FAULT DETECTION AND DIAGNOSIS USING CORRELATION COEFFICIENTS

MAK WENG YEE

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Faculty of Chemical and Natural Resources Engineering Universiti Teknologi Malaysia

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To my beloved parents, brother and sister.

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ABSTRACT

Accurate process fault detection and diagnosis (FDD) at an early stage of a chemical process is very important to modern chemical plant in overcoming challenges such as strict requirements on product quality, low consumption of utility, environmentally friendly and safe operation. The use of the Contribution Plots (CP) for fault diagnosis in previous methods in Multivariate Statistical Process Control (MSPC) is not suitable since it is ambiguous due to no confidence limit in the CP. This research is to formulate a FDD algorithm based on MSPC via correlation coefficients. A fractionation column from a palm oil fractionation plant is chosen as the case study and the model of the case study is simulated in Matlab. Data collected with a process sampling time, T_{MSPC} , of 4.6 hours and following the normal distribution are used as Nominal Operation Condition (NOC) data. Normal Correlation (NC), Principal Component Analysis (PCA) and Partial Correlation Analysis (PCorrA) are used to develop the correlation coefficients between the selected key process variables with the quality variables of interest in the process from the NOC data. Faults considered in the research are sensor faults, valve faults and controller faults generated in the fault data (OC). Shewhart Control Chart and Range Control Chart together with the developed correlation coefficients are used for fault detection and diagnosis. Results show that the method based on PCorrA (overall FDD efficiency = 100%) is more superior than the method based on NC (overall FDD efficiency = 67.82%) and the two analysis methods based on PCA (overall FDD efficiency = 67.82%).

ABSTRAK

Pengesanan dan diagnosis kecacatan proses (FDD) yang tepat untuk suatu proses adalah penting bagi mengatasi cabaran-cabaran seperti kawalan kualiti produk yang ketat, pengunaan utiliti yang rendah, kesan kepada alam sekitar yang minima dan operasi yang mempunyai aspek keselamatan yang tinggi. Pengunaan Carta Sumbangan (CP) bagi mendiagnosis punca kecacatan dalam kaedah yang lepas dengan Kawalan Proses Multipembolehubah Statistik (MSPC) adalah tidak sesuai. Ini kerana ketiadaan batas kawalan dalam CP yang menyebabkan keputusan diagnosis yang tidak menyakinkan. Kajian ini ialah untuk membangunkan algoritma FDD berdasarkan MSPC melalui pekali korelasi. Sebuah menara penyulingan daripada loji penyulingan kelapa sawit dipilih sebagai kes kajian dan model kes kajian ini disimulasi di dalam Matlab. Data dikumpul dengan masa penyampelan, T_{MSPC} , bersamaan 4.6 jam dan data yang mempunyai taburan normal yang dikenali sebagai data "Nominal Operation Condition" (NOC). Korelasi Normal (NC), Analisa Komponen Prinsipal (PCA) dan Analisa Korelasi Separa (PCorrA) diguna untuk menerbitkan pekali-pekali korelasi di antara pembolehubah proses yang terpilih dengan pembolehubah kualiti yang dikaji daripada data NOC. Kecacatan proses yang dikaji dalam kajian ini ialah kecacatan injap, kecacatan pengesan dan kecacatan pengawal yang dijanakan dalam data kecacatan (OC). Carta Kawalan Shewhart dan Carta Kawalan Julat digunakan bersama dengan pekali-pekali korelasi yang telah diterbitkan untuk pengesanan dan diagnosis kecacatan proses. Keputusan menunjukkan kaedah berdasarkan PCorrA (pekali keseluruhan FDD = 100%) adalah lebih baik prestasi persembahannya berbanding kaedah NC (pekali keseluruhan FDD = 67.82%) dan kedua – dua kaedah analisis PCA (pekali keseluruhan FDD = 67.82%).

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LIST OF SYMBOLS

A_B	Bottom column area
$A_i B_i C_i$	Antoine constants for component- <i>i</i>
A^{*},B^{*},C^{*},D^{*}	Constants for liquid heat capacity
A_P	Pumparound drum area
A_R	Reflux drum area
A_t	Tray active area
a_{ij}	Wilson constant
a	Number of factors in the PLS regression
В	Bottom flow rate
B_{ii}	Virial coefficient for component- <i>i</i>
B_{ij}	Virial coefficient for component- <i>i</i> and
	component-j
b_i	<i>i</i> -th regression coefficient
C_{ik}	Correlation coefficient
D	Distillate flow rate
Ε	Residual matrix of X
F	Residual matrix of Y
h	Matrix and vector index
h_b	Enthalpy for bottom stream
H_N	Vapor enthalpy for stage-N
h_N	Liquid enthalpy for stage-N
h_{ow}	Over weir height
K_i	Vapor-liquid distribution ratio for component- <i>i</i>
L	Liquid stream flow rate from reflux drum
L_{f}	Liquid feed flow rate

$L_{H,B}$	Bottom column liquid level
$L_{H, N}$	Liquid level at stage-N
$L_{H,P}$	Pumparound drum liquid level
$L_{H,R}$	Reflux drum liquid level
L_N	Liquid flow rate leaving stage-N
M	Number of components
M_B	Bottom column molar holdup
M_P	Pumparound drum molar holdup
M_R	Reflux drum molar holdup
N	Number of stages
Р	Pumparound flow rate
P_{tot}	Total pressure of the system
P_i^{sat}	Vapor pressure of component- <i>i</i>
p_i	Loading vectors of the <i>i</i> -th PLS factor
Q_R	Reboiler duty
q_i	Loading vectors of the <i>i</i> -th PLS factor
R	Universal gas constant
Re	Reflux flow rate
<i>r</i> _i	<i>i</i> -th prediction error
r _{ij}	Correlation between variable <i>i</i> and <i>j</i>
S	Sidedraw flow rate
Т	Temperature
T_b	Normal boiling point
T_{ci}	Critical temperature for component-i
T _{cij}	Critical temperature for component- <i>i</i> and
	component-j
Т	Transpose vector
t_i	Latent score vectors of the <i>i</i> -th PLS factor
u_i	Latent score vectors of the <i>i</i> -th PLS factor
V_N	Vapor flow rate leaving stage- N
V _{ci}	Critical volume for component-i
V_{cij}	Critical volume for component-i and
	component-j

V_i	Liquid molar volume of component- <i>i</i>
-------	--

- W_L Weir length
- w Weight used in PLS regression
- X Cause data matrix
- x_i *i*-th input variable
- $x_{f,i}$ Liquid feed mole fraction for component-*i*
- x_i Liquid phase mole fraction for component-*i*
- $x_{D,i}$ Distillate mole fraction for component-*i*
- $x_{P,i}$ Pumparound mole fraction for component-*i*
- $x_{R,i}$ Reflux mole fraction for component-*i*
- $x_{S,i}$ Sidedraw mole fraction for component-*i*
- Y Effect data matrix
- y_i *i*-th output variable
- y_i Vapor phase mole fraction for component-*i*
- Z_{ci} Critical compressibility factor for component-*i*
- Z_{cij} Critical compressibility factor for component-*i* and component-*j*
- χ^2 Chi square
- ρ Liquid density
- ω_i Accentric factor for component-*i*
- ω_i Accentric factor for component-*i* and component-*j*
- Λ_{ij} Wilson binary interaction parameters for component-*i* and *j*
- γ_i Liquid phase activity coefficient for component-*i*
- ϕ_k Vapor fugacity coefficient for component-*i*
- ΔH_{vap} Heat of vaporization
- $\Delta H_{vap, n}$ Heat of vaporization at normal boiling point

LIST OF ABBREVIATIONS

Abbreviation	Meaning
CSTR	Continuous Stirred Tank Reactor
DPLS	Dynamic Partial Least Squares
DPCA	Dynamic Principal Component Analysis
ERD	Empirical Reference Distribution
ICA	Independent Component Analysis
MSPC	Multivariate Statistical Process Control
ms-PCA	Multi-scale Principal Component Analysis
NC	Normal Correlation
PLS	Partial Least Squares
PCorrA	Partial Correlation Analysis
PCA	Principal Component Analysis
PCR	Principal Component Regression
QTA	Qualitative Trend Analysis
RLS	Recursive Least Squares
RPLS	Recursive Partial Least Squares
SPC	Statistical Process Control
SPE	Square Prediction Error
MESH	Mass, Equilibrium, Summation and Heat

MSPC	Multivariate Statistical Process Control
MW	Molecular Weight

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CHAPTER I

INTRODUCTION

1.1 Introduction

Chemical industries are facing a lot of challenges. The industries have to keep sustainable production and within the quality specifications for the products. The whole production process has to operate at the minimum production of waste, minimum consumption of utilities, minimum cost of re-work and re-processing. If the chemical industries are able to do so, the industries can achieve a better competitive position in the world market and gain great revenue. In order to achieve these targets, modern chemical plants need to operate as fault free as possible because faults that present in a chemical process increase the operating cost due to the increase in waste generation and product having undesired specifications. Therefore, an efficient fault detection and diagnosis method need to be developed to detect faults that are present in a process and pinpoint the cause of the detected faults. Multivariate Statistical Process Control (MSPC) is a fault detection and diagnosis method which has gained wide applications in the chemical industries (Kourti *et al.*, 1996).

This research is aimed to formulate a fault detection and diagnosis algorithm based on MSPC. The functions of this algorithm are to ensure safe operation, better understanding of the process behavior and to prevent continuously producing offspecification products. The developed algorithm can be applied to any unit operation in the chemical industry. A distillation column is chosen as the case study.

1.2 Research Background

Multivariate Statistical Process Control (MSPC) is an extension of univariate Statistical Process Control (SPC). This extension enables MSPC to become applicable in chemical industries which are multivariable in nature. MSPC monitoring method consists of collecting nominal operation condition process data, building process models by using multivariate projection methods and comparing the incoming process measurements against the developed process models.

The present MSPC method has several weaknesses in detecting and diagnosing faults. According to Yoon and MacGregor (2000), MSPC is a very powerful tool for fault detection but its main limitation lies in the ability to isolate or diagnose the actual causes of the detected fault. Although contribution plots are use to diagnose the faults, they tend to be noisy and ambiguous. The contribution plots also do not have confidence limit, making it difficult to determine whether a situation is normal or abnormal.

From the previous paragraph, the major weakness of MSPC lies in its ability to diagnose the actual causes of the detected faults. Therefore, this research is trying to solve this problem by introducing new elements into the fault detection and diagnosis method in MSPC. The new elements are:

- a) A new fault detection procedure based on correlation coefficient between the quality variables of interest and the selected key process variables.
- b) Fault diagnosis using statistical control charts with control limits showing clearly the status of a situation.
- c) Formulation of the correlation coefficient based on Normal Correlation (NC), Partial Correlation Analysis (PCorrA) and Principal Component Analysis (PCA).

1.3 Objectives of the Research

- To formulate a new fault detection and diagnosis algorithm based on the correlation coefficient between quality variables of interest and the selected key process variables.
- 2) To study the efficiency of the developed fault detection and diagnosis algorithm in detecting faults and diagnosis the causes of the detected faults.

1.4 Scopes of Research

Scopes of the research consist of:

- A distillation column from plant simulated data (**Appendix B**) is used as the case study. The dynamic models for the column are developed. The distillation column models will be used to describe the column behavior.
- A dynamic simulation algorithm is formulated based on the developed distillation column dynamics models. Later, the dynamic simulation algorithm is developed using Matlab software.
- The performance of the developed dynamic simulation program is assessed. The Matlab simulation results are compared to the simulation results from the plant simulated data (**Appendix B**).
- Controllers tuned and installed for stable operation of the column program.
- Selection of quality variables of interest and key process variables
 - Linoleic Acid composition (*x*₈) and Oleic Acid composition (*x*₉) in the bottom stream are chosen as the quality variables of interest.

• Key process variables selected are process variables that are highly correlated with the two selected quality variables of interest. Process variables that have a Normal Correlation (NC) of 0.1 or more with the two quality variables of interest are selected as key process variables. The selected key process variables are feed flow rate (L_f) , feed temperature (T_f) , reflux flow rate (Re), pumparound flow rate (P), reboiler duty (Q_r) and bottom temperature (T_{bot}) .

Determination of Process Sampling Time, T_{MSPC}

- An autocorrelation test based on Wetherill and Brown (1991) was used to determine the suitable **Process Sampling Time**, T_{MSPC} of the process. The T_{MSPC} is determined at a value of 4.6 hours. In this research, T_{MSPC} refers to the time used to sample a data from the process into the data set used for calculation of correlation coefficients.
- Generation of Data
 - Data (values of the selected key process variables and quality variables of interest) are sampled from the process using the determined T_{MSPC} . The collected data are mean-centered and variance-scaled. This data are checked of its average, standard deviation, kurtosis and skewness to establish its normal distribution properties. Once the data follow the normal distribution, it is further checked to determine whether it is the desired Nominal Operation Condition Data (NOC).
 - Nominal Operation Condition (NOC) data are a set of data in which, the selected quality variables and key process variables have values within the statistical control limits of their statistical control charts. The statistical control charts used in this research are Shewhart Control Chart and Range Control Chart. For NOC, the statistical control limits are $\pm 3\sigma$ for the quality variables and $\pm 3\sigma/C_{ik}$ for selected key process variables (C_{ik} is the correlation coefficients between the selected key process variables with the quality variables of interest).

- Fault Data (OC) are a set of data in which, the selected quality variables and key process variables have values outside the statistical control limits of their statistical control charts in certain times. Fault Data are also sampled from the process using the determined T_{MSPC} .
- Formulating fault detection and diagnosis (FDD) algorithm based on Normal Correlation (NC), Principal Component Analysis (PCA) and Partial Correlation Analysis (PCorrA). The procedures in formulating the algorithm are shown as follow:
 - a) Develop the correlation coefficients using NC, PCA and PCorrA.
 - b) Develop the fault detection tools.
 - c) Develop the fault diagnosis tools.
- The developed FDD algorithm is used with Shewhart Control Charts (SCC) and Range Control Charts (RCC) for fault detection and diagnosis on the generated set of Fault Data.
- The performance of the FDD algorithm is evaluated. The results for fault detection and diagnosis are discussed in depth.

1.5 Contributions of the Research

The contributions of this research can be summarized as follows:

- The introduction of the correlation coefficient between quality variables of interest and the selected key process variables in formulating the FDD algorithm.
- The derivation of the correlation coefficient based on Normal Correlation (NC), Principal Component Analysis (PCA) and Partial Correlation Analysis (PCorrA).

3) The application of Partial Correlation Analysis (PCorrA) as an important analysis tool in MSPC.

1.6 Layout of thesis

This thesis contains six chapters: introduction, literature review, distillation column modeling and simulation, methodology, results and discussion and conclusions and recommendations. The first chapter comprises of the introduction of the research, objectives of the research, research background and research's scopes and contributions.

Chapter II elaborates the literature review concept of Multivariate Statistical Process Control (MSPC), Principal Component Analysis (PCA), Partial Correlation Analysis (PCorrA) and the development of MSPC.

Chapter III presents the dynamic modeling of a distillation column as the case study, formulation and establishment of the dynamic simulation program, the tuning of controllers in the column and the evaluation of the performance of the developed simulation program.

Chapter IV mainly consists of the procedures in formulating the fault detection and diagnosis (FDD) algorithm based on NC, PCA and PCorrA. The introduction of the correlation coefficient between the quality variables of interest and the selected key process variables were also presented in this chapter.

Chapter V presents the results obtained from the developed FDD algorithm and the discussion of these results.

Chapter VI gives the conclusions that can be made from the results obtained and also recommendations for future work.

robustness of the statistical control charts and the number of false alarms that happens on the number of rules to be used when using Shewhart Control Chart.

Aside from Shewhart Control Chart and Range Control Chart, there are numerous other types of control charts that can be used with the proposed correlation coefficients in this research such as Exponentially-Weighted Moving Average Control Chart (EWMA), Cumulative-Sum Control Chart (CUSUM) and Moving Average Control Chart (MA) (Wachs and Lewin, 1999). By applying the developed correlation coefficients on these control charts, the results of the FDD of the fault data set will certainly be different.

In this research, three techniques of correlation analysis were used: NC, PCA and PCorrA. For future work, techniques such as Partial Least Squares (PLS) and Independent Component Analysis (ICA) can be used to develop the correlation coefficients between the variables of the data matrix. Chemical processes tend to change continuously and the correlation coefficients developed from history data may not truly represent the relationship between process variables. Therefore, online updating of the data matrix used to develop the correlation coefficients can take account into process dynamics and give better FDD qualities of the developed FDD method based on correlation coefficients.

Finally, the author hopes that this research work can be a platform for future studies on the field of fault detection and diagnosis using Multivariate Statistical Process Control (MSPC) via correlation coefficients.

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