE process	√	Kini & Madakyaru [242]

66	2019	WT	KFDA	~	~		~		TE process	~	Nor et al. [243]
67	2021	WT	PCA	~					AHWR	√	Yellapu et al. [244]
68	2021	WT	ICA	~				~	NE, QTP, DC	1	Kini & Madakyaru [245]
69	2021	WT	РСА	~					NE, TE process	~	Sheriff et al. [246]

Name of Issue: (A*)-fault detection, (A)- multiscale methods for quality relevant process monitoring, (B)- multiscale methods for nonlinear process monitoring, (C)- multiscale methods for dynamic process monitoring, (D)- multiscale methods for incipient fault detection, (E)- multiscale methods for fault diagnosis, (F)- multiscale methods for batch process monitoring, (G)-multiscale methods for non-Gaussian data.

2.8.1 Multiscale methods for quality-related process monitoring

MSPM methods are more beneficial for extracting meaningful information from the highly correlated process and quality variables because quality variables are measured at lower frequencies and typically have significant time delays [247]. Monitoring quality variables is essential for preventing system breakdowns and substantial financial losses. A few researchers have also developed a quality-related multiscale process monitoring technique.

Partial least squares (PLS) is the MSPM method associated with quality-relevant monitoring, and it finds a relationship between the process and quality variables [248]. Teppola and Minkkinen [191] proposed a quality-related multiscale process monitoring scheme combining wavelets with PLS. The PLS model is constructed based on filtered measurements obtained by removing low-frequency scales in this approach. Lee et al. [216] proposed a multiscale technique combining PLS and WT for sensor fault detection. The feasibility of the proposed technique was confirmed by using the real industrial dataset from the biological wastewater treatment process. The monitoring results were also compared to those of the standard PLS method.

Madakyaru et al. [235] proposed a MSPLS model based on generalized likelihood ratio (GLR) tests. In this approach, a modeling framework is created by integrating WT with PLS, and then GLR testing is used to improve fault detection. The proposed methodology proved immensely influential in the early detection of minor faults with incipient behaviour in distillation columns. Similar work is proposed by Botre et al. [236], where efficiency and robustness are demonstrated through simulated CSTR system and TE process.

Zhang and Hu [223] proposed a multiscale KPLS (MSKPLS) method combining kernel PLS (KPLS) and wavelet analysis for investigating the multiscale nature of the nonlinear process. The feasibility of the proposed method was tested for a real industrial data set, and the process monitoring abilities were compared with the standard KPLS method.

2.8.2 Multiscale methods for nonlinear process monitoring

Multiscale process monitoring frameworks using conventional MSPM methods have been used effectively in the process industry. Conventional MSPM methods underperform in complex industrial processes with nonlinear features due to their assumption of linear correlations in the process data. Nonlinear process monitoring has become a significant area of research in this field in recent years, and some nonlinear multiscale approaches have been developed and discussed in this subsection.

Shao et al. [192] proposed a multiscale NLPCA process monitoring approach based on an input-training neural network (IT-NN) where non-parametric control limits were employed instead of linear control limits to improve online performance monitoring. This technique was modified using multi-level wavelet decomposition to enhance process monitoring [195]. Geng and Zhu [130] proposed an adaptive multiscale NLPCA approach to monitor slow and weal changes in process variables. Maulud et al. [37,203] have developed a new multiscale approach using optimal wavelet decomposition and the orthogonal NLPCA. They only use approximation and highest detail functions, simplifying the overall model structure and improving interpretation at each scale. This work determined the optimal decomposition level by a PCA-based graphical method.

The kernel learning methods recently received significant attention in the chemical industry and have been coupled with conventional MSPM process monitoring methods [139, 249-251]. Several researchers have proposed KPCA and KPLS based multiscale nonlinear process monitoring methods [34,214,252]. Choi et al. [214] proposed a new multiscale nonlinear process monitoring technique using KPCA to detect and identify faults. This approach has been extended by Deng and Tian [252] to nonlinear dynamic processes that can effectively extract autocorrelation, cross-correlation, and nonlinearity from the process data. Zhang and Ma [34] further developed this approach to improve diagnostic capabilities. The further study proposed a nonlinear system monitoring approach based on KPLS at different levels. Zhang and Hu [223] have extended this approach to monitoring online processes in nonlinear processes.

The FDA does better than the PCA approach to classification problems in many cases. Although it shows limited performance in nonlinear systems due to its linearity, it is better suited to classification problems [253]. Liu et al. [218] proposed a multiscale classification method to obtain the most discriminatory characteristics of the scale. The effects of feature extraction investigated the classifier performance, and a multiscale classifier was developed to classify the faults better. This method can be applied to relatively large multi-class issues. Nor et al. [230] proposed a novel multiscale approach by combining KFDA with wavelets for nonlinear process monitoring, where XmR and T^2 statistics were used for fault detection. This approach was further extended to enhance the performance of fault classification and developed a robust multiscale feature extraction and fault classification method [24].

2.8.3 Multiscale methods for dynamics process monitoring

Due to random noise and process disturbances, a dynamic relationship exists among process variables in modern chemical processes. Information on this dynamic behaviour is not included in conventional process monitoring methods, leading to misleading results. Changes in dynamic relationships among process variables can not be investigated efficiently, resulting in significant process failure due to dynamic relationships, intermittent noises, and other disturbances. Substantial research has improved monitoring performance in dynamic industrial processes in recent years.

Haitoa et al. [193] proposed a multiscale framework for monitoring dynamic multivariate processes at different scales by combining wavelets and PCA. This framework enhances the suitability of PCA for monitoring processes based on autocorrelated data. Yoo et al. [199] have developed a multiscale approach to dynamic processes using dynamic PCA for WWTP. Similar faults have been detected and isolated by incorporating D statistics into the algorithm. Alabi et al. [204] have developed a multiscale dynamic process monitoring approach by integrating WT with a generic dissimilarity measure (GDM) to improve performance monitoring. Kini and Madakyaru [242] developed a multiscale DPCA framework where T^2 and SPE statistics were used for fault detection. The effectiveness of this framework is demonstrated by using dynamic multivariate data acquired from the TE process.

2.8.4 Multiscale methods for incipient fault detection

Early detection of incipient faults in modern chemical process systems is increasingly becoming important, as these faults can slowly develop into severe abnormal events, which lead to the failure of critical equipment. It is critical to detect even the most minor irregularities to ensure the safety of the process and the highest level of product quality. Detecting minor or incipient anomalies in modern chemical process systems is essential for process safety and maintaining product quality. These faults are difficult to detect early because they are obscured by noise and process control. They are common in complex processes and may quickly increase if no action is taken.

Kano et al. [198] proposed a multiscale method for incipient fault detection using dissimilarity analysis (DISSIM). Although DISSIM is mathematically comparable to PCA, its statistical index differs from T^2 . A new multiscale fault detection method based on ensemble empirical mode decomposition (EEMD) is proposed, effectively detecting three specific faults in the TE process that were previously undetectable using previously reported methods [239]. In this method, fault signatures are extracted using EEMD based PCA, and then half-normal probability and Cumulative Sum (CUSUM) are used for fault detection. The proposed method is further extended where CUSUM based on T^2 and SPE statistics improves fault detection [240]. Žvokelj et al. proposed multivariate and multiscale fault detection methods to detect the incipient failure of large slewing bearings based on Acoustic Emission signals by integrating EEMD with PCA [219], KPCA [220] and ICA [232].

2.8.5 Multiscale methods for fault diagnosis

Multiscale methods for fault detection have been thoroughly reviewed in previous sections. Although fault diagnosis is essential in process monitoring, it is relatively limited while employing multiscale methods. It is challenging to analyze the simultaneous impact of multiscale variables on monitoring statistics. Generally, fault diagnosis is accomplished via fault identification and classification. In fault identification, the faulty variables are identified based on their influence on the value of the statistical index. Identifying faulty variables is beneficial for highly integrated, large-scale, and complex plants [8]. There is no need for fault information for diagnosis through fault identification. If prior knowledge about the fault is available, the learning problem would be finding the boundary between normal and faulty samples. This learning problem is related to fault classification, and the three common approaches are similarity factors, discriminant analysis, and support vector machines (SVM).

Contribution plots are the most popular tool for identifying which variables push the statistics beyond control limits. Shao et al. [192] proposed a wavelet-based nonlinear PCA algorithm for process monitoring and applied differential contribution plots to find faulty variables of an industrial drying process. Many researchers have also used contribution plots with MSPCA process monitoring approaches to determine faulty variables [31,128,222]. Zhiqiang and Quanxiong [201] used contribution plots for fault identification in the wavelet-based adaptive MSPCA method. Many researchers applied contribution plots to identify the faulty variables using kernel-based nonlinear multiscale techniques [34,214,223]. A similarity factor was integrated with MSPCA to identify the fault type and reveal the fault source [213,252].

Lau et al. [132] have implemented Adaptive Neuro-Fuzzy Inference System (ANFIS) fault classification with MSPCA to diagnose selected fault cases in the TE process. Nor et al. [243] proposed a new multiscale fault diagnosis method by combining the multiscale KFDA and the ANFIS classification model. The fault classification performance was evaluated using the TE process data, and the results indicated that the proposed multiscale KFDA-ANFIS framework improved over the multiscale PCA-ANFIS and FDA-ANFIS.

SVM is a well-known classification tool, proposed initially by Cortes and Vapnik [254]. Liu et al. [218] proposed a multiscale fault diagnosis method and applied the SVM classifier based on classification distance, using 4-fold to obtain the optimal parameters. Nor et al. [24] incorporated the SVM classifier with multiscale KFD, and

the performance accuracy was compared to the multiscale KFD-GMM of the faults in the TE process.

2.8.6 Multiscale methods for batch process monitoring

Batch processes often operate in different phases of operation. The batch operations are becoming increasingly complicated due to frequent start-ups and shutdowns. As a result, monitoring tasks in batch processes are more challenging to perform. Multiway PCA [255] and multiway PLS [183] are still used to monitor batch processes.

Lee et al. [133] proposed a multiway MSPCA approach for batch processes that combines WT and multiway PCA and has been effectively used in the sequencing batch reactor process for biological wastewater treatment. The proposed approach aids in detecting early faults and detecting less apparent faults. Alawi and Morris [209] proposed a multiscale multi-block modeling approach for batch process monitoring and compared it with the conventional MPCA approach using simulated data obtained from the penicillin fermentation simulation benchmark.

2.8.7 Multiscale methods for non-gaussian data

Contrary to the eminent advances in MSPCA and MSPLS fault detection methods, ICA has received significantly less attention in the field of wavelet-based process monitoring despite ICA being a better choice for monitoring non-Gaussian data. A few researchers have also developed multiscale process monitoring methods to handle non-Gaussian data.

Salahshoor and Kiasi [215] proposed a multiscale-ICA technique by integrating with wavelet analysis and ICA for non-gaussian data. They used Daubechies 3 (db3) up to level 3 and found that the proposed technique effectively used TE process data. Zvokelj et al. [232] proposed a new multiscale process monitoring technique combining EEMD with ICA. They found that this technique is also suitable for detecting incipient faults in large slewing bearing systems. Kini and Madakyaru [245] proposed a wavelet-based multiscale fault detection technique by combing wavelets with ICA. The

effectiveness of the proposed technique was illustrated by using three different case studies and found that this technique can enhance the detection rate in noisy process environments.

2.9 Research gap

A few future research prospects in the field are identified based on the discussion of multiscale fault detection and diagnosis methods in section 2.8. The most crucial and challenging task in the process industry is efficient quality control, which ensures product quality, maximizes profitability, and prioritizes safety in real-time processes. Real-time process monitoring is essential for effective process control. It has been identified that in the existing multiscale fault detection diagnosis frameworks, the wavelet decomposition of process signals was performed by offline signals, which limits the requirements for real-time applications. The current literature does not have enough knowledge related to real-time process monitoring.

After fault detection, fault identification is a critical step in determining the root cause of the fault. It has been identified from the literature that the contribution plot is used to identify faulty variables. It is a popular tool that is often used to identify faulty variables. However, it is well known that this approach suffers from the smearing effect, which may mislead the faulty variables of the detected faults. The finding revealed that the highlighted aspects had not been covered extensively.

Many chemical processes exhibit nonlinear behaviour and it is difficult to detect fault by using linear approaches. In addition to nonlinearity problems, the performance of fault detection and diagnosis in single-scale approaches is not well performed due to the smearing effect. Thus, there is a need to develop multiscale fault detection and diagnosis framework that can be used to handle these issues.

2.10 Summary

The literature review covers two major categories of fault detection and diagnosis methods: Model-based approaches and data-based approaches, as well as current

improvements in data-driven fault detection and diagnosis approaches for various industrial applications. The comparison of these methods has also been discussed in detail, along with the fault detection and diagnosis characteristics. Statistical process monitoring has a broader aspect, which has been demonstrated in section 2.7. It covers the univariate and multivariate statistical process monitoring techniques. Recent developments in MSPM methods have also been discussed in this section. A detailed discussion on multiscale fault detection and diagnosis has been covered in section 2.8. The available literature on multiscale fault detection and diagnosis has been divided into seven parts based on the issues discussed in it. These issues are quality-related process methods, nonlinear process monitoring, dynamic process monitoring, batch process monitoring and fault diagnosis. Finally, Table 2.1. provides a comprehensive overview of multiscale fault detection and diagnosis methods in terms of all aspects, including method used, issue addressed, case study, and the type used.
CHAPTER 3

METHODOLOGY

3.1 Chapter overview

This chapter describes the research methodology and case studies used in this thesis to achieve the research objectives delineated in Chapter 1. This chapter is divided into five main sections. The overall research methodology is described in section 3.2. The algorithms, tools, and formulas used to develop the proposed fault detection, and diagnosis framework are presented in sections 3.3 and 3.4. The development of fault detection and diagnosis framework for the real-time processes has been presented in detail in section 3.5. This framework for fault detection and diagnosis is achieved through the algorithms and formulas presented in sections 3.3 and 3.4. Section 3.6 describes the case studies such as the continuous stirred tank reactor (CSTR) system and Tennessee Eastman (TE) process. The types of faults and their description are also explained in the section.

3.2 Overall methodology of research

The overall methodology of research is shown in Figure 3.1. The overall methodology consists of four main steps to cater to the research objectives specified in chapter 1. The data collection, multiresolution analysis using wavelet transforms, feature extraction using the reference model and fault detection and diagnosis. In addition, the multiresolution analysis step consists of further two steps which are wavelet decomposition and wavelet reconstruction step. However, a detailed description of fault detection and diagnosis framework development has been presented in the following subsections.



3.2.1 Data collection

The normal and faulty datasets have been obtained from the process system under normal and different faulty conditions. The normal dataset is the training dataset and is used to develop the fault detection and diagnosis framework. The faulty datasets are known as testing datasets and are used to evaluate the developed framework's performance.

3.2.2 Multiresolution analysis

Multiresolution analysis refers to breaking up a signal into components, which produce the original signal exactly when added back together. To be useful for data analysis, how the signal is decomposed is important.

3.2.3 Dimensionality reduction

Dimensionality reduction, or dimension reduction, is the transformation of data from a high-dimensional space into a low-dimensional space so that the lowdimensional representation retains some meaningful properties of the original data, ideally close to its intrinsic dimension.

3.2.4 Fault detection and diagnosis

3.2.4.1 Fault Detection

Fault detection is the first step in process monitoring and determines whether an abnormal event occurs in the process. A fault alert should be raised whenever monitoring data results exceed their respective control limits. The first goal of fault

detection systems is to reduce the false alarm rate and the missed alarm rate to ensure the processing system's dependability.

3.2.4.2 Fault Identification

After detecting a process fault, the goal of fault identification is to determine its direction and size. The typical value of the faulty data set can be retrieved once a flaw has been recreated. In addition, we may analyze the comprehensive fault details, which are highly useful for the subsequent fault isolation and process recovery procedures. Furthermore, fault reconstruction is critical, mainly when this faulty parameter is utilized for additional reasons such as process control, soft sensor modelling, and quality assessment. Without fault reconstruction, the findings may be misconstrued, possibly causing another defect in the process.

3.2.4.3 Fault Diagnosis

After detecting a fault in the process, we may wish to identify which section or subsystem is aberrant. It contributes to the fault diagnosis procedure, which can identify the underlying cause of the identified fault. The diagnosis outcome may be typically traced to a specific section of the process or even a sensor/actuator. However, distinct processing parameters are constantly connected, and the fault might affect many variables and spread to other sections of the process. As a result, providing reliable fault diagnostic results remains challenging in the process monitoring field.

3.3 Wavelet Transforms

Wavelet transforms (WT) is a way of displaying how a signal changes over time. Alfred Haar conducted the first work on the WT in 1909, and it was Jean Morlet and Alex Grossman who developed the wavelet concept and gave it the name wavelet [256].

To do this, the WT utilizes a wavelet function's correlation with translation and dilation. It shows a signal as a mix of wavelets of different sizes and places, which

allows for long time intervals for low-frequency information and short time intervals for high-frequency information. This process is shown in Figure 3.2.



Figure 3.2: The fundamental principle of wavelet transforms [257]

Continuous wavelet transform (CWT) and discrete wavelet transform (DWT) are the two main types of WTs. Calculating wavelet coefficients at every possible scale as implemented in CWT is a fair amount of work, and it generates an awful lot of data. Usually, the researchers obtain such an analysis from DWT from a denoising viewpoint. The definition of DWT is given by

$$C(a,b) = \sum_{n \ge Z} x(n) g_{j,k}(n)$$
 3-1

where C(a,b) are dyadic wavelet coefficients, *a* is the dilation or scale $(a=2^{-j})$, b is translation $(b=k\times2^{-j})$, x(n) is the input signal, and $g_{j,k}(n)$ is the discrete wavelet.

When the input signal is decomposed to a certain level using the DWT, a set of wavelet coefficients is correlated to the high-frequency components (low-scale) while the other wavelet coefficients are correlated to low-frequency components (high-scale).

The detailed wavelet decomposition and reconstruction process is shown in Figure 3.3. In the first step, the initial signal (S) is processed by two complementary filters, a low-pass filter and a high-pass filter, yielding two signals, approximations, and details. The first-level approximation coefficient (cA1) is obtained by a low-pass filter with down sampling, while the first-level detail coefficient (cA1) is obtained by a high-pass filter with down sampling (cD1). The low-pass and high-pass filtering methods are

equivalent to convolving the signal with a scaling function and a wavelet function, respectively. The most relevant component is the low-frequency content (cA), whereas the high-frequency content (cD) is noise. Inputting the cA1 into the filters yields the second-level approximation coefficient (cA2) and the second-level detail coefficient (cD2). This is equivalent to diluting the original scaling and wavelet functions before convolving with the cA1. The process is repeated until the desired final level approximation is obtained, as well as the detail coefficients. It has three breakdown stages, as indicated in Figure.3.3. When decomposition is taken into account, the denoising process may be utilized. If no changes are required, the reconstruction operation will be finished immediately. The reconstructed signal, including the last level approximation and all level details, accurately replicates the original signal, indicating optimal reconstruction. In the reconstruction process, each coefficient is up sampled prior to refiltering.



Figure 3.3: Wavelet decomposition and reconstruction process

Conventional WT play a Important role in multiscale process monitoring, but they can't meet real-time application needs. The moving window could help us figure out how to deal with this issue. A moving-window technique is used in WT to extract the process signals by adding a step of sample time to the process signals as they change over time. Following this, we keep an eye on the process and figure out what's going to happen next. These steps are repeated for all the extra steps of sample time, which

would make it easier for the management to make decisions about what to do next. As shown in Figure 3.4, this is how moving the window process works. Moving windows are added to the wavelet transformation in this study to get around this problem. In this way, the process data is broken down into a moving window that is dyadic in length, because the most recent sample is in the window as well. When you add a moving window into the wavelet decomposition method, you can monitor real-time process changes.



Figure 3.4: Moving window technique used in wavelet transforms

3.4 Kernel principal component analysis

PCA is a common way to reduce the number of dimensions in data. It compresses high-dimensional data into a low-dimensional subspace with little data loss. If two data points have a linear relationship to each other, PCA can only look at that relationship. Because most chemical process data has a lot of nonlinear features, the PCA method has a lot of problems when it comes to computing nonlinear data. KPCA is a nonlinear PCA method based on kernel functions and the main idea to use KPCA is to use a nonlinear mapping to map the input data into a feature space, then use a linear approach to look at the feature space data. In this way, the nonlinear problem of the original space is changed into the linear problem of the feature space [258].

Suppose a data matrix X (where m is the number of variables and n is the number of observations) as

$$X = (x_1, x_2, \dots, x_n) = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{pmatrix}$$
3-2

with

$$x_{i} = \frac{x_{i}^{*} - (1/n)\sum_{i=1}^{n} x_{i}^{*}}{\sqrt{(1/n-1)(x_{i}^{*} - (1/n)\sum_{i=1}^{n} x_{i}^{*})^{2}}}$$
3-3

where $x_i (i = 1, 2, ..., n)$ is the n observations normalized from the n training samples $x_i^* (i = 1, 2, ..., n)$ of the input space. using nonlinear mapping Φ , the measured inputs are extended into the high dimensional feature space as follows:

$$\Phi: x \in \mathbb{R}^m \to \Phi(x) \in F \tag{3-4}$$

The covariance matric in the feature space can be constructed as

$$C = \frac{1}{n} \sum_{i=1}^{n} \Phi(x_i) \Phi(x_i)^{T}$$
3-5

Where C is the connivance matrix of non-zero eigenvalues

To perform PCA in the feature space

$$\lambda v = Cv \tag{3-6}$$

Where λ is the eigenvalues and V is the eigenvectors of the covariance matrix C

$$Cv = \left(\frac{1}{n}\sum_{i=1}^{n} \Phi(x_i)\Phi(x_i)^T\right)v$$
$$= \frac{1}{n}\sum_{i=1}^{n} \langle \Phi(x_i), v \rangle \Phi(x_i)$$
3-7

Where $\langle x, y \rangle$ is the dot product between x and y. This implies that all solutions v with $\lambda \neq 0$ must lie in the span of $\Phi_1, \Phi_2, ..., \Phi_n$. Hence $\lambda v = Cv$ is equivalent to

$$\lambda \langle \Phi(x_i), v \rangle = \langle \Phi(x_i), Cv \rangle, i = 1, 2, ..., n$$
3-8

For any $\lambda \neq 0$, there exists coefficients $\alpha_i (i = 1, 2, ..., n)$, such that

$$v = \sum_{i=1}^{n} \alpha_i \Phi(x_i)$$
 3-9

Combining eqs. (3.7) and (3.8), we have

$$\lambda \sum_{i=1}^{n} \alpha_i \left\langle \Phi(x_k), \Phi(x_i) \right\rangle$$

= $\frac{1}{n} \sum_{i=1}^{n} \alpha_i \left\langle \Phi(x_i) \sum_{i=1}^{n} \Phi(x_j) \right\rangle \left\langle \Phi(x_j), \Phi(x_i) \right\rangle, k = 1, 2, ..., n$
3-10

To obtain the coefficients α_i (i = 1, 2, ..., n), a kernel matrix K of dimension $n \times n$ is defined, and its elements are determined by virtue of kernel tricks.

$$K_{ij} = \Phi(x_i)^T \Phi(x_j) = \left\langle \Phi(x_i), \Phi(x_j) \right\rangle = k(x_i, x_j)$$
3-11

where $k(x_i, x_j)$ is the calculation of the inner product of two vectors in F with a kernel function.

A number of kernel functions exist. According to Mercer's theorem of functional analysis, there exists a mapping into a space where a kernel function acts as a dot product if a kernel function is a continuous kernel of a positive integral operator. The requirement of the kernel function is to therefore satisfy Mercer's theorem. The representative kernel functions are as follows:

Polynomial kernel

$$k(x, y) = \langle x, y \rangle^d$$
 3-12

Sigmoid kernel

$$k(x, y) = \tanh(\beta_0 \langle x, y \rangle + \beta_1)$$
3-13

Radial basis kernel

$$k(x, y) = \exp(-\frac{\|x - y\|^2}{c}$$
 3-14

where d, $\beta 0$, $\beta 1$ and c are specified a priori by user. The polynomial kernel and radial basis kernel always satisfy Mercer's theorem while the sigmoid kernel satisfies it only for some values of β_0 and β_1 . The specific choice of a kernel function implicitly determines the mapping φ and the feature space F. If one has a nonlinear information of process, it could be used to select the kernel function among kernels in KPCA. Before applying KPCA, mean centring and variance scaling in high-dimensional space should be performed.

Then the left hand side of Eq. 3.9 can be simplified to

$$\lambda \sum_{i=1}^{n} \alpha_i \left\langle \Phi(x_k), \Phi(x_i) \right\rangle = \lambda \sum_{i=1}^{n} \alpha_i K_{ki}$$
3-15

Since k =1,...,n, Eq 3.14 can be written as $\lambda K \alpha$.

The right hand side of Eq 3.9 can be expressed as

$$\frac{1}{n} \sum_{i=1}^{n} \alpha_{i} \left\langle \Phi(x_{k}), \sum_{j=1}^{n} \Phi(x_{j}) \right\rangle \left\langle \Phi(x_{j}), \Phi(x_{i}) \right\rangle$$
$$= \frac{1}{n} \sum_{i=1}^{n} \alpha_{i} \sum_{j=1}^{n} K_{kj} K_{ki}$$
3-16

Since k=1,...n, Eq 3.15 can be written as $(\frac{1}{n})K^2\alpha$.

Combining Eq 3.14 and 3.15, we have

$$n\lambda K\alpha = K^2 \alpha \qquad \qquad 3-17$$

where $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)^T$ identifies the eigenvector *V* after normalization.

Notice that before applying KPCA, we have to perform mean centering procedure since the gram matrix used for the above eigenvalue problem is not mean-centered. The centered gram matrix \overline{K} can be easily obtained by

$$K = K - EK - KE + EKE$$
 3-18

with

$$E = \frac{1}{n} \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} \in \mathbb{R}^{n \times n}$$
3-19

From (3.14)–(3.16), the final eigenvalue problem in KPCA approach is to solve

$$n\lambda\alpha = \overline{K}\alpha \tag{3-20}$$

The coefficient α should be normalized to satisfy $\|\alpha\|^2 = 1/n\lambda$, which corresponds to the normality constraint $\|v\|^2 = 1$ of eigenvector.

Cumulative percent variance (CPV) is utilized to determine number of PC,

$$CPV(d) = \frac{\sum_{i=1}^{d} \lambda_i}{\sum_{i=1}^{n} \lambda_i}$$
3-21

Then the dimension reduction can be achieved by retaining the first d eigenvectors. After constructing the PCs in the feature space F, the score vector of the kth observation in the training data set can be obtained by projecting the centred value $\overline{\Phi}(x)$ onto the eigenvectors V_k in F of the new sample x, where k = 1, 2, ..., d, such that

$$t_{k} = \left\langle v_{k}, \overline{\Phi} \right\rangle = \sum_{i=1}^{n} \alpha_{k,i} \left\langle \overline{\Phi}_{i}, \overline{\Phi} \right\rangle = \sum_{i=1}^{n} \alpha_{k,i} \overline{K}(x_{i}, x)$$
3-22

where the mapping of x is simply noted as $\Phi(x) = \Phi$. Using (3.18), we finally obtain a score vector $t = (t_1, t_2, ..., t_d)^T$ for x. For the special case in which $\Phi(x) = x$, KPCA is equivalent to linear PCA. From this viewpoint, KPCA can be regarded as a generalized version of linear PCA.

3.4.1 Fault detection and diagnosis methods

3.4.1.1 Fault detection

Besides, the Hotelling's T^2 and SPE statistics that in the linear PCA are used to monitor processes, in the feature space can be interpreted in the same way. Thus, a measure of the variation within the KPCA model is given by Hotelling's T^2 statistic, which is calculated as follows [175,259]:

$$T^{2} = [t_{1}, \dots, t_{l}]\Lambda^{-1}[t_{1}, \dots, t_{l}]^{T}$$
3-23

The T^2 threshold can be calculated as [175].

$$T_{\rm lim}^2 = \frac{l(m-1)}{m-l} F_{l,m-l,\alpha}$$
 3-24

The SPE monitors the variation in the residual subspace and can be computed as [175,259]:

$$SPE = \left\| \Phi(x) - \hat{\Phi}(x) \right\|^{2} = \left\| \hat{\Phi}(x) - \hat{\Phi}(x) \right\|^{2}$$

$$= \hat{\Phi}_{n}(x)^{T} \hat{\Phi}_{n}(x) - 2 \hat{\Phi}_{n}(x)^{T} \hat{\Phi}_{p}(x) + \hat{\Phi}_{p}(x)^{T} \hat{\Phi}_{p}(x)$$

$$= \sum_{j=1}^{n} t_{j} v_{j}^{T} \sum_{k=1}^{n} t_{k} v_{k} - 2 \sum_{j=1}^{n} t_{j} v_{j}^{T} \sum_{k=1}^{p} t_{k} v_{k} + \sum_{j=1}^{p} t_{j} v_{j}^{T} \sum_{k=1}^{p} t_{k} v_{k}$$

$$= \sum_{j=1}^{n} t_{j}^{2} - 2 \sum_{j=1}^{n} t_{j}^{2} + \sum_{j=1}^{p} t_{j}^{2}$$

$$= \sum_{j=1}^{n} t_{j}^{2} - \sum_{j=1}^{p} t_{j}^{2}$$

$$3-25$$

Where $t_j v_j^T = 1$ when j = k, $v_k v_j^T = 0$ otherwise. The threshold for SPE is determined as [175].

$$SPE_{lim} \approx gx_h^2$$
 3-26

This limit is based on the box's equation achieved by adjusting the weighted distribution of the reference distribution utilizing training [260]. Taking into account *a*

and *b* the estimated mean and variance of the SPE. *g* and *h* are the weight assigned to the SPE size and degree of freedom, respectively and are computed using, g = b/2a and $h = 2a^2/b$.

3.4.1.2 Fault identification

Once the system detects a fault, the numerical method of the RBC model identifies the variable contribution rate.

In a system with n sensors, when a fault happens in sensor xi, the faulty measurement is $x \in \Re n$ and the direction of the fault is ξi . The reconstructed vector along direction ξi is

$$z_i = x - \xi_i f_i \tag{3-27}$$

where fi is the estimated fault magnitude. The fault detection index of the reconstructed sample zi is

$$Index(zi) = z_i^T M zi = ||zi||_M^2 = ||x - \xi i fi||_M^2$$
3-28

which should be minimized. The least-squares solution for f_i is

$$f_i = \left(\xi_i^T M \xi_i\right)^{-1} \xi_i^T M x \tag{3-29}$$

Then, the RBC of variable xi to the fault detection index is defined as

$$RBC_i^{Index} = \left\| \xi_i f_i \right\|_M^2$$
 3-30

which is the amount of reconstruction along the ith variable direction that minimizes the fault detection index. The substitution of eq 3.29 in eq 3.30 gives

$$RBC_i^{Index} = \left\| \xi i (\xi_i^T M \xi i)^{-1} \xi_i^T M x \right\|_M^2$$
3-31

$$RBC_i^{Index} = x^T M \xi_i (\xi_i^T M \xi_i)^{-1} \xi_i^T M x$$
3-32

The control limits for the RBCs can also be determined using the results of Box,26 because they have the quadratic form as well. Because of the smearing effect in the RBCs, nevertheless, the control limits cannot be utilized to identify which variable is the cause of the fault. The fault isolation task can only be achieved based on the magnitudes of the RBCs. In the case of single-sensor faults, variable xi with the largest RBC_i Index is identified as the most likely faulty variable

3.5 Multiscale KPCA based fault detection and diagnosis framework

The primary objective of the proposed multiscale fault detection and diagnosis framework is to develop an online process monitoring model for detecting faults in highly correlated multivariate data. A multiscale KPCA based fault detection framework is developed, and T^2 and SPE control charts were used to detect the fault present in the process data. After detecting the fault, an RBC-based fault diagnosis framework is developed for the SPE control chart for fault identification and isolation. The proposed fault detection and diagnosis framework is mentioned in Figure 3.5.

First, the normal datasets are decomposed to level 4 using wavelet transforms, and then wavelet coefficients for approximation and all detail functions are reconstructed. In WT, a moving-window technique is used to dynamically extract the process signals by adding the step of sample time. It is followed by monitoring and predicting the next situation of the process. These steps are repeated for all the added steps of sample time, which would ease out the decisions of the management. The KPCA model is developed using the approximation matrix of the last level. In the end, fault detection indices have developed based on conventional monitoring indices such as T^2 and SPE. After successful detection, the performance evaluation of the proposed framework is done using various performance indices. Lastly, the fault diagnosis framework is developed based on RBC for the SPE control chart.



Figure 3.5: Proposed fault detection and diagnosis framework

Table 3.1 outlines the overall procedure adopted to develop the proposed fault detection and diagnosis framework using MSKPCA and RBC.

Table 3.1: Proposed fault detection and diagnosis framework using multiscale KPCA and RBC.

Model	development stage
1.	Generate a fault-free dataset representing normal operating conditions and a faulty dataset representing different faulty scenarios.
2.	Each variable in the fault-free data matrix is decomposed into wavelet coefficients by applying the moving window-based wavelet transformation and then reconstructing the approximation and details matrices from the wavelet coefficients.
3.	Normalize the approximation and details matrices obtained using zero mean and unit variance.
4.	Calculate the kernel matrix

- 5. Calculate the number of principal components and residual subspaces
- 6. Compute the T^2 and SPE control limits.

Fault detection and diagnosis

- 1. Collect the faulty data
- 2. For faulty data, each variable is decomposed into wavelet coefficients by applying the moving window-based wavelet transformation and then reconstructing the approximation and details matrices from the wavelet coefficients.
- 3. Normalize the approximation and details matrices obtained after wavelet decomposition using the mean and standard deviation of the fault-free dataset that has already been computed.
- 4. Compute the T^2 and SPE decision functions.

- 5. Calculate the kernel matrix
- 6. Centralized the kernel matrix
- 7. Combining the reference model values of the fault-free condition, calculate the new data statistics.
- 8. Check whether the T² and SPE statistics exceed the control limit. If one of the control limits is exceeded, it indicates that the process has a fault condition: otherwise, it is identified as normal and then returned to step 1 to continue to detect a new set of process datasets.
- 9. Evaluate the performance using performance indices

3.5.1.1 Data normalization

It is of significant implication to normalize the data before applying KPCA. The main reason for data normalization is that the attributes with a higher numerical range may affect the lower numerical range. Normalization is an essential preprocessing step as it can decrease the computational time and ensure that the weightage is equally distributed among the variables. One of the scaling techniques is auto scaling which rescales the original data to have a mean of 0 and a variance of 1 as given by

$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i$$
$$\sigma = \sqrt{\frac{1}{m-1} \sum_{i=1}^{n} (x_i - \mu)^2}$$
$$\overline{x}_i = \frac{x_i - \mu}{m-1}$$

where

 σ

 μ = mean

σ = standard deviation

 \overline{x}_i = re-scaled data point to $\mu = 0$ and $\sigma = 1$

3.5.1.2 Fault evaluation

After detecting a fault, the evaluation of faults plays a significant role in assessing the performance of the proposed model.

1. Fault detection rate

FDR is the percentage of fault samples identified correctly. It was computed as

$$FDR = \frac{n_{fc}}{n_{tf}} \times 100$$
 3-33

where n_{fc} denotes the number of fault samples identified correctly, and n_{tf} is the total number of fault samples.

2. Detection delay

Detection delay is the difference between fault occurrence and fault detected.

3.6 Case studies

This thesis considers two case studies to evaluate the performance of the proposed fault detection and diagnosis algorithm. The first case study is CSTR system. The second case study is TE process.

3.6.1 Case Study 1- Continuous stirred tank reactor system

The CSTR system is widely used to test fault detection methods' performance. A schematic diagram of the CSTR system with the cascade control system is shown in Figure 3.6. In this CSTR system, the reactant A flows into the reactor, and then a first-order irreversible exothermic reaction occurs in this system:

$$A \rightarrow B$$
 3-34

Product B flows out as an outlet stream. The cooling liquid in the jacket removes the heat from the exothermic reaction. The liquid level and temperature in the reactor are controlled by manipulating the outlet flow and cooling liquid flow, respectively.

Based on the mass, energy and component balances, the dynamic model of this CSTR system can be constructed as

$$\frac{dh}{dt} = \frac{F_i - F}{A}$$
 3-35

$$\frac{dC}{dt} = \frac{C_i F_i - CF}{Ah} - k_0 \exp\left(\frac{E_A}{RT}\right)C$$
3-36

$$\frac{dT}{dt} = \frac{F_i T_i - FT}{Ah} + \frac{k_0 \exp\left(\frac{E_A}{RT}\right) C\left(-\Delta H\right)}{\rho C_p} + \frac{U A_c (T_c - T)}{\rho C_p Ah}$$
3-37

$$\frac{dT_c}{dt} = \frac{F_c \left(T_{ci} - T_c\right)}{V_c} + \frac{UA_c \left(T_c - T\right)}{\rho_c C_{pc} V_c}$$
3-38



Figure 3.6: CSTR system with cascade control

The description of parameters and their values under normal operating conditions for CSTR system is listed in Table. 3.2. Process variables involved in the CSTR system are listed in Table 3.3. Fault free and faulty process data are generated by simulating CSTR with a period of one min for normal and faulty operating conditions. One thousand fifty samples of fault-free process data were recorded with normal operating conditions. Six fault scenarios were simulated, and 1050 samples were recorded for each fault pattern. Table 3.4 details the simulated fault scenarios, including process disturbances, sensor bias, and process faults. The proposed MSKPCA fault detection and identification framework was used to detect and identify faults in the CSTR system, and its performance was compared to PCA and KPCA methods.

Model parameters	Parameter descriptions	Parameter values	
А	Reactor cross-sectional area	0.1666 m ²	
UA _C	Heat-transfer coefficient	$5 \times 10^4 \text{J} \cdot \text{min K}$	
V _C	The capacity of the cooling jacket	10 L	
ρ	The density of reactor contents	$\rho C_p = 239 \text{ J L K}$	
Cp	Heat capacity of reactor contents		
ρς	Density of coolant	$\rho_C C_{pC} = 4175 \text{ J L K}$	
C _{pC}	Heat capacity of the coolant		
ΔΗ	Reaction heat	$-5 imes 10^4 \text{ J mol}^{-1}$	
E ₀ /R	Activation energy	8750 K	
k ₀	Preexponential factor	$7.2 \times 10^{10} \text{ min}^{-1}$	
Fi	Reactor feed flow rate	100 L min ⁻¹	
Ti	The temperature of the reactor feed stream	320 K	
C _{Ai}	The concentration of species A in the reactor feed stream	$1.0 \text{ mol } L^{-1}$	
F	Reactor outlet flow rate	100 L min ⁻¹	
Т	Reactor temperature	402.35 K	
C _A	Concentration of species A in reactor	0.037 mol L ⁻¹	
T _{Ci}	The temperature of the coolant feed	300 K	
T _C	The temperature of the coolant in the cooling jacket	345.44 K	
Fc	Coolant flow rate	15 L min ⁻¹	
h	Reactor liquid level	0.6 m	

 Table 3.2: parameter description and parameter values under normal operating conditions for CSTR system.

Number	Variable	Variable description
1	Fi	The flow rate of the feed stream
2	T_{i}	The temperature of the feed stream
3	Ci	The initial concentration of reactant A in the feed stream
4	F	The flow rate of the outlet stream
5	Т	The temperature in the reactor
6	С	The concentration of reactant A in the reactor
7	T _{ci}	Cooling liquid temperature
8	T _c	The cooling liquid temperature in the cooling jacket
9	F _c	The flow rate of cooling liquid
10	h	Liquid level in the reactor

Table 3.3: process variables of the CSTR system measured for fault detection.

Table 3.4: Fault patterns	in the CSTR case study.
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Fault number	Fault description	Fault variable	Change value
1	The step-change in reactor feed flow rate	Fi	Input disturbance
2	Ramp change in initial concentration	Ci	Input disturbance
3	step-change in reactor temperature	Т	Sensor bias
4	Ramp change in the temperature of coolant feed	TC _i	Sensor bias
5	Ramp change in catalyst activation energy	E ₀ /R	Process fault
6	Ramp change in the heat-transfer coefficient	U _{AC}	Process fault

3.6.2 Case Study 2- Tennessee Eastman process

The Tennessee Eastman (TE) process, which was developed by Downs and Vogel, is considered a benchmark case in the field of process engineering [261]. In this work, the TE process was used as a case study for a proposed framework for detecting and diagnosing faults. It has been used as a case study for many plant-wide process control issues, such as process monitoring and fault detection [261,262]. The simulation data

were generated by Rieth, C. A., et al. [263] and can be downloaded at <u>https://dataverse.harvard.edu/dataset.xhtml?persistentId=doi:10.7910/DVN/6C3JR1</u>. This case consists of five major unit operations: a reactor, a condenser, a compressor, a separator, and a product stripper. From A to H there are eight chemical compounds G and H are made from gaseous reactants that are mixed with inert B and gaseous A, C, D and E, and the by-product material F is made from gaseous F [261].

The exothermic reactions are:

$A(gas) + C(gas) + D(gas) \rightarrow G(liq)$	3-39
$A(gas) + C(gas) + E(gas) \rightarrow H(liq)$	3-40
$A(gas) + E(gas) \rightarrow F(liq)$	3-41
$3D(gas) \rightarrow 2F(liq)$	3-42

The process has 22 (X_1 to X_{22}) continuous process measurements (such as temperatures, pressures, flow rates, and levels), 19 (X_{23} to X_{41}) composition measurements and 11 (X_{42} to X_{52}) manipulated variables, as listed in Table 3.5. In the original description, there were 20 faulty scenarios, and these are listed in Table 3.6. Faults 1 to 7 are linked to step changes in connected variables, whereas faults 8 to 12 are linked to random fluctuations in certain variables. Slow drift in response kinetics is related with fault 13, whereas sticky valves are associated with faults 14, and 15, and faults 16 to 20 are unknown faults with unknown root causes.



Figure 3.7: Tennessee Eastman Process system [190]

Identification	Description	Туре	Identification	Description	Туре
X ₁	A feed stream 1	measured	X ₂₇	Component E stream 6	measured
X ₂	D feed stream 2	measured	X ₂₈	Component F stream 6	measured
X ₃	E feed stream 3	measured	X ₂₉	Component A stream 9	measured
X4	A and D feed stream 4	measured	X ₃₀	Component B stream 9	measured
X5	Recycle flow stream 8	measured	X ₃₁	Component C stream 9	measured
X ₆	Reactor feed rate stream 6	measured	X ₃₂	Component D stream 9	measured
X ₇	Reactor pressure	measured	X ₃₃	Component E stream 9	measured
X ₈	Reactor level	measured	X ₃₄	Component F stream 9	measured
X9	Reactor temperature	measured	X35	Component G stream 9	measured
X ₁₀	Purge rate stream 9	measured	X ₃₆	Component H stream 9	measured
X ₁₁	Product separator temperature	measured	X ₃₇	Component D stream 11	measured
X ₁₂	Product separator level	measured	X ₃₈	Component E stream 11	measured
X ₁₃	Product separator pressure	measured	X ₃₉	Component F stream 11	measured
X ₁₄	Product separator underflow stream 10	measured	X_{40}	Component G stream 11	measured
X ₁₅	Stripper level	measured	X41	Component H stream 11	measured

Table 3.5: Measured and manipulated variables of the Tennessee Eastman process

X ₁₆	Stripper pressure	measured	X ₄₂	D feed flow stream 2	manipulated
X ₁₇	Stripper underflow stream 11	measured	X ₄₃	E feed flow stream 3	manipulated
X ₁₈	Stripper temperature	measured	X44	A feed flow stream 1	manipulated
X19	Stripper steam flow	measured	X45	Total feed flow stream 4	manipulated
X ₂₀	Compressor work	measured	X_{46}	Compressor recycle valve	manipulated
X ₂₁	Reactor cooling water outlet temperature	measured	X47	Purge valve stream 9	manipulated
X ₂₂	Separator cooling water outlet temperature	measured	X48	Separator pot liquid flow stream 10	manipulated
X ₂₃	Component A stream 6	measured	X49	Striper liquid product flow stream 11	manipulated
X ₂₄	Component B stream 6	measured	X50	Stripper steam valve	manipulated
X ₂₅	Component C stream 6	measured	X ₅₁	Reactor cooling water flow	manipulated
X ₂₆	Component D stream 6	measured	X ₅₂	Condenser cooling water flow	manipulated

Fault ID	Description	Туре
1	A/C feed ratio, B composition constant (Stream 4)	Step
2	B composition, A/C ratio constant (Stream 4)	Step
3	D feed (Stream 2)	Step
4	Reactor cooling water inlet temperature	Step
5	Condenser cooling water inlet temperature	Step
6	A feed loss (Stream 1)	Step
7	C header pressure loss – reduced availability (Stream 4)	Step
8	A, B and C composition (Stream 4)	Random variation
9	D feed temperature (Stream 2)	Random variation
10	C feed temperature (Stream 4)	Random variation
11	Reactor cooling water inlet temperature	Random variation
12	Condenser cooling water inlet temperature	Random variation
13	Reaction kinetics	Slow drift
14	Reactor cooling water valve	Sticking
15	Condenser cooling water valve	Sticking
16	Unknown	Unknown
17	Unknown	Unknown
18	Unknown	Unknown
19	Unknown	Unknown
20	Unknown	Unknown

Table 3.6: Fault patterns in the Tennessee Eastman process

The proposed fault detection and diagnosis framework was used to test and analyze all of the faults in the CSTR system and TE process in this work. The simulated CSTR model was developed and data for all six designated faults were introduced at various operating conditions. For each fault, data was collected to include ten different types of variables which are listed in Table 3.3. Faults were set to occur after 500 samples, and the specifications for each fault are listed in Table 3.4. In the TE process, there are total 52 process variables, including 11 manipulated variables and 41 measured variables.

These variables are recorded throughout both normal and abnormal conditions, which are triggered by 20 different fault types. The sampling interval is 3 min and there was total 500 samples in fault free dataset and 960 samples in faulty datasets. The fault occurs at the 161st sampling time in each fault scenario. Table 3.5 contains a detailed description of all 52 variables, while Table 3.6 contains a list of the designated process faults. The previously discussed framework in section 3.5. was applied to datasets to determine performance in terms of fault detection and identification.

3.7 Summary

The development of the proposed fault detection and diagnosis framework is presented in this chapter which serves as the key building blocks for the implementation of the research objectives of this thesis as presented in chapter 1. The first part presented the overall research methodology, formulation, and the mathematical structures required to develop the proposed methodology. The development of wavelet-based fault detection and diagnosis framework is presented as the second major part of this chapter. The essential steps of fault detection and diagnosis model development are wavelet decomposition and reconstruction, KPCA model development, fault detection, and diagnosis. In the last part of the chapter, two case studies are presented. The list of various variables for both case studies is presented.

Furthermore, process faults are explained in detail and selected for detection and diagnosis in this research. Six types of fault scenarios are selected for the CSTR system including input disturbances, sensor biases and process faults. Twenty fault scenarios are selected for the TE process including step changes, random variations, slow drift, sticking and unknown faults. Using the proposed framework described in this chapter, the corresponding results and discussion are presented in Chapter 4.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Chapter Overview

This chapter presents the findings of this study on the three main objectives of the current research work: (1) fault detection in the CSTR system, (2) fault diagnosis in the CSTR system, (3) Evaluation of fault detection, and diagnosis framework using TE process faults. The MATLAB version used in this study was released in 2018a running on window 10 Intel Core i5 processor. This chapter is divided into two main sections. The results based on the proposed MSKPCA based fault detection framework are presented in section 4.2. It also comprises the performance evaluation of the fault detection framework. The fault diagnosis results based on the RBC method are presented in section 4.3.

4.2 Fault diagnosis results and analysis

To verify the superiority of the proposed framework for fault detection and diagnosis the proposed framework is used to analyze the cause of the faults under different fault types.

4.2.1 Fault detection results

This section presents the performance of the proposed MSKPCA fault detection framework developed in chapter 3. The Hotelling T^2 and SPE indices were used to detect the faults of the CSTR and TE process databases. The models were developed

utilizing the fault free data (training data) obtained under normal operating conditions, while the fault data (testing data) has been used to evaluate the detection results.

4.2.1.1 Case study 1-Continuous stirred tank reactor

CSTR has wide applications in the process industry and embodies many features of other reactors. This section presents the performance of the proposed fault detection framework. The proficiencies of the process monitoring statistics are investigated for fault detection and compared with conventional methods for fault detection. Performance of fault detection statistics are evaluated, and the results based on fault detection rate is presented in Tables 4.1.

Table 4.1: Comparison of fault detection rate of different methods in the CSTR

Method	Method PCA method KPCA method		PCA method	MSKPCA m	ethod	
Statistics	T ²	SPE	T ²	SPE	T^2	SPE
Fault num	ber	ł				
1	100	100	100	100	100	100
2	5.2	5.6	18.8	15.2	61.2	35.4
3	0	13.2	13	100	100	100
4	54	41.8	63.4	85	11.6	100
5	32.2	19.4	35.6	52.2	74.2	67.4
6	1.2	34.2	35.4	67.6	71	84.4

system.	•
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The FDR values have been computed and tabulated in Table 4.1 related to all fault scenarios of the CSTR system. In this table, statistics having the higher FDR value are shown in yellow colour. Fault scenarios 1 and 3 are the step changes, and it can be observed from Table 4.1 that the proposed MSKPCA method can detect the fault effectively at the 501st sample, where the FDR is 100% on both control charts (T^2 and SPE). In Fault 1, the FDR for PCA and KPCA based methods is 100% for both control charts. In the case of Fault 3, no fault is observed in the T^2 chart for the PCA-based method, whereas SPE hardly detects this fault. The FDR for the SPE control chart is 13.20%.

Compared with the step-change faults, the indication of abnormality presence on the ramp-change fault is difficult to observe, which is confirmed by the FDR values listed in Table 4.1. For fault pattern 2, the FDR was 61.20% and 35.40% in T^2 and SPE control charts of the MSKPCA method. These FDR values are much higher as compared to PCA and KPCA based methods. For the PCA-based method, the FDR value was 5.20% in the T^2 control chart and 5.60% in the SPE control chart. A slight increase in FDR values was observed in KPCA based method, where FDR values increased to 18.80% and 15.20% in the T^2 and SPE control charts, respectively. For fault pattern 4, the FDR values were 11.60% and 100% in T^2 and SPE control charts. In this fault pattern, the FDR value in the T^2 control charts of the proposed method was less than the FDR values in the T^2 control charts of the comparative methods (PCA and KPCA).

Faults 5 and 6 are complex and are difficult to detect because these faults can also disturb the other variables. For fault pattern 5, the proposed MSKPCA method shows FDR 74.20% and 67.40% on T^2 and SPE charts, respectively. The FDR values were higher than that of other comparative methods. For the KPCA method, the FDR values were 35.60% and 52.20% on T^2 and SPE charts, respectively. The FDR values were 32.30% and 19.40% for the PCA method on T^2 and SPE charts, respectively. For fault pattern 6, the proposed MSKPCA method shows FDR 71.00% and 84.40% on T^2 and SPE charts, respectively. For the KPCA method, the FDR values were 35.60% on T^2 and SPE charts, respectively. For the KPCA method, the FDR values were 32.30% and 19.40% for the PCA method shows FDR 71.00% and 84.40% on T^2 and SPE charts, respectively. For the KPCA method, the FDR values were 35.40% and 67.60% on T^2 and SPE charts, respectively. For the PCA method, the fault was hardly detected in the T^2 control chart, and its FDR value was only 1.20%, whereas, in the SPE control chart, its value was 34.20%.

The FDR of the proposed method is much higher than that of traditional PCA and KPCA methods for all fault patterns. PCA and KPCA are unable to identify slight variations in measured variables, however the proposed framework can. When wavelet analysis and KPCA are used together, the measured variables provide more fault information and improved detection outcomes.

To illustrate the detection effects, three different fault scenarios are selected as specific cases.

Scenario 1-Fault 2

This scenario is associated with Fault 2, where the ramp change is introduced in the reactant's initial concentration (C_i). Figures 4.1-4.3 illustrate the fault detection results for this scenario using the proposed MSKPCA and other comparing methods. As shown in Figure 4.1, the fault is observed at the 784th sample on both control charts of the PCA-based detection method. It can also be observed that, despite the existence of the fault, the majority of the monitoring statistic values on both control charts are below the detection limit after the fault is detected. For the KPCA method, as shown in Figure 4.2, a distinct change is observed on the T² and SPE control charts around the sample numbers 783 and 832, respectively. However, after the fault is detected, some of the monitoring statistic values on both charts remain below the detection limits. In this case, the detection point of fault on the T² control chart is almost the same as the T² chart of the PCA-based method, but there is a delay in detection observed on the SPE control chart.

In contrast, early and noticeable fault detection is observed in the proposed MSKPCA method, as shown in Figure 4.3. The monitoring statistic values in the T^2 and SPE control charts of the proposed MSKPCA-based fault detection method, as shown in Figure 4.3, exceed the detection limit around sample numbers 605 and 753, respectively. In the T^2 control chart (see Figure 4.3a), a few monitoring statistic values remain below the detection limit before sample number 813, and after that, all monitoring statistic values are above the detection limit. The SPE control chart (see Figure 4.3b) shows that the monitoring statistic values after sample number 871 are above the detection limit. In this case, after detecting the fault, a few samples were still below the detection limit till sample number 870. As a result of the control chart comparison, the proposed MSKPCA method can provide an earlier and more noticeable fault indication for fault 2. Therefore, the MSKPCA method had a better fault detection performance than other methods.



Figure 4.1: PCA based monitoring charts for fault 2



Figure 4.2: KPCA based monitoring charts for fault 2.



Figure 4.3: MSKPCA based monitoring charts for fault 2.

Scenario 2- Fault 5

This scenario is associated with Fault 5, in which the ramp change is introduced in the activation energy (E/R). The comparison of fault detection results for this scenario using the proposed MSKPCA and other methods is shown in Figures 4.4-4.6. As seen in Figure 4.4, a delay in fault detection was observed in both control charts when using the PCA-based method. In this case, the monitoring statistic values cross the detection limit at sample numbers 820 and 859 on T² and SPE control charts, respectively. In the T² control chart (see Figure 4.4), almost all monitoring statistic values were above the detection limit after the detection of fault, whereas in the SPE control chart (see Figure 4.4), some portion of the monitoring statistic values remained below the detection limit. For the KPCA method, as shown in Figure 4.5, the monitoring statistic values cross the detection limits around sample numbers 785 and 692 on the T² and SPE control charts, respectively. In this case, a few monitoring statistic values remained below the detection limit after detecting the fault.

In contrast, it can be seen from Figure 4.6 that the proposed MSKPCA method shows an early fault detection than the PCA and KPCA methods. The monitoring statistic values in the T^2 and SPE monitoring charts of the proposed MSKPCA-based fault detection method exceed the detection limit around sample numbers 617 and 646, respectively. After detecting a fault in both control charts, almost all monitoring statistic values were above the detection limits. The above comparison concludes that the proposed MSKPCA method is capable of earlier fault detection than PCA and KPCA methods regarding fault 5. The fault detection results verified the effectiveness of the proposed method.



Figure 4.4: PCA based monitoring charts for fault 5.



Figure 4.5: KPCA based monitoring charts for fault 5.



Figure 4.6: MSKPCA based monitoring charts for fault 5.

Scenario 3-Fault 6

This scenario is associated with Fault 6, where the ramp change in the heat transfer coefficient (UA_c) is introduced. The fault detection results for the proposed MSKPCA and other comparative methods such as PCA and KPCA for this scenario are shown in Figures 4.7-4.9. In the case of PCA based fault detection method, as shown in Figure 4.7, a delay in fault detection was observed. In the T² control chart (see Figure 4.7), an indication of any fault is completely missing before sample number 993, whereas on the SPE control chart (see Figure 4.7), and the monitoring statistic values cross the detection limit around sample number 788. It can also be seen that after the fault is detected, most of the monitoring statistic values before the sample number 830 are below the detection limit, despite the presence of the fault. For the KPCA method, as shown in Figure 4.8, much early fault detection is observed than the PCA-based method. It can be seen from Figure 4.8 that the sample number greater than 739 and 634 cross the detection limits on T² and SPE control charts, respectively. In this case, most of the monitoring statistic values were above the detection limit after detecting fault in both control charts.

In contrast, in the proposed MSKPCA method, a quick and sharp change in fault detection on both control charts was observed, as shown in Figure 4.9. In this case, almost all the monitoring statistical values cross the detection limits from the sample numbers 604 and 585 on T^2 and SPE control charts, respectively. In the T^2 control chart (see Figure 4.9), a few samples remained below the detection limit, whereas in the SPE control chart (See Figure 4.9), almost all monitoring statistic values crossed the detection limits after the detection. As a result of the control chart comparison, the proposed MSKPCA method can provide an earlier and more noticeable fault indication for fault 6. The fault detection results for fault 6 further verified the effectiveness of the proposed method.


Figure 4.7: PCA based monitoring charts for fault 6.



Figure 4.8: KPCA based monitoring charts for fault 6.



Figure 4.9: MSKPCA based monitoring charts for fault 6.

Detection delay is another criterion that is used to show the effectiveness of the proposed method. The delay in detection in sample numbers for all 6 fault scenarios is calculated and tabulated in Table 4.2. In this table, statistics with the least detection delay are shown in yellow. It can also be seen that the T^2 and SPE statistics based on the proposed MSKPCA performed better as compared to statistics based on other methods in terms of smaller detection delays.

For fault pattern 1, there was no delay observed for the proposed method and other comparative methods. For fault pattern 3, the proposed method detects the fault as it was introduced, whereas there was a delay in detecting was observed using the PCA and KPCA methods. For the PCA method, there was no indication of any fault in the T^2 control chart. The proposed method performs better with less detection delay than the other comparative methods for faults where a ramp change is introduced. For fault 4, the detection delay for this fault 219 samples for the MSKPCA- T^2 control chart. However, the T^2 control charts of the KPCA method can detect the fault much more rapidly than the MSKPCA (91 vs. 219 samples). As fault patterns 5 and 6 are complex faults, they can be transmitted to other variables. The proposed method detects these faults much early as compared to PCA and KPCA based methods. It can be observed from Table 4.2 that PCA based fault detection method hardly detect these fault patterns.

Furthermore, it can be seen from Table 4.2. that the proposed method has performed even better than the other methods in most cases. Only T^2 control of the KPCA method for fault pattern 4 gives the least detection delay than the proposed method. The SPE control chart of the proposed method for all fault scenarios shows the least detection delay.

The detection results in Table 4.2. are based on the approximations of the highest level of decomposition. The detection results based on all details are presented in appendix C.

Method	ethod PCA method		КРСА	method	MSKPC	A method				
Statistics	T^2	SPE	T ²	SPE	T^2	SPE				
Fault numbe	Fault number									
1	0	0	0	0	0	0				
2	283	283	282	331	104	252				
3	-	40	40	0	0	0				
4	223	225	91	43	219	0				
5	319	358	284	191	116	145				
6	492	287	239	134	103	64				

Table 4.2: Comparison of detection delay of different methods in the CSTR system.

4.2.1.2 Tennessee Eastman process

The TE process, developed by Downs and Vogel, was chosen as a case study for the proposed fault detection and diagnosis framework. Process monitoring performance is quantified for the purposes of statistical analysis and comparison. For fault detection statistics, the quantitative criteria are based on the fault detection rate is presented in Tables 4.3.

Table 4.3 shows the FDR achieved by the proposed approach and comparable monitoring methods (PCA and KPCA) for all TE process faults. Table 4.3 shows that the MSKPCA-based control charts tend to have the highest FDRs on both control charts. It shows that the proposed method can identify small variations in measured variables that PCA and KPCA are unable to detect. For faults 4, 5, 8, 10, 11, 16, and 17, the proposed method provides the best FDR in both control charts. In 15 of the 17 faults, the SPE control chart was the best, and the T² control chart was the best in 8 of them. A total of 16 of 17 faults were found by the proposed method, but a slight failing only in the detection of fault 1. All the methods almost had the same FDR for this one. The average detection rates for all fault scenarios were found to be 45.85% and 82.51% for T² and SPE monitoring charts. The detection rates for other comparative methods such as PCA (45.11% and 49.51% on T² and SPE monitoring charts) and KPCA

(47.93% and 71.66% on T^2 and SPE monitoring charts). In this way, it can be said that the proposed method had a much better detection rate, especially when it came to the SPE control chart. Because wavelet analysis and KPCA work better together, they get more information from the data and find more faults.

The analysis of the proposed method presented in Table 4.3 is only focused on approximations discarded the details coefficients. The approximation function capture low frequency information which contains the important underlying deterministic features. The detail functions, capture high frequency information which are mainly noises. Wavelets can be used to filter out unwanted noise from a data set. The fault detection analysis of the detail functions of all levels (D1, D2, D3 and D4) is shown in Appendix C.

Method	PCA method		КРСА	method	MSKPCA method		
Statistics	Statistics T ² SPE		T^2	SPE	T ²	SPE	
Fault number	•						
1	99.13	99	99.25	99.75	99.13	99.63	
2	98.13	98	98.25	99.13	98.25	99	
3	0	0	0	4.88	0	26.5	
4	0	0	1	100	26.13	100	
5	12.38	22.5	22.13	27.75	27.88	89.63	
6	98.5	98.88	98.75	100	98.38	100	
7	100	88.5	100	100	99.88	100	
8	78.75	81.75	85.25	97	90	98.13	
9	0	0	0	5.25	0	28	
10	6.88	22	14.63	72.25	19.75	90.63	
11	18.63	16.75	35	91	38.63	96.38	
12	69.38	98.63	99.63	99.13	97.75	99.13	
13	69.38	98.5	99.5	99.13	94	96.13	
14	99.75	99.63	99.75	100	16.5	100	
15	0	0	0	7	0	29.5	
16	0	3.88	2.88	43.38	3.13	67.25	
17	54.38	63.63	67.25	94.13	83.5	97.38	
18	86.88	88.25	23.13	89.75	22.38	91.5	
19	0	0	0	39.25	0	59.25	
20	10	10.25	12.13	64.38	1.63	82.25	

Table 4.3: Fault detection rates for the TE process data.

Faults 4, 7, 8, 11 and 14 were chosen as particular examples to demonstrate the strengths and weaknesses of each statistic.

Scenario 1-Fault 4

Fault 4, a step-change in the reactor cooling water flow rate, was the first scenario. The monitoring charts of the proposed MSKPCA and other comparative methods such as PCA, KPCA are shown in Figures 4.10-4.12. PCA method was unable to detect this fault as both control charts did not show any evidence, as shown in Figure 4.10. The KPCA method detected fault samples on both control charts, as shown in Figure 4.11. The T² control chart did not give consistent detection, and only a few samples crossed the control limit. The SPE control chart was provided better fault detection, and all faulty samples were detected successfully. The FDR in T^2 and SPE control charts were 1.00% and 100%, respectively. A much better fault detection was observed in the T^2 control chart of the proposed MSKPCA based method, as shown in Figure 4.12. In the T^2 control chart, the fault was detected at sample number 163, but after detecting a fault, most of the monitoring statistic values remained below the detection limit even though the fault was present. The SPE control again successfully detected all faulty samples like KPCA based SPE control chart. The FDR were 26.13% in the T² control chart and 100% in the SPE control chart. Therefore, it can be concluded that for fault 4, the MSKPCA method had a better fault detection performance than other methods.



Figure 4.10: PCA based fault detection results for fault 4.



Figure 4.11: KPCA based fault detection results for fault 4.



Figure 4.12: MSKPCA based fault detection results for fault 4.

Scenario 2-Fault 7

The next scenario is associated with a step-change in the inlet temperature of the condenser cooling water. The comparison of fault detection results for this scenario using the proposed MSKPCA and the conventional PCA and KPCA methods are shown in Figures 4.13-4.15. All the methods can identify the fault within few samples after the fault occurred. As shown in Figure 4.13, the T^2 and SPE control charts of the PCA based method detect the fault within few samples after the fault occurred. It can be seen that, in SPE control chart, after the sample number 515, a few monitoring statistic

values remained blow the detection limit. The FDR was 100% in the T^2 control chart, while it was dropped to 88.50% in the SPE control chart. For the KPCA based method, as shown in Figure 4.14, It can be seen that both control charts detected the fault successfully, and the FDR was 100% in both control charts. As shown in Figure 4.15, both control charts showed almost the same behaviour as the KPCA method. The FDR was 100% in both control charts.



Figure 4.13: PCA based fault detection results for fault 7.



Figure 4.14: KPCA based fault detection results for fault 7.



Figure 4.15: MSKPCA based fault detection results for fault 7.

Scenario 3-Fault 8

Another Scenario is fault 8, a random variation in stream 4 composed of A, B and C. Regarding this fault, the fault detection results using the proposed MSKPCA, and other comparative methods (PCA and KPCA) are illustrated in Figures 4.16-4.18. The fault detection results using the PCA-based method are shown in Figure 4.16. The fault was detected around 250th sample in both control charts. In the T² control chart, a few samples were remained below the detection limit even though the fault was present. The FDRs were 78.75% and 81.75% in T² and SPE control charts, respectively. The KPCA-based method shows better fault detection than the PCA-based method, as illustrated in Figure 4.17. In the T^2 control chart, the monitoring statistic vales crossed the threshold limit at sample number 183, and after that, some samples remain below the threshold limit. The SPE control chart gave much better detection results, and it was detected the fault at sample number 176. The FDRs were 85.25% and 97.00% in T² and SPE control charts, respectively. As shown in Figure 4.18, the proposed method shows much better performance in terms of fault detection. Both control charts detected the fault around the same detection point as the KPCA method. The FDRs were 90.00% and 98.13% in T² and SPE control charts, respectively. The fault detection results for fault 8 further verified the effectiveness of the proposed method.



Figure 4.16: PCA based fault detection results for fault 8.



Figure 4.17: KPCA based fault detection results for fault 8.



Figure 4.18: MSKPCA based fault detection results for fault 8.

Scenario 4-Fault 11

The next scenario is about fault 11, a random variation in the reactor's cooling inlet temperature. The fault detection results using the proposed MSKPCA, and other comparative methods (PCA and KPCA) are illustrated in Figures 4.19-4.21. Regarding this fault, the control charts of PCA based method are shown in Figure 4.19. The fault was detected in both control charts around the 185th sample, but after that almost all monitoring statistic values remained below the detection threshold after detecting the fault. The FDRs were only 18.63% and 16.75% in the T² and SPE control charts, respectively. Much better detection results were achieved by using KPCA based method, as shown in Figure 4.20. in this case, the fault was also detected around 185th sample, but in this case more monitoring statics values crossed the detection threshold. The FDRs were raised to 35.00% in the T² control chart and 91.00% in the SPE control chart.

On the other hand, the MSKPCA based fault detection results are presented in Figure 4.21. The T^2 control chart gave a slightly better detection result. This control chat detected the fault at sample number 182, and after the detection of a fault, most samples could not cross the detection threshold. The SPE control chart detected the fault within a few samples after it occurred, and after that, only a few samples remained below the detection threshold. The FDRs were 38.63% in the T^2 control chart and 96.38% in the SPE control chart. The proposed MSKPCA-based method gives significantly better results than the PCA and KPCA-based methods. The output value always stays higher than with the PCA and KPCA-based methods.



Figure 4.19: PCA based fault detection results for fault 11.



Figure 4.20: KPCA based fault detection results for fault 11.



Figure 4.21: MSKPCA based fault detection results for fault 11.

Scenario 5-Fault 14

The next scenario is about fault 14 that is associated with the reactor cooling water valve. The fault detection results using proposed MSKPCA, and other comparative methods such as PCA and KPCA illustrated in Figures 4.22-4.24. The control charts of all the methods identified the fault within few samples after the fault occurred, except the SPE control chart of the MSKPCA method. The FDRs were almost the same, close to 100% in both control charts of the PCA and KPCA based methods. In the case of MSKPCA based method, as shown in Figure 4.24, There was a delay in detection in the T² control chart, and the fault was detected at sample number 241, where the FDR was only 16.75%. The SPE control chart successfully detected the fault as it was occurred, and the FDR was 100%. Although poor fault detection was observed in the T² control chart of the MSKPCA method, this method still performs better than PCA and KPCA based methods.



Figure 4.22: PCA based fault detection results for fault 14.



Figure 4.23: KPCA based fault detection results for fault 14.



Figure 4.24: MSKPCA based fault detection results for fault 14.

The detection delays were measured as the first time the threshold was exceeded. Table 4.4 summarizes the detection delay in terms of sample counts for all 20 fault scenarios. The statistic with the lowest detection delay is highlighted in yellow. Table 4.4 shows that employing the proposed MSKPCA-based method may reduce detection delays when compared to PCA and KPCA methods. PCA based method was unable to detect faults 3, 4, 9, 15, and 19 in both monitoring charts. The KPCA based method perform better than PCA method and the detection delays were smaller than PCA method. Furthermore, it is seen that the SPE based statistics of the proposed MSKPCA method have performed even better than the other comparative control charts. Another important point to note here that SPE control chart of the KPCA and proposed MSKPCA method were able to detect fault 3, 9 and 15, whereas T² control chart was not able to detect these faults. In conclusion, from the detection delay results presented

in Table 4.4, it can be seen that SPE control chart of the proposed MSKPCA based method showed smaller detection delays as compared to other comparative methods.

Method	PCA 1	nethod	KPCA	method	MSKPCA method					
Statistics	T^2	SPE	T ²	SPE	T^2	SPE				
Fault number										
1	7	8	6	2	7	3				
2	15	16	14	7	14	8				
3	-	-	-	42	-	32				
4	-	-	2	0	76	0				
5	1	2	0	0	4	0				
6	12	9	10	0	13	0				
7	0	0	0	0	1	0				
8	87	84	23	16	24	15				
9	-	-	0	42	-	32				
10	22	27	26	31	112	31				
11	23	25	6	4	22	3				
12	8	5	4	3	9	3				
13	8	5	4	3	48	31				
14	1	1	1	0	81	0				
15	-	-	-	42	-	32				
16	-	108	216	32	84	32				
17	24	21	21	15	22	15				
18	97	94	92	42	89	33				
19	-	-	-	4	-	4				
20	67	63	63	31	116	31				

Table 4.4: Comparison of detection delay for TE process data

In effort to demonstrate the superiority the proposed MSKPCA based fault detection framework, a comparison was made to the fault detection results of the PCA, DPCA, KPCA and DKPCA, which were proposed by Russel et al. [264] and Sumana et al. [265]. The comparison of detection rates is shown in Table 4.5, and it is apparent

that the proposed framework has the highest average in detection rates for the SPE control chart (82.51%) compared to PCA (63.79%), DPCA (66.15%), KPCA (68.85%) and DKPCA (64.25%).

	Russell et al., (2000)			Sı	ımana e	t al. (201	Proposed	MSKPCA		
Method	PC	CA	DP	CA	KP	CA	DKPCA		Toposcu	
Statistic	T^2	SPE	T ²	SPE	T ²	SPE	T ²	SPE	T ²	SPE
Fault Number										
1	99.20	99.70	99.40	99.50	99.01	99.38	99.38	99.46	99.13	99.63
2	98	98.60	98.10	98.50	97.14	81.30	98.38	98.26	98.25	99
3	0.20	0.90	0.90	1	3.76	10.26	6.66	5.41	0	26.50
4	4.40	96.20	6.10	100	7.63	60.38	18.04	55.08	26.13	100
5	22.50	25.40	24.20	25.20	28.26	31.26	29.43	28.05	27.88	89.63
6	98.90	100	98.70	100	99.25	99.38	99.38	99.5	98.38	100
7	91.50	100	84.10	100	45.38	100	99.76	100	99.88	100
8	96.60	97.6	97.20	97.50	88	97.38	97.26	97.5	90	98.13
9	0.60	1.90	0.50	0.60	3.26	91.01	6.79	6.4	0	28
10	33.40	34.1	42	33.50	40.38	56.76	54.96	54.7	19.75	90.63
11	20.60	64.4	19.90	80.70	9.01	58.63	38.44	58.34	38.63	96.38
12	97.10	97.5	99	97.60	89.62	98.64	98.62	98.62	97.75	99.13
13	94	95.50	95.10	95.10	92.88	94.38	94.38	94.38	94	96.13
14	84.20	100	93.90	100	38.88	100	100	100	16.50	100
15	1.20	2.70	3.60	2.40	8.88	17.88	16.29	14.54	0	29.50
16	16.60	24.50	21.70	29.20	25.88	41.38	40.06	39.07	3.13	67.25
17	74.10	89.20	76	94.70	61.51	87.76	82.36	86.86	83.50	97.38
18	88.70	89.90	88.90	90	88.14	89.13	89	89.24	22.38	91.50
19	0.40	12.70	0.70	26.50	1.88	4.75	2	5	0	59.25
20	29.90	45	35.60	51	31.12	57.38	51.70	54.58	1.63	82.25

Table 4.5: Comparison of fault detection rates of the TE process

The effectiveness of the proposed framework further demonstrates by comparing the detection delays which were proposed by Russel et al. [264] and Sumana et al. [265]. The comparison is shown in the Table 4.6, and it can be seen that the proposed framework is capable of early fault detection as compared to other methods.

	Russell et al., (2000)		Sumana et al. (2012)				Proposed MSKPCA			
Method	PC	CA	DP	CA	KP	CA	DK	PCA	Toposcu	
Statistic	T ²	SPE	T ²	SPE	T ²	SPE	T ²	SPE	T^2	SPE
Fault Number	Detect	Detection delay based on the number of samples								
1	7	3	6	5	8	6	6	5	7	3
2	17	12	16	13	24	16	14	15	14	8
3	-			-	358	84	84	84	-	32
4	-	3	151	1	60	8	58	8	76	0
5	16	1	2	2	15	12	12	1	4	0
6	10	1	11	1	7	6	6	5	13	0
7	1	1	1	1	3	1	0	0	1	0
8	23	20	23	21	11	22	23	21	24	15
9	-	-	-	-	230	6	4	1	-	32
10	96	49	101	50	24	20	16	23	112	31
11	304	11	195	7	296	52	141	48	22	3
12	22	8	3	8	24	8	7	7	9	3
13	49	37	45	40	51	46	46	46	48	31
14	4	1	6	1	45	1	1	1	81	0
15	-	740	-	-	616	576	576	576	-	32
16	312	197	199	196	225	197	192	35	84	32
17	29	25	28	24	32	27	28	27	22	15
18	93	84	93	84	96	88	89	87	89	33
19	-	-	-	82	100	100	100	100	-	4
20	87	87	89	84	82	80	82	80	116	31

Table 4.6: Comparison of detection delays of TE process

4.2.2 Fault diagnosis results

In the above section, the results obtained by the proposed MSKPCA fault detection framework has been presented. After the detection of fault, the proposed fault diagnosis is implemented to diagnose the root cause of process faults in the CSTR system and TE process. The section discusses the application of the proposed fault diagnosis framework for the process faults diagnosis in the CSTR system and TE process. As it is clear from the fault detection results that the SPE control chart give better fault detection performance than T^2 control chart. Therefore, for fault diagnosis purpose SPE control chart was utilized.

Case study 1-Continuous stirred tank reactor

After the detection of all six fault scenarios in the CSTR system, the RBC method is used to diagnose the detected faults and find out the root cause of the fault. Table 4.7. list the root variable corresponding to each fault in the CSTR system. Three types of faults including input disturbance, sensor bias and process faults were simulated in the CSTR system. In the detection stage about three fault scenarios including input disturbance, sensor bias and process were selected. These three types of fault diagnosis results and root cause variables are described in detail.

Fault	Type of fault	Number faulty variables	fault variables
1	Input disturbance	4	1, 4, 8, 9
2	Input disturbance	3	3,8,9
3	Sensor bias	1	5
4	Sensor bias	1	7
5	Process fault	3	6,8,9
6	Process fault	3	4,8,9

Table 4.7: The root fault variables 6 faults of CSTR system

Scenario 1: fault 2

The RBC contribution plot for the first scenario which is about Fault 2 where a ramp change is introduced in initial concentration of the reactant (C_i) is shown in Figure 4.25. In this scenario, the associated faulty variables are variables 3, 8 and 9.

Fault 2 involves a ramp change in initial concentration of the reactant. As the initial concentration of the reaction increased the reaction rate increased. Therefore, the temperature in the reactor would be changed. Since the temperature was regulated by the cooling water flowrate, the temperature in the reactor would be brought back to its set point after a short period of time. The cooling water flow rate adopted a new steady state condition which change induced the cooling outlet temperature to become lower than its normal operating value due to the excessive cooling flow rate. The fault trajectories of the initial concentration of the reactant, cooling liquid flow rate and cooling liquid temperature is plotted in Figure 4.26.



Figure 4.25: Fault diagnosis result for fault 2 in CSTR system



Figure 4.26: Plot of the root cause variables of fault 2 in the CSTR system

Scenario 2: fault 5

The RBC contribution plot for the second scenario which is about Fault 5 where a ramp change in the activation energy (E/R) is shown in Figure 4.27. In this scenario, the associated faulty variable is 6.

Fault 4 involves a ramp change in the activation energy (E/R), which is a complex fault, and this fault would also be propagated to other variables. The proposed method identifies this fault correctly and the major faulty variable was variable 6, whereas other variables were also deviate from the normal conditions. The fault trajectories of the

concentration of A in the reactor, cooling liquid temperature and flowrate of cooling liquid is plotted in Figure 4.28.



Figure 4.27: Fault diagnosis result for fault 5 in CSTR system



Figure 4.28: Plot of the root cause variables of fault 5 in the CSTR system

Scenario 3: fault 6

The RBC contribution plot for the third scenario which is about Fault 6 where a ramp change in the heat transfer coefficient is introduced as shown in Figure 4.29. In this scenario, the associated faulty variables are 4, 8 and 9.

Fault 6 involves a ramp change in the heat transfer coefficient. This is a complex fault and it disturb the other variables as follows: As the value of heat transfer coefficient decreased which increased the flowrate of the outlet stream. With the increase of the outlet stream flowrate, the temperature in the reactor decreased. As temperature in the reactor is controlled with the cooling water flowrate, the flowrate decreased to brought back the temperature to its set point. The temperature of the cooling water increased as a result of decreased in the cooling water flowrate. The fault trajectories of the flowrate of the outlet stream, cooling water flow rate and cooling water outlet temperature is plotted in Figure 4.30.



Figure 4.29: Fault diagnosis result for fault 6 in CSTR system



Figure 4.30: Plot of the root cause variables of fault 6 in the CSTR system

4.2.2.1 Case study 2-Tenessee Eastman process

After the detection of all twenty fault scenarios in the TE process, the RBC method is used to identify the detected faults and find out the root cause of the fault. Table 4.8 lists the root variable associated with each fault in the TE process. Though the SPE control chart for faults 3, 9, and 15 indicates higher FDR values for the proposed framework, the fault patterns would not be evaluated for fault identification and root cause diagnosis.

Fault Number	Fault Number Type of fault		Fault variables
1	Step	2	16, 44
2	Step	4	10, 28, 34, 31
3	Step	-	-
4	Step	1	51
5	Step	4	11,18,50,52
6	Step	2	1,44
7	Step	1	45
8	Random	5	4,10,14,30,47
9	Random	-	-
10	Random	4	18,19,20,50
11	Random	2	9,51
12	Random	7	7,11,13,16,50,20,38
13	Slow drift	7	7,13,18,19,20,38,51
14	Sticking	3	9,21,51
15	Sticking	-	-
16	Unknown	2	18,19,50
17	Unknown	1	21
18	Unknown	7	7,13,16,20,43,46
19	Unknown	2	5,46
20	Unknown	3	13,20,46

Table 4.8: The fault variables of TE process

Scenario 1: fault 4

The RBC contribution plot for Fault 4, which involved a step-change in the inlet temperature of the reactor cooling water is provided in Figure 4.31. In this scenario, the main variable that cause Fault 4 is variable 51 (Reactor cooling water flow).

Fault 4 involves a step change in the reactor cooling water inlet temperature. A significant effect of Fault 4 is to induce a step change in the reactor cooling water flowrate (X_{51}) . This abnormality directly affected the reactor temperature (X_9) as the fault occurs and there is a sudden temperature increase is observed. The feedback controller acted quickly before the other variables responded. The flow rate of the reactor cooling water (X_{51}) was adjusted to return the reactor to its set-point temperature. Because of the good controller performance, the adjustment was efficient, and the reactor temperature (X_9) quickly reverted to normal. The other variables still show a normal status after the fault occurs. The trajectories of two process variables, reactor temperature (X_9) and reactor cooling water flowrate (X_{51}) are plotted Figure 4.32. Figure 4.32 shows that X_{51} is the only process variable that contributes consistently to this fault, whereas X_9 is only significant at the first time point after the fault has been detected.



Figure 4.31: Fault diagnosis result for fault 4 in TE process



Figure 4.32: Plot of the root cause variables of fault 4 in the TE process

Scenario 2: fault 7

The RBC contribution plot for Fault 7, which involved by a step-change in C header pressure loss is provided in Figure 4.33. which indicates that the opening of the valve for stream 4 (X_{45}) was the only problematic variable, and the controller was successful in bringing the process to a steady state. There are several minor faulty variables (X_4 , X_7 , X_{13} , X_{27} , X_{31} , X_{33}), which are shown in Figure 4.33.

The cause of fault 7 can be clarified as when the total feed flow rate on stream 4 changes, the process variable reactor pressure and the product separation pressure are measured separately. So, to compensate for the reduced C header pressure, the total feed flow rate is increased by adjusting the flow valve on stream 4, which in turn will affect the reactor pressure and product separation pressure in the process. Although there are several minor faulty variables but the Figure 4.34. shows the trajectories of three process variables, flow rate of stream 4 (X_4), product separator pressure (X_{13}) and

total feed volume (X_{45}). At the 160th sample, the fault 7 was triggered, which resulted in a sudden drop in the flow rate of stream 4 (X_4). As soon as the major faulty variable (X_{45}) reached a new steady state, the process controller adjusted the minor faulty variables.



Figure 4.33: Fault diagnosis result for fault 7 in TE process



Figure 4.34: Plot of the root cause variables of fault 7 in the TE process

Scenario 3: fault 8

The RBC contribution plot for Fault 8, which involved by a step-change in C header pressure loss is provided in Figure 4.35. In this scenario, the main variables that cause fault 8 is variables 4, 10, 24, 30 and 47.

The fault identification results shows that the major variable that causes this fault is variable 47 (purge valve). The cause of fault 8 can be clarified as when the purge valve fails the total feed flow rate on stream 4 disordered. The purge rate and component B in the stream 6 and 9 will also be abnormal. The trajectories of these process variables, total feed (X₄), purge rate (X₁₀) and component B, stream 6 (X₂₄), component B, stream 9 and purge value (X₄₇) are plotted Figure 4.36 and Figure 4.37.



Figure 4.35: Fault diagnosis result for fault 8 in TE process



Figure 4.36: Plot of the root cause variables of fault 8 in the TE process



Figure 4.37: Plot of the root cause variables of fault 8 in the TE process

Scenario 4: fault 11

The RBC contribution plot for Fault 11, which involved by a random variation in reactor cooling water inlet temperature is provided in Figure 4.38. In this scenario, the main variables that cause fault 11 are variable 9 (total feed volume) and variable 51 (reactor pressure).

This fault is similar to Fault 4 where the fault induces in the reactor cooling water inlet temperature. The fault in this scenario is a random variation. The cause of this fault is a random variation in the reactor cooling water flowrate (X_{51}) , which caused the reactor temperature (X_9) to fluctuate as a result of this change. Although, it is possible for the control loops to compensate the change in the reactor temperature after a longer time has elapsed, the fluctuations in both variables affected early after the introduction of the fault were correctly identified. The other variables may remain close to the set

point and behave normally. The trajectories of two process variables, reactor temperature (X_9) and reactor cooling water flowrate (X_{51}) are plotted in Figure 4.39.



Figure 4.38: Fault diagnosis result for fault 11 in TE process



Figure 4.39: Plot of the root cause variables of fault 11 in the TE process

Scenario 5: fault 14

The RBC contribution plot for Fault 11, which involved by a random variation in reactor cooling water inlet temperature is provided in Figure 4.40. In this scenario, the main variables that cause fault 11 are variable 9 (total feed volume) and variable 51 (reactor pressure).

Fault 14 is due the reactor cooling water valve sticking, and it occurs as follows. The temperature of the reactor cooling water is reduced as a result of valve sticking, increasing the cooling effect on the reactor. Thus, a drop in the reactor temperature (X₉) is observed. The controller will reduce the condenser cooling water flow (X₅₁) rate to maintain the equilibrium. Additionally, the viscous reactor cooling water valve directly affects the temperature of the reactor cooling water outlet (X₂₁). The trajectories of three process variables, reactor temperature (X₉), reactor cooling water outlet temperature (X₂₁) and reactor cooling water flowrate (X₅₁) are plotted in Figure 4.41.



Figure 4.40: Fault diagnosis result for fault 14 in TE process



Figure 4.41: Plot of the root cause variables of fault 14 in the TE process

4.3 Chapter Summary

In this chapter, the proposed fault detection and diagnosis framework has been investigated and analyzed using two case studies including CSTR system and TE process. This chapter presents the results of the research objectives listed in Chapter 1 of this thesis. The fault free data has been used to develop the proposed framework whereas the fault data has been used to validate the performance of the performance.

The proposed MSKPCA based fault detection framework is found to be very efficient for the detection of faults in the CSTR system. From these results, it can be concluded that the developed framework is adequate for the representation of system behavior, and thus appropriate for efficient fault detection. This framework gives a viable result for an effective fault detection method for CSTR system. Three different types of faults such a process disturbance, sensor bias and process fault have selected for comparison. The proposed framework showed a better fault detection result than that of PCA and KPCA methods. The reliability of the fault detection framework is measured with the FDR and DD, since it is crucial in the application of fault detection and diagnosis method in real time processes.

Furthermore, the effectiveness of the proposed framework has been validated by using the TE process data. Finally, five different types of faults were selected for comparison. Proposed MSKPCA fault detection framework has better detection results the comparative methods including PCA and KPCA.

The fault detection results has been compared to the results presented in literature. The proposed framework shows a better FDR than the other methods including PCA, DPCA, KPCA and DKPCA. The proposed framework shows a higher fault detection on both control charts (T^2 and SPE) compared to other comparative methods. The proposed framework has the highest average in detection rates for the SPE control chart (82.51%) compared to PCA (63.79%), DPCA (66.15%), KPCA (68.85%) and DKPCA (64.25%).

In addition to fault detection, a proposed fault diagnosis framework based on RBC has been evaluated to diagnosis faults in the CSTR system and TE process. For fault detection, T^2 and SPE control charts were used and from these two charts SPE chart shows better fault detection rate. Thus, for fault diagnosis, SPE based RBC framework has been used for fault diagnosis and root cause fault variables of each fault are obtained. Three types of faults consistent with fault detection results and for types of faults are consistent with the detection results with TE process are selected for fault diagnosis. In addition, the cause of the fault is also distinguished for the faults that contain the relationship of the fault variables. The results show that the SPE-MSKPCA
framework and the RBC model for real-time chemical process faults have a high detection and identification effect.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Real-time process monitoring is preferred for efficient quality control of final products and process optimization. The work reported in the literature used offline data to build the model then modified it for the real-time data. In this study, wavelet analysis and KPCA were used to establish a framework for fault detection and diagnosis for real-time process data.

The following conclusions can be derived from this study:

A MSKPCA based fault detection framework has been developed by integrating wavelets with KPCA. The objective of the developed MSKPCA framework is to use the wavelet-based multiscale representation of data to enhance the effectiveness of the KPCA based fault detection method. In wavelet transforms, a moving window technique is introduced, which is helpful in real-time process monitoring. In the developed framework, the KPCA model will be constructed using the highest-level wavelet coefficients, and then T² and SPE control charts were used to detect the faults present in the process. Six different fault scenarios have been studied to observe the abnormal behaviour of the CSTR system. The normal data set is used to develop the model, while faulty detests are used for testing and validation.

Fault detection rate and detection delay evaluated the performance of the proposed fault detection framework. Faults 1 and 3 are step changes from all six fault patterns, and faults 2, 4, 5 and 6 are random variations. The FDR for 1 and 3 was high compared to other faults as these fault patterns are easy to detect. Faults 5 and 6 were process faults and are difficult to detect as these faults disturb the other variables also. Similarly,

detection delays were also calculated for each fault pattern to evaluate the fault detection framework. It was found that the proposed framework accurately detected step-change fault patterns as the fault was introduced, and early fault detection was also observed for ramp change fault patterns. The average fault detection rate for the CSTR system's faults is found to be 69.67% and 81.20% for T^2 and SPE control charts, respectively. The results revealed that the proposed framework was found to be efficient.

A comparison of the proposed fault detection framework was also done with other established methods such as PCA and KPCA. It would be observed that FDR of the proposed method was higher than that of the comparative methods (PCA and KPCA). It was found that the SPE control chart has higher FDR values for all six fault patterns whereas T^2 control chart has higher FDR values in 5 fault patterns out of all 6. In this fault pattern, T^2 statistic based on KPCA method shows better FDR. Overall, it would be observed that the performance of the proposed framework was satisfactory.

A fault diagnosis framework has been developed using MSKPCA and RBC model, and the root cause of faulty variables of each fault is obtained. Three types of faults consistent with the detection results are selected for find out he root cause. In addition, the cause of the fault is also distinguished for the faults that contain the relationship of the fault variables.

The MSKPCA framework is also applied to the TE process. The results show that the MSKPCA framework can accurately detect faults and the RBC model determines the cause and propagation path of the fault. Under fault conditions, the MSKPCA framework is compared with conventional PCA and KPCA methods in terms of FDR and detection delays. The FDR of the proposed framework is higher in 19 fault patterns out of 20 fault patterns, which shows the proposed framework's effectiveness in fault detection. For fault pattern 1, not much difference is observed in the proposed framework and the conventional PCA and KPCA. The TE process, the average fault detection rate for all faults is found to be 45.85% and 82.51% for T² and SPE control charts, respectively.

In the case of the TE process, five types of fault patterns consistent with the detection results are selected to identify the faulty variables, and the cause of the fault is also distinguished for the faults that contain the relationship of the fault variables.

5.2 Recommendations

Based on the findings of the proposed research work, a few potential recommendations and research directions have emerged for future consideration that would further improve the current research work.

These includes:

1. Detection of small variations

The current study comprises various fault patterns in the CSTR system and TE process. It would be interesting some fault patterns are not detected or sometimes delay in detection is observed by using the proposed framework and other comparative methods. Although, faults were present in the system, but the variations are so small, and the fault detection methods does not detect these small variations. These faults may lead to a huge damage to the plant if not detected in time. An adaptive fault detection framework is required for this type of fault in nonlinear processes.

2. Real-time plant data

The current research is based on the simulated data of the CSTR system and TE process. The next step is more interesting to develop adaptive fault detection and diagnosis framework based on real-time plant data to evaluate the performance of the proposed framework on the real working system.

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APPENDIX A

STATISTICAL ANALYSIS OF MULTISCALE PROCESS MONITORING



Figure A.1: Name of method used

Various fault detection and diagnosis techniques have been used for multiscale process monitoring. These include conventional process monitoring methods such as (CUSUM and EWMA), multivariate (PCA and PLS), and their various extensions. Figure A.1 shows the most widely used methods involved in multiscale process monitoring. PCA is the most widely used method in multiscale process monitoring, followed by KPCA, PLS, KPLS, NLPCA and KFDA.





Validation of multiscale process monitoring approaches has been done using various applications. Figure A.2 illustrates the most often used applications in this field of study. The TE process is widely used by researchers, with a share of about 22.22%. The CSTR system, Industrial processes, and simulated numerical data are the next most used application areas, with 15.15%, 16.16%, and 14.14%, respectively.



Figure A.3: Type of case study used

The performance of the multiscale process monitoring methods was evaluated using process data from various diverse application areas. Figure A.3 shows the distribution of data types used in multiscale process monitoring. Two types of datasets have been used for multiscale process monitoring, including real-time and simulated data. Figure A.3 shows that the portion of the real-time dataset used is only 24.21%, acquired from either industrial processes or pilot plants. On the other hand, the rest of the portion includes simulated datasets. The characteristics of simulated datasets usually are known, which can help highlight the effectiveness of a specific method.

APPENDIX B

SELECTION OF MOTHERWAVELET TYPE AND DECOMPOSITION LEVEL



Figure B.4: Proposed methodology to select optimal mother wavelet and fault detection at various levels

A comparative study was conducted based on the simulated CSTR system data to select the optimal mother wavelet (MWT) basis function and level of decomposition. The proposed methodology is shown in Figure B.4. The best MWT was determined in the first part of the methodology, and the optimal wavelet decomposition level for the best MWT was identified in the second part. Twenty-three (23) MWTs were utilized in this work to evaluate their compatibility, including Daubechies (db2-db10), Symlets (sym2-sym10), and Coiflets (coif1-coif5). The best MWT is determined by the rates of fault detection and false alarms. Throughout the process, the level of decomposition was kept at 3. The result is presented in Tables B.1-B.3 showed that db2, sym2, sym8, coif2 and coif4 have the best results. Although, sym8, coif2 and coif4 have the highest value of fault detection rates they also have the false alarm rates. On the other hand, db2 and sym2 showed the same detection rates and there was no false alarm rate for both of them. Daubechies (db2) was identified as the best of the 23 MWTs used in this study since it provides the best results based on the above-mentioned criteria. After determining the best MWT, the decomposition level was determined using the approach shown in Figure B.4. The optimal MWT has been investigated with decomposition levels ranging from 3 to 8. As per the results in Table B.4, the number 4 was found to be the best level of signal decomposition since it had the highest fault detection rate and the lowest false alarm rate. Table B1-B4 contains the complete results for identifying the best mother wavelet type and decomposition level.

Mother wavelet	Type of mother	Fault detection rate (%)/Missed detection rate (%)				
	wavelet	MSPCA-T ²	MSPCA-SPE	Average		
	db2	<mark>68.80/0.00</mark>	<mark>61.60/0.00</mark>	<mark>65.20/0.00</mark>		
	db3	54.60/0.00	43.60/0.00	49.10/0.00		
	db4	68.20/0.00	62.00/0.00	65.10/0.00		
	db5	57.20/0.00	50.00/0.00	53.60/0.00		
Daubechies	db6	68.20/0.00	62.00/0.00	65.10/0.00		
	db7	62.00/0.00	58.20/0.00	60.10/0.00		
	db8	<mark>68.20/0.00</mark>	<mark>62.00/0.00</mark>	<mark>65.10/0.00</mark>		
	db9	63.20/0.00	60.60/1.00	61.90/0.50		
	db10	67.40/0.00	62.60/0.00	65.00/0.00		

Table B.1.Fault detection rates for scenario 1 using Daubechies mother wavelet

Table B.2. Fault detection rates for scenario 1 using Symlets mother wavelet

Type of	Fault detection rate (%)/Missed detection rate (%)			
mother wavelet	MSPCA-T ²	MSPCA-SPE	Average	
<mark>sym2</mark>	<mark>68.80/0.00</mark>	<mark>61.60/0.00</mark>	<mark>65.20/0.00</mark>	
sym3	54.60/0.00	43.60/0.00	49.10/0.00	
sym4	62.80/0.00	60.80/0.60	61.80/0.30	
sym5	64.20/0.00	61.40/0.80	62.80/0.40	
sym6	72.00/0.00	58.20/0.00	65.10/0.00	
Sym7	65.40/0.00	62.40/1.20	63.90/0.60	
sym8	<mark>72.00/0.00</mark>	<mark>69.00/1.40</mark>	<mark>70.50/0.70</mark>	
sym9	65.80/0.00	62.80/0.80	64.30/0.40	
sym10	66.80/0.00	63.20/1.00	65.00/0.50	
	Type of mother wavelet sym2 sym3 sym4 sym5 sym6 Sym7 sym8 sym9 sym9	Type of mother Fault detection r MSPCA-T ² sym2 68.80/0.00 sym3 54.60/0.00 sym4 62.80/0.00 sym5 64.20/0.00 sym6 72.00/0.00 sym8 72.00/0.00 sym9 65.80/0.00 sym10 66.80/0.00	Type of mother wavelet Fault detection rate (%)/Missed det MSPCA-T ² sym2 68.80/0.00 61.60/0.00 sym3 54.60/0.00 43.60/0.00 sym4 62.80/0.00 60.80/0.60 sym5 64.20/0.00 61.40/0.80 sym6 72.00/0.00 58.20/0.00 Sym7 65.40/0.00 62.40/1.20 sym8 72.00/0.00 69.00/1.40 sym9 65.80/0.00 63.20/1.00	

Table B.3. Fault detection rates for scenario 1 using Coiflets mother wavelet

Mother wavelet	Type of mother wavelet	Fault detection rate (%)/Missed detection rate (%)			
		MSPCA-T ²	MSPCA-SPE	Average	
Coiflets	coif1	57.80/0.00	52.40/0.00	55.10/0.00	
	coif2	71.80/0.00	68.40/1.00	70.10/0.50	
	coif3	61.40/0.00	60.00/1.40	60.70/0.70	
	<mark>coif4</mark>	72.00/0.00	69.20/0.80	70.60/0.40	
	coif5	59.00/0.00	58.60/0.00	58.80/0.00	

Mathan Wavalat	Decomposition	Fault detection rate (%)/False alarm rate (%)			
wiother wavelet	level	MSPCA-T ²	MSPCA-SPE	Average	
Daubechies	3	68.80	61.60	65.20	
	<mark>4</mark>	<mark>73.20</mark>	<mark>68.20</mark>	<mark>70.70</mark>	
	5	60.00	51.20	55.60	
	6	62.60	54.00	58.30	
	7	71.80	64.00	67.90	
	8	69.20	63.40	66.30	

Table B.4. fault detection rate using optimal wavelet at different levels

APPENDIX C

FAULT DETECTION RATES FOR TE PROCESS

Method	D1		D2		D3		D4	
Statistics	T ²	SPE	T^2	SPE	T ²	SPE	T^2	SPE
Fault number	1			1	1		1	
1	5.38	5.38	7	18.63	4.5	44.5	22.75	67.75
2	0	0	0	2.13	0	28	0	58
3	0	0	0	1.38	0	24.75	0	55.88
4	0	0	0	1.75	0	26	0	57
5	3.63	3.13	5.5	10.63	4	37.5	18.63	65.88
6	1.88	3.63	2.38	22.38	1.5	33	6.75	43.38
7	21.63	20.75	22	30.38	19.38	52.88	34.13	71.75
8	22.38	31.13	33.5	67.38	36.25	92.5	82.13	98.25
9	0	0	0	1.63	0	26.63	0	57.38
10	1.63	1.63	1.5	13.13	3	57.88	8.25	85.88
11	1.88	1.38	21.13	64.88	21.13	95.5	38.25	100
12	86.63	83.63	91.75	98.25	96.63	99.63	98.88	100
13	31.13	37.38	35.13	59	22.75	76.38	56.75	94.25
14	99.88	100	99	100	0	100	0	72.38
15	0	0	0	2.75	0	29.88	0	60.5
16	5.25	4.38	5.25	42.13	6.38	80	16.63	95
17	15.13	27.88	24.38	67.88	40.38	93.38	71.38	98.63
18	18.25	18.5	18.25	21.38	17.25	31.5	20.88	44
19	0.25	33.13	0	78.5	0.5	90.5	0	91.75
20	12.88	11.88	17.38	31.38	30	70.13	21.38	92.38

Table C.5: Fault detection rates of Details (D1, D2, D3 and D4) for the proposed method

Table C.5 shows the FDR values for all Details, including D1, D2, D3, and D4. It can be noticed that the FDR values for 17 fault patterns are less than 25% for detail level 1 (D1). On both monitoring charts, the FDR value for fault #14 was close to 100 percent. On the T^2 monitoring chart, it was 86.63 percent, and on the SPE monitoring chart, it was around 83.63 percent. There was no indication of any disturbance for faults #2, 3,4, 9 and 15. A much better detection rate was observed for detail of level 2 (D2). In this situation, the FDR values for faults 12 and 14 were greater than 80% on both monitoring charts. On the SPE monitoring chart, FDR values for faults 8, 11, 17, and 19 exceeded 60. On both monitoring charts, the FDR value for defect #12 is larger in the case of detail level 3 (D3). On SPE charts, the detection rates for faults #7, 8, 10,

11, 13, 14, 17, 19, and 20 were much greater than those for D1 and D2. In the detail of level 4, detection rates were substantially higher (D4). Almost all fault patterns had larger FDR values than the other detail functions. The approximation function was the underlying signal in the wavelet decomposition, and it included important information in the data. These are the details for all levels and noises in the data. As a result, the FDR values are not consistent across all details.

LIST OF PUBLICATIONS

- Muhammad Nawaz, Abdulhalim Shah Maulud, and Haslinda Zabiri, Humbul Suleman, and Lemma Dendena Tufa, "Multiscale Framework for Real-Time Process Monitoring of Nonlinear Chemical Process Systems," Industrial & Engineering Chemistry Research, 2020 (Impact Factor 2021=4.326)
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- Muhammad Nawaz, Abdulhalim Shah Maulud, and Haslinda Zabiri, Humbul Suleman, "Review of multiscale methods for process monitoring, with an emphasis on applications in chemical process systems, "IEEE Access (Impact Factor 2021=3.476)
- Muhammad Nawaz, Abdulhalim Shah Maulud, and Haslinda Zabiri, "Analysis of multiscale process monitoring in industrial processes from a bibliometric perspective, "Computers & Chemical engineering (Under Review) (Impact Factor 2021=4.130)
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