DEVELOPMENT OF MULTIPLE-INPUT MULTIPLE-OUTPUT (MIMO) AND MULTIPLE-INPUT SINGLE-OUTPUT (MISO) NEURAL NETWORK MODELS FOR CONTINUOUS DISTILLATION COLUMN

Comment [ZA1]: MODEL

by

ZALIZAWATI BINTI ABDULLAH

Thesis submitted in fulfillment of the requirements for the degree of Master of Science

NOVEMBER 2008

ACKNOWLEDGEMENTS

Alhamdulillah. All praises to almighty Allah who has made it possible for me to complete my thesis.

I would like to express my utmost gratitude to my supervisors, Dr. Norashid Aziz and Dr. Zainal Ahmad for their ideas, guidance and support. I would like also to thank the Ministry of Science, Technology and Innovation (MOSTI) for granting me the NSF scholarship that made it possible for the realization of this work.

My special acknowledgment goes to the Dean of the School of Chemical Engineering and to the Deputy Dean of Postgraduate Studies and Research & Development for their support towards my postgraduate affairs. Not forgetting all the staff and technicians of the School of Chemical Engineering for their invaluable help and concern during the completion of my research.

In addition, I would like to acknowledge everyone all people that have polished my mind. Special thanks to all my control colleagues especially to Ramesh, Zahrah, Siti Asyura and Asobri for their help and support. To all my friends, Kak Jia, Kak Min, Kak Airene, Aziah, Tijah, Jusliha, Kak Nida, Kak Un, Kak Shitah, Abir, Pakaq, Fadhil, Abang Syed, Huda, Kak Midah, Dilla, Nora and others: my deepest gratitude to all of you for your help, motivation, support and laughter that healed me during my hard times.

Last but not least, I would like to express my sincere appreciation to my beloved parents, Mr. Abdullah Abu Bakar and Mrs Juliah Malek, for their endless love and blessings. To my great brothers and sisters: thanks for all the love, support and care.

To those who directly and indirectly contributed to this research, your kindness will never be forgotten. Thank you.

TABLE OF CONTENTS

Comment [ZA2]: Recommendations

LIST OF TABLES

LIST OF FIGURES

LIST OF PLATES

LIST OF ABBREVIATIONS

ANN	Artificial neural network
ARX	Autoregressive with exogenous input
ASYM	asymptotic
CDU	Crude oil distillation unit
CPI	Chemical processing industry
DAE	Differential–algebraic equation
GNN	Group neural network
H-BEST	Hammerstein Block-oriented Exact Solution Technique
IMC	Internal model control
LM	Levenberg–Marquardt
MIMO	Multiple-input multiple-output
MISO	Multiple-input single-output
MLP	Multilayer Perceptron
MPC	Model predictive control
N/A	Not Available
NARMAX	Nonlinear autoregressive moving average with exogenous inputs
NARX	Nonlinear autoregressive models with exogenous inputs
NEQ	Nonequilibrium
NN	Neural network
NNFS	Neural network fuzzy system
ODE	Ordinary differential equations
ORB	Overall rate-based
PCA	Principle Component Analysis
PE	Processing elements
PID	Proportional–integral–derivative

Comment [ZA3]: New Added

PLS	Partial Least Squares
RBF	Radial Basis Function
RDNN	Recurrent dynamic neuron network
SOM	Self-Organizing Maps
SSE	Sum Squared Error
SVM	Support vector machine
TSK	Takagi-Sugeno-Kang
UNIFAC	Universal Functional Activity Coefficient
XOR	Exclusive or

LIST OF SYMBOLS		Unit
a	Parameters for pure component	-
a_{mn}	Net energy of interaction between groups m and n	-
B	Bottom product flowrate	kmol/sec
b	Parameters for pure component	-
b_k	Bias	-
D	Distillate flowrate	kmol/sec
$\bar{f}_i$	Fugacity of a species i in a mixture	-
F	Feed flowrate	kmol/sec
h_i	Entalphy of liquid on stage i	kJ/mol
H_i	Enthalpy of vapor on stage i	kJ/mol
L_i	Liquid flowrate on stage i	kmol/sec
$\bar{L}_i$	Past liquid flowrate value	kmol/sec
LT	Level transmitter	-
M_B	Liquid holdup in reboiler	kmol
M_i	Liquid holdup on stage I	kmol
N_F	Feed stage number	-
N_T	Total number of stages	-
P	Pressure	Pa
PT	Pressure transmitter	-
Q_B	Reboiler duty	kW
Qc	Condenser duty	kW
q_i	Surface area parameter of species i	-
$Q_{k/m/n}$	Surface parameters of group k/m/n	-
QR	Reboiler heat input	kW
R	Correlation coefficient	-

R	Reflux rate	kmol/sec
R	Gas constant	m^3.Pa/(mol.K)
$r_{i/j}$	Volume parameter of species i/j	-
T	Temperature	K
T10	Temperature tray 10	^oC
T14	Temperature tray 14	^oC
T2	Temperature tray 2	^oC
T4	Temperature tray 4	^oC
TB	Reboiler temperature	^oC
TC	Temperature controller	-
TD	Condenser temperature	^oC
TT	Temperature transmitter	-
u_{mn}	Interaction energy between groups m and n	-
V_i	Vapor boilup rate on stage i	kmol/sec
$\bar{V}_i$	Past vapor flowrate value	kmol/sec
V_{NT}	Vapor boilup rate on top stage	kmol/sec
w_i	Weight	-
xB	Bottom product composition	mol/mol
x_B	Bottom product composition	mol/mol
xD	Top product composition	mol/mol
x_D	Top product composition	mol/mol
x_F	Feed composition	mol/mol
x_i	Input	-
x_i	Liquid composition on stage i	mol/mol
$x_{i/j}$	Moles of pure liquid species i/j	mol/mol
$X_{m/n}$	Mole fraction of group m/n in mixture	mol/mol
y_i	Output	-

y_i	Vapor composition on stage i	mol/mol
y_{NT}	Vapor composition on top stage	mol/mol
Z	Compressibility factor	-
β	Hydraulic time constant	-
γ_i	Activity coefficient of species i	-
θ_i	Area fraction for species i	-
φ_i	Molar weighted segment for species i	-
$\upsilon_k^{(i)}$	Numbers of k groups present in species i	-
∇_θ	Parameter increment	-
$\Gamma_k^{(i)}$	Residual contribution to the activity coefficient of group k in a pure fluid of species i molecules	-

PEMBANGUNAN MODEL RANGKAIAN NEURAL BERBILANG-MASUKAN BERBILANG-KELUARAN (MIMO) DAN BERBILANG-MASUKAN SATU-KELUARAN (MISO) UNTUK TURUS PENYULINGAN BERTERUSAN

ABSTRAK

Turus penyulingan banyak digunakan dalam proses-proses kimia dan mewakili kira-kira 95 peratus sistem pemisahan dalam industri. Turus penyulingan merupakan sistem berbilang pembolehubah kompleks dan mempunyai kelakuan dinamik tak linear kerana hubungan keseimbangan wap-cecair tak linear, tatarajah proses yang kompleks dan ketulenan keluaran yang tinggi. Untuk mendapatkan kualiti keluaran yang lebih baik dan mengurangkan penggunaan tenaga oleh turus penyulingan, sistem kawalan berasaskan model tak linear yang berkesan diperlukan untuk membenarkan proses dijalankan di atas julat pengendalian yang besar. Kebolehsediaan model tak linear yang sesuai adalah penting dalam pembangunan kawalan berasaskan model. Dalam kajian ini, model tak linear untuk meramal komposisi keluaran atas dan bawah untuk loji pandu turus penyulingan metanol-air dibangunkan menggunakan teknik rangkaian neural.

Data masukan-keluaran untuk model rangkaian neural dijana daripada model am prinsip pertama yang disahkan. Berdasarkan analisis masukan-keluaran, haba masukan pengulang didih, aliran refluks dan suhu-suhu dulang dipilih sebagai masukan untuk model rangkaian neural. Tujuh profil haba masukan pengulang didih dan kadar aliran refluks yang berbeza-beza direkabentuk untuk menguja model prinsip pertama bagi menjana data masukan-keluaran. Set-set data ini dibahagikan kepada data latihan, pengesahan dan ujian.

Dua struktur model rangkaian neural telah dibangunkan iaitu model berbilang-masukan berbilang-keluaran (MIMO) dan sepasang model berbilang-masukan satu-keluaran (MISO) dengan masukan 16 dan 24 untuk setiap model. Kesan neuron tersembunyi dan data masukan sejarah lalu terhadap model juga dinilai. Didapati bahawa model MISO lebih hebat berbanding model MIMO. Di samping itu, didapati bahawa 16 masukan ke dalam model rangkaian neural mengatasi 24 masukan untuk kedua-dua model MISO dan MIMO. Diperhatikan bahawa struktur rangkaian yang optimum tidak semestinya terdiri daripada bilangan neuron yang terbanyak dan pemilihan yang berhati-hati terhadap data sejarah lalu diperlukan bagi menyediakan masukan yang sesuai ke dalam model rangkaian neural. Sepanjang kajian ini, prestasi model-model ditentukan berdasarkan nilai-R dan SSE. Model MISO-1 yang terdiri daripada 19 neuron dan 20 neuron dipilih sebagai model terbaik berdasarkan prestasinya dengan nilai-R yang lebih tinggi daripada 0.996 dan SSE yang lebih rendah daripada 6.86×10^{-4} semasa proses pengesahan dan ujian.

Pengesahan model yang dibangunkan dengan data sebenar adalah penting untuk memastikan kebolehan model tersebut untuk mewakili proses sebenar yang dipertimbangkan. Maka, kerja ujikaji telah dijalankan untuk memisahkan campuran methanol air di dalam loji pandu turus penyulingan berterusan. Keputusan menunjukkan bahawa model prinsip pertama dan model rangkaian neural yang dibangunkan berada dalam persetujuan yang baik dengan data ujikaji. Keputusan yang diperolehi dalam kajian ini membuktikan bahawa model rangkaian neural yang dibangunkan boleh digunakan bagi mewakili proses penyulingan.

DEVELOPMENT OF MULTIPLE-INPUT MULTIPLE-OUTPUT (MIMO) AND MULTIPLE-INPUT SINGLE-OUTPUT (MISO) NEURAL NETWORK MODEL FOR CONTINUOUS DISTILLATION COLUMN

ABSTRACT

Distillation columns are widely used in chemical processes and account for approximately 95 percent of the separation systems in industries. A distillation column is a complex multivariable system and exhibits nonlinear dynamic behavior due to the nonlinear vapor-liquid equilibrium relationships, the complexity processing configurations and high product purities. In order to gain better product quality and lower the energy consumption of the distillation column, an effective nonlinear model based control system is needed to allow the process to be operated over a larger operating range. The availability of a suitable nonlinear model is crucial in the development of a nonlinear model based control. In this study, a nonlinear model to predict the top and bottom product compositions of a methanol-water pilot plant distillation column was developed using the neural network technique.

The input-output data for the neural network model was generated from the validated general first principle model. Based on the input-output analyses, reboiler heat duty, reflux flowrate and tray temperatures were selected as the inputs for the neural network model. Seven different profiles were designated to excite the first principle model to generate the input-output data. These sets of data were then divided into training, validation and testing data.

Two neural network model structures were developed i.e. a multiple-input multiple-output (MIMO) model and a pair of multiple-input single-output (MISO)

Comment [ZA4]: run

Comment [ZA5]: crucial important

models with 16 and 24 inputs for each model respectively. The effect of hidden neurons and past historical input data on the model performance was also evaluated. It was found that the MISO model was superior to the MIMO model. In addition, it was found that the 16 inputs to the neural network model outperformed the 24 inputs for both the MISO and the MIMO models. It was also observed that the optimum network structure did not necessarily consist of the highest number of neurons and the careful selection of historical data was required in order to provide suitable input to the neural network model. Throughout the study, the performance of the models was determined based on their R-values and SSE. The MISO-1 model consisted of 19 neurons and 20 neurons was selected as the best model based on its performance with R-value which was higher than 0.996 and SSE which was lower than 6.86×10^{-4} during the validation and testing processes.

The validation of the developed model with real data was important in order to ensure the ability of the model to represent the real processes being considered. Therefore, experimental works was carried out to separate the methanol water mixture in a continuous pilot plant distillation column. The results showed that the first principle and the neural network models which were developed were in good agreement with the experimental data. The results obtained in this study proved that the neural network model which was developed could be used to represent the distillation process.

CHAPTER 1

INTRODUCTION

1.1 Research Background

Many chemical processes in industries are inherently nonlinear due to the nature of the process itself. In many situations, the dynamic behavior of the process system is known to be nonlinear due to the complex thermodynamic relations or reaction kinetics of the processes.

In distillation process, the nonlinear dynamics behavior occurs due to the nonlinear vapor liquid equilibrium relationships, the complexity of the processing configurations (e.g., prefractionators, sidestreams, and multiple feeds) and high product purities (Luyben, 1987).

Comment [ZA1]: In the vapor liquid separation process, also known as the distillation process

Research by the Industrial Info Resources in 2007 reported that distillation columns are key components for hundreds of chemical processing industry (CPI) plants. They are often found to be the nucleus of a petrochemical plant on which everything in the plant ultimately depends on for feed or output. The distillation column is often the most significant and most common separation technique used in the processing of chemical feedstock in petrochemical plants (Marketwire, 2007). It comprises 95 percent of the separation processes for the refining and chemical industries (Riggs, 2006). The increasing demand for highly integrated chemical plants, tight product quality specifications and tough environmental regulations require an effective control system of the distillation plant (Kumar and Daoutidis, 2002). It was also reported that an effective control of the distillation column is the best way to reduce the operating costs of existing units since the distillation process

Comment [ZA2]: (CPI) plants and are

Comment [ZA3]: (Marketwire, 2007); it consumes enormous amounts of energy both in terms of cooling and heating requirements. It also contributes to more than 50 percent of the plant operating costs (Tham, 2006).

In general, the distillation process presents crucial control problems such as delays and for multivariable systems, the interaction among the loops could become serious problem. Furthermore, the nonlinear dynamic behavior of the distillation process may cause problems in designing a control system. This is because optimal control performance cannot be achieved through the conventional PID control system. As an alternative, one can use a model based approach to control the system. A model of a system is a tool that needs to be used to answer questions about the system without having to perform experiments. Model based control strategies such as the internal model control (IMC) and the model predictive control (MPC) have shown to be better control systems when compared to the conventional method because of their ability to satisfy tight performance whenever required (Qin and Badgwell, 1998). In the absence of a reasonably accurate model, these processes are fairly difficult to control.

Comment [ZA4]: could serious become serious problem.

Comment [ZA5]: conventional control system

Comment [ZA6]: have been shown to be

Comment [ZA7]: satisfy strict performance which is required

Conventional process control systems utilize linear dynamic models. However, the linear model fails to provide satisfactory performance especially when the process is operated away from the nominal operating region. For highly nonlinear systems, control techniques which are directly based on nonlinear models are expected to provide significantly improved performance. For the modeling of the nonlinear process, three different model structures can be used: white box models, also called fundamental models which are derived based on mass, energy and momentum balances of the process; empirical models which are derived from the

Comment [ZA8]: cannot

input-output data of processes like neural networks, fuzzy models and block oriented models; and hybrid models which combine both the fundamental and the empirical model.

Applications which utilize the neural network based strategies are widely used in nonlinear chemical processes such as the polymerization process (Fernandes and Lona, 2005; Bomberger *et al*., 2001), the bioprocess (Eiken *et al*., 2001) and the fermentation process (Chen *et al*. 2004). As approximators, their capacity to learn from example offers a cost-effective method of developing useful process models.

The main aim of this research is to develop a nonlinear model by using a neural network technique which is able to represent the continuous distillation column. This is based on the distinct capability of the model to capture the complex dynamic and static interactions of the input-output pattern of the distillation column.

1.2 Problem Statement

Model based control has significant advantages over structured PID control loops and has become the most widely used multivariable control strategy in the chemical industry (Brosilow and Joseph, 2002; Abu-Ayyad and Dubay, 2007). Process modeling has become the most essential procedure for the implementation of a model based control algorithm. However, the difficulty in developing the process model is closely related to the system behavior which is not well understood and hard to be modeled precisely particularly for a complex nonlinear dynamic system such as the distillation column. At present, many industrial controllers use a linear process model such as first-order-plus-dead-time or pure-integrator-plus-dead-time models (Nikolaou and Misra, 2003). Since many processes are nonlinear, control

Comment [ZA9]: Model based control has significant advantages over structured PID control loops and has become the most widely used multivariable control strategy in the chemical industry.

systems which are based on these linear models perform poorly when the operating condition change. In order to deal with this phenomenon, good control of the distillation column requires a nonlinear model based controller.

The development of a suitable nonlinear model for the process is critical and has become one of the most time-consuming activities in the development of the nonlinear model based control. Although a lot of fundamental models have been developed, these models tend to involve many equations. In addition, the models obtained may be too complex to be used for nonlinear model based control design and may increase the computational burden of the controller. At present, a lot of data available in the industries has led to the growth of the data driven model or the empirical model.

Comment [ZA10]: the industries have led

The neural network technique is one of the most useful data driven models that can be utilized in developing a nonlinear model based control system. The neural network provides powerful analysis properties such as the complex processing of large input-output information arrays which represent complicated nonlinear associations among the data and the ability to generalize.

Previously, several nonlinear neural network models have been developed to represent distillation process for both the binary and multicomponent systems. However, the best neural network model has yet to be discovered due to several inadequacies such as lack of reliable data processing which cause the effectiveness of the model cannot be accurately obtained and the stability of the neural network in control scheme is still an open question. The flexibility of the neural network architecture opens the scope for further development of the neural network model for

Comment [ZA11]: yet to be undiscovered due

Comment [ZA12]: However, the best neural network model has yet to be discovered due to several inadequacies.

continuous distillation column. In addition, the selection of the input-output of the neural network, which has become one of the major successes in developing the neural network model, is still indecisive. Furthermore, only a few neural network models which are based on past and current input that have been found to be useful in light of the dynamic systems have been applied to the continuous distillation column. These issues have led to this research which focused on improving the development of neural network model for a continuous distillation column.

In this study, two different neural network structures were developed: the multiple-input multiple-output (MIMO) model and a set of multiple-input single-output (MISO) model to describe the nonlinear behavior of the distillation column. The sets of training, testing and validation data for the neural network were generated from the simulation of the validated first principle model. The first principle model was also used to analyze the relationship between the key variables in the distillation column in order to study the dynamics of the distillation process and to select the best input-output for the neural network model. Finally, validation with actual data from experiments was carried out in order to verify the capability of the neural network model in predicting the real process. In this study, the separation of water methanol binary system is chosen as the case study since it is inherently dynamic and nonlinear in nature (Ramasamy and Aziz, 2003).

1.3 Objectives of the Research

The objective of this research is to develop a nonlinear neural network model for distillation column. The specific objectives of this project are as follows:

1. To develop a general code of the first principle model that can be used for binary and multicomponent systems. This model will be used to study the relationship within the distillation process and to generate the data set for the development of the neural network model.

2. To study the relationships among the key variables in the distillation column in order to select the best input-output for the neural network model

3. To develop the MIMO and MISO neural network models for the distillation process and to optimize the architecture of the models based on the number of hidden neurons.

4. To compare the performance of the models which have been developed based on network structures and historical input data and to select the best neural network model to predict the top and bottom product composition.

5. To validate the neural network model with experimental results in order to observe the accuracy and effectiveness of the neural network model as compared to the pilot distillation plant.

Comment [ZA13]: To develop the general first principle model

1.4 Organization of Thesis

This thesis is divided into five chapters.

Chapter 1 describes the existence of nonlinear behaviors in chemical processes particularly in the distillation process. It also discusses the importance of model

Comment [ZA14]: a nonlinear behavior development in chemical processes. In addition, this chapter also outlines the problem statement and the objectives of the research.

Chapter 2 provides an overview of the distillation column, its behaviors and its sensitivity. It also gives details about the need of a nonlinear model in advanced control strategies. A review of several approaches which have been applied in the development of nonlinear models of distillation column is also given. This is followed by a discussion on the development of empirical model utilizing neural network approaches. Finally, the advantages of the neural network approach are highlighted.

Chapter 3 outlines the methodology of this work. This chapter is divided into two main sections: the first section explains the methodology used in the modeling of the first principle and the neural network models. The procedure to optimize the neural network model is also highlighted. The second section covers the experimental part of the work. It also explains the chemicals and equipment used in the experiment as well as the experimental procedures in this work.

Chapter 4 presents the results and discussions obtained from simulation and experimental work. It covers the simulation results obtained from the general first principle model for the behavior of the distillation column and the sensitivity analysis studies. The generation of simulation data for neural network model development is also presented. The chapter also discusses the results of the neural network model. The performance of the neural network models is evaluated based on the number of hidden neurons, the structures and the historical input data. The

Comment [ZA15]: of

extrapolation ability of the models is also demonstrated. Finally, the validation of the neural network model with the pilot plant data is discussed.

Chapter 5 contains the conclusions of the present work. Some recommendations for future research are also proposed in this chapter.

CHAPTER 2

LITERATURE REVIEW

2.1 Distillation Column

Distillation columns play a key role to separate an input stream of chemical species into two or more output streams of desired and useful chemical species. This process is widely used in the beverage industry, chemical processing, petrochemicals, and natural gas processing. It is usually the most economical method utilized for separating liquids and consists of a process of multi-stage equilibrium separations.

2.1.1 Operation

Distillation is used to separate miscible liquid mixtures. The basic concept of the distillation column is to separate a mixture of two or more liquids with different boiling points by heating the mixture to a temperature between their respective boiling points (Rousseau, 1987; Felder and Garrett, 2003; Goodwin *et al*., 2006). The basic principle is the preferential vaporization of low boiling point components away from high boiling point components when heat energy is applied to the mixture. The low boiling point component will boils and transforms into vapor while the high boiling point component will remain as a liquid. This phenomenon is usually quantified by the relative volatility of the components.

Comment [ZA16]: boil and transform

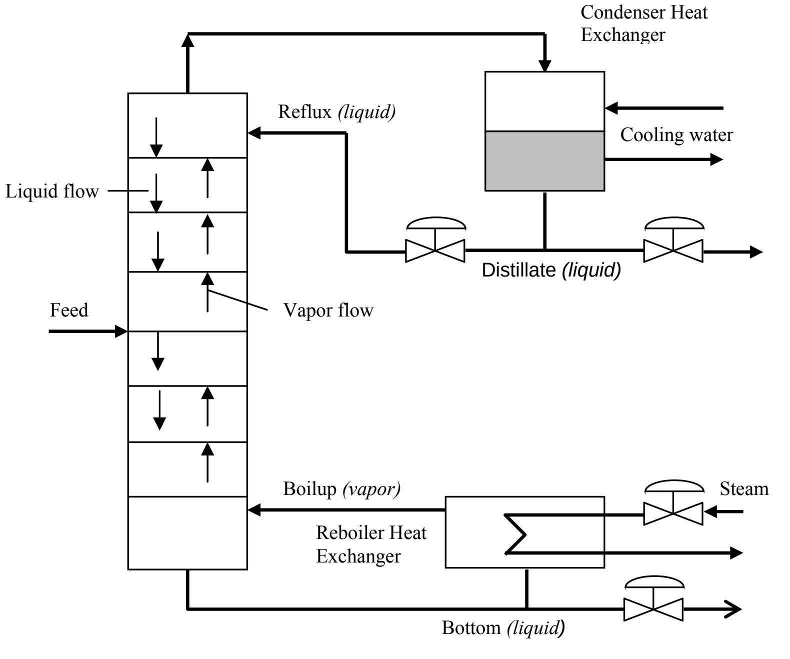

Figure 2.1: A schematic diagram of a distillation column

Figure 2.1 shows a schematic diagram of a distillation column. In the distillation column, the feed containing the mixture of components enters the column at one or more points. The liquid flows over the plates and vapor bubbles up through the liquid via holes in the plates. As the liquid travels down the column, vapor comes in contact with it. The liquid and vapor are kept in contact with each other for a sufficient period to ensure the chemical components are transferred between phases until equilibrium is reached. The liquid and vapor phases are brought into contact because as one molecule of high boiling point component converts from vapor to the liquid phase by energy release, another molecule of the low boiling point component utilizes the free energy to convert from the liquid to vapor phase. At equilibrium, all compositions of all phases stop changing i.e thermal, pressure and chemical potential are in equilibrium. As the system moves toward equilibrium, each species establishes a different concentration in each zone and the new liquid and vapor phases are separated.

The base of the distillation column contains a large volume of liquid which is mostly the liquid with the high boiling point component. Some of this liquid is heated in the reboiler and returned to the column and this is called the boilup. The remaining liquid is removed as a bottom product. The vapor follows its way to the top of the column and enters a reflux drum. In the drum, the vapor is cooled until it becomes a liquid. Part of the product is returned to the column as reflux and the remainder of the product leaves the column as distillate.

2.1.2 Nonlinear Dynamic Behavior

Many chemical processes in industries are inherently nonlinear. The nonlinear behavior of the process can be characterized as mildly nonlinear, strongly nonlinear or intermediate nonlinear (Pearson, 2003). The dynamics of the distillation column that is variations in time constants resulting from the size and direction of an input changes made are caused by a mixture of very fast vapor flowrate changes, moderately fast liquid flowrate changes, slow temperature changes and very slow composition changes (Luyben, 2002).

Comment [ZA17]: with the size and direction of an input change

According to Pearson (2003), the observation of one of the following phenomena in the distillation process shows the existence of the nonlinear dynamic behavior:

a) Asymmetric responses to symmetric input changes i.e. violation of the odd symmetry of linear systems (ASYM)

b) Generation of harmonics in response to a sinusoidal input i.e. change of shape without changing the periodicity (HARM)

c) Observation of input multiplicity (IM)

d) Observation of output multiplicity (OM)

e) Generation of subharmonics in response to any periodic input i.e. lengthening of the fundamental period (SUB)

f) Highly irregular responses to simple inputs i.e. impulses, steps, or sinusoids (CHAOS)

g) Input-dependent stability (IDS).

These phenomena are divided into three subsets:

a) Mildly nonlinear behavior which consists of ASYM, HARM and IM and corresponds to behavior that can be expected from almost any nonlinear dynamic model.

b) Strongly nonlinear behavior which consists of OM, SUB and CHAOS and it requires models exhibiting nonlinear feedback.

c) Intermediate nonlinearity which consists of IDS.

2.1.3 Sensitivity

The sensitivity of the process shows the influence of various variables on the system behavior in the distillation process. The variables are feed rate, vapor rate, heat input, pressure, temperature and reflux (Felder and Garrett, 2003). Descriptions on how these variables ~~impacted~~affected the distillation column behaviors are given below.

i. Feed rate

Comment [ZA18]: a)ASYM: asymmetric responses to symmetric input changes (i.e. violation of the odd symmetry of linear systems)
b)HARM: generation of harmonics in response to a sinusoidal input (i.e. change of shape without changing the periodicity)
c)IM: observation of input multiplicity
d)OM: observation of output multiplicity
e)SUB: generation of subharmonics in response to any periodic input (i.e. lengthening of the fundamental period)
f)CHAOS: highly irregular responses to simple inputs (i.e. impulses, steps, or sinusoids)
g)IDS: input-dependent stability.

Comment [ZA19]: i.Mildly nonlinear behavior will be defined as ASYM, HARM and IM and corresponds to behavior that can be expected from almost any nonlinear dynamic model.
ii.Strongly nonlinear behavior corresponds to OM, SUB and CHAOS and it requires models exhibiting nonlinear feedback.
iii.Intermediate nonlinearity corresponds to IDS.

Comment [N20]: Impacted or affected?

Comment [ZA21]: Following is an explanation of the term.

The feed is introduced to the column at the point that closely matches its concentration at the feed stage. If the feed composition changes and deviates from the feed stage concentration, the composition of the overhead and bottom products will be affected as the vapor liquid equilibrium established within the column are perturbed.

Comment [ZA22]: The feed is introduced to the column at the point that matches the concentration of the components being separated. If the feed composition changes and is no longer the same as the feed point liquid composition, the composition of the overhead and bottom products will be affected because the separation is less efficient.

On the other hand, changes in the feed rate causes the vapor and liquid rates within the column to change in order to maintain the material balance. A feed rate that is too high or too low can lead to inefficient vapor-liquid contact on the trays which affect the separation performance. The change in feed rates also has an effect on the column temperatures and pressures at different points due to the change in the component concentration.

Comment [ZA23]: The feed rate to the column should be constant. As the feed rate changes, the vapor and liquid rates within the column must change in order to maintain a material balance. A feed rate that is too high or too low can lead to inefficient liquid-vapor contact on the trays which may affect the effectiveness of the separation

ii. Vapor rate

In the distillation column, the vapor velocity must be sufficient in order to overcome the pressure drop across each tray which must not be too high leading to liquid entrainment to the next tray. At high feed rates, the reflux can be reduced to stabilized vapor velocity but more likely at the expense of the increased high boiling point component in the top product stream. If reflux is reduced too much, the separation of the high boiling component will become unsatisfactory.

Comment [ZA24]: create the desired pressure drop across each tray but not too high and entrain liquid to the next tray.

iii. Heat input

In a reboiler located at the base of the column, a portion of the liquid is converted to vapor, which serves as the major heat input into the column. The latent heat energy added in the reboiler creates the vapor flow moving upwards from tray to tray right to the top of the column. The amount of heat added to the reboiler determines the amount of the liquid vaporized which corresponds to the vapor flow rate rising up the column.

Comment [ZA25]: In a heated reboiler (at the base of the column), a portion of the liquid is converted to vapor, which is usually the major heat input into the column. The latent heat energy added in the reboiler creates the vapor flow from tray to tray up the length of the column. The amount of heat added to the reboiler determines the amount of the liquid vaporized and the vapor rate up the column

iv. Pressure

Pressure has two effects on the column operation:

a) An increase in pressure increases the boiling point of the liquids, therefore the overall operating temperature of the column is increased. A decrease in pressure lowers the boiling point, thus, giving an opposite effect to the overall operating temperature in the column.

Comment [ZA26]: of a column goes up as pressure is increased. A decrease in pressure lowers the boiling point, thus, the overall operating temperature drops

b) Pressure increases or decreases vapor density, which has an effect on vapor-liquid contact.

The columns are designed to operate at a fixed head pressure in order to maintain constant base and head temperature, which are the boiling point of the top and bottom streams. The column differential pressure (pressure drop) is also important as a measure of the vapor flow from the bottom to the top of the column. A higher or lower differential column pressure than the normal one may indicate possible column interior problems.

v. Temperature

The top temperature is the lowest temperature in the column and is the boiling point temperature of the vapor leaving the column and fed to the condenser. It is essentially the boiling point of the top stream column and defines the low boiling point component content of the top stream. The top temperature is used to monitor the composition of the top stream.

Comment [ZA27]: head

A profile of the temperature is measured across the column between the top and bottom. This temperature profile can also be used as indication on the separation performance within the various segments inside the column. The temperature profile could also be used to determine the concentrations of the components inside the column on each tray. An increase in temperature at constant pressure represents an increase in the high boiling point component concentration and a decrease in temperature at constant pressure represents an increase in the low boiling point concentration.

Comment [ZA28]: A profile of the temperature is measured along the column between the bottom and the top. This temperature profile is an indication of the low and high boiling point components separation performance up and down the column

Comment [ZA29]: The temperature profile across a distillation column represents the boiling points. It also determines the concentrations of the components up and down the column on each tray

Base temperature is measured at or very near to the bottom of the column. This is the highest temperature point in the column and reflects the high boiling point concentration in the bottom product stream. The base temperature is important as it changes with a change in the column pressure drop and the composition profile. A high base temperature could indicate excessive pressure drop inside the column and it could affect the thermal stability of the bottom product stream.

Comment [ZA30]: The base temperature is very important in the efficiency of the column separation as it changes with a change in the column pressure drop. A high base temperature raises a concern about excessive pressure drop because it is related to the thermal stability of the bottom product stream.

An increase in the heat added to the reboiler increases the vapor rate and increases the temperature on the trays. As the temperature of the tray liquid increases, the liquid contains more of the high boiling point component. On the other hand, if the amount of reflux is increased, the amount of liquid which enters the tray through the downcomer increases. Therefore, increasing the reflux rate lowers the temperature of the liquid on the tray. As the temperature of the tray liquid decreases, the liquid contains more of the low boiling point components.

vi. Reflux

The vapor velocity up the column can be stabilized at different feed rates by recycling a portion of the overhead condensate. The total feed to a column can also be stabilized by the reflux flowrate. Reflux serves a second purpose of increasing the low boiling component concentration overhead by sending the high boiling component back down the column.

Comment [ZA31]: This is essence, is a way to maintain a constant feed rate to the column

When the product from a distillation contains higher boiling point component than is desired, an increase in the flow of reflux can be used to wash this material out of the vapor in the top of the column. The top column temperature is a very good indication of high boiling point component content in the condensate.

Comment [N32]: Change has been made

Reflux is also the means of controlling the temperature profile in the column. Increasing the amount of reflux flow lowers the temperature in the column whereas decreasing the reflux flow raises the column temperatures. Changing the temperature by the reflux rate is the result of changing the concentration of high and low boiling point components.

2.1.4 Methanol-Water System: A Case Study

In this study, a distillation column for methanol-water separation is taken as a case study in this research since this system is a nonlinear dynamic process.

Ramasamy and Aziz (2003) studied a simple binary distillation column and verified that the nonlinear dynamic behavior is present even in a simple binary distillation column. They found that this process is mildly nonlinear based on the existence of several criteria as proposed by Pearson (2003). Ramesh *et al.* (2006) in their study proved that the methanol water system sufficiently represented the nonlinear dynamic system. From the simulation of methanol water separation, they obtained the asymmetric responses in top product for the symmetric input changes of manipulated variables. This is an indication of the violation of the add symmetry of the linear system. They also found the non-elliptical form of the response. The result obtained from the study is evidence of the existence of a dynamic nonlinear behavior in methanol-water system.

2.2 Control

Distillation columns have several inputs and outputs therefore, they present multivariable control problems. The effective control of distillation columns can improve product yield, reduce energy consumption, increase capacity, improve product quality and consistency, reduce product giveaway, increase responsiveness and improve process safety. Therefore, an effective control system for the column is required but their nonlinear behavior and ill-conditioned nature and factors such as hydraulic, separation, heat transfer, pressure and temperature constraints cause difficulties in the control design of the distillation column.

Model based control strategies can be used to overcome some of the limitations of traditional control systems. The performance of model-based controller is mostly determined by its model. If the model is accurate and if its inverse exists then process dynamics can be cancelled by the inverse model. As a result, the output of the process is always equal to the desired output. This means that the model based control design has the potential to provide perfect control (Willis and Tham, 2007). In a model-based controller, a model of the process is used in one of three ways:- (i) explicit model in control algorithm; (ii) adaptive change to control algorithm based

Comment [ZA33]: will always be

on the model; (iii) a combination of sensor data with models to provide improved estimates of the process performance used by the control algorithm (MACC, 2007).

2.3 Modeling

One of the major challenges in developing a model based control strategy is to construct a model that can be utilized to describe the process and this issue has been noted by several researchers (Qin and Badgewell, 1998; Pearson, 2003).

Comment [ZA34]: which is

At present, many industrial controllers use a linear process model such as the first-order-plus-dead-time model or the pure-integrator-plus-dead-time model. The linear model is applied to the estimation of the linearity and the dynamic range of the process. However, in general, the satisfactory performance of this linear model is achieved over a narrow operating range. This is because it is only able to approximate the system close to a given operating point but when a wide range of process operations with tight specifications on product composition is required, the nonlinearities become more critical and control performance is sacrificed (Mahfouf *et al*., 2002).

Since many of the processes are nonlinear, the process industries require operating systems which are closer to the boundary of the admissible operating region. In these cases, linear models are inherently incapable of describing an enormous range of important dynamic phenomena (Findeisen and Allgower, 2002; Pearson, 2003).

The difficulty in developing the nonlinear model arises from several sources and the following two are fundamental: the fact that model utility can be measured in general, in a conflicting way and the class of nonlinear models does not exhibit unity. There are four important measures of model utility (Pearson, 2003):

i. approximation accuracy
ii. physical interpretation
iii. suitability for control
iv. ease of development

2.4 Type of Model

Several models can be used for the distillation column and these models can be categorized into three major groups: fundamental models, empirical models and hybrid models.

2.4.1 Fundamental Model

Fundamental models are derived based on mass, energy and momentum balances of the process. Heat and mass transfer occurring in a real column distillation process is translated into a quantitative mathematical model. These knowledge-based models, which are also referred as the first principle models, tend to involve the order of 10^2–10^3 nonlinear differential equations and a comparable number of algebraic relations (Michelsen and Foss, 1996). Due to the very large number of equations needed for the rigorous description, calculations are made with the help of a personal computer by using an integration method. Examples of fundamental models are the differential algebraic model, the low order model or the reduced order model and the rate based model or the nonequilibrium model.

The fundamental model is the most accurate method to represent the nonlinear dynamic behavior of the distillation column. However, fundamental models are highly constrained with respect to their structures and parameters. The model parameters can be estimated from laboratory experiments and routine operating data. As long as the underlying assumptions remain valid, fundamental models can be expected to extrapolate at operating regions which are not represented in the data set used for the model development (Henson, 1998).

The main advantage is that a model obtained on the basis of fundamental principles would be globally valid and are usually more accurate and would give a more complete process understanding. However, the fundamental model is too complex for controller design and the process characteristics for fundamental model development are based on assumptions which may be wrong (Pearson, 1995). Such models are often not suitable for direct application in model based control strategies. Table 2.1 shows a summary of several fundamental models that have been developed for the continuous distillation column.

Table 2.1: Fundamental models applied in distillation column

No	Model	Distillation system	Reference
1	Dynamic model	Methanol/water	Can *et al.*, 2002
2	Differential algebraic equation model	Benzene /toluene	Bansal *et al.*, 2000
3	Differential algebraic first principle model	Methanol/n-propanol	Diehl *et al.*, 2003
4	Dynamic model	Methanol/water/ impurities	Olsen *et al.*, 1997
5	Low order modeling	N/A	Balasubramhanya and Doyle III, 1995
6	Reduced order model	Methanol/water	Yang and Lee, 1997
7	Reduced-order models	N/A	Kumar and Daotidis, 1999
8	Reduction model	N/A	Hahn and Edgar,

Comment [ZA35]: Benzane /toulene

			2002
9	Low order dynamic model	Methanol/ethanol/1-propanol	Kienle, 2000
10	Nonlinear wave model	Benzane/toulene	Bian and Henson, 2006
11	Overall rate based stage model	Acetone/methanol/2-propanol /water	Muller and Segura, 2000
12	Nonequilibrium model	Ethanol/ water/cyclohexane	Higler *et al*., 2004

As can be seen in Table 2.1, the dynamic model and the differential algebraic equation model can be classified as rigorous dynamic models. These models were developed using the equilibrium model which consisted of mass, component and energy balances for each tray, reboiler, condenser and reflux drum. The low order model, the reduced order model, the reduction model, the low order dynamic model and the nonlinear wave model can all be classified as reduced order models and they are the most preferable approach used to develop the fundamental model. Several techniques have been utilized to reduce the order of the rigorous model such as orthogonal collocation and cubic spline method, singular perturbation analysis, balancing of empirical gramians and nonlinear wave propagation. The rate-based or the non-equilibrium model is more complicated to develop as compared to the equilibrium model, thus, only a few researchers have developed this model to represent the continuous distillation column. A detailed discussion of this can be found in Abdullah *et al.* (2007).

Comment [ZA36]: Zalizawati *et al.* (2007).

2.4.2 Empirical Model

The empirical models, also known as black-box models can be obtained in the absence of a priori physical knowledge. The most valuable information comes from the input-output data collected during the operation (i.e. the measurements). These models describe the functional relationships between system inputs and system outputs. A detailed process understanding is not required, therefore, model complexity can be avoided and the computational burden on the controller can be alleviated. According to Eikens *et al*. (2001), the empirical model can accurately represent a nonlinear relationship in the domain reflected by the data even if unmeasured disturbances are present.

The results of the models depend not only on the accuracy of the measurements but also on the similarities between the situation to be analyzed and the situation where the measurements are carried out. Some examples of empirical models are the Hammerstein model, the Volterra model, the nonlinear autoregressive moving average with exogenous inputs (NARMAX) model, the artificial neural network model and the partial least squares (PLS) model. Several empirical models that have been developed for the continuous distillation column, excluding the neural network model, are summarized in Table 2.2.

Table 2.2: Empirical models applied in distillation column

No	Model	Distillation system	Reference
1	Wiener model	Not mentioned	Zhu, 1999
2	Weiner model	C2 splitter	Norquay *et al*., 1999
3	Wiener model	N/A	Bloemen *et al*., 2001
4	Simple Hammerstein model	Ammonia/water	Nugroho *et al*., 2004
5	Continuous time Hammerstein model	N/A	Bhandari and Rollins, 2004
6	Block-oriented model	methanol and ethanol	Gomez and Baeyens, 2004
21	NARMAX model	Gasoline/butane	Fortuna *et al*. 2005
22	Soft sensing model	N/A	Yan *et al*., 2004
23	TSK piece wise linear fuzzy model	N/A	Mahfouf *et al*., 2002
24	Polynomial type nonlinear autoregressive models with exogenous inputs (NARX)	Methanol/ ethanol	Sriniwas *et al*., 1995
25	PLS model	Alcohol/water/ether	Kano *et al*., 2000
26	PLS model	Methanol/ethanol/ propanol/n-butanol	Kano *et al*., 2003
27	PLS model	Methanol/ethanol/ propanol/n-butanol	Showchaiya *et al*., 2001
28	PLS model	C7	Park and Han, 2000

As can be seen in Table 2.2, it is found that several approaches have been used to develop the nonlinear model for the continuous distillation column. The Wiener and Hammerstein models, also known as block-oriented model, are built from the combination of linear dynamic and nonlinear static functions. In the early 2000s, several PLS models were developed to represent the continuous distillation column. These models were developed based on the partial least squares regression technique which generalized and combined features from principal component analysis and multiple regressions. The neural network approach, which is the most attractive and widely used method to develop the empirical model, will be discussed at the end of this chapter.

2.4.3 Hybrid Model

Hybrid models are developed by combining both the empirical model and the fundamental model. These models are summarized in Table 2.3. Knowledge of the process can go to the fundamental model while the input output models can be developed for those parts of the process which are hardly formulated.

A common method for developing the hybrid model is either to use empirical models in order to estimate the unknown function in the fundamental model or to use a fundamental model to capture the basic process characteristic and then use a nonlinear empirical model to describe the residual between the plant and the model (Henson, 1998).

Table 2.3: Hybrid models applied in distillation column

No	Model	Distillation system	Reference
1	Hybrid wave-nets	Water-ethanol	Safavi and Romagnoli,

	model		1997
2	Hybrid model	Water - ethanol	Safavi *et al*., 1999
3	Gray box model	Methanol/propanol	Pearson and Pottmann, 2000
4	Nonlinear Balanced model	N/A	Hahn *et al*., 2000
5	Reduced DAE model	Cyclohexane/heptane	Sun and Hahn, 2005

As shown in Table 2.3, it can be observed that only a handful of studies on the development of the hybrid model have been implemented in the continuous distillation column. The neural networks together with the fundamental model have become the most preferable approach used to develop the hybrid model.

2.5 Neural Network

2.5.1 Introduction to Neural Networks

Neural networks appeal to many researchers due to their closeness to the structure of the brain, a characteristic not shared by more traditional systems. The neural network system works like the biological neural system. In an analogy to the brain, an entity which is made up of interconnected neurons is similar to the neural networks which are made up of interconnected processing elements, called units, which respond in parallel to a set of input signals. The unit is the equivalent of its brain counterpart, the neuron (Stergiou and Siganos, 2006). This is shown in Figure 2.2.