MODELING AND SIMULATION OF DISTILLATION COLUMN

IVY WONG FUI ANN

BACHELOR OF CHEMICAL ENGINEERING
UNIVERSITI MALAYSIA PAHANG

Thesis Access Form

No_________________________Location__________________________________

Author : ………………………………

Title : ………………………………

Status of access OPEN / RESTRICTED / CONFIDENTIAL

Moratorium period:___________ years, ending_________/______200____

Conditions of access proved by: DR RAMESH KANTHASAMY

Supervisor (Signature)………………………………………………

Faculty: ………………………………

Author’s Declaration: *I agree the following conditions:*

OPEN access work shall be made available (in the University and externally) and reproduced as necessary at the discretion of the University Librarian or Head of Department. It may also be copied by the British Library in microfilm or other form for supply to requesting libraries or individuals, subject to an indication of intended use for non-publishing purposes in the following form, placed on the copy and on any covering document or label.

*The statement itself shall apply to **ALL** copies:*

This copy has been supplied on the understanding that it is copyright material and that no quotation from the thesis may be published without proper acknowledgement.

Restricted/confidential work: All access and any photocopying shall be strictly subject to written permission from the University Head of Department and any external sponsor, if any.

Author's signature…………………………………….Date: ………………………………

users declaration: for signature during any Moratorium period (Not Open work):
I undertake to uphold the above conditions:

Date	Name (CAPITALS)	Signature	Address

MODELING AND SIMULATION OF DISTILLATION COLUMN

IVY WONG FUI ANN

Thesis submitted in partial fulfilment of the requirements
for the award of the degree of
Bachelor of Chemical Engineering

Faculty of Chemical & Natural Resources Engineering
UNIVERSITI MALAYSIA PAHANG

JAN 2014

SUPERVISOR'S DECLARATION

We hereby declare that we have checked this thesis and in our opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Bachelor of Chemical Engineering.

Signature :
Name of main supervisor : DR. RAMESH KANTHASAMY
Position : SENIOR LECTURER
Date : JAN 2014

STUDENT'S DECLARATION

I hereby declare that the work in this thesis is my own except for quotations and summaries which have been duly acknowledged. The thesis has not been accepted for any degree and is not concurrently submitted for award of other degree.

Signature :
Name : IVY WONG FUI ANN
ID Number : KA10002
Date : JAN 2014

Dedication To

My dearest parent,
My beloved sibling,
My fellow lecturers,
My friends

For all your concern, support and faith in me.

ACKNOWLEDGEMENT

I would like to thanks the following people and organisations;

- My supervisors Dr. Ramesh Kanthasamy for their guidance through an effective well-arranged weekly meeting.
- Centre of Graduate Studies UMP for providing their full support and co-operation to make this study possible.

ABSTRAK

Kertas ini membentangkan pemodelan dan simulasi kajian kolum penyulingan. Kajian ini adalah untuk menjalankan simulasi kolum penyulingan “sieve tray” (rate-based model) dan khususnya untuk proses berbilang komponen dengan menggunakan Aspen Hysys . Kepentingan ekonomi pemisahan telah menjadi motivasi untuk penyelidikan dalam prosedur sintesis selama lebih daripada 30 tahun. Penyulingan mencakupi hampir 90% daripada sistem pemisahan yang digunakan dalam industri proses kimia. Cara terbaik untuk mengurangkan kos operasi unit yang sedia ada adalah untuk meningkatkan kecekapan dan operasi mereka melalui pengoptimuman proses dan kawalan. Simulasi menjana satu atau lebih trajektori (tingkah laku yang mungkin dari model peringkat tinggi), dan mengumpul statistik daripada trajektori ini untuk menganggarkan prestasi atau langkah-langkah yang dikehendaki. Pemodelan dan simulasi turus penyulingan sudah banyak dikaji tetapi pemodelan dan simulasi kolum berganda untuk berbilang komponen masih belum yang komersial diperkenalkan kepada industri. Dalam projek ini , jenis berbilang komponen yang terkenal (n- butane , n- pentane dan benzene) dipilih sebagai contoh untuk menjalankan simulasi ini dengan menggunakan kolum penyulingan berganda. Dengan memasukkan butir-butir dan spesifikasi di Aspen Hysys , proses penyulingan berbilang komponen dirangsang di bawah keadaan mantap . Berdasarkan keputusan yang diperolehi, pengiraan seperti komposisi, suhu , keseimbangan jisim dan keseimbangan tenaga boleh dilakukan langkah demi langkah. Komposisi , nilai k , suhu dan kadar aliran akan terus dijelaskan dalam perbincangan. Selain daripada itu, batasan teknik keadaan mantap dibincangkan , dan keperluan menggunakan simulasi dinamik untuk pemilihan akhir adalah strategi yang boleh digunakan dan yang teguh digambarkan .

ABSTRACT

This paper presents modeling and simulation studies of distillation column. This study is to stimulate sieve tray distillation (rate based model) and specifically for multiple columns process by using Aspen Hysys. The economic importance of distillation separations has been a driving force for the research in synthesis procedures for more than 30 years. Distillation accounts for almost 90% of the separation systems used in chemical process industries. The best way to reduce operating costs of existing units is to improve their efficiency and operation via process optimization and control. Simulation generates one or more trajectories (possible behaviors from the high-level model), and collects statistics from these trajectories to estimate the desired performance or dependability measures. Modeling and simulation of distillation column might already be very familiar but modeling and simulation of multicomponent distillation in multiple columns still yet being commercially introduced to the industries. In this project, the well known kind of multi components (n-butane, n-pentane and benzene) is chosen as the example to run this simulation by using multiple distillation columns. By inserting the details and specifications in Aspen Hysys, multicomponents distillation process is stimulated under steady state condition. From the result gained, calculations such as compositions, temperature, mass balance and energy balance can be done step by step. The composition, k values, temperature and flowrate will be further explained in discussion. Other than that, the limitations of steady state techniques are discussed, and the need for rigorous dynamic simulation for final selection of a workable and robust strategy is illustrated.

Table of Contents

LIST OF FIGURE

LIST OF TABLE

CHAPTER 1

INTRODUCTION

1.1 Background of Proposed Study

The study of multi components distillation in multiple columns has been one of the most interesting and challenging topics of process simulation in chemical industries. In a typical chemical plant, distillation columns and their support facilities can account for about one-third if the capital cost and more than half of the total energy consumption (Julka, Chiplunkar, & O'Young, 2009). Consequently, the design and optimization of the distillation train have a critical impact on the economics of the entire process.

Distillation is defined as a process of liquid or vapor mixture with two or more substances is separated into its desired component fractions by application and removal of heat(Tham, 2007). Some substances have components that vaporise at different temperatures and thus can be separated by condensing their vapors in turn. Distillation is also used as purification process in which non-volatile components are separated from volatile ones. Practically, distillation can be carried out by two methods. The first method is based on the production of a vapour by boiling the liquid mixture to be separated and condensing the vapour without allowing any liquid to return to the still and there is no reflux. The second method is based on the return of the part of the condensate to the still under such conditions that is returning liquid is brought into the intimate contact with the vapours on their way to condenser(Kaushik , 2011).

Distillation column is where the process of distillation occurs. Kaushik (2001) claims that in a distillation column, the more volatile or lighter components are removed from the top of the column, and the less volatile or heavier components are removed from the lower part of the column. There are many types of distillation column used in the industry nowadays such as packed tower and tray tower.

The models of the distillation process can be rate-based or equilibrium. In this study, it will be rate-based simulation for sieve tray distillation. A process with a time dependent behavior is called dynamic (Luyben, 1990) while steady state cannot model variations in variables over time.

1.2 Motivation and Statement of Problem

Simulation by using computer program is a numerical solution of a set of differential equations that are intended to model the way in which particular system evolves in time (Kulakowsk et al., 2007). Process simulation allows one to predict the behavior of a process by using basic engineering relationships, such as mass balance, energy balance, phase equilibrium and chemical equilibrium.

In previous works, it shows that dynamic simulation is more preferable than steady state simulation because dynamic simulation can identify bottlenecks and inefficiencies which are unable to be done in steady state simulation. Distillation inevitably consumes extra large amount of energy and also, due to significant interactions, it has been known as a nontrivial process to control. For this reason, distillation has been considered as one of the major challenges for advanced control and on-line optimization in chemical engineering (Mahdipoor et al., 2007).

Realistic performance (dynamic) of an actual distillation column by simulation is being introduced to the industries recently but unfortunately lots of them were just limited to certain cases and also conditions. Furthermore, some industries are still depending on the steady state simulation while running their process as the dynamic simulation provided was not reliable enough. An effective dynamic simulation for distillation column is supposed to have the flexibility to apply on both in terms of research and development as well as solving practical problems. Besides, the exists of dynamic model should be numerically robust and able to solve large industrial problems (Ganti et al., 1840). The simulation packages that were used to carry out the simulations in this study are Aspen Hysys by Aspen Technology, Inc..

1.3 Objectives

The following are the objectives of this research:

- To determine the behavior of sieve tray distillation column
- To stimulate the distillation process by using rate-based model.
- To study the multicomponents distillation process by using Aspen Hysys

1.4 Scope of Study

The following are the scope of this research:

i) Further study of behavior of distillation column
ii) Verify the pilot scale data by using Aspen Hysys
iii) Analyse steady state distillation process
iv) Specify the process for multicomponents distillation

1.5 Main Contribution of Study

The following are the contributions:

i) Improve steady state modeling and simulation from previous works
ii) To be able to stimulate multicomponents distillation process
iii) Help out the industries by solving their problems using Aspen Hysys simulation

1.6 Organisation of This Thesis

The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provides a detailed knowledge about distillation and also description of the types of distillation column. The process models available and description about the chosen process model are presented. This chapter also provides some basic informations about multicomponents distillation process, mentioning about the way to separate it. A summary of the previous experimental work on simulation for distillation column is also presented.

Chapter 3 gives a review on how the multicomponents distillation works. Besides, detailed information are also presented in this chapter, the pilot scale data which is taken from previous research and will be used in the simulation. Some important assumptions for azeotropic process are also listed. This chapter also provides the equations that will be used and some explanation on that. Clear procedures are also shown.

Chapter 4 is the results and discussion of this study. It is the work of running simulation in steady state using Aspen Hysys. Results will be shown in graphs and some appropriate discussions are also included in this chapter.

Chapter 5 gives an overall conclusion of this study. The objectives or aims of this study will be proved to be achieved from the results gained.

CHAPTER 2

LITERATURE REVIEW

2.1 Overview

Identification of the best measurement is necessary before the plant is fully operating and simulation is one of the most suitable and easy ways. This can increase agility in decision making, improve reliability and lower operating cost (Schumann & Davis, 2008). There are very few publications on dynamic modeling of distillation in the literature and the dynamic behaviour of distillation is poorly understood (Jianjun et al., 2003). In order to have a better simulation, a deeper understanding of distillation is a must. Other than the study the basics of distillation, a need of knowing the needs of the industry is also compulsory. A real distillation process can be complicated by many factors. There might be many components. The component to be separated out has neither the highest nor lowest boiling point. Feeds of different mixture can come in several stages (Brooks, 1993).

2.2 Introduction

The subtopic below shows the detailed information of distillation, multicomponents, distillation column, process model, thermodynamics model, steady state and also simulation and dynamic modeling.

2.2.1 Distillation

The history of distillation dated back to centuries ago. Forbes has chronicled the full history of distillation in 1948. Reputedly, it was the Chinese who discovered it during the middle of Chou dynasty. It was later introduces to India, Arabic, Britian and the rest of the world (Hoon et al., 2011). Distillation is probably the most popular and important process studied in the chemical engineering literature. Distillation is used in many chemical processes for separating feed streams and for purification of final and intermediate product streams (Luyben, 1990). Although distillation is the most economical separating method for liquid mixtures, it can be energy intensive (Hoon, Ling, & Jaya, 2011). One of the solution of this was to increase the efficiency of the operations. A real distillation process can be complicated by many factors. There might be components. The component to be separate out has neither the highest nor lowest boiling. Seader (1998) claimed that this separation process requires three things. First, a second phase must be formed so that both liquid and vapor phases are present and can contact each other on each stage within a separation column. Secondly, the components have different extent. Lastly, the two phases can be separated by gravity or other mechanical means.

2.2.2 Multicomponents

Multi component distillation, which is the most dominant separation process, utilizes the latter method. It is the separation of a liquid mixture based on the differences in the volatilities of liquid constituents (Afolabi et al., 2004). Synthesis of multi component separation sequences is an important process design problem in chemical industry. It is concerned with the selection of a separation method and the selection of the best sequence of separators to split a multi component mixture into several products, relatively pure species (Ay et al., 2011). In our study, a mixture of butane, pentane and benzene is used to be the multi component feed for the multiple columns.

2.2.3 Distillation Column

Many types of distillation columns are designed to be different in terms of complexity in order to perform specific types of separations. Distillation columns can be classified into how they are operated: batch columns and continuous columns. In batch operation, the feed to the column is introduced batch-wise. When the desired task is achieved, a next batch of feed is introduced. As for continuous columns, it is a process that includes continuous feed stream. They are capable of handling high throughputs and are most common in industry (Tham, 2007). Continuous columns can be further classified according to the extra feed exits (extractive or azeotropic) and also they type of column internals (packed tower or tray tower). According to Tham (2007), extractive distillation is where the extra feed appears in the bottom product while azeotropic distillation is where the extra feed appears at the top product stream. Norrie (2010) claims that packed tower is a vertical, steel column which contains 'Beds' of packing material which are used to bring the rising vapors into intimate contact with falling liquid within the tower. As for tray tower, it is also a tall, cylindrical column which a series of trays are placed inside, one above another. The tray is used to bring the rising vapor and falling liquid into intimate contact (Norrie, 2010). There are various types of tray in use, for example, bubble cap, valve and also sieve trays. In our study, we choose to have a further study on sieve trays distillation column. Distillation columns are made up of several components, each of which is used either to transfer heat energy or enhance material transfer (Adeleke et al., 2013). A typical distillation unit contains the following major components:

i. A vertical shell where the separation of liquid is carried out.
ii. Column internals such as trays or plates and/or packing which are used to enhance component separations.
iii. A reboiler to provide the necessary vaporization for the distillation column.
iv. A condenser to cool and condense the vapour leaving the top of the column so that liquid (reflux) can be recycled back to the column.

Distillation processes can use one or more distillation columns. For instance, to efficiently separate multicomponent mixtures into more than two product streams using distillation, a sequence of distillation columns is required (Shenvi et al., 2012).. Multiple columns consist of combinations of two distillation columns. In our study, the bottoms of the first column will be the feed of the second distillation column. Figure 2.1 shows the sieve trays distillation column and Figure 2.2 shows the configuration of distillation columns. In this study, the simulation method is applied to a separation process of n-butane, n-pentane and benzene.

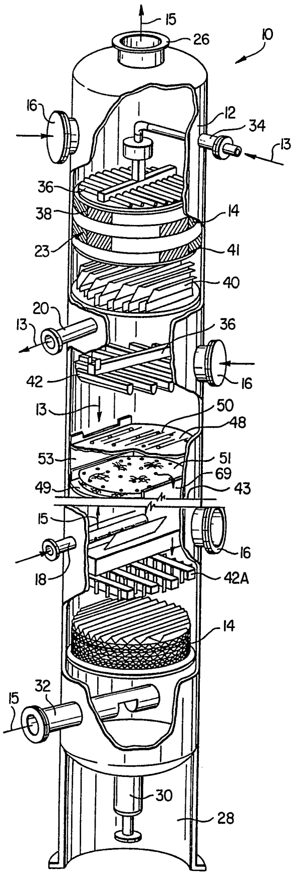


Figure 2-1 Sieve Tray Distillation Column

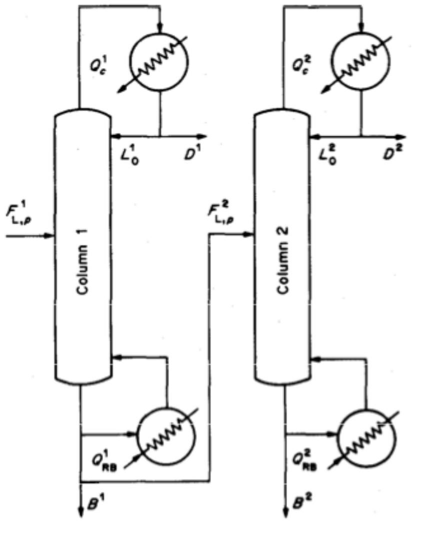


Figure 2-1 Configurations of Multicomponents Distillation

2.2.4 Process Model

There are two kind of models in distillation process, namely rate-based and equilibrium model. The rate-based model is a model in which the finite mass transfer rates across the vapor-liquid interface are accounted for (Baur et al., 2000). Baur et al. also mention that the equilibrium model is a model in which the vapor and liquid phases are assumed to be in thermodynamic equilibrium. The non-equilibrium model or denoted as rate-based model was initially presented by Krishnanmurthy and Taylor (1985) for conventional distillation process and consists of a set of mass and energy balances for vapor and liquid phases, along with rate equations for the evaluation of mass and heat transfer. This model use the Maxwell-Stefan equations for description of vapor-liquid mass transfer and it requires information about parameters such as mass and heat transfer coefficients and vapor-liquid interfacial area (Duran et al., 2010). Duran et al. (2010) also mentioned that this method requires the evaluation of the mass and heat transfer processes for both phases seperately. The rate-based model is much more complicated than the equilibrium model and also more difficult to converge (Peng et al., 2002). It was found that there is a relationship between the equilibrium model and the rate-based model. When the number of segments in the rate-based model is chosen to be the same as the number of theoritical stages in the equilibrium model and the vapor-liquid interfacial area is increased, the profiles from the rate-based model approach those from the equilibrium model. When the vapor-liquid interfacial area is about 100 times as large as the real area, the profile from the rate-based model are almost identical to those from the equilibrium model (Peng et al., 2002). Seader (1985) had provided an elegant history of the first century of equilibrium stage modeling by creating the equilibrium stage model for the distillation of alcohol. But in real distillation process, normally it does not operate at equilibrium stage.

In order to have a simulation which is more feasible, rate-based model is being chosen as the model in this study. Previously, simulations based on non-equilibrium or rated-based model were considered impractical due to their complexity. However, with the ever-increasing computing power, these simulations are not only feasible, but in some circumstances they should be regarded as mandatory (Taylor et al., 2003). Innumerous articles have been published on this subject, simulation of distillation column. Roat et al. (1986) discussed dynamic simulation of reactive distillation using an equilibrium model. Ruiz et al. (1995) developed a generalized equilibrium model for the dynamic simulation of multicomponent reactive distillation. A rate-based simulation for sieve tray distillation is developed by Mortaheb and Kosuge (2003). In this study, the mostly used distillation process which is rate-based simulation for sieve tray distillation has been chosen. The data and some useful informations from the previous works can be a reference to produce an advanced model.

2.2.5 Thermodynamic Model

UNIQUAC models UNIQUAC (Universal Quasi Chemical) is an activity coefficient model used in description of phase equilibria (Abrams Prausnitz, 1975). The model is a so-called lattice model and has been derived from a first order approximation of interacting molecule surfaces in statistical thermodynamics. The model is however not fully thermodynamically consistent due to its two liquid mixture approach. In this approach the local concentration around one central molecule is assumed to be independent from the local composition around another type of molecule.

It has been shown that while the local compositions are correlated, ignoring this correlation gives little effect on the correlation of activity coefficients (McDermott, 1976). Today the UNIQUAC model is frequently applied in the description of phase equilibra (i.e. liquid solid, liquid-liquid or liquid-vapour equilibrium). The UNIQUAC model also serves as the basis of the development of the group contribution method UNIFAC, where molecules are subdivided in atomic groups.

The UNIFAC method is a semi-empirical system for the prediction of non-electrolyte activity estimation in non-ideal mixtures. UNIFAC uses the functional groups present on the molecules that make up the liquid mixture to calculate activity coefficients. By utilizing interactions for each of the functional groups present on the molecules, as well as some binary interaction coefficients, the activity of each of the solutions can be calculated.

The calculated activity coefficient can be used for steady state simulation of distillation column. But Aspen provides some inbuilt property models which can be used as per the requirement of the problem. Hence we don’t need supplying the property methods from outside.

In this study, UNIQUAC is being chosen instead of UNIFAC as the thermodynamic model of the simulation.

2.2.6 Steady State

Steady state process models have long been used to assist the control engineer in designing control strategies for distillation columns. However, with the large number of industrial columns still operating in manual or with ineffectual controls, there remains a need for sound distillation column control design techniques. Steady state models are easily manipulated and provide robust solutions(Mohanty & Purkait, 2012). In order to make a change to the solution conditions, only a few changes need to be made to the model input file. The model input file is then submitted to the software which finds a new solution. Generally, very little time is spent getting converged solutions, which allows us to efficiently generate the large number of case studies necessary for this design procedure. Ay et al. (2009) also claimed that the steady state target must satisfy the requirements of system safety, energy and technical conditions.

2.2.7 Simulation and Modeling

Process simulation models can offer significant capabilities for operating personnel to analyze and troubleshoot current performance and to develop optimum responses in a proactive manner(Schumann & Davis, 2008). Steady state techniques have been used for decades to develop control strategies for distillation columns (Mahoney & Freuhauf, 2011). To accurately assess the performance and suitability of alternative control schemes, rigorous dynamic simulation is required. A complete dynamic model of a distillation column must include material balance and flow, energy balance and flow, liquid to or from vapour flow within a stage, temperature, pressure and hydrauluc dynamics, system, constraints and chemical reactions(Brooks, 1993).

The Key ostensible difference between the steady state models and dynamic models is the ability to take into account variation over time(Matzopoulos, 2011). However, as can seen below the difference is not simply the addition of a time dimension; dynamic modeling often brings a whole different approach that results in dynamic models being a much truer-to-life representation of the process in many respects. While steady state analysis is mainly used for process flowsheet design, usually to determine mass and energy balances and approximate equipment sizes, or perhaps stream propeerties, the ability of dynamics models to transient behaviou opens up a whole new world of application. Matzopoulos (2011) also mentioned that typical applications of dynamic models are as follows:

- analysis of transient behavior, including performance during start-up, shut-down, and load change;
- regulatory (i.e., PID) control scheme analysis and design;
- design of optimal operating procedures – for example, to optimize transition between product grades;
- design of batch processes;
- design of inherently dynamic continuous processes – for example, pressure swing adsorption;
- fitting data from nonsteady-state operations – for example, dynamic experiments, which contain much more information than steady-state experiments, or estimation of process parameters from transient plant data;
- safety analysis – for example, the determination of peak pressures on compressor trip;
- inventory accounting and reconciliation of plant data;
- online or offline parameter re-estimation to determine key operating parameters such as fouling or deactivation constants;
- online soft-sensing;
- operator training.

In this study, Aspen Hysys is being used. Further Aspen Hysys makes it easy to build and run the process simulation model by providing with a comprehensive system of online process modeling(Kaushik , 2011). It enables one to run many cases, conduct 'what if' analysis and perform sensitivity analysis and optimisation runs.

2.3 Previous Work

From the Table 2-1, it is clearly show that there are lots of researches or works doing on both rate-based model and also equilibrium model. Besides, people also tend to choose distillation other than multicomponents distillation. Obviously, simulation on multicomponents distillation process is needed to be studied in advanced.

Table 2-1 Previous Work

No.	Model Name	Simulation	References
1	Rate-based model	sieve tray distillation	Mortaheb and Kosuge (2003)
2	Rate-based model	three phase distillation	Eckert et al. (2001)
3	Equilibrium model	heteroazeotropic distillation	Kurooka et al. (2000)
4	Equilibrium model	extractive distillation	Llano-Restrepo et al. (2002)
5	Equilibrium model	heat integrated distillation	Ho et al. (2009)
6	Rate-based model and Equilibrium model	heteroazeotropic distillation	Denes et al. (2009)
7	Rate-based model and Equilibrium model	extractive and azeotropic distillation	Kiss et al. (2012)
8	Rate-based model and Equilibrium model	multicomponent distillation	Pelkonen et al. (2000)
9	Rate-based model	three phase distillation	Gutierrez-Oppe et al. (2013)
10	Equilibrium model	packed distillation	Kasiri and Dorj (2012)

2.4 Summary

This paper presents a study of simulation for multicomponents distillation with sieve trays column by rate-based model using Aspen Hysys. The basics theory and some important knowledge which we need to understand before proceeding to the next step, simulation are provided in this chapter.

CHAPTER 3

METHODS

3.1 Overview

This paper presents a simulation and dynamic modeling of multicomponents distillation process for n-butane, n-pentane and benzene. Sieve tray distillation column and rate-based model were chosen for this study. The pilot scale data is also shown below. The simulation results will be discussed with the attachment of graphs.

3.2 Data

Table below is the details and specifications of the distillation columns to insert into the Aspen Hysys for simulation.

Table 3-1 Detail and Specifications of Distillation Columns

Variable		Column 1	Column 2
Number of actual plates		20	20
Number of components		3	3
Plate efficiency		100%	100%
Number of effective plates simulated		20	20
Actual feed plate position		11	18
Plate spacing (cm)		60	60
Plate diameter (cm)		183	183
Type of condenser		Total	Total
Type of reboiler		Total	Total
Feed condition		Bubble point	Bubble point
Feed temperature (K)		316.1	316.1
Feed flow rate (kmol/h)	**Liquid phase**	226.8	226.8
	Vapor phase	-	-
Feed enthalpy (kcal/kmol)	**Liquid phase**	1106.9	1106.9
	Vapor phase	-	-
Feed composition (total)	**n-Butane**	0.3867	
	n-Pentane	0.4190	
	Benzene	0.1943	
Reboiler heat duty (Gcal/h)		2.760	2.760
Reflux rate (kmol/h)		429.0	429.0

3.3 Assumptions

The suppositions below were made to simplify the model (Ferreiro , 2011) :

- **i.** There are no heat losses; the column is adiabatic.
- **ii.** The condenser is complete, so therefore the vapor flowing from the top of the column will be the same as that of the reflux and distillate current.
- **iii.** Total pressure loss of the column is distributed linearly among all the plates
- **iv.** Each phase is perfectly mixed in each segment.
- **v.** Vapour-Liquid equilibrium is only assumed at the interface
- **vi.** The condenser and the reboiler are treated as equilibrium stages.
- **vii.** The heat transfer coefficients are assumed to be constant for all segments.

3.4 Procedures

To start of the initial setup, a new case was opened in Aspen Hysys. Butane, Propane and Benzene are selected as the components. As for the fluid package, UNIQUAC is being chosen.

Next is to set up the distillation columns with the details and specifications before run. Since this is a multi component distillation in 2 distillation columns, 9 process streams are needed. 5 material streams are placed for the feed, the distillates and the bottoms. Another 4 energy streams are for reboilers and condensers. Rename the distillation columns, material and energy streams for each stream in order to make the simulation easy to follow. After that, distillation columns are placed. Just need to click the Distillation Column button in the simulation toolbar, and place it to the simulation window. When the columns are ready to be hooked up to the process and energy streams. “Distillation Column Input Wizard” is being brought up by double click on the distillation column. The flows, the streams is set by referring to Figure 1. Started off with Distillation Column 1 and followed by Distillation Column 2. The streams are being hooked up to their appropriate locations. The specifications and details showed in Table 1 are being filled.

Lastly, to get ASPEN HYSYS to start actively running the simulation and solving for unknown properties, the solver is being activated. Because of having two columns which is related, the bottoms of the Distillation Column 1 will be the feed of the Distillation Column 2, the first distillation column should be converged before the second one. To stimulate, click on the “Run” button. The streams turned to dark blue which signifying that ASPEN HYSYS had successful solved for those streams. After the first distillation column, continued with the second distillation column by repeating the same steps.

The figures below show some steps for simulation in Aspen Hysys. Figure 3-1 is the distillation columns and arrangement of the columns. Figure 3-2 is the specifications of distillation column 1 while Figure 3-3 is the specifications of distillation column 2.

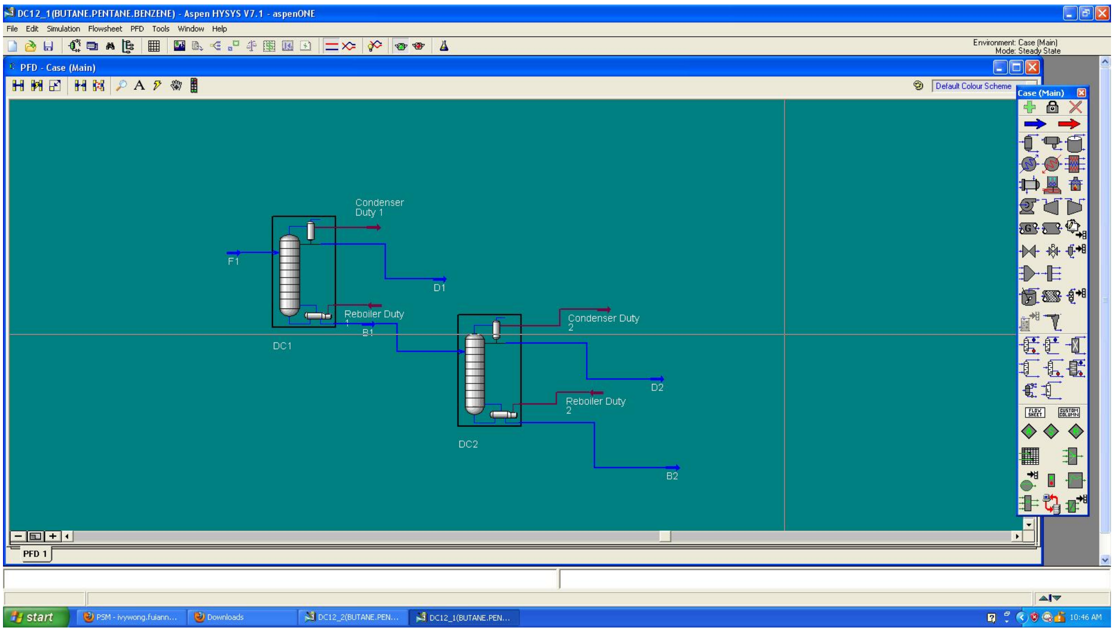
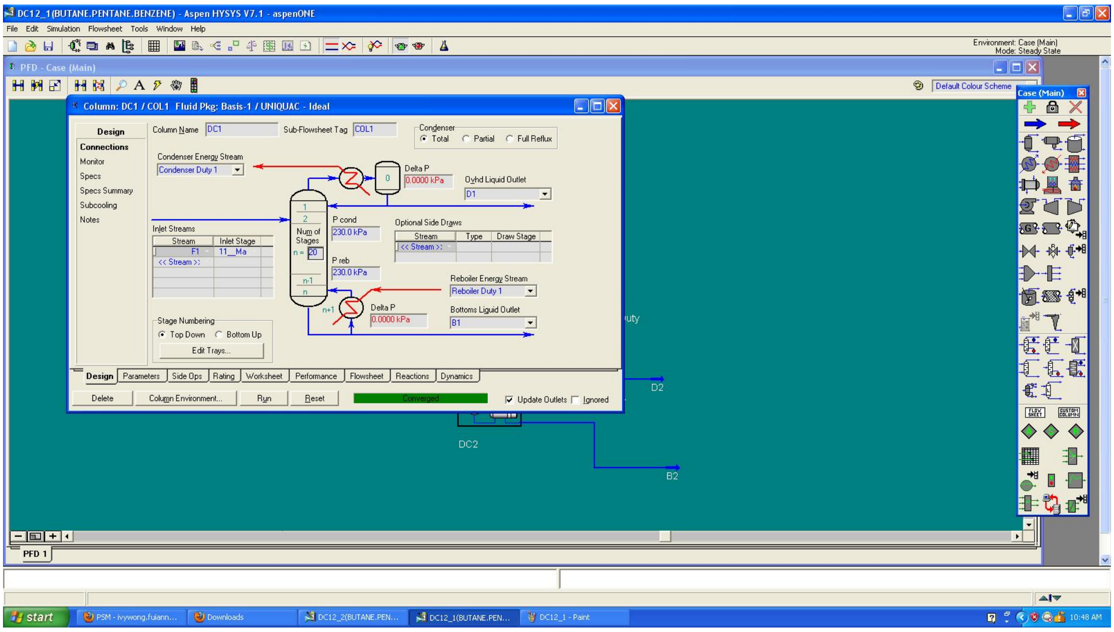


Figure 3-1 Distillation Columns in Aspen Hysys


DC12_1(BUTANE.PENTANE.BENZENE) - Aspen HYSYS V7.1 - aspenONE

Column: DC1 / COL1 Fluid Pkg: Basis-1 / UNIQUAC - Ideal

Column Name: DC1
Sub-Flowsheet Tag: COL1
Condenser: ● Total ○ Partial ○ Full Reflux
Condenser Energy Stream: Condenser Duty 1
Delta P: 0.0000 kPa
Ovhd Liquid Outlet: D1
Num of Stages: n = 20
P cond: 230.0 kPa
P reb: 230.0 kPa

Inlet Streams

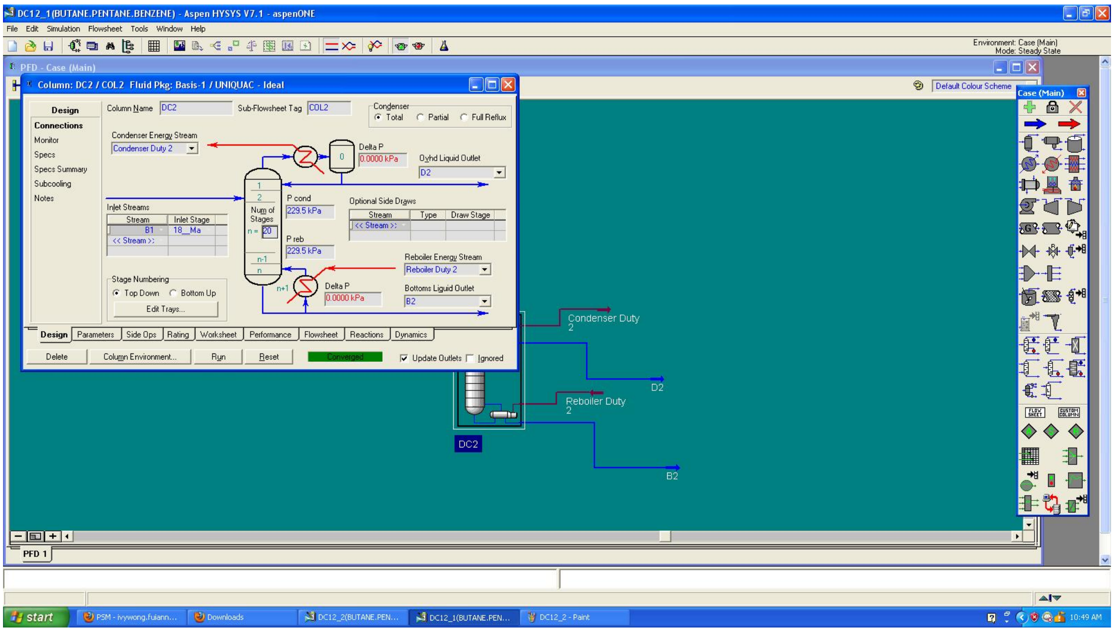
Stream	Inlet Stage
F1	11__Ma
<< Stream >>	

Optional Side Draws

Stream	Type	Draw Stage
<< Stream >>		

Reboiler Energy Stream: Reboiler Duty 1
Delta P: 0.0000 kPa
Bottoms Liquid Outlet: B1
Stage Numbering: ● Top Down ○ Bottom Up
Converged
☑ Update Outlets ☐ Ignored

Figure 3-2 Specifications in Distillation Column 1


DC12_1(BUTANE.PENTANE.BENZENE) - Aspen HYSYS V7.1 - aspenONE

Column: DC2 / COL2 Fluid Pkg: Basis-1 / UNIQUAC - Ideal

Column Name: DC2
Sub-Flowsheet Tag: COL2
Condenser: ● Total ○ Partial ○ Full Reflux
Condenser Energy Stream: Condenser Duty 2
Delta P: 0.0000 kPa
Ovhd Liquid Outlet: D2
Num of Stages: n = 20
P cond: 229.5 kPa
P reb: 229.5 kPa

Inlet Streams

Stream	Inlet Stage
B1	18__Ma
<< Stream >>	

Optional Side Draws

Stream	Type	Draw Stage
<< Stream >>		

Reboiler Energy Stream: Reboiler Duty 2
Delta P: 0.0000 kPa
Bottoms Liquid Outlet: B2
Stage Numbering: ● Top Down ○ Bottom Up
Converged
☑ Update Outlets ☐ Ignored

Figure 3-3 Specifications in Distillation Column 2

3.5 Summary

This paper presents methods to stimulate the azeotropic distillation. The data, assumptions and equations provided are used in the simulation process. The procedures of simulation and modeling of distillation column are included in this chapter as well.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Overview

In this chapter, the results obtained will be further discussed and explained. From the succeed simulation, the graph of temperature, k values, flowrates and composition versus stages can be obtained.

4.2 Results of Simulation under Steady State

The results below is obtained by simulating the data in steady state. As for discussion, it will be separated into distillation column 1 and distillation column 2 for detailed explanation.

4.2.1 Distillation Column 1

For Distillation Column 1, Figure 4-1 showed the graph of temperature versus stages and Figure 4-2 showed the graph of flowrate versus stages. From Figure 4-1, temperature in the distillation column is showed to be increasing from the upper part (stage 1) to the bottom (stage 20) among the stages. The temperature in condenser and reboiler is 23.59°c and 69°c respectively. Flowrates of vapor and bulk liquid can be found in Figure 4-2. The vapor flowrate is decreasing from the stage 1 to stage 20 in a range of 518.910 kgmol/h to 457.042 kgmol/h. There is no vapor flowing in condenser while in reboiler, there is still 446.529 kgmol/h of flowrate. As for bulk liquid flow, the graph shows a different trend before and after stage 11. This is because the feed is being placed from stage 11. The flowrate is decreasing from stage 1 to stage 10 and a sudden increase to 585.458 kgmol/h in stage 11. The trend of flowrate of bulk liquid is then going up until it come to 583.434 kg/mol in stage.

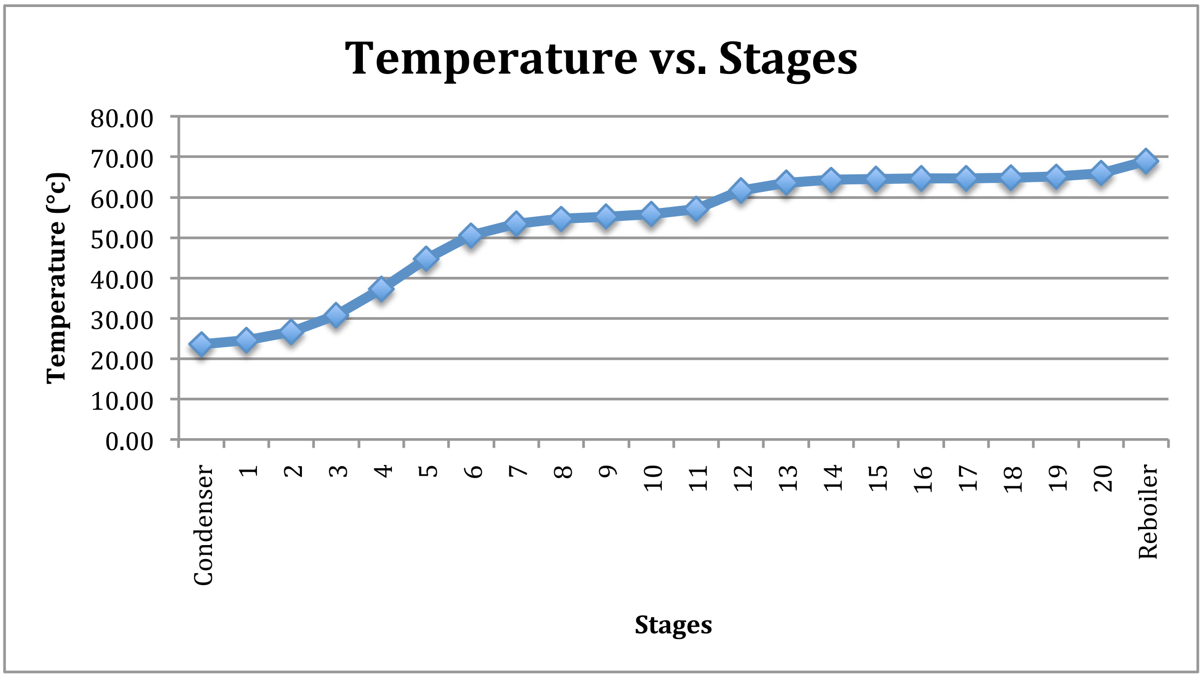


Figure 4-1 Temperature vs. Stages (Distillation Column 1)

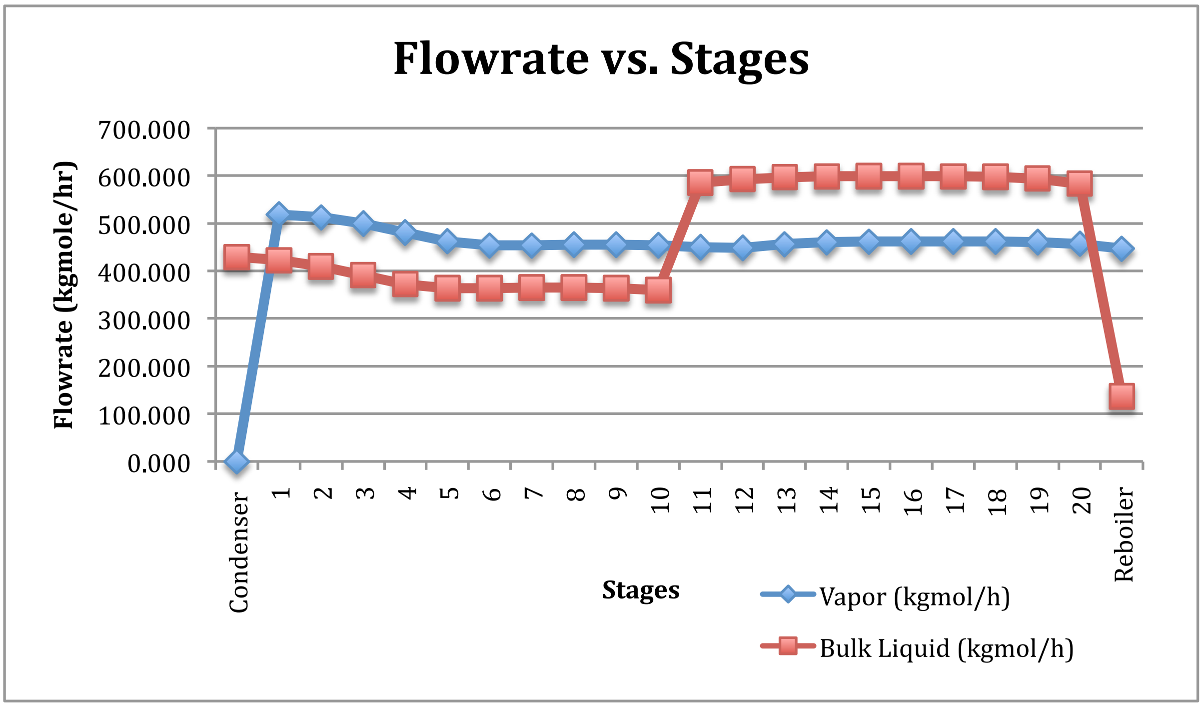


Figure 4-2 Flowrate vs. Stages (Distillation Column 1)

Besides that, Figure 4-3 showed the composition versus stages graph. From the graph, n-butane is having higher composition at the upper part of the columns as the composition goes from 0 up to 0.9309 (stage 20 to stage 1). On the other way, n-pentane is being opposite way of n-butane. The composition of n-pentane goes from 0.8194 to 0.0244 (stage 20 to stage 1). Besides, benzene is also increased from top of the column to bottom with a little amount of composition. To conclude from this graph, n-butane is the distillate product while the rest (n-pentane and benzene) is the bottoms product which will be the feed for Distillation Column 2. Figure 4-4 showed the K values of each components between stages. Each components showed a increasing trend of values from stage 1 to stage 20, this is because the temperature in the bottom of the distillation column increased as well.

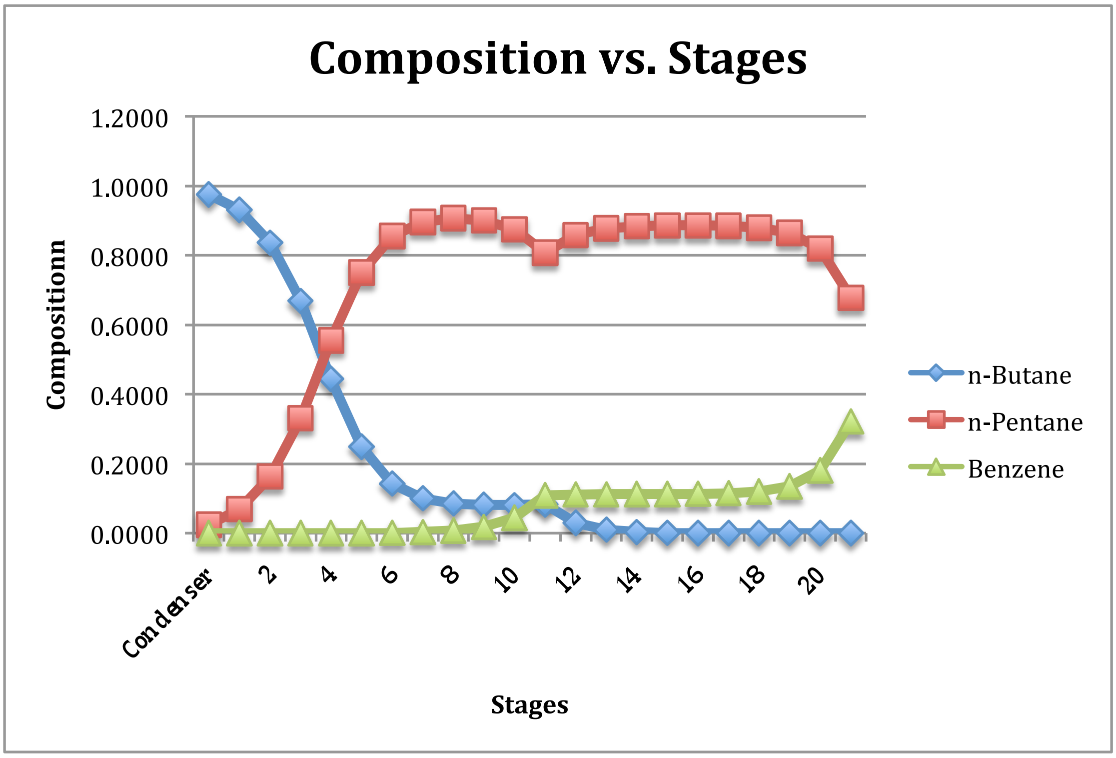


Figure 4-3 Composition vs. Stages (Distillation Column 1)

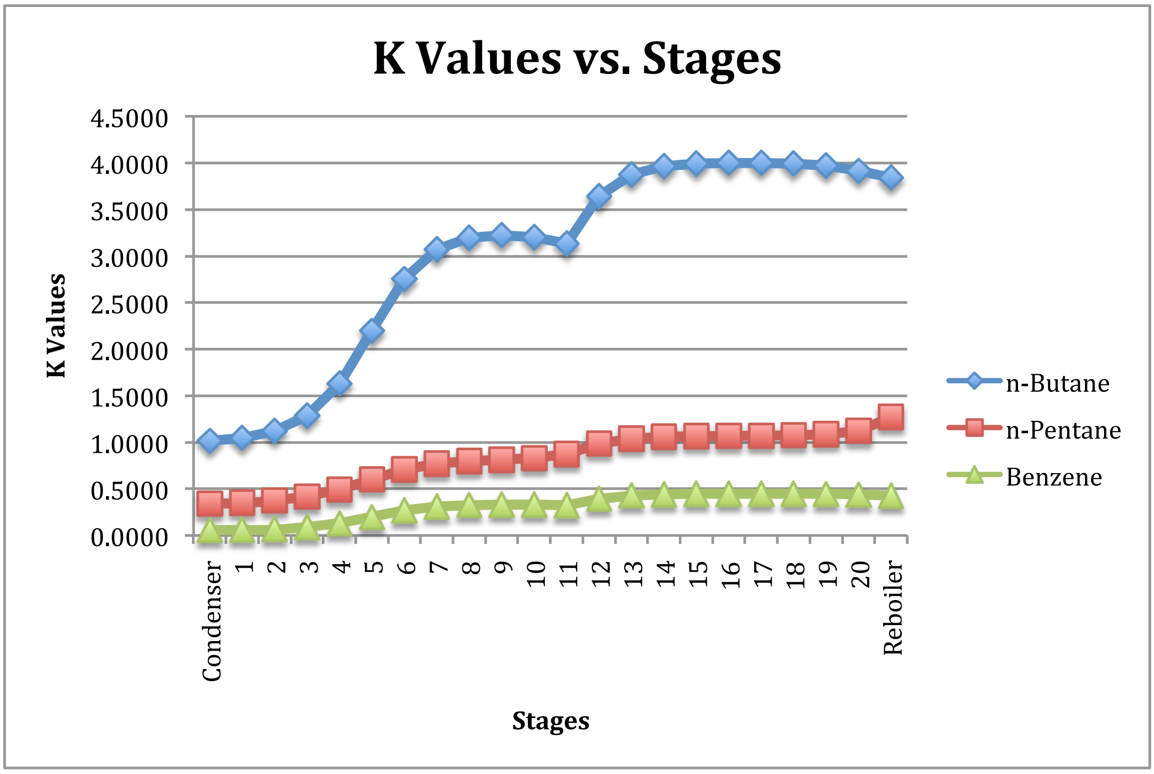


Figure 4-4 K Values vs. Stages (Distillation Column 1)

4.2.2 Distillation Column 2

For Distillation Column 2, Figure 4-5 showed the graph of temperature versus stages and Figure 4-6 showed the graph of flowrate versus stages. From Figure 4-5, temperature in the distillation column is showed to be in constant of 62.46°c from stage 1 to stage 9 and started to increased from stage 10 to stage 20. The temperature in condenser and reboiler is 62.46°c and 72.39°c respectively. Flowrates of vapor and bulk liquid can be found in Figure 4-6. The vapor flowrate is slightly decreasing from the stage 1 to stage 20 in a range of 470.8692 kgmol/h to 451.9466 kgmol/h. There is no vapor flowing in condenser while in reboiler, there is still 435.3409 kgmol/h of flowrate. As for bulk liquid flow, the graph shows a different trend before and after stage 18. This is because the feed is being placed from stage 18. The flowrate is decreasing in very slight differences from stage 1 to stage 17 and a sudden increase to 552.8371 kgmol/h in stage 18. The trend of flowrate of bulk liquid is then going up until it come to 530.4220 kg/mol in stage 20.

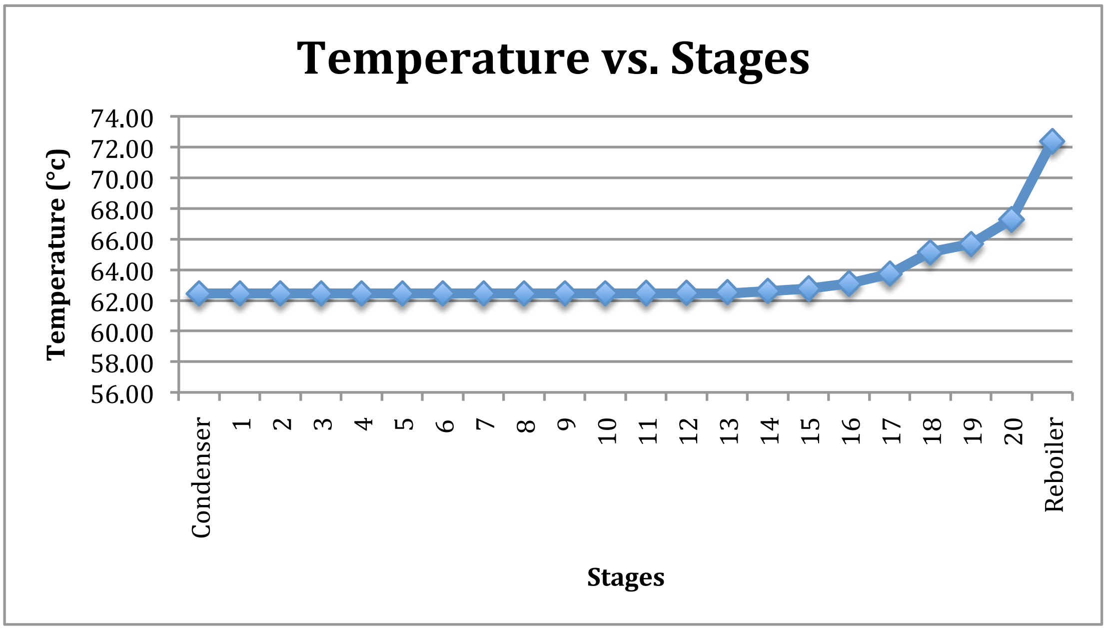


Figure 4-5 Temperature vs. Stages (Distillation Column 2)

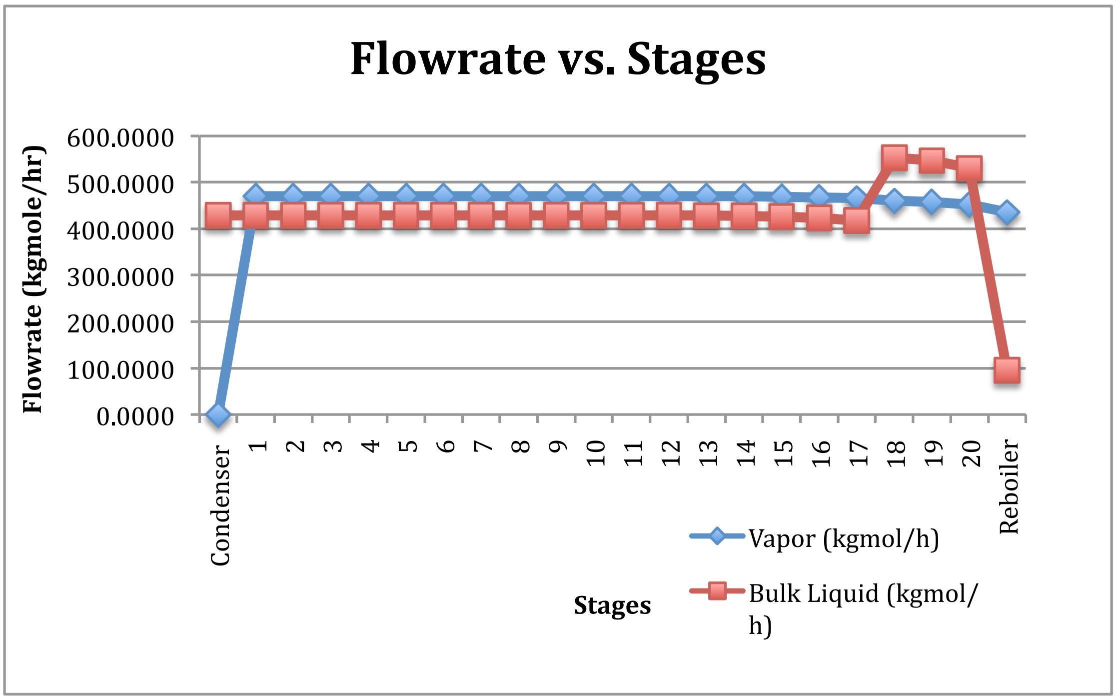


Figure 4-6 Flowrate vs. Stages (Distillation Column 2)

Furthermore, Figure 8 showed the composition versus stages graph. From the graph, n-butane which being separate as distillate product doesn't have any composition left in this distillation column. On the other hand, the composition of n-pentane goes from 1 to 0.537 (stage 1 to stage 2). From stage 1 to stage 9, there is no existence of any benzene until it comes to stage 10. Benzene is having 0.247 at the very last stage

(stage 20). To conclude from this graph, n-pentane is the distillate product while the leftover (0.753 of n-pentane and 0.247 of benzene) is the bottoms. Figure 5 showed the K values of each component between stages.

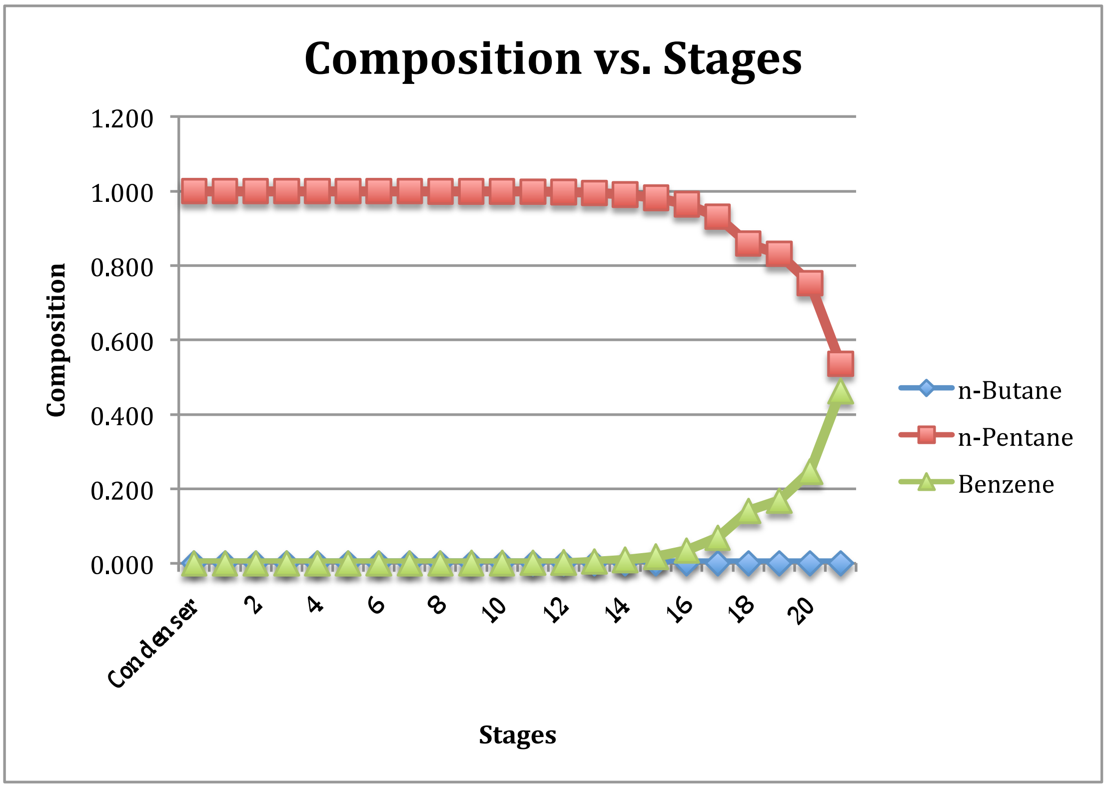


Figure 4-7 Composition vs. Stages (Distillation Column 2)

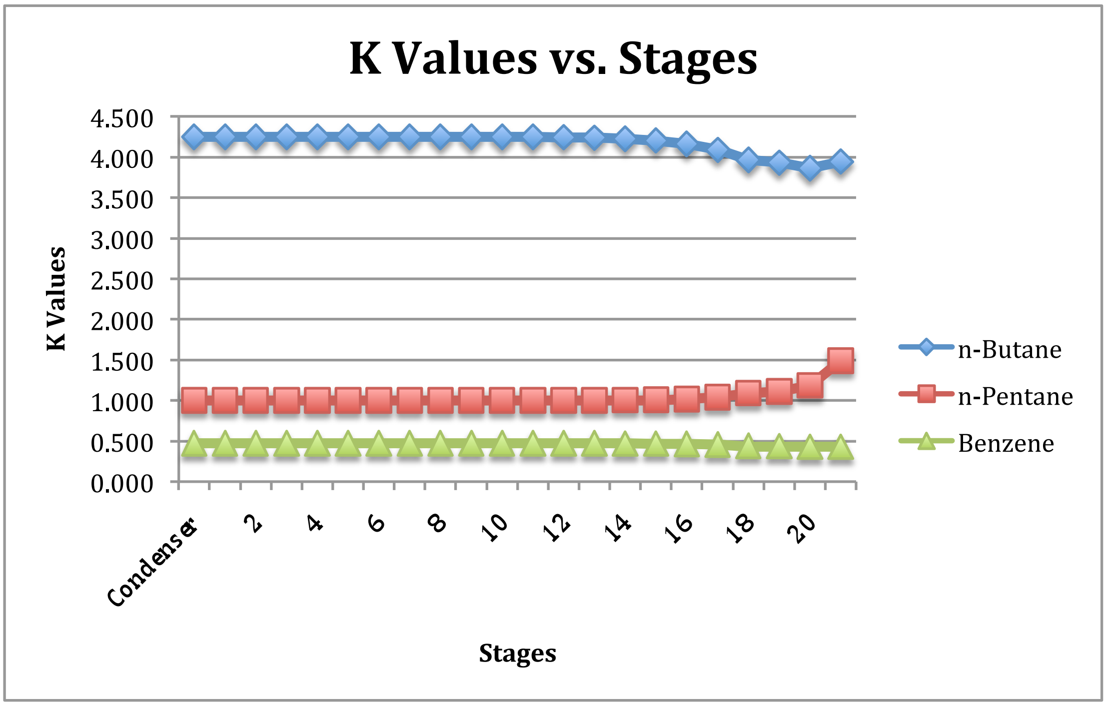


Figure 4-8 K Values vs. Stages (Distillation Column 2)

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Aspen Hysys makes it easy to build and run the process simulation model by providing with a comprehensive system of the online process modeling. After process simulation allows one to predict the behaviour of a process by using basic engineering relationships, such as mass and energy balances, and phase and chemical equilibrium. From the obtained results, we observe that with simulation; one can design better plants and increase the profitability in the existing plants. Process simulation is helpful throughout the entire life of a process, from research and development through process design to production.

By stimulating multicomponents in multiple columns in steady state by using Aspen Hysys, able to find out the conditions of the separation throughout the stages of distillation columns. The heat duty, mass balance or even some specific conditions can be solved as well. From this simulation, we knew that n-butane can be separated with high purity as a distillate product of Distillation Column 1 while n-pentane can be separated with high purity also as a distillate product of Distillation Column 2. But steady state simulation had it own limitations. To accurately assess the performance and suitability of alternative control schemes, rigorous dynamic simulation is required.

5.2 Recommendation

For further improvements in simulation and modeling of distillation column, recommendations are needed.

5.2.1 Dynamic Modeling and Simulation

Instead of stimulate only in steady state, the work should be studied under dynamic simulation as well. Dynamic modeling and simulation of distillation column can bring up a better understanding of the behavior under the considerations of changes with time. Besides, comparisons between steady state and dynamic should also be presented. Parameters such as feed flow rate, feed composition, reboiler heat load and reflux flow rate will be change in order to simulate under dynamic condition.

5.2.2 Control Strategies

The purity of distillate should be controlled using two strategies as below:

- **i.** Tray temperature control.
- **ii.** Composition control.

The tray temperature and composition controllers are basically a PI controller which is tuned by the Tyreus–Luyben method. The tray temperature controller uses temperature as process variable and reboiler heat input as a manipulated variable. Composition controller uses mole fraction of one of the component as the process variable and reboiler heat input as a manipulating variable. Cascade controller if used, uses both the temperature and composition controllers together, where the tray temperature controller is the secondary controller. The purity of distillate for both servo and regulatory type situation is also controlled.

REFERENCES

Adeleke, A. E., Aiyedun, P. O., Waheed, M. A., Olawale, O. A., Dairo, O. U., & Sanni, L. O. (2013). A New Simulation Model for Design of Distillation Column in a Bio-ethanol/Water System: Effect of Reflux Ratio. British Journal of Applied Science & Technology (3), 508-517.

Afolabi, & Jolaade, T. (2004). A General Approach To Multicomponent Distillation Column Design. 381-394.

Ay, S., & Karacan, S. (2011). Decoupling Constrained Model Predictive Control of Multi Component Packed Distillation Column. World Applied Sciences Journal (3), 517-530.

Brooks, B. A. (1993). Modeling of Distillation Column using Bond Graphs. 1-214.
Chou, T.-L. (2004, April). Kinetics of Salt Formation Using Terephthalic Acid and N-Methyl-2-Pyrrolidinone , 1-80.

Chemical Engineering Science. A Spray Reactor Concept for Catalytic Oxidation of p-xylene to Produce High-purity Terephthalic Acid (104), 93-102.

D. S. Abrams, Prausnitz J. M., “Statistical Thermodynamics of Liquid Mixtures”, A New Expression for The Excess Gibbs Energy of Partly or Completely Miscible System, AIChE. 21(1), 116-128, 1975

Ferreiro , A. R. (2011). Dynamic Modeling and Simulation with Ecosimpro of an Ethanol Distilltion Column In the Sugar Industry .

Gani, R., Ruiz, C. A., & Cameron, I. T. (1985, October 7). Model Description and Applications . A generalized model for distillation columns , 181-198.

Hoon, C. Y., Ling, A. L., & Jaya, A. (2011, February). Distillation Column Selection and Sizing . Practical Engineering Guidelines for Processing Plant Solutions . Johor Bahru, Malaysia: KLM Technology Group .

Julka, V., Chiplunkar, M., & O'Young, L. (2009, March). Selecting Entrainers for Azeotropic Distillation. Reactions and Seperations , 47-53.

Kaushik , V. (2011). Dynamics and Control of Distillation using Aspen. National Institute of Technology Rourkela , Department of Chemical Engineering .

Kim, J. K., Wankat, P. C., 2004. Quaternary Distillation Systems with less than N-1 Columns. Ind. Eng. Chem. Res. 43, 3838.

Li, C. T. (2004, April). KINETICS OF SALT FORMATION USING TEREPHTHALIC ACID AND N-METHYL-2-PYRROLIDINONE .

Li, M., Niu, F., Zuo, X., Metelski, P. D., Busch, D. H., & Subramaniam, B. (2013). ￼ A spray reactor concept for catalytic oxidation of p-xylene to produce high-purity terephthalic acid. Chemical Engineering Science , 93-102.

Linninger, A. (2009). Distillation. Senior Desgin CHE 396 , 1-30.

Luyben, W. L. (1990). Process Modeling, Simulation and Control for Chemical Engineers (2nd Edition ed.). Singapore: McGraw-Hill Publishing Company.

Mahoney, D. P., & Freuhauf, P. S. (2011). An Integrated Approach for Distillation Column Control Design Using Steady Stare and Dynamic Simulation. 1-12.

Matzopoulos, M. (2011). Dynamic Process Modeling: Combining Models and Experimental Data to Solve Industrial Problems. (M. C. Georgiadis, J. R. Banga, & E. N. Pistikopoulos, Eds.) Process Systems Engineering , VII, 3-33.

Mohanty, K., & Purkait, M. K. (Eds.). (2012). Membranes Technologies and Applications. CRC Press.

Norrie. (2010). Distillation Columns (or Towers). LNG production , Department of Training Programmes fir Libyan, Libya.

Production of Terephthalic Acid. (2006). Retrieved 2013 from Design Thesis: http://www.sbioinformatics.com/design_thesis/Terephthalic_acid/Terephthalic-2520acid.htm

Qinbo, W., Li, X., Wang, L., Cheng, Y., & Xie, G. (2005). KINETICS, CATALYSIS, AND REACTION ENGINEERING. Kinetics of p-Xylene Liquid-Phase Catalytic Oxidation to Terephthalic Acid (44), 261-266.

Saboo, M., & Kumar, D. D. (2008, May). Manufacture of Terephthalic Acid. 1-68.
Schumann, D., & Davis, G. (2008). Application of Simulation Models in Operations. A Success Story , 1-7.

Seader, J. & Henley, E. Separation Process Principles. John Wiley & Sons, 1998, Chapters 7 and 8.

Shenvi, A. A., Shah, V. H., & Agrawal, R. (2012). New Multicomponent Distillation Configurations with SImultaneous Heat and Mass Integration. AIChE , 59, 272-282.

Skogestad, S. (1977). Dynamics and control of distillation columns - a critical survey . Modeling, Identification and Control , 18, 177-217.

Tham, M. T. (2007, June 22). Distillation. (R.C. Costello and Associates, Inc.) Retrieved March 7, 2013 from Newcastle University Swot Shop: http://lorien.ncl.ac.uk/ming/distil/reboil.htm

Wang, Q., Li, X., Wang, L., Cheng, Y., & G. X. (2005). KINETICS, CATALYSIS, AND REACTION ENGINEERING . Kinetics of p-Xylene Liquid-Phase Catalytic Oxidation to Terephthalic Acid (44), 261-266.

Zhao, W., Mou, Q., Zhang, X., Shi, J., Sun, S., & Zhao, C. (2013). Preparation and characterization of sulfocated polyethersulfone membranes by a facile approach. European Polymer Journal (49), 738-751.

APPENDIX A

STEADY STATE SIMULATION RESULT
(DISTILLATION COLUMN 1)

Temperature vs. Stages

	Temperature(°c)
Condenser	23.59
1	24.56
2	26.68
3	30.80
4	37.27
5	44.77
6	50.51
7	53.44
8	54.65
9	55.24
10	55.86
11	57.14
12	61.69
13	63.63
14	64.32
15	64.56
16	64.65
17	64.70
18	64.81
19	65.11
20	66.01
Reboiler	69.00

Flowrate vs. Stages

	Vapor (kgmol/h)	Bulk Liquid (kgmol/h)
Condenser	0.000	429.015
1	518.910	422.338
2	512.233	409.728
3	499.623	391.037
4	480.931	372.445
5	462.340	363.509
6	453.403	363.473
7	453.368	364.958
8	454.852	365.192
9	455.087	363.890
10	453.785	359.889
11	449.783	585.458
12	448.553	592.827
13	455.921	596.843
14	459.938	598.309
15	461.404	598.827
16	461.922	598.856
17	461.951	598.495
18	461.589	597.360
19	460.455	593.947
20	457.042	583.434
Reboiler	446.529	136.905

Composition vs. Stages

	n-Butane	n-Pentane	Benzene
Condenser	0.9756	0.0244	0.0000
1	0.9309	0.0691	0.0000
2	0.8367	0.1633	0.0000
3	0.6690	0.3310	0.0000
4	0.4447	0.5552	0.0001
5	0.2492	0.7504	0.0004
6	0.1427	0.8561	0.0012
7	0.1002	0.8967	0.0030
8	0.0855	0.9071	0.0075
9	0.0810	0.9009	0.0181
10	0.0806	0.8754	0.0440
11	0.0827	0.8083	0.1090
12	0.0296	0.8590	0.1114
13	0.0099	0.8779	0.1121
14	0.0033	0.8843	0.1125
15	0.0011	0.8862	0.1127
16	0.0003	0.8863	0.1133
17	0.0001	0.8849	0.1150
18	0.0000	0.8799	0.1201
19	0.0000	0.8649	0.1350
20	0.0000	0.8194	0.1806
Reboiler	0.0000	0.6781	0.3219

K Values vs. Stages

	n-Butane	n-Pentane	Benzene
Condenser	4.252	1.000	0.473
1	4.252	1.000	0.473
2	4.252	1.000	0.473
3	4.252	1.000	0.473
4	4.252	1.000	0.473
5	4.252	1.000	0.473
6	4.252	1.000	0.473
7	4.252	1.000	0.473
8	4.252	1.000	0.473
9	4.251	1.000	0.473
10	4.250	1.000	0.473
11	4.249	1.001	0.473
12	4.246	1.001	0.473
13	4.240	1.002	0.472
14	4.228	1.005	0.471
15	4.206	1.010	0.469
16	4.165	1.019	0.465
17	4.090	1.040	0.457
18	3.967	1.091	0.444
19	3.931	1.114	0.439
20	3.864	1.187	0.431
Reboiler	3.946	1.492	0.431

APPENDIX B

STEADY STATE SIMULATION RESULT
(DISTILLATION COLUMN 2)

Temperature vs. Stages

	Temperature(°c)
Condenser	62.46
1	62.46
2	62.46
3	62.46
4	62.46
5	62.46
6	62.46
7	62.46
8	62.46
9	62.46
10	62.47
11	62.48
12	62.50
13	62.54
14	62.63
15	62.79
16	63.10
17	63.75
18	65.15
19	65.69
20	67.29
Reboiler	72.39

Flowrate vs. Stages

	Vapor (kgmol/h)	Bulk Liquid (kgmol/h)
Condenser	0.0000	429.0452
1	470.8692	429.0449
2	470.8690	429.0440
3	470.8681	429.0429
4	470.8669	429.0413
5	470.8654	429.0388
6	470.8629	429.0347
7	470.8588	429.0274
8	470.8515	429.0137
9	470.8378	428.9879
10	470.8119	428.9385
11	470.7626	428.8437
12	470.6678	428.6615
13	470.4856	428.3091
14	470.1331	427.6233
15	469.4474	426.2804
16	468.1044	423.6050
17	465.4290	418.1106
18	459.9347	552.8371
19	457.7560	547.0278
20	451.9466	530.4220
Reboiler	435.3409	95.0811

Composition vs. Stages

	n-Butane	n-Pentane	Benzene
Condenser	0.000	1.000	0.000
1	0.000	1.000	0.000
2	0.000	1.000	0.000
3	0.000	1.000	0.000
4	0.000	1.000	0.000
5	0.000	1.000	0.000
6	0.000	1.000	0.000
7	0.000	1.000	0.000
8	0.000	1.000	0.000
9	0.000	1.000	0.000
10	0.000	0.999	0.001
11	0.000	0.999	0.001
12	0.000	0.998	0.002
13	0.000	0.995	0.005
14	0.000	0.991	0.009
15	0.000	0.982	0.018
16	0.000	0.965	0.035
17	0.000	0.931	0.069
18	0.000	0.859	0.141
19	0.000	0.832	0.168
20	0.000	0.753	0.247
Reboiler	0.000	0.537	0.463

K Values vs. Stages

	n-Butane	n-Pentane	Benzene
Condenser	4.252	1.000	0.473
1	4.252	1.000	0.473
2	4.252	1.000	0.473
3	4.252	1.000	0.473
4	4.252	1.000	0.473
5	4.252	1.000	0.473
6	4.252	1.000	0.473
7	4.252	1.000	0.473
8	4.252	1.000	0.473
9	4.251	1.000	0.473
10	4.250	1.000	0.473
11	4.249	1.001	0.473
12	4.246	1.001	0.473
13	4.240	1.002	0.472
14	4.228	1.005	0.471
15	4.206	1.010	0.469
16	4.165	1.019	0.465
17	4.090	1.040	0.457
18	3.967	1.091	0.444
19	3.931	1.114	0.439
20	3.864	1.187	0.431
Reboiler	3.946	1.492	0.431