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

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To my beloved parents, siblings and friends

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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.

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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.

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A: Process System

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

$k_{p.x}$ = Reaction rate, m^3/kg .

A = Ethylene.

B = Oxygen.

C = Ethylene Oxide.

D = Carbon Dioxide.

E = Water.

C_{Ai} = Input Concentration of Ethylene (mol/m^3)

C_{Bi} = Input Concentration of Oxigen (mol/m^3)

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)

C_A = Concentration of Ethylene (mol/m^3)

C_B = Concentration of Oxigen (mol/m^3)

C_C = Concentration of Ethylene Oxide (mol/m^3)

C_D = Concentration of Carbon Dioxide (mol/m^3)

C_E = Concentration of Water (mol/m^3)

T = Reactor Temperature (K)

F	= Reactants/ Products flowrate (m^3/s)
Tc	= Coolant Temperature (K)
Fc	= Coolant flowrate(m^3/s)
ρ	= Density, kg/m^3
V	= System Volume, m^3
t	= Time, s
F	= Volumetric flowrate, m^3/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
ρ_{mix}	= Density for mixture, kg/m^3
ρ_b	= Catalyst's density , kg/m^3
U_h	= Overall heat transfer coefficient, W/m^2K
D	= Reactor diameter, m
γ_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^3)

$C_{Ethylene\ Oxide}$ = Output Concentration of Ethylene Oxide (mol/m^3)

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)
$\mathbf{P}$	= principals component loadings,
$\mathbf{T}$	= principals component scores.
P	= number of variable
m	= NOC data size
n	= New observe sample size
$\mathbf{Z}$	= Standardized matrix,
$\boldsymbol{X}$	= Input data matrix,
$\overline{X}_i$	= Sample mean scalar for each particular variable,
S_i^2	= Standard Derivation scalar for each particular variable.
α	= Level of significance,
F	= F-distribution.
v_j	= Eigenvector for j^{th} variable,
λ_j	= Eigenvalue for j^{th} variable.
C	= Contribution Score

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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^2-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^2 Score Contribution Chart,
   b) C_{ik} Score Contribution Chart
   c) T^2 Score Contribution Chart with Signal Cumulating,
   d) C_{ik} 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.

1. Since the proposed MSPC method has shown promising performance over the conventional MSPC method, the incoming step is to develop a user-friendly 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.

3. 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.

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