ABSTRACT

The current method for composition measurement of an industrial distillation column specifically offline method, is slow, tedious and could lead to inaccurate results. Among the advantages of using online composition designed are to overcome the long time delay introduced by laboratory sampling and provide better estimation, which is suitable for online monitoring purposes. Principal component and partial least square analysis are used to determine the important variables surrounding the column prior to implementing the neural network. It is due to the different types of data available for the plant, which requires proper screening in determining the right input variables to the dynamic model. Statistical analysis is used as a model adequacy test for the composition prediction of n-butane and i-butane in the column. Simulation results showed that the Artificial Neural Network (ANN) can reliably predict the online composition of the column. The major contribution of the current research is the development of composition prediction of n-butane and i-butane using equation based neural network (NN) models. Based on statistical analysis, the results indicate that neural network equation, which is more robust in nature, predicts better than the PLS equation and RA equation based methods. The temperature predictions using neural network equation are also compared with partial least square (PLS) and regression analysis (RA) equations methods. A new technique for nonlinear system, which is based on hybrid neural network modeling, is proposed. The hybrid model consists of combination of residual composition and residual temperature with first principle in terms of mass and energy balance. Hybrid neural network equation performs better than the hybrid neural network, and neural network predictions to estimate composition and temperature for the column. The use of an inverse neural network and forward neural network are used for the direct control of a distillation column. The neural network used for the control strategy to track the set point of the top and bottom temperature. Neural network
estimators are used to track the set point of the top and bottom composition together with disturbances. There are two types of controller used for control strategies which are the direct inverse control (DIC) and internal model controller (IMC). Based on the results, IMC and DIC were found to perform better in controlling the temperature with respect to set point changes and disturbances compared to conventional PID controllers.
ABSTRAK

ACKNOWLEDGEMENTS

First of all, I would like to express my gratitude to Allah S.W.T for His Blessings and giving me strength to complete my PhD study for 5 years at University of Malaya. I would like to take this opportunity to thank University of Malaya for giving me an opportunity to complete my PhD here.

My sincere and heartfelt thanks to my supervisors, Prof Ir Dr Mohd Azlan Hussain and Dr Badrul Mohamed Jan in the Chemical Engineering Department, Faculty of Engineering for enlightening supervision and countless hours spent in sharing their insightful understanding, profound knowledge and valuable experiences throughout my PhD study.

A grateful thanks to all staff of PP(T)SB especially to Process Technology and Control Department (PTCD) staff members who are involved directly and indirectly in making my PhD study a valuable and beneficial experience for me.

Last but not least, I would also like to express a special thank to UTP for providing financial assistance to undergo my PhD study at University of Malaya.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>iii</td>
</tr>
<tr>
<td>Abstrak</td>
<td>v</td>
</tr>
<tr>
<td>Acknowledgement</td>
<td>vii</td>
</tr>
<tr>
<td>Table of Contents</td>
<td>viii</td>
</tr>
<tr>
<td>List of Figures</td>
<td>xiii</td>
</tr>
<tr>
<td>List of Tables</td>
<td>xxii</td>
</tr>
<tr>
<td>List of Symbols and Abbreviations</td>
<td>xxiv</td>
</tr>
<tr>
<td>List of Appendices</td>
<td>xxvi</td>
</tr>
</tbody>
</table>

## CHAPTER 1: INTRODUCTION

1.1 Problem statement and motivation                                     2
1.2 Objectives                                                           6
1.3 Scope of work                                                        7
1.4 Novelty                                                              8
1.5 Dissertation organization                                            8

## CHAPTER 2: LITERATURE REVIEW

2.1 Introduction                                                         10
2.2 Neural network introduction                                           10
2.3 Types of artificial neural network                                    11
    2.3.1 Feedforward network                                              12
    2.3.2 NARX network                                                    12
2.4 Learning paradigms learning task                                     12
CHAPTER 3: PLANT DESCRIPTION AND CASE STUDY OF THE
DEBUTANISER COLUMN

3.1 Introduction

3.2 Plant description

3.3 Data generation: open loop, closed loop, extract close loop

3.4 Steady state and dynamic state

3.5 Open loop response

3.5.1 Step test overhead pressure

3.5.2 Step test reflux flow rate

3.5.3 Step test reboiler flow rate
CHAPTER 4: NEURAL NETWORK PROCESS MODEL FOR COMPOSITION AND TEMPERATURE

4.1 Introduction.................................................................81
4.2 Methodology for modelling.............................................81
4.3 Model adequacy test for neural network to determine the hidden layer........83
4.4 Neural network prediction of n-butane composition (MIMO model)........85
   4.4.1 With partition into 3-------------------------------------87
   4.4.2 Validate based on close loop data for n-butane.............93
4.5 Model data generation..................................................101
   4.5.1 Neural network, Partial least square (PLS) and Regression Analysis (RA) data sets..............................................................101
   4.5.2 Neural network n-butane equation based model..............103
   4.5.3 PLS analysis............................................................105
   4.5.4 Regression analysis..................................................105
   4.5.5 Analysis of variance (ANOVA) n-butane.......................107
   4.5.6 Comparison NN, PLS and RA......................................109
   4.5.7 Residual analysis....................................................118
4.6 Neural network design................................................120
   4.6.1 Neural network top and bottom temperature (MIMO model).........121
4.7 Neural network, PLS and RA modeling temperature prediction...........127
4.7.1 Neural network equation based………………………………………127
4.7.2 PLS model………………………………………………………..128
4.7.3 Regression model………………………………………………..129
4.7.4 Analysis of variance (ANOVA) results for neural network model…..130
4.7.5 Comparison NN, PLS and RA…………………………………..131
4.7.6 Residual analysis………………………………………………..137

CHAPTER 5 : HYBRID NEURAL NETWORK TO ESTIMATE COMPOSITION AND TEMPERATURE FOR THE COLUMN…………………………140
5.1 Introduction…………………………………………………………140
5.2 Hybrid model construction…………………………………………141
5.3 Hybrid simulation of the distillation column……………………….142
5.4 Mathematical modelling of the distillation column…………………..143
5.5 Hybrid neural network (HNN) approach…………………………..148
5.6 Neural network hybrid modelling…………………………………149
5.7 Residual neural network n-butane…………………………………156
5.7.1 With partition into 3…………………………………………..158
5.8 Residual top and bottom temperature neural network……………161
5.8.1 With partition into 3……………………………………………163
5.9 Hybrid modelling of n-butane……………………………………167

CHAPTER 6 : ADVANCED PROCESS CONTROL…………………………175
6.1 Introduction…………………………………………………………175
6.2 Neural network based control strategies…………………………177
6.2.1 Direct Inverse Control (DIC) method…………………………178
6.2.2 Internal Model Control (IMC) method…………………………179
LIST OF FIGURES

Figure 2.1: General procedure to obtain the suitable neural network model............17
Figure 2.2: Notation used in PCA.........................19
Figure 2.3: A geometric illustration of a PCA model with two principal components \( t_1 \) and \( t_2 \).................................................................21
Figure 2.4: The X variables is defined as factors and Y variables are called responses.24
Figure 3.1: Flow chart for the refinery process.............................................49
Figure 3.2: Debutaniser column configuration.............................................50
Figure 3.2a: Simulation flow chart...............................................................52
Figure 3.2b: Flow chart to extract close loop to obtain open loop data...............56
Figure 3.3: top temperature........................................................................57
Figure 3.4: bottom temperature..................................................................57
Figure 3.5: receiver bottom temperature.....................................................57
Figure 3.6: light naphtha temperature.........................................................57
Figure 3.7: reboiler outlet temperature.........................................................58
Figure 3.8: feed temperature.......................................................................58
Figure 3.9: receiver overhead pressure.........................................................58
Figure 3.10: top temperature.................................................................59
Figure 3.11: bottom temperature............................................................59
Figure 3.12: receiver bottom temperature...................................................59
Figure 3.13: light naphtha temperature.......................................................59
Figure 3.14: reboiler outlet temperature......................................................59
Figure 3.15: feed temperature.................................................................59
Figure 3.16: receiver overhead pressure......................................................59
Figure 3.17: top temperature.................................................................60
Figure 4.13: Actual and simulated n-butane top composition line plot validation……..90
Figure 4.14: Actual and simulated n-butane bottom composition line plot validation...90
Figure 4.15: Actual and simulated n-butane top composition line plot testing……………90
Figure 4.16: Actual and simulated n-butane bottom composition line plot testing……..90
Figure 4.17: Manipulated variable reboiler and reflux flow rate………………………90
Figure 4.18: Actual and simulated n-butane top composition training…………………..94
Figure 4.19: Actual and simulated n-butane bottom composition training…………………94
Figure 4.20: Actual and simulated n-butane top composition validation………………….94
Figure 4.21: Actual and simulated n-butane bottom composition validation………………94
Figure 4.22: Actual and simulated n-butane top composition testing…………………….95
Figure 4.23: Actual and simulated n-butane bottom composition testing…………………95
Figure 4.24: Actual and simulated n-butane top composition line plot training………….95
Figure 4.25: Actual and simulated n-butane bottom composition line plot training………95
Figure 4.26: Actual and simulated n-butane top composition line plot validation………..96
Figure 4.27: Actual and simulated n-butane bottom composition line plot validation…96
Figure 4.28: Actual and simulated n-butane top composition line plot testing……………….96
Figure 4.29: Actual and simulated n-butane bottom composition line plot testing………96
Figure. 4.30: Prediction versus actual value neural network equation top
composition n-butane………………………………………………………………….110
Figure. 4.31: Prediction and actual value for top composition n-butane line plot……….111
Figure 4.32: Prediction versus actual value neural network equation bottom
composition n-butane………………………………………………………………….112
Figure. 4.33: Prediction and actual value for bottom composition n-butane line plot..112
Figure. 4.34: Prediction versus actual value PLS equation top composition n-butane.113
Figure. 4.35: Prediction and actual value for top composition n-butane line plot……….113
Figure. 4.36: Prediction versus actual value PLS equation bottom position n-butane..114
Figure 4.37: Prediction and actual value for bottom composition n-butane line plot. 115
Figure 4.38: Prediction versus actual value RA equation top composition n-butane. 115
Figure 4.39: Prediction and actual value for top composition n-butane line plot. 116
Figure 4.40: Prediction versus actual value RA equation bottom composition n-butane. 117
Figure 4.41: Prediction and actual value for bottom composition n-butane line plot. 117
Figure 4.42: Residual analysis for neural network equation, PLS equation and regression analysis equation top composition n-butane. 119
Figure 4.43: Residual analysis for neural network equation, PLS equation and regression analysis equation bottom composition n-butane. 119
Figure 4.44: Neural network architecture for top and bottom temperature. 121
Figure 4.45: Profile of the RMSE training. 122
Figure 4.46: Profile of the RMSE validation. 123
Figure 4.47: Profile of the RMSE testing. 123
Figure 4.48: Actual and simulated top temperature training. 123
Figure 4.49: Actual and simulated bottom temperature training. 123
Figure 4.50: Actual and simulated top temperature validation. 124
Figure 4.51: Actual and simulated bottom temperature validation. 124
Figure 4.52: Actual and simulated top temperature testing. 124
Figure 4.53: Actual and simulated bottom temperature testing. 124
Figure 4.54: Actual and simulated top composition line plot training. 124
Figure 4.55: Actual and simulated bottom composition line plot training. 124
Figure 4.56: Actual and simulated top temperature line plot validation. 125
Figure 4.57: Actual and simulated bottom temperature line plot validation. 125
Figure 4.58: Actual and simulated top temperature line plot testing. 125
Figure 4.59: Actual and simulated bottom temperature line plot testing. 125
Figure 4.60: Prediction versus actual value neural network equation top temperature………………………………………………………………………………………………131
Figure 4.61: Prediction and actual value for top temperature line plot………………132
Figure 4.62: Prediction versus actual value neural network equation bottom temperature………………………………………………………………………………………………132
Figure 4.63: Prediction and actual value for bottom temperature line plot………………133
Figure 4.64: Prediction versus actual value PLS equation top temperature……………133
Figure 4.65: Prediction and actual value for top temperature line plot………………134
Figure 4.66: Prediction versus actual value PLS equation bottom temperature………134
Figure 4.67: Prediction and actual value for bottom temperature line plot……………135
Figure 4.68: Prediction versus actual value RA equation top temperature……………135
Figure 4.69: Prediction and actual value for top temperature line plot………………136
Figure 4.70: Prediction versus actual value RA equation bottom temperature………136
Figure 4.71: Prediction and actual value for bottom temperature line plot……………137
Figure 4.72: Residual analysis for neural network equation, PLS equation and regression analysis equation top temperature………………………………………………138
Figure 4.73: Residual analysis for neural network equation, PLS equation and regression analysis equation bottom temperature………………………………………………138
Figure 5.1: Two approaches used in HNN with FPM……………………………………142
Figure 5.2: Hybrid model for the composition n-butane and temperature………………156
Figure 5.3: Neural network architecture for residual n-butane…………………………157
Figure 5.4: Profile of the RMSE of n-butane training……………………………………158
Figure 5.5: Profile of the RMSE of n-butane validation……………………………………158
Figure 5.6: Profile of the RMSE of n-butane testing……………………………………158
Figure 5.7: Actual and simulated n-butane top residual composition training………159
Figure 5.8: Actual and simulated n-butane bottom residual composition training……159
Figure 5.32: Actual and simulated bottom residual temperature line plot validation...............................................................166

Figure 5.33: Actual and simulated top residual temperature line plot testing........167

Figure 5.34: Actual and simulated bottom residual temperature line plot testing......167

Figure 5.35: Top composition n-butane first principle model.................................168

Figure 5.36: Bottom composition n-butane first principle model...........................168

Figure 5.37: Top temperature first principle model.................................................169

Figure 5.38: Bottom temperature first principle model...........................................169

Figure 5.39: Hybrid model, neural network and actual top composition n-butane.....170

Figure 5.40: Hybrid model, neural network and actual bottom composition n-butane170

Figure 5.41: Hybrid model, neural network and actual top temperature..................172

Figure 5.42: Hybrid model, neural network and actual bottom temperature.........172

Figure 6.1: Control loop of neural network based Direct Inverse Model Control (DIC)..............................................................................................................................177

Figure 6.2: Control loop of neural network based Internal Model Controller (IMC)...178

Figure 6.2a: Forward and inverse models to control temperature.........................183

Figure 6.3: Set point top temperature.................................................................186

Figure 6.4: Set point bottom temperature.........................................................186

Figure 6.5: Manipulated variable temperature neural network.............................187

Figure 6.6: Manipulated variable temperature PID..............................................187

Figure 6.7: Disturbances top temperature..........................................................189

Figure 6.8: Disturbances bottom temperature....................................................189

Figure 6.9: Manipulated variable temperature neural network disturbances........190

Figure 6.10: Manipulated variable temperature PID disturbances.......................190

Figure 6.11: Neural network estimator for the top composition............................191

Figure 6.12: Neural network estimator for the bottom composition......................192

Figure 6.13: Manipulated variable composition for PID.....................................192
Figure 6.14: Top composition disturbances…………………………………………193
Figure 6.15: Bottom composition disturbances……………………………………194
Figure 6.16: Manipulated variable composition PID due to disturbances………..194
Figure 6.17 Steady state error top temperature………………………………………194
Figure 6.17 Steady state error bottom temperature…………………………………195
LIST OF TABLES

Table 3.1: Debutaniser column specification ..................................................48
Table 3.2: Tag name description of the column ...............................................49
Table 3.3: Composition at the feed .................................................................53
Table 3.4: Properties of the compounds ..........................................................53
Table 3.5: Controller setting and set point .......................................................54
Table 3.6: Important variables involved in the PCA analysis .............................70
Table 3.7: Data pretreatment after PCA and PLS .............................................77
Table 3.8: Data pretreatment after PCA and PLS .............................................78
Table 3.9: Important variables for neural network prediction of n-butane ........79
Table 3.10: Important variables for neural network prediction of i-butane .........79
Table 4.1: Important variables for neural network prediction ............................85
Table 4.2: Neural network architecture ............................................................86
Table 4.3: Statistical analysis for n-butane composition prediction ......................92
Table 4.4: Statistical analysis for online n-butane composition prediction ..........97
Table 4.5: ANOVA of the n-butane top composition .......................................108
Table 4.6: ANOVA of n-butane bottom composition .......................................109
Table 4.7: Variables involved in the PLS analysis, regression analysis and neural
network n-butane ..............................................................................................110
Table 4.8: n-butane statistical analysis of NN equation, PLS equation and RA
equation .........................................................................................................118
Table 4.9: Important variables for neural network prediction ............................121
Table 4.10: Neural network architecture ...........................................................122
Table 4.11: Statistical analysis for temperature with 3 partition........................126
Table 4.12: ANOVA of the n-butane top temperature .......................................130
Table 4.13: ANOVA of n-butane bottom temperature ......................................130
Table 4.14: Variables involved in the PLS analysis, regression analysis and neural
Network

Table 4.15: Statistical analysis of NN equation, PLS equation and RA equation

Table 5.1: Important variables for neural network prediction

Table 5.2: Neural network architecture

Table 5.3: Important variables for neural network prediction

Table 5.4: Neural network architecture

Table 5.5: Statistical analysis for composition prediction n-butane

Table 5.6: Statistical analysis for temperature prediction

Table 5.7: Statistical analysis for robustness analysis variable Temp 6

Table 6.1: PID tuning

Table 6.2: Controller performance during set point changes

Table 6.3: Controller performance during disturbance changes

Table 6.4: Computing time
# LIST OF SYMBOLS AND ABBREVIATIONS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIC</td>
<td>Akaike information criterion</td>
</tr>
<tr>
<td>ANN</td>
<td>Artificial neural network</td>
</tr>
<tr>
<td>ANOVA</td>
<td>Analysis of variance</td>
</tr>
<tr>
<td>BIC</td>
<td>Bayesian information criteria</td>
</tr>
<tr>
<td>CDC</td>
<td>Correct Directional Change</td>
</tr>
<tr>
<td>IAE</td>
<td>Integral absolute error</td>
</tr>
<tr>
<td>ISE</td>
<td>Integral square of error</td>
</tr>
<tr>
<td>LM</td>
<td>Levenberg-Marquardt</td>
</tr>
<tr>
<td>MAPE</td>
<td>Mean Absolute Percentage Error</td>
</tr>
<tr>
<td>MS</td>
<td>Mean of square</td>
</tr>
<tr>
<td>NARX</td>
<td>Nonlinear autoregressive network with exogenous inputs</td>
</tr>
<tr>
<td>PCA</td>
<td>Principal component analysis</td>
</tr>
<tr>
<td>PLS</td>
<td>Partial least square</td>
</tr>
<tr>
<td>R²</td>
<td>Coefficient of determination</td>
</tr>
<tr>
<td>RMSE</td>
<td>Root Mean Square Error</td>
</tr>
<tr>
<td>SS</td>
<td>Sum of square</td>
</tr>
<tr>
<td>At</td>
<td>Actual value</td>
</tr>
<tr>
<td>Cp</td>
<td>Person correlation co-efficient</td>
</tr>
<tr>
<td>Di</td>
<td>Product $y_i \times \bar{y}_j$</td>
</tr>
<tr>
<td>$E_a$</td>
<td>Actual value</td>
</tr>
<tr>
<td>$E_p$</td>
<td>Predicted value</td>
</tr>
<tr>
<td>$\bar{E}_a$</td>
<td>Average actual value</td>
</tr>
<tr>
<td>$\bar{E}_p$</td>
<td>Average predicted value</td>
</tr>
<tr>
<td>$F_i$</td>
<td>Predicted value</td>
</tr>
<tr>
<td>K</td>
<td>Number of free model parameters</td>
</tr>
<tr>
<td>MSE</td>
<td>Mean square error</td>
</tr>
<tr>
<td>N</td>
<td>Number of observation</td>
</tr>
<tr>
<td>$R^2$</td>
<td>R squared</td>
</tr>
<tr>
<td>T</td>
<td>Number of parameters</td>
</tr>
<tr>
<td>df</td>
<td>Degree of freedom</td>
</tr>
<tr>
<td>F</td>
<td>Statistical F value</td>
</tr>
<tr>
<td>$x_{measured}$</td>
<td>Measure value</td>
</tr>
<tr>
<td>$x_{predicted}$</td>
<td>Predicted</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>---------------------------------------</td>
</tr>
<tr>
<td>$y_i$</td>
<td>Difference actual and average actual</td>
</tr>
<tr>
<td>$\bar{y}_i$</td>
<td>Difference predicted and average predicted</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>Variance</td>
</tr>
</tbody>
</table>
LIST OF APPENDICES

Appendix 1.1: Results for i-butane.................................................................213
Appendix 1.2: Neural network programming.............................................245