

# 10360397

# IMPROVED MULTIVARIATE STATISTICAL PROCESS CONTROL FOR CHEMICAL PROCESS FAULT DETECTION AND DIAGNOSIS

## LAM HON LOONG

A thesis submitted in fulfilment of the requirements for the award of the degree of Master of Engineering (Chemical)

Faculty of Chemical and Natural Resources Engineering
Universiti Teknologi Malaysia

**NOVEMBER 2004** 

To my beloved parents, siblings and friends

## **ACKNOWLEDGEMENTS**

Growing up in a small town in rural Machang, Kelantan, I dreamed of attending institute of higher education and participating in the discovery of new theories and technologies that would further extend the boundaries of science and engineering. I consider myself extremely fortunate to have that dream becoming a reality. However, the level of success that any individual achieves in life is dependent upon the guidance and support of family, friends, supervisor and advisors.

Firstly, I would like to express my sincere gratitude to my supervisor, Associate Professor Dr Kamarul Asri bin Ibrahim, the current Deputy Dean of *Unit Pengurusan Program Kerjasama* Universiti Teknologi Malaysia (UTM), for his dedication, support and guidance throughout the whole period of this research work. His knowledge and experience in the field of Multivariate Statistical Process Control (MSPC) has enlightened me to be involved in this relatively new area. I also appreciate his guidance on the research and the freedom that he has given me in exploring the scope for my research.

I also extend my most heartfelt thanks to my father and mother who sacrificed so much, asked for so little and inspired so often. Throughout my life their guidance and teaching has provided wisdom that no university could match. I also thank my brother and sister, who remain one of my biggest supporters despite the torment I dished out throughout our childhood. I also thank my grandma who challenged a young child to explore all that education and life may present.

I am grateful to The Ministry Of Science, Technology and the Environment for providing the IRPA (Intensified Research Priority Area) research grant and National Science Fellowship (NSF) scholarship for this project.

Thank are also due to my friend Lee Lean Eng, who work together in MSPC research group who always gave me a hand when I get into troubles, and also my senior Chiah Yoke Lin who helped me solve the simulation programming problem.

I also wish to thank my good friends in the debate team and my housemates. Without their friendship, I could not have survived my life as a graduate student.

Finally, I would like to thank my darling for her support and understanding during my difficulties.

#### **ABSTRACT**

This thesis demonstrates the application of Multivariate Statistical Process Control (MSPC) monitoring method that is capable of detecting and diagnosing process faults. Conventionally,  $T^2$  Control Chart and Contribution Chart, which have been widely used for these purposes, are not accurate and sensitive enough to detect and diagnose abnormal changes in operating conditions. In order to overcome these problems, the objective of this research is to develop new approaches, which can improve the performance of the present conventional MSPC methods. Three new approaches have been developed i.e., the Outline Analysis Approach for examining the distribution of Principal Component Analysis (PCA) scores, the Correlation Coefficient  $(C_{ik})$  Approach for detecting changes in the correlation structure within the variables, and the Signal Cumulating Approach for gathering more information regarding the fault. In order to implement the three new approaches, this research proposed PCA Outline Analysis Control Chart and Correlation Coefficient  $(C_{ik})$ Control Chart for fault detection; and the  $T^2$  Score Contribution Chart, the  $C_{ik}$  Score Contribution Chart,  $T^2$  Score Contribution Chart with Signal Cumulating Approach and the  $C_{ik}$  Score Contribution Chart with Signal Cumulating Approach for fault diagnosis. The results from the conventional method and new approaches were compared based on their accuracy and sensitivity. Based on the results of the study, the new approaches generally performed better compared to the conventional approaches, particularly the PCA Outline Analysis Control Chart and  $C_{ik}$  Score Contribution Chart with Signal Cumulating Approach.

#### **ABSTRAK**

Tesis ini menengahkan penggunaan kaedah pemantauan Kawalan Statistik Berbilang Angkubah, (MSPC) sebagai teknik bagi mengesan dan mengenalpasti kehadiran kesilapan dalam proses. Secara konvensional, Carta kawalan  $T^2$  dan Carta Penyumbangan banyak digunakan tetapi tidak tepat dan kurang sensitif untuk mengesan dan mengenalpasti perubahan tidak normal yang berlaku dalam proses. Bagi mengatasi kelemahan ini, objektif penyelidikan ini adalah untuk membangunkan beberapa kaedah baru yang dapat mempertingkatkan prestasi kaedah MSPC konvensional yang sedia ada. Tiga pendekatan baru telah dicadangkan, iaitu Kaedah Analisis Garis Bentuk yang dapat mengkaji corak taburan nilai Analisis Komponen Utama (PCA); Kaedah Pemalar Hubungan,  $C_{ik}$ , yang dapat mengesan perubahan struktur kolerasi antara angkubah; dan Kaedah Konggokan bagi mengumpul maklumat mengenai kesilapan. Untuk mengaplikasikan tiga kaedah baru ini, penyelidikan ini mencadangkan, Carta Kawalan Analisis Garis Bentuk PCA dan Carta Kawalan  $C_{ik}$  untuk mengesan kehadiran kesilapan. Bagi mengenalpasti punca kesilapan pula, Carta Penyumbang Nilai  $T^2$ , Carta Penyumbang Nilai  $C_{ik}$ , Carta Penyumbang Nilai  $T^2$  secara Konggokan dan Carta Penyumbang Nilai  $C_{ik}$  secara Konggokan disyorkan. Keputusan dari kaedah konvensional dan kaedah baru yang dicadangkan akan dibandingkan berdasarkan ketepatan dan kepekaan. Keputusan daripada kajian ini menunjukkan prestasi kaedah baru yang dicadangkan adalah lebih baik berbanding dengan kaedah konvensional, terutamanya, Carta Kawalan Analisis Garisan Bentuk PCA dan Carta Penyumbang Nilai  $C_{ik}$  Konggokan.

# **TABLE OF CONTENTS**

CHAPTER	TITLE	PAGE
	Title	i
	Declaration	ii
	Dedications	iii
	Acknowledgement	vi
	Abstract	vi
	Abstrak	vii
	Table of Content	viii
	List of Tables	xiv
	List of Figures	xv
	List of Symbol	xviii
	List of Appendices	xxvi
	1 INTRODUCTION	1
	1.1 Research Background of the Project.	1
	1.2 Problem Statement.	2
	1.3 Research Objective.	3
•	1.4 Scope of Research.	3
	1.5 Research Contribution.	5
	1.6 Organization of The Thesis	5

2 L	ITERATURE REVIEW	7
2.	1 Process Fault Detection and Diagnosis	7
	2.1.1 Characteristics of Process Fault Detection	8
	and Diagnosis System (PFDD).	
	2.1.2 Classification of PFDD System	1
	2.1.3 Development and Application of Process	13
	Fault Detection and Diagnosis.	·
2.2	2 Multivariate Statistical Process Control As The	15
	Fault Detection and Diagnosis Tool	
	2.2.1 Development and Implementation of	16
	MSPC in Chemical Process.	
	2.2.2 Explaining the Relation Between	17
	Variables via Principal Component	
	Analysis (PCA).	20
	2.2.3 PCA Extensions.	23
	2.2.4 Multivariate Control Chart.	30
	2.2.5 Fault Diagnosis via Contribution Chart.	33
2.3	Conclusions	33
B PR	OCESS MODELING AND DATA	35
SIN	MULATION	
3.1	Introduction	35
3.2	Motivation for Process Modeling and	35
	Simulation.	
3.3	Ethylene Oxide Reaction System.	36
3.4	Cooled Tubula r Reactor for EO Production.	37
3.5	Model Formulating	39
	3.5.1 Total Mass Balance	41
	3.5.2 Components Balance	41
	3.5.3 Energy Balance for Reactor.	11

	3.5.4	Energy Balance for Cooling System	46
3.6	5 Data	Generation and Collection	50
	3.6.1	The Mathematical Solution for Model's	
		Differential Equations.	50
	3.6.2	Simulation Data with Fault Appearance	52
3.7		mary	57
4 M	ЕТНО:	DOLOGY	58
4.1	Intro	duction.	58
4.2	Obtai	ining The Statistical Relationship Between	58
	the C	ollected Data via Eigenvector-Eigenvalue	
	Deco	mposition Principal Component Analysis,	
	(PCA	).	
	4.2.1	Data Sampling.	60
	4.2.2	Data Standardization.	61
	4.2.3	Eigenvalue Decomposition.	61
4.3	Corre	lation or Relation Coefficient Between	
	Varia	bles Based on PCA Calculation.	63
4.4	Contr	ol Chart.	67
	4.4.1	Hypothesis Testing Formulation.	68
	4.4.2	Standardized Normal Distribution	
		Control Chart: Extended from	69
		Hypothesis Testing Formulation.	
4.5	Conve	entional PFDD Mechanisms.	72
	4.5.1	Conventional T <sup>2</sup> Statistics.	73
	4.5.2	Conventional Contribution Chart via	
		Eigenvector-eigenvalue PCA.	75
4.6	Modif	ied Process Fault Detection and Diagnosis	77
	Mecha	nisms.	
	4.6.1	Outline Analysis Approach.	78
	4.6.2	Cross-Variable Correlation Approach.	80

		4.6.3	Signal Cumulating Approach.	82
	4.7	Sumn	nary	83
5	RE	SULT	ANALYSIS AND DISCUSSION	84
	5.1	Introd	luction	84
	5.2	Simul	ation Result: Normal Operating Condition	85
		(NOC	) and Out-of-control Operating Condition	
		(OC)	Data.	
		5.2.1	Data Normality.	90
		5.2.2	Data Sample Class Size.	95
	5.3	Princi	pal Component Analysis.	98
	5.4	Multiv	variate Fault Detection Control Chart.	101
		5.4.1	Fault Detection Control Chart	101
			Performance: Superficial Result	
		5.4.2	Result Analysis and Discussion for	112
			Fault Detection Control Chart.	
		5.4	2.2.1 Conventional PCA Based T <sup>2</sup> -	112
			Control Chart.	
		5.4	.2.2 Result Analysis and Discussion for	118
			$C_{ik}$ Control Chart.	
		5.4	.2.3 Performance of Outline Analysis	121
			Control Chart.	
	5.5	Fault I	Diagnosis Via Contribution Chart.	128
		5.5.1	General Advantages of Contribution	128
			Chart.	
		5.5.2	Result Analysis and Discussion for Fault	130
			Diagnosis.	
		5.5.2	2.1 Case Study 1: Significant Fault	131
			Diagnosis	
		5.5.2	2.2 Case Study 2: Insignificant Fault	135
			Diagnosis.	

# LIST OF TABLES

1

TAB	LE NO. TITLE	PAGE
2.1	Summary of The Important Work and Research Interest in Fault Detection and Diagnosis.	14
2.2	Summary of the Important Work in PCA Extension Development.	26
3.1	Nomenclature for The Cooled Tubular Reactor System	38
3.2	Nomenclature for The Symbol Used in Mass and Energy Balance	40
3.3	Simulation Parameters.	51
3.4	Estimated Parameters for Initial Conditions.	51
3.5	Description of Different Sources of Faults	54
3.6	Fault Appearance In OC Data	55
4.1	Eigenvector and Eigenvalue for Particular Variables	71
5.1	Statistics Calculation Element's Value for Normal Operating Condition.	85
5.2	Significant Fault Appearances in Case Study 1.	87
5.3	Significant Fault Appearances in Case Study 2.	88
5.4	Significant Fault Appearances in Case Study 3.	89
5.5	Data Sampling Scheme with Difference Sample Class Size	95
5.6	Summary Results for Sampling Size Test.	96
5.7	Principal Component Analysis Eigenvector and	
	Eigenvalue	98
5.8	Fault Detection for Case Study 1.	106

5.9	Fault Detection for Case Study 2.	107
5.10	Fault Detection for Case Study 3.	108
5.11	Performance of PCA Based T <sup>2</sup> Control Chart in Each	114
	Case Study.	•••
5.12	Analysis: The Relationship Between the PCA Mean And	117
	T <sup>2</sup> Score.	• • • •
5.13	Performance of $C_{ik}$ Profile Control Chart in Each Case	120
	Study.	
5.14	The Relationship Between the Distribution Normality and	120
	Fault Detection Result.	
5.15	Performance of Outline Analysis Control Chart in Each	122
	Case Study.	
5.16	The Relationship Between the PCA Mean And T <sup>2</sup> Score.	125
5.17	Fault Diagnosis Result for Case Study 1.	131
5.18	Fault Diagnosis Result for Case Study 2.	135
5.19	Fault Diagnosis Result for Case Study 3.	140

# **LIST OF FIGURES**

FIGU	JRE NO. TITLE	PAGE
2.1	Schematic Diagram of Difference between Feedback	10
	Control System and PFDD System	10
2.2.	Classification of PFDD Approach	12
2.3	General Function of Multivariate Statistical Process	16
	Control	16
2.4	Relationship Between Original Data with Obtained PCs.	21
2.5	Graphical Interpretation of Principal Component Analysis	22
2.6	Data Matrix Unfolding.	24
2.7	Data Matrix Array for Multiblock PCA	24
2.8	Modified Input Matrix	25
2.9	T <sup>2</sup> -control Chart with UCL.	32
3.1	The Principles and Motivation for Process Modeling	36
3.2	Schematic Diagram of Cooled Tubular Reactor System for EO Production	38
3.3	Dynamic Simulation Algorithm	49
3.4	Indication of The Different Sources of Fault in The System	53
4.1	Summary of Methodology Sequence.	59
4.2	Schematic Diagram for Data Sampling.	60
4.3	PCA Model Schematic Diagram	63
4.4	Hypothesis Testing Formulation.	69
4.5	Standardized Normal Distribution	
		69
4.6	Hypothesis Testing Formulation Extended to Croi Control	72

	Chart	
4.7	Schematic Diagram for T <sup>2</sup> -Analysis via Control Chart.	76
4.8	Schematic Diagram for Contribution Chart Development.	77
4.9	Two Different Data with The Same Mean Profile.	78
4.10	Linear Relationship Between Incoming Variables and $C_{ik}$ Profile.	81
5.1	Ethylene Oxide Concentration, $C_{EO}$ Profile during Normal	
	Operating Condition for First 100 <sup>th</sup> Data.	86
5.2	CEO Profile During Case Study 1.	87
5.3	C <sub>EO</sub> Profile During Case Study 2.	88
5.4	$C_{EO}$ Profile During Case Study 3.	90
5.5	Statistical Summary of Concentration of Ethylene, $C_{Eth}$ Data	92
5.6	Statistical Summary of Concentration of Ethylene Oxide, $C_{EO}$ Data	92
5.7	Statistical Summary of Input Temperature, T Data	93
5.8	Statistical Summary of Cooling System Temperature, <i>Tc</i> Data	93
5,9	Statistical Summary of Cooling Water Flow Rate, Fc Data	94
5.10	Statistical Summary of Input Flow Rate, F Data	94
5.11	T <sup>2</sup> Control Chart Results for Several Sampling Size: 25, 50,100, and 150.	96
5.12	Principal Component Vs Covered Variation Plot	99
5.13	Parameter Complexity Reduction By Principals Component Analysis.	99
5.14	Outline T <sup>2</sup> Control chart with Difference Number of	
	Principal Component. (a) with 3 principal components, (b)	100
	with 6 principal components.	
5.15	Fault Detection Result for Case Study 1	102
5.16	Fault Detection Result for Case Study 2	103
5.17	Fault Detection Result for Case Study 3	104

5.18	Pictorial Representation of Multivariate Data Undergoing a	110
	Mean Shift and Covariance Shift.	110
5.19	PCA Score Plot for NOC Area and 50 <sup>th</sup> Sample in Case	113
	Study 1.	113
5.20	Process Monitoring for 1st 500 Incoming Data of Case	116
	Study 1.	110
5.21	Linear Relationship Between The Input Variables and	119
	Quality Interested Variable.	117
5.22	Process Monitoring for 2000 <sup>th</sup> – 2500 <sup>th</sup> Incoming Data of	126
	Case Study 3.	120
5.23	PCA Score Contribution Chart for Case Study 1.	129
5.24	T <sup>2</sup> Score Contribution Chart for Case Study 1	130
5.25	C <sub>ik</sub> Score Contribution Chart for Case Study 1	130
5.26	Multivariate and Univariate Approached Contribution	132
	Chart.	132
5.27	PCA Score Contribution Chart for Case Study 2	134
5.28	T <sup>2</sup> Score Contribution Chart for Case Study 2	134
5.29	Cik Score Contribution Chart for Case Study 2	135
5.30	Improved PCA Contribution Chart via Signal Cumulating	136
	Approach	150
5.31	Improved T <sup>2</sup> Profile Contribution Chart via Signal	137
	Cumulating Approach	137
5.32	Improved T <sup>2</sup> Profile Contribution Chart via Signal	137
	Cumulating Approach	157
5.33	PCA Score Contribution Chart for Case Study 3	139
5.34	C <sub>ik</sub> Score Contribution Chart for Case Study 3	139

## LIST OF SYMBOL

## A: Process System

 $(\Delta H)_{p,x}$  = Reaction heat, kJ/mol.

 $k_{p.x}$  = Reaction rate, m<sup>3</sup>/kg.

A = Ethylene.

B = Oxygen.

C = Ethylene Oxide.

D = Carbon Dioxide.

E = Water.

 $C_{Ai}$  = Input Concentration of Ethylene (mol/m<sup>3</sup>)

 $C_{Bi}$  = Input Concentration of Oxigen (mol/m<sup>3</sup>)

Ti = Input Reactor Temperature (K)

Fi = Input Reactants/ Products flowrate (m $^3$ /s)

Tci = Input Coolant Temperature (K)

Fci = Input Coolant flowrate(m<sup>3</sup>/s)

 $C_A$  = Concentration of Ethylene (mol/m<sup>3</sup>)

 $C_B$  = Concentration of Oxigen (mol/m<sup>3</sup>)

 $C_C$  = Concentration of Ethylene Oxide (mol/ $\mathbb{R}^3$ )

 $C_D$  = Concentration of Carbon Dioxide (mol/m<sup>3</sup>)

 $C_E$  = Concentration of Water (mol/m<sup>3</sup>)

T = Reactor Temperature (K)

```
F = Reactants/ Products flowrate (m<sup>3</sup>/s)
```

Tc = Coolant Temperature (K)

Fc = Coolant flowrate(m<sup>3</sup>/s)

 $\rho$  = Density, kg/m<sup>3</sup>

 $V = \text{System Volume, m}^3$ 

t = Time, s

F = Volumetric flowrate, m<sup>3</sup>/s

n = mol, kmol

h = Enthalpy, kJ/kg

E = Activation energy, J

U = Initial Energy, J

K = Kinetic Energy, J

PE = Potential energy, J

Q = Heat transferred to the system from its surroundings, W

 $W_s$  = Work done on the system by its surroundings, W

i = Input species

j = Output species

 $\rho_{mix}$  = Density for mixture, kg/m<sup>3</sup>

 $\rho_b$  = Catalyst's density, kg/m<sup>3</sup>

 $U_h$  = Overall heat transfer coefficient, W/m<sup>2</sup>K

D =Reactor diameter, m

 $\gamma_p = E_p/RT_{R,}$  dimensionless activation energy.

 $p_e = E_X/E_P$ , active energy ratio.

 $S'_{XP} = dX_X/dX_P$ , differential reciprocal selectivity ratio.

## **B:** Statistical Analysis

 $C_{Ethylene i}$  = Input Concentration of Ethylene (mol/m<sup>3</sup>)

 $C_{Ethylene\ Oxide}$  = Output Concentration of Ethylen? Oxide (mol/m<sup>3</sup>)

Ti = Input Reactor Temperature (K)

Fi = Input Reactants/ Products flowrate (m $^3$ /s)

Tci = Input Coolant Temperature (K)

Fci = Input Coolant flowrate(m $^3$ /s)

P = principals component loadings,

T = principals component scores.

P = number of variable

m = NOC data size

n = New observe sample size

**Z** = Standardized matrix,

X = Input data matrix,

 $\overline{X}_i$  = Sample mean scalar for each particular variable,

 $S_i^2$  = Standard Derivation scalar for each particular variable.

 $\alpha$  = Level of significance,

F = F-distribution.

 $v_j$  = Eigenvector for  $j^{th}$  variable,

 $\lambda_i$  = Eigenvalue for  $j^{th}$  variable.

C = Contribution Score

# LIST OF APPENDICES

Appendix	TITLE	PAGE
<b>A.</b>	<b>Process Modeling &amp; Simulation Code</b>	
A.1	Model Differential Equation Function	156
A.2	Model Simulation	158
В.	Statistical Analysis Programming Code	
B.1	PCA Model Generation	160
B.2	T <sup>2</sup> Control Chart	162
B.3	Outline Analysis	164
B.4	Cik Control Chart	167
B.5	PCA Score Contribution Chart	169
B.6	T2 Score Contribution Chart	171
B.7	Cik Score Contribution Chart	174
B.8	PCA Score Contribution Chart with Signal	176
	Cumulating Approach	
B.9	T <sup>2</sup> Score Contribution Chart with Signal	179
	Cumulating Approach	
B.10	C <sub>ik</sub> Score Contribution Chart with Signal	182
	Cumulating Approach	

## CHAPTER 1:

#### INTRODUCTION

Chemical process systems are highly sensitive to abnormal changes in operating condition. So that, to attain the maximum possible yield in chemical process, it is necessary to ensure that the process is maintained around the desired limit. As a direct consequence, the accuracy and the sensitivity of the process monitoring tool is very important. The Multivariate Statistical Process Control (MSPC) method has been applied because it provided a wide range of tools to perform process monitoring and also very effective at extracting hidden information in problems with multiple correlated variables (Louwerse and Smilde, 2000). This research demonstrates the application of the MSPC method to provide a monitoring tool, which is capable of detecting and diagnosing the process fault.

# 1.1 Research Background of the Project.

Most of the Statistical Process Control (SPC) techniques involve operations on single response variables such as weight, pH, temperature, specific gravity, concentration and pressure. This is natural because one is usually interested in a problem involving a single response. Normally, the fault in the process is sought through the usage of the SPC control chart, but in practice, most of the SPC control charts are based on charting only a small number of variables, usually the final product of quality variables. These approaches are often inadequate for modern and complex process industries. For this reason, a multivariate approach is applied in the SPC realm to detect the fault condition in the large number of variable observations.

There are however, a number of occasions when more than one response variable (multivariate) are of importance to a problem, and these variables should be studied collectively in order to take advantage of the information about the relationship among the data. With the advance of process sensors and data acquisition systems, today's chemical processes are becoming better instrumented. In many cases, this instrumentation provides an abundance of data, some of which can be classified as redundant for example, the measurements are highly correlated. Multivariate method such as Principal Component Analysis (PCA) can express the essential information contained in these measurements in term of relatively "small dimension" of new variables without losing the previous information. By applying the MSPC, this new strategy of monitoring fault and diagnosis process operating condition can predict process degradation and equipment failure; thus it can improve the chemical plant production process using the diagnosis through this method.

Fault detection and the monitoring of process performance is an integral part for a successful operation. The MSPC chart can be used to monitor the performance of any given process. The main function of this control chart is to compare the current state of the process against the "Normal Operating Condition (NOC)". The "NOC" condition exists when the process or product variables remain close to the desired values. In contrast, the "Out of Control (OC)" occurs when fault appears in the process. The fault or malfunction is designated when the process departs from an acceptable range of observed variables.

#### 1.2 Problem Statement.

The present conventional MSPC has several weaknesses in process fault detection and diagnosis. Some researchers in this field had commented that the MSPC is a powerful tool for data complexity reduction and fault detection in the significant fault appearance data. According to Manabu and his research partner, (2000), the current fault detection and diagnosis method via MSPC is limited to significant faults and does not point put the insignificant ones accurately. Qin

(2001) also commented that the contribution chart does not have a control limit, making it difficult to determine what is the root cause of the abnormal operating condition.

As a summary of summary other researchers, the weakness of the conventional MSPC can be briefly concluded into three disadvantages. First of all, the complicated control charts are not "user-friendly", secondly, the conventional MSPC fault detection tools are easily rise up to noisy-fault-signals and lastly, the conventional fault diagnosis is not ready with a proper control limit, thus it cannot determine the root cause of the fault, especially multiple faults. In order to improve the limitation of MSPC, this research should focuses on the alternative, which can solve the disadvantages mentioned above.

## 1.3 Research Objective.

To develop new approaches those improve the conventional MSPC based fault detection and diagnosis methods performance.

## 1.4 Scope of Research.

- i) Matlab is used to run the dynamic model simulation of a typical Ethylene Oxide reaction system (Westerterp and Ptasinski, 1984).
- ii) Generate a set of normal operating condition (NOC) data.
- iii) Generate several sets of out-of-control condition (OC) data that contains various multiple appearance disturbance and small operation condition change.

- iv) Develop conventional MSPC on-line monitoring systems for process fault detection (conventional PCA based T<sup>2</sup>-control chart) and diagnosis (conventional PCA score contribution chart).
- v) Develop modified MSPC on-line monitoring systems for process fault detection and diagnosis (PFDD).
- vi) Develop new approaches:
  - a) Outline Analysis Approach
  - b) Cross-variable Correlation,  $C_{ik}$  Approach
  - c) Signal Cumulating Approach
- vii) Formulate the fault detection by implementing new approaches such as:
  - a) PCA Model Profile Outline Analysis Control Chart,
  - b)  $C_{ik}$  Control Chart,
- viii) Improving the conventional contribution chart for fault diagnosis purpose.

  These contribution chart are:
  - a) T<sup>2</sup> Score Contribution Chart,
  - b) C<sub>ik</sub> Score Contribution Chart
  - c) T<sup>2</sup> Score Contribution Chart with Signal Cumulating,
  - d) C<sub>ik</sub> Score Contribution Chart with Signal Cumulating.
  - ix) All of these proposed methods and conventional methods are compared in terms of sensitivity and accuracy in:
    - a) Multiple fault identifiability,
    - b) Insignificant fault identifiability,

## 1.5 Research Contribution.

In this research, effort mainly concentrates on breaking through the current limitation and the further application of MSPC on a multivariable continuous chemical process. The main contributions of this research are:

- i) Application of MSPC tools on the fault detection and diagnosis for tubular reactor in a chemical plant.
- ii) An Eigenvalue-eigenvector PCA (EPCA) approach had been used for developing Principals Components model instead of the conventional NIPALS algorithm.
- iii) Modified Process Fault Detection and Diagnosis, PFDD mechanisms are also developed based on the Outline Analysis, Cross-variable Coefficient, and Signal Cumulating approaches.

## 1.6 Organization of The Thesis

This thesis contains six chapters: introduction, literature review, process modeling, research methodology, results analysis and discussion, and conclusion as well as recommendations. The first chapter of this thesis mainly presents about the introduction of the research projects, which consists of the research background, problem statement, research objectives and scopes.

Second chapter, covers the literatures review. This chapter presents the development of Process Fault Detection and Diagnosis and MSPC methods. While, Chapter III will then presented the outline of reactor modeling procedures and the way multiple cooled tubular reactor modeling has been adopted.

In the following chapter, the methodology for the research project will be proposed. The proposed methodologies are described and presented step by step.

Chapter V mainly focuses on results analysis and discussion. The suggested fault detection and diagnosis results are presented and compared to the results obtained by means of conventional approach.

Finally, this thesis wrap up with the conclusion and recommendations for future researches.

- Since the proposed MSPC method has shown promising performance over the conventional MSPC method, the incoming step is to develop a userfriendly computer interface, which enables the application of this new method.
- 2. Except the reaction process, the proposed MSPC approach can be applied to various kinds of unit operations in the chemical industries. Such as separation unit operation, mixing operations and so on. In addition, the future research can focuses on the application of MSPC for batch system and semi batch system.
- Other tools can be implemented to get the relationship between the correlated variables instead of PCA. The incoming researchers can try to implement other extension of PCA such as Dynamic PCA, Non-linear PCA, Multiblok-PCA or other techniques as well, such as Projection Latent Structures, PLS
- 4. As this research only focuses to the application of MSPC for single unit operation monitoring, the future research activities can study on the application of the proposed approach to plant-wide system. Such as the MSPC plant wide monitoring for a simulation plant, real plant or pilot plant.
- 5. On the other hand, MSPC can be applied in other engineering field, which deal with a large input and out put data. As an example, MSPC can formulate the statistical model, control limit and optimum condition for process safety monitoring, environmental control and process design.

## Reference

Akbaryan, F., & Bishnoi, P. R. (2000). "Smooth Representation of Trends by A Wavelet-based Technique." *Computer Chem. Eng.*, **24**,1913–1943.

Akbaryan, F., & Bishnoi, P. R. (2001). "Fault Diagnosis of Dynamic Multivariate Chemical Processes Using Pattern Recognition, and Smooth Representation of Trends by A Wavelet-based Technique." *Computer Chem. Eng.*, **25**,1313–1339.

Alt, F.B. (1985). "Multivariate Quality Control.": Encyclopedia of Statistical Sciences 6, New York., John Wiley& Sons.

Arsene. P (1998) "Fault Detection Methods for Process Control." University Politehnical Bucuresti: Unpublished PhD thesis.

Ashton S. A., Shields D. and Daley S, (1999) "Application of A Fault Detection Method for Pipelines." *Systems Science*, Vol. 23 (2), pp 97-109.

Baffi, G., Martin, E.B. and Morris, A.J., (1999), "Non-linear Projection to Latent Structures Revisited - The Neural Network PLS Algorithm", Computers and Chemical Engineering, 23, pp.1293-1307.

Bakshi, B.R, (1998). "Multiscale PCA with Application to Multivariate Statistical Process Monitoring." *AIChE Journal*, **44-7**. 1596-1610.

Chen K. H., Boning D. S., and Welsch R. E.(2001) "Multivariate Statistical Process Control and Signature Analysis Using Eigenfactor Detection Methods,"

The 33rd Symposium on the Interface of Computer Science and Statistics, Costa Mesa, CA.

Christie J. G. (1995). "Transport Process and Unit Operations", Third Edition, USA, Prentice Hall.

Clark.R, F. P and Patton R, (1989), "Fault Diagnosis in Dynamic System." New York, Prentice Hall.

Dash, S and Venkat V, (2000). "Challenges in The Industrial Application of Fault Diagnostic Systems." Computer and Chemical Engineering 24 (2000). 785-791.

David, L.M. and David M. U. (1994) "Fault Diagnosis and Computer Integrated Manufacturing Systems." Engineering Management, Vol. Jan. 1-29.

David, A.W. (2001). "Multivariate Analysis of Spectral Measurements for the Characterization of Semiconductor Process." MIT, PhD. Thesis.

Dayal, B. S. and MacGregor, J. F. (1997) "Recursive Exponentially Weighted PCA and Its Application to Adaptive Control and Prediction." *J. Proc. Cont.*, **7(3)**, 169-179.

Dong, D., and McAvoy, T.J. (1996). "AIChE Journal A Institute of Chemical Engineering Journal, 42(8). 2199-2208.

Dutta,S and Gualy, R, (1999). "General Reactor Model Improves HPI Applications." *Archive* Vol 78(July).7.

Fisher H., (1980). "The Large-Sample Behavior of Transformation to Normality," Journal of American Statistical Association, 75. 855-861.

Fjalestad, K., Gravklev, J.A., Mjaavatten, A. and Salid, S. (1994). "A Total Quality Management System for Reduction of Industrial Discharge", *Computer and Chemical Engineering*, **18(1994)** .369-373.

Fogler, H.S (1992). "Elements of Chemical Reaction Engineering",2<sup>nd</sup> Edition, New York. Prentice Hall International Series.

Gavy, E.F., Warren, W.F., Susan, A. and Bob, M. (1995). "Process Control of Stepper Overlay Using Multivariate Techniques". *OCG Interface* '95.1-17

Goodlin B., Sawin H., D. Boning, and B. Wise. (2002) "Simultaneous Fault Detection and Identification for Plasma Etching Processes," 201st Meeting of the Electrochemical Society, International Symposium on Plasma Processing XIV, paper 413.

Ha, T.C (1999). "Feedback Control of Cooled Tubular Reactor for Multiple Reaction." Universiti Teknologi Malaysia: Undergraduate Thesis.

Hawkins, C and Wood, M. (2000). "The Application of MSPC to BASF's Continuous Manufacturing Process". *MDC Technology Technical Report*. (2000).

Himmelblau, D. M. (1978). "Fault Detection and Diagnosis in Chemical and Petrochemical Process". Amsterdam: Elsevier. Hofling, T(1996). 343-393.

Huang, H.W. (1996). "Adaptive and Predictive Modeling for Real-Time Statistical Process Control". Department of Electrical Engineering and Computer Sciences, University of California: Master of Science Thesis Report.

Huang Y. J., Reklaitis G. V., and Venkatasubramanian V. (2002) "A Model-Based Fault Accommodation System", *Ind Eng Chem Res*, **41**(16), 3806-3821.

Johan, A. W. (1998) "Contribution Plots in Statistical Process Monitoring", Department of Chemical Engineering, University of Amsterdam, Netherlands: PhD Thesis Proposal.

Johnson, R.A. and Wichern D.W., (1996) "Applied Multivariate Statistical Analysis". 3<sup>rd</sup> Edition, Prentice Hall International Inc, USA.

Kamarul Asri Ibrahim. (1996). "Active Statistical Process Control" Newcastle University, England. Unpublished PhD. Thesis

Kenson, R. E. and Lapkin, M. (1986) "Kinetics and Mechanism of Ethylene Oxidation. Reactions of Ethylene and Ethylene Oxide on a Silver Catalyst". *Canadian Journal of Chemical Engineering*, Vol. 62. 1493-1502.

Kourti, T and MacGregor, J.F (1995) "Analysis, Monitoring and Fault Diagnosis of Batch Processes Using Multiblock and Multiway PCA." *Journal Proc. Control*, Vol. 5. 277-281.

Kourti, T and MacGregor, J.F (1996) "MSPC Methods for Monitoring Process and Product P erformance." *Journal of Quality Technology*, Vol. 28. 409-428.

Kourti, T, Lee, J. and MacGregor, J.F(c) (1996) "Experiences with Industrial Applications of Projection Methods for MSPC." Computer and Chemical Engineering, 20(1996) .S745-S748.

Kroschwitz, Jacqueline I. And Howe-Grant, Mary (1994). "Kirk-Othmer Encyclopedia of Chemical Technology." New York, John Wiley & Sons. 915-951.

Ku, W., Storer, R.H, and Georgakis, C. (1995). "Disturbance Detection and Isolation by Dynamic PCA." *Computer and Chemical Engineering*, Vol.7 (1995) .2269-2279.

Kupka Karel. (1999). "Statistical Techniques for Real Data from Production and QC". TriloByte Statistical Software, Pardubice, Czech Republic.

Lam H.L. and Kamarul A.I, (2002) (a) "Improved Multivariate Statistical Process Control for Chemical Process Fault Detection and Diagnosis via Outline Analysis Approach" World Engineering Congress, 2002, Chemical and Process Engineering, 39-43.

Lam H.L. and Kamarul A.I, (2002) (b). "Improved Multivariate Statistical Process Control for Chemical Process Fault Detection and Diagnosis via Cross Variable Correlation Coefficient Approach" Regional Symposium on Chemical Engineering, RSCE/SOMChem 2002, Vol. 2, 1637-1644.

Lane S., Martin E. B., Koijimans R. and Morris A. J. (2001). "Performance Monitoring of a Multi-Product Semi-Batch Process." *Journal of Process Control*. **Vol 11**. 1-11.

Lennox, B., Hiden, H.G, Montague, G.A., Kornfeld, G., Goulding, P.R. (2000) "Application of Multivariate Statistical Process Control to Batch Operations." Computer and Chemical Engineering, Vol.24 (2000) .291-296.

Levy, G. and Piccinini, N. (1984) "Ethylene Oxide Reactor: Safety According to Operability Analysis." *Canadian Journal of Chemical Engineering*, **Vol. 62**. 547-558.

Lin, W. Qian, Y., Li, X. (2000) "Nonlinear Dynamic PCA for On-line Process Monitoring and Diagnosis." *Computers and Chemical Engineering*, Vol. 53. 1225-1235.

Louwerse, D. J. and Smilde, A. K. (2000) "Multivariate Statistical Process Control of Batch Processes Based on Three-way Models." *Computers and Chemical Engineering*, Vol. 24, 423-429.

Luca Z. (1996) "Validation and Verification of Continuous Operating Modes Using Multivariate Statistical Methods." *Computer and Chemical Engineering*, **Vol. 20** (1996). 683 – 688.

Manabu, K. N., Shinji H., Iori H., Hiromu O., Ramon S. and Bakshi B. (2000) (a). "Comparison of Statistical Process Monitoring Methods: Application to The Eastman Challenge Problem." *Computer and Chemical Engineering*, Vol. 24 (2000). 175-181.

Manabu K., Segawa T., Ohno H. (2000) (b). "Identification of Fault Situations by Using Historical Data Sets" Proceedings of International Symposium on Design, Operation and Control of Next Generation Chemical Plants (PSE Asia 2000). Kyoto, Japan. 345-350.

Manabu K., Hasebe S., Hashimoto and Ohno H. (2000) (c). "Fault Detection and Identification Based on Dissimilarity of Process Data." IFAC Symposium on Advance Control of Chemical Process (ADCHEM), Pisa, Italy. 231-236.

Manabu K, Hasebe S, Hashimoto I., and Ohno H., (2004). "Evolution of Multivariate Statistical Process Control: application of Independent Component Analysis and External Analysis." *Computer and Chemical Engineering* 28. 1157 – 1166.

Martin, E and Morris, A. (1996) "An Overview of Multivariate Statistical Process Control in Condition in Continuous and Batch Process Performance Monitoring." *Trans Inst MC*, **18**, 51-60

Martin E. B. and Morris, A. J. (1999), "Manufacturing Performance Enhancement Through Multivariate Statistical Process Control." *Annual Review In Control.* **23**. 35-44.

Mason, R.L, Tracy, N.D, and Young, J.C., (1995) "Decomposition of T<sup>2</sup> for Multivariate Control Chart Interpretation." *Journal of Quality Technology*, Vol. 27, 99-108.

McKetta, J.J. and Cunningham, W.A. (1983) "Encyclopedia of Chemical Processing and Design (Volume 20)." New York, Marcel Dekker, Inc. 282-303.

Milan Pauls and Ivan Dvorak. (1991) "Singular Value Decomposition in Attractor Reconstruction: Pitfalls and Precautions." Physica D 55 (1991) 221-234.

Montgometry, D.C (1996), "Introduction to Statistical Quality Control." John Willey & Sons, New York, USA.

Morris A. J. (2000). "Bioprocess Performance Monitoring – A Novel Perspective." World Pharmaceutical Development: Inviting Paper.

Nash, J.C. and Lefkovitch, L.P. (1976) "Principal Component and Regression by SVD on a Small Computer." Apply Statistics (1976) 25, No. 3, 210-216.

Neal B.G., Barry M.W., Stephanie W.B., Daniel D., White, Jr. and Gabriel G. B. (2000) "Development and Benchmarking of Multivariate Statistical Control Tools for A Semiconductor Etch Process: Improving Robustness Through Model Updating." Eigenvector Research, Inc., USA.

Nedumaran, G. and Pignatiello, J.J (1999) "On constructing T<sup>2</sup>-Control Charts for Online Process Monitoring." *IIE Transactions* **31**, 529-536.

Nomikos, P. and MacGregor, J. (1994) "Monitoring Batch Process Using Multiway Principal Component Analysis", *AIChemJ*, **40**, 1361-1375.

Qian, Y., Lin, W. Li, X. (2001) "Nonlinear Dynamic PCA for On-line Process Monitoring and Diagnosis." *Computers and Chemical Engineering*, Vol. 53. 1225-1235.

Qin, S.J, S. Valle (2001). "On Unifying Multi-block Analysis with Application to Decentralized Process Monitoring." *J. Chemometrics*. **2001**.

Qin Yu.(2001), "An Integrated Process Operation System Platform and Fault Diagnosis for The Lubricating Oil Dewaxing Process" South China University of Technology, Guangzhou: Master of Science Thesis Report.

Rengaswamy R. and Venkatasubramanian V. (1995)"A Syntactic Pattern Recognition Approach for Process Monitoring and Fault Diagnosis", *Eng Appl Artif Intel*, **8**(1), 35-51, 1995.

Robetson and Lee Jay H, (1998) "A Method for The Estimation of Infrequent Changes in Non-linear System". *Autimatical*, **34**, 261-270.

Rollins D.K., Cheng Y. and Chen V.C.P. (1996) "Detection of Equipment Faults in Automatically Controlled Process" *AIChem* **42**, 1642-1647.

Shields D. N. and Du S. (2000) "A Fault Detection Method for A Three-Tank System." System Science. 26 (2), pp 27-41

Shoichiro. N, (1996), "Numerical Analysis and Graphic Visualization with Matlab", Prentice Hall, USA.

Smith J.M., Van Ness, H.C., Abbott, M.M., (1996) "Introduction to Chemical Engineering Thermodynamics", McGraw-Hill, Singapore.

Stephanopoulos and Han.G (1996). "Intelligent System in Process Engineering: A Review." Computer and Chemical Engineering, Vol. 20(2000), 743-791.

Marlin T. E. (2000), "Process Control: Designing Process and Control System for Dynamic Performance", McGraw-Hill, USA.

Vedam H. and Venkat V., (1997) "Signed Digraph-based Multiple Fault Diagnosis", *Comput Chem Eng*, **21** ( in the Proceedings of ESCAPE-7), S655-S660.

Venkat V., Rengaswamy R., Yi K, Surya N. K. (2003), "A review of Process Fault Detection and diagnosis Part I: Quantitative Model-based Method". *Computers and Chemical Engineering* **27**. 293 – 311.

Verrill.S.and Johnson R.A,. (1988). "Tables and Large-Sample Distribution Theory for Censored-Data Correlation Statistics for Testing Normality." Journal of American Statistics Association, 83. 1192-1197.

Westerterp K.R. and Ptasinsky K.J. (1984) (a), "Safety Design of Cooled Tubular Reactions for Exothermic, Multiple Reaction; Parallel Reactions-I: Development of Criteria", *Chemical Engineering Science*, vol. 39, No. 2, 235-244.

Westerterp K.R. and Ptasinsky K.J. (1984) (b), "Safety Design of Cooled Tubular Reactions for Exothermic, Multiple Reaction; Parallel Reactions-II: The Design and Operation of An Ethylene Oxide Reactor", *Chemical Engineering Science*, vol. 39, No. 2. 245-252.

Wise, B. M., and Gallagher (1996), "The Process Chemometric Approach to Chemical Process Fault Detection and Supervision". *Journal of Process Control*, 6(6), pp. 329-348.

Wu J., Tan S., and Tso S. K. (2002) "Fault Detection and Diagnosis Techniques for Liquid-Propellant Rocket Engines" 53<sup>rd</sup> International Astronautical Congress, Taxas. IAC-02-S.108.

Wu J., Tan S., and Tso S. K. (2002) "Fault Detection and Diagnosis Techniques for Liquid-Propellant Rocket Engines Health Monitoring- A Survey" 52<sup>nd</sup> International Astronautical Congress, France. IAF-01-S.107.

Young, J.J. (1997). "Mathematical Model for Optimal Allocation of Statistical Process Control". Department of Mechanical Engineering, Boston University: Master of Science Thesis Report.

Yoon Seongkyu, J. F. MacGregor. (2000) "Statistical and Causal Model-based Approaches to Fault Detection and Isolation.". American Institute of Chemical Engineers, *AIChE Journal*, V 46, Issue 9, 1813 – 1824.

Zhang, Gongxu (1997), "Multivariate Diagnosis with Two Kinds of Quality", China Quality, **No. 2**, pp.36-39.

Zheng, L. L., McAvoy T. J., Huang, Y. and Chen, G. (2001), "Application of MSPC in Batch Process." *Ind. Eng. Chem. Res.*, **40**, 1641-1649.