## A PRECUT COLUMN DESIGN AND CONTROL USING ASPEN

NOR SYAZWANI BINTI SUKRI

UNIVERSITI MALAYSIA PAHANG

BORANG PENC	GESAHAN STATUS TESIS "
JUDUL: A PRECUT COLUMN I	DESIGN AND CONTROL USING ASPEN
SESI PI	ENGAJIAN: <u>2007/2008</u>
Saya NOR SYAZWANI BINTI SUK (HURUF BESAR) mengaku membenarkan kertas projek ini disimpa seperti berikut:	<b>RI</b> n di Universiti Malaysia Pahang dengan syarat-syarat kegunaan
<ol> <li>Hak milik kertas projek adalah di bawah dibiayai oleh UMP, hak miliknya adalah</li> <li>Naskah salinan di dalam bentuk kertas at papulia</li> </ol>	nama penulis melainkan penulisan sebagai projek bersama dan kepunyaan UMP. tau mikro hanya boleh dibuat dengan kebenaran bertulis daripada
<ol> <li>penulis.</li> <li>Perpustakaan Universiti Malaysia Pahan</li> <li>Kertas projek hanya boleh diterbitkan de yang dipersetujui kelak.</li> <li>*Saya membenarkan/tidak membenarkan pertukaran di antara institusi pengajian ti</li> <li>**Sila tandakan ( √ )</li> </ol>	g dibenarkan membuat salinan untuk tujuan pengajian mereka. ngan kebenaran penulis. Bayaran royalti adalah mengikut kadar n Perpustakaan membuat salinan kertas projek ini sebagai bahan nggi.
SULIT (Mer seper	ngandungi maklumat yang berdarjah keselamatan atau kepentingan rti yang termaktub di dalam AKTA RAHSIA RASMI 1972)
TERHAD (Me orga	ngandungi maklumat TERHAD yang telah ditentukan oleh nisasi/badan di mana penyelidikan dijalankan)
TIDAK TERHAD	
	Disahkan oleh
(TANDATANGAN PENULIS) Alamat tetap: G-2 Tingkat 3-G, Jalan Lama Kg Kijing, 21600 Marang,	(TANDATANGAN PENYELIA) Cik Rohaida binti Che Man Nama Penyelia
Terengganu Tarikh: 28 April 2008	Tarikh:
CATATAN: * Potong yang tidak berkenaan. ** Jika tesis ini SULIT atau TERH berkuasa/organisasiberkenaan d sebagai SULIT atau TERHAD. U Tesis dimaksudkan sebagai tesis disertasi bagi pengajian secara ku (PSM).	AD, sila lampirkan surat daripada pihak engan menyatakan sekali sebab dan tempoh tesis ini perlu dikelaskan bagi Ijazah Doktor Falsafah dan Sarjana secara penyelidikan, atau erja kursus dan penyelidikan, atau Laporan Projek Sarjana Muda

"I/We hereby declare that I/We have read this thesis and in my/our opinion this thesis is sufficient in terms of scope and quality for the award of the Degree of Chemical Engineering."

> Signature: ..... Name of Supervisor I: ....ROHAIDA BINTI CHE MAN...... Date: ....

\*Delete as necessary

A PRECUT COLUMN DESIGN AND CONTROL USING ASPEN

### NOR SYAZWANI BINTI SUKRI

A thesis submitted in fulfillment of the requirements for the award of the degree of Bachelor of Chemical Engineering

Faculty of Chemical Engineering & Natural Resources Universiti Malaysia Pahang

**APRIL 2008** 

I declare that this thesis entitled "A Precut Column Design and Control Using ASPEN" is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is concurrently submitted in candidature of any other degree.

> Signature : ..... Name : NOR SYAZWANI BINTI SUKRI Date : ....

To my beloved family, especially to my precious mother and father. You are everything for me and you my entire all

### ACKNOWLEDGEMENT

In order to complete this research, I was in contact with many peoples, researchers, academicians and practitioners. All of them have assisted me in many ways towards completing this research. They also have contributed towards my understanding and thoughts. I would like to express my sincere appreciation to my main supervisors, Miss. Rohaida binti Che Man and Miss Noorlisa binti Harun for their encouragement, guidance, critics and friendship during in finishing my research.

I also would like to thanks the personnel of Faculty of Chemical Engineering and Natural Resource (FKKSA), especially lecturers for their assistance and cooperation. Not forgotten to Dr Chin, Mr Noor Asma Fazli and Mr Izirwan for their advices, motivation and ideas. Without their continued support and interest, this research would not have been the same as presented here.

My sincere appreciation also extends to all my colleagues and others who have provided assistance at various occasions. Their views and tips are useful indeed. Your kindness is really appreciate and always in my mind forever. Thank you.

### ABSTRACT

A pre-cut column from the Palm Oil Fractionation Plant is one approach to the distillation of fatty acids. This research aim to develop dynamic Pre Cut Column model using ASPEN and incorporate control system into distillation column model. The scope of this study is to learn how to use dynamic simulators by simulating Pre Cut Column in steady-state condition and moving to a dynamic simulation, then applying PID (proportional-integral-derivative) control system as an effective control system for continuous processes. For designing the precut column, the method that must be concerned are specifying chemical components and physical properties, specifying stream properties and specifying equipment parameters before running the simulation. PID controllers are the controller of choice for controlling the precut column because PID system is a balancing act with all terms interacting. Integral feedback Element (I) is added to the proportional element to provide a means for eliminating a changing offset in a non linear system and to slow down the reaction to allow for the time delays in the system. Derivative feedback element (D) is added to provide a means of reducing sudden changes in the output and will provide a faster response to step functions and transients. The result was in steady state simulation of precut column and the parameters of controllers were identified from dynamic responses. Dynamic simulation has become increasingly important as processes become more complex and are designed and operated closer to constraints.

### ABSTRAK

Salah satu pendekatan kepada penyulingan asid lemak adalah melalui 'Precut kolom' daripada Pelan Pemecahan Kelapa Sawit. Matlamat projek ini adalah untuk membangunkan dinamik kolom Precut menggunakan ASPEN Model dan menggabungkan sistem kawalan kepada Model kolum penyulingan. Skop pembelajaran ini adalah untuk mempelajari bagaimana menggunakan simulasi dinamik dengan mensimulasikan kolom Precut dalam keadaan fasa tetap dan memindahkan keadaan tersebut kepada fasa dinamik. Selepas itu mengaplikasikan system kawalan 'PID "(proportional-integral-derivative)" sebagai sistem kawalan efektif untuk process berterusan. Bagi rekaan kolom Precut, cara-cara rekaan mestilah diambil kira dari segi menspesifikasikan komponen-komponen kimia dan sifat fizikal, menspesifikasikan sifat aliran serta parameter alatan sebelum menjalankan simulasi. Kawalan PID merupakan pilihan terbaik untuk mengawal kolom Precut kerana sistem PID dapat mengimbangi penetapan dan terma pengaruh. Elemen "Integral" (I) ditambah kepada elemen "Proportional" (P) untuk meghasilkan pertengahan dan mengelakkan perubahan keseimbangan dalam sistem tidak linear serta memperlahankan reaksi untuk memberikan kelambatan masa dalam system. Ini akan mengurangkan 'overshoot' dalam system kawalan Proportional secara praktikal. "Derivative" (D) elemen ditambah untuk menghasilkan pertengahan bagi mengurangkan perubahan yang mendadak pada output serta menghasilkan tindakbalas yang cepat kepada fungsi pergerakan dan sementara. Keputusan terhasil adalah rekaan yang dispesifikasikan dengan alatan diperlukan untuk kolom Precut.dan parameter kawalan diperkenalkan daripada respon dinamik. Simulasi dinamik menjadi semakin penting sejajar dengan proses yang semakin komplek serta rekaan dan operasi yang terbatas.

# TABLE OF CONTENTS

CHAPTER	TITTLE	PAGE
	TITLE PAGE	i
	ACKNOWLEDGEMENT	iv
	ABSTRACT	v
	ABSTRAK	vi
	TABLE OF CONTENT	vii
	LIST OF TABLES	xi
	LIST OF FIGURES	xii
	LIST OF ABBREVIATIONS	xiv

1	INTI	INTRODUCTION	
	1.1	Introduction	1
	1.2	Problem Statement	3
	1.3	Research Objectives	3
	1.4	Scopes of Research	4

## 2 LITERATURE REVIEW

3

2.1	Distill	lation	5
	2.1.1	Application of distillation	6
2.2	Pre- C	Cut Column	7
	2.2.1	Process description of precut column	8
2.3	Dynai	mic simulation	10
2.4	Asper	n software	12
	2.4.1	Aspen dynamics	13
2.5	PID c	ontrol systems	15
	2.5.1	PID controller theory	17
		2.5.1.1 Proportional term	17
		2.5.1.2 Integral term	18
		2.5.1.3 Derivative term	19
		2.5.1.4 Summary	20
2.6	Sensit	tivity analysis	21

MET	HODOLOGY	23
3.1	Introductions	23
3.2	Data collection	24
	3.2.1 The information of Precut column	25
3.3	Simulation process	27
	3.3.1 Steady-state simulation	28

	3.3.1.1 New Simulation Configuration	28
	3.3.1.2 Chemical Components Specifications	29
	3.3.1.3 Stream Properties and Physical Properties Specifications	29
	3.3.1.4 Equipment parameters Specifications	31
	3.3.1.5 Running the Simulation	31
3.3.2	Dynamic Simulation	32
	3.3.2.1 Aspen Dynamics Control	34
	3.3.2.2 Performance evaluation	35
Comp	varison of Simulation Results	36

37

# 4 RESULTS AND DISCUSSION

3.4

4.1	Stead	Steady-state Simulation Using ASPEN Plus	
	4.1.1	Precut Column Description	38
	4.1.2	Steady-state Simulation Results	41
	4.1.3	Comparison Results by ASPEN and Palm Oil Fractionation Plant	46
4.2	Dynai	mic Simulation using ASPEN Dynamics	49
	4.2.1	Tuning	50

		4.2.1.1 Tuning of Distillate Level Controller	51
		(LC1)	
		4.2.1.2 Tuning of Bottom Level Controller (LC2)	54
		4.2.1.3 Tuning of Vent Level Controller (LC1)	57
		4.2.1.4 Summary	59
4.3	Perfor	mance Controller Evaluation	60
	4.3.1	Effect of Set Point Tracking	60
	4.3.2	Disturbance Changes	64

# 5 CONCLUSION AND TECOMMENDATION 67

5.1	Conclusion		67

5.2	Recommendations	68	3

REFERENCES	69

72

# LIST OF TABLES

TABLE NO	TITLE	PAGE

2.1	List of available software for simulation	12
3.1	Specification of the precut column	25
3.2	Components composition and condition of the precut	26
	column	
3.3	Physical property of the fatty acid component	30
3.4	Configuration of controller for flow-driven dynamic	34
	simulation	
4.1	Comparison between actual plant results with simulated	47
	results	

# LIST OF FIGURES

FIGURE NO	TITLE	PAGE
2.1	Schematic diagram of fractionation process	8
2.2	Schematic diagram of pre cut column	10
2.3	A simple feedback system	15
3.1	Flow Chart for Simulated Pre Cut Column	24
3.2	Relation of process input to process output	27
3.3	Aspen Plus startup	28
3.4	Input Stream data	30
3.5	Ready-to-run message	31
3.6	Control Panel	32
3.7	Aspen dynamic flowsheet	33

4.1	Flow diagram steady state simulation of precut column	39
4.2	Information of Control Panel	40
4.3	Graph of Temperature and Pressure Profile	43
4.4	Graph of Mass Flowrate Profile	44
4.5	Graph of Molar Flowrate Profile	45
4.6	Flow Diagram Dynamic Simulation of Precut Column	49
4.7	Distillate Level Controller Response at $Kc=10$ ; $\tau i = 60$	51
4.8	Distillate Level Control Response: (a) $Kc = 12$ ; (b) $Kc = 8$	52
4.9	Distillate Level Control Response: (a) $\tau_i = 72$ ; (b) $\tau_i = 48$	53
4.10	Bottom Level Controller Response at Kc=10; $\tau i = 60$	54
4.11	Bottom Level Control Response: (a) $Kc = 13$ ; (b) $Kc = 7$	55
4.12	Bottom Level Control Response: (a) $\tau_i = 78$ ; (b) $\tau_i = 42$	56
4.13	Pressure Controller Response at $Kc=20$ ; $\tau i = 12$	57
4.14	Pressure Control Response: (a) $Kc = 24$ ; (b) $Kc = 16$	58

4.15	Bottom Level Control Response: (a) $\tau_i = 14.4$ ; (b) $\tau_i = 9.6$	59
4.16	Control performance plots in set point tracking of PC1	61
	a) original set point (sp); b) +20% original sp; c) -20% original sp	
4.17	Control performance plots in set point tracking of LC1 a) original set point (sp); b) +20% original sp; c) -20% original sp	62
4.18	Control performance plots in set point tracking of LC2 a) original set point (sp); b) +20% original sp;c) -20% original sp	63
4.19	Dynamic responses for 5 % disturbances in feed flowrate	65
4.20	Dynamic responses for 5 % disturbances in feed temperatures	66

## LIST OF ABBREVIATION

SYMBOL	DESCRIPTION
e	$\operatorname{Erro}\mathbf{r} = SP - PV$
Iout	Integral output
Iout	Integral output
K <sub>d</sub>	Derivative Gain, a tuning parameter
<i>K</i> <sub><i>i</i></sub> :	Integral Gain, a tuning parameter
$K_p$	Proportional Gain, a tuning parameter
MV	Manipulated Variable
PD	Proportional-Derivative
PI	Proportional-Integral
PID	Proportional-integral-derivative
Pout	Proportional output
PV	Process Variables
QC	Quality Control
SP	Set Point

SSE	steady-state error
t	Time or instantaneous time (the present)
τ	Time in the past contributing to the integral response

**CHAPTER 1** 

### INTRODUCTION

### 1.1 Introduction

Distillation is and will remain in the twenty-first century the premier separation method in the chemical industries. Distillation represents the backbone of what distinguishes chemical engineering and uniquely under the purview of chemical engineers. The analysis, design, operation, control and optimization of distillation columns have been extensively studied for almost a century (Luyben, 2002).

Initially most engineers wrote their own programs to solve both nonlinear algebraic equations that describe the steady-state operation of distillation column and the nonlinear ordinary differential equations that describe its dynamic behavior. The advancements in computer technology provide the very fast computers requirements so; lots of commercial steady-state simulators and dynamic simulators were developed (Luyben, 1990).

Aspen software is a simulation tool for multi-engineering purposes to enable users to develop dynamic models quickly for their processes. Aspen is designed to operate as automatically as possible, while allowing the user to have some control over the Quality Control (QC) methods. For instance, as soon as the user selects a sounding file for processing, the data is brought into Aspen and automatically analyzed. If the processing needs to be modified, the user can change the QC parameters and reprocess the data as many times as necessary.

Dynamic simulation is generally used to make stability, operability and control analysis. So, dynamic simulation is a rational way to consider dynamic interactions and the design of modern control system. It also helps managers and engineers link business operations to process operations. It uses simulation to guide in developing the optimum economic steady-state design of distillation systems. Then it uses simulation to develop effective control structures for dynamic control. Questions are addressed as where to locate temperature control trays and how excess degrees of freedom should be fixed (Luyben, 2006).

The objective of performing the design and control analyses is to optimize the economics of the project in evaluating the enormous number of alternatives. The hierarchical design procedure proposed by Douglas (1988) is a way to approach this task. The control engineer then must devise the control strategies to ensure stable dynamic performance and to satisfy the operational requirements. The objective is to operate the plant in the face of potentially known and unknown disturbances, production rate changes and transition from production to another.

#### **1.2 Problem Statement**

In this work the phenomena consisting on heat and mass transfer occurring in a real column distillation process is translated into a quantitative mathematical model. This is because of the very large number of equations needed for the rigorous description the calculations are made, with the help of a personal computer and by using some integration method. Therefore, the simulator can mimic the nonlinear behavior of that system which can use it as an unknown plant which needs to be controlled.

Process simulation with Aspen Plus allows used to predict the behavior of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium and reaction kinetics. Given reliable thermodynamic data, realistic operating conditions and the rigorous Aspen Plus equipment models, they can simulate actual plant behavior. This application delivers the benefits of dynamic modeling throughout the plant operation and engineering organizations. Increased operability, safety and productivity can be achieved because Aspen Dynamics reproduces the dynamics of real plant operation.

### 1.3 Research Objectives

The main objectives of this research are to develop dynamic Pre Cut Column model using Aspen software and to incorporate control system into distillation column model using Aspen Dynamics.

### 1.4 Scopes of Research

The scopes of the research are:-

- a) To learn how to use dynamic simulators by starting with the basic simulation by simulating Pre Cut Column in steady-state condition. Then go through the learning the basic operations of moving from steady-state simulation to a dynamic simulation.
- b) To develop a process design which are "conceptual design", preliminary design and "detailed design".
- c) Applying PID (proportional-integral-derivative) control system as an effective control system for continuous processes that performs two control tasks.

**CHAPTER 2** 

### LITERATURE REVIEW

### 2.1 Distillation

The separation process known as distillation is a method for separating the various components of a liquid solution which depends upon the distribution of these components between a vapor phase and a liquid phase. All components are present in both phases. The vapor phase is created from the liquid phase by vaporization at the boiling point (Geankoplis *et al.*, 2003).

Distillation accounts for approximately 95% of the separation system used by the refining and chemical industry (Hurowitz *et al.*, 2003). It has a major impact upon the product quality, energy consumption and plant throughout of these industries. Maintaining the product quality within specification is the usual policy in industry and it is very difficult to control the process at the desired target. The sensitivity of product quality to disturbances decreases as impurities are reduced. According to Shinskey (1984), 40 percent of the energy consumed in the plant allocated to distillation. Distillation columns are fairly complex units. Their dynamics are a mixture of very fast liquid flowrate changes, slow temperature changes and very slow composition changes. The manipulated variables often have constraints because of column flooding limitations or heat exchanger limitations (Luyben, 2002).

Distillation control is a challenging endeavor due to (Hurowitz et al., 2003):

- a) The inherent nonlinearity of distillation.
- b) Severe coupling present for dual composition control.
- c) Non-stationary behavior.
- d) The severity of disturbances.

More work has appeared in the chemical engineering literature on distillation column control than on any other unit operation. The long term popularity of distillation control is clear evidence that this is a very important and challenging area of process control. Most chemical plants and all petroleum refineries use distillation columns to separate chemical components. Distillation is undisputed king of the separation processes (Luyben *et al.*, 1999).

#### 2.1.1 Application of Distillation

Distillation is a method of separating chemical substances based on differences in their volatilities in a boiling liquid mixture. Distillation usually forms part of a larger chemical process, and is thus referred to as a unit operation.

Commercially, distillation has a number of uses. It is used to separate crude oil into more fractions for specific uses such as transport, power generation and heating. Water is distilled to remove impurities, such as salt from sea water. Air is distilled to separate its components notably oxygen, nitrogen and argon for industrial use. The use of distillation on fermented solutions to produce distilled beverages with higher alcohol content is perhaps the oldest form of distillation, known since ancient times (Banks, 1998).

The application of distillation can roughly be divided in four groups: laboratory scale, industrial distillation, distillation of herbs for perfumery and medicinal (herbal distillate) and food processing. The latter two are distinct from the former two, in that in the distillation is not used as a true purification method, but more to transfer all volatiles from the source materials to the distillate. Large scale industrial distillation applications include both batch and continuous fractional, vacuum, azeotropic, extractive and steam distillation. The most widely used industrial applications of continuous, steady-state fractional distillation are in petroleum refineries, petrochemical and chemical plants and natural gas processing plants.

#### 2.2 Precut Column

Different approaches to the distillation of fatty acids have been reported in literature and patents and have successfully been practiced in the production scale. The aims of the existing technologies is to separate different kinds of by-products from the fatty acids, namely partial glycerides from incomplete fat splitting and other high boilers, metals (e.g. from catalysts), color bodies and odor substances.

The present invention provides a new process for obtaining fatty acids with improved color, odor and heat stability. In a first step the crude acids are fed to a precut column in order to remove low boiling by-products being present in the starting material as a top fraction. In a second step the bottom fraction of the precut rectification column is fed to a sidestream column in order to obtain the pure fatty acids as the side fraction, to remove low boiling by-products which have been formed in the course of the first distillation as a top fraction and to remove high boiling by-products, either being present from the starting material or formed during the first distillation, with the residue. Preferably, the precut rectification column and the side column each comprise a rectifying section and a stripping section. (Lausberg and Nataly, 2006).

### 2.2.1 Process Description of Precut Column

The Fatty Acid fractionation unit consists of a Precut column, Light Cut column, Middle Cut column, Still and Residue Still connected in series. The feed to the plant is either Palm Kernel Oil (PKO) or Palm Stearine. All the distillation columns operate at highly vacuum condition generated using steam ejectors. The columns are packed with structured packing to provide the desired separation properties. The schematic diagram of the plant is presented in the Figure 2.1.



Figure 2.1: Schematic diagram of fractionation process

The Dehydrated Crude Fatty Acid (DCFA) from PKO contains all fatty acid fractions from C6 to C18, plus a residue. The various fractions are separated into the following components:

- a) C10 and lighter cut, recovered as distillate in the Precut Column
- b) C12 cut, recovered as distillate in the Light Cut Column
- c) C14 cut, recovered as distillate in the Middle Cut Column
- d) Mixed C16 and C18 cut, recovered as distillate in the Still
- e) Pitch, recovered as bottoms in the Residue Still (the Residue Still Distillate being recycled to the Still).

A pre-cut column from the Palm Oil Fractionation Plant is chosen as a study column. The hydrogenated DCFA feed from the Hydrogenated Unit or from storage is filtered and heated successively by DCFA in a preheater and by hot oil in a feed heater and put through a dryer-deaerator where air and water are removed by vacuum. It is then flashed into the Precut column. The vapours, consisting of C6, C8 and C10 fractions, are condensed by direct contact in the pumparound section of the column. The condensed distillate is pumped by the reflux pump and cooled by cooling water in the condenser before being returned to the top of the pumparound section. Part of the hot distillate is sent as reflux to the rectification section of the column. The net distillate is pumped to storage under level control. The bottoms are pumped by the bottom pump and heated by the hot oil, under pressure to suppress vaporization in the reboiler. The net bottom product is pumped, to the Lights Cut Column. Vacuum is maintained at the top of the column by the second stage of the Precut column ejector. Figure 2.2 shows schematic diagram of precut column (Chen, 2005).



Figure 2.2: Schematic diagram of pre cut column

#### 2.3 Dynamic Simulation

Simulation is the construction and use of a computer- based representation or *rigorous model*, of some part of real world as a substitute vehicle for experimental and behavior prediction. Digital simulation is recognized as a powerful tool for solving the equations that represent a real system. Over the years specialist simulation software has been developed and is extensively marketed by commercial organizations. In theory, these simulation languages relieve the engineer of knowing anything about numerical integration. Therefore, these packages make it easier for the engineer to set up and solve the problems (Basualdo, 1990).

Dynamic Simulation has become increasingly important as processes more complex and are designed and operated closer to constraints. Increasing yields and suppressing the formation of undesirable and environmentally friendly by-products are often achieved by using complex flow sheets with many recycle streams. Increasing energy costs keep pushing design engineers towards more heat integration. All of these trends make dynamic control more difficult and dynamic simulation more important (Luyben, 2002).

Ideally the dynamics of the process should be considered at very early stages of the development of a process. Certainly at the pilot-plant stage, trade-offs between design and control should be explored, and basic regulatory control structure should be developed and tested. The engineering time expended at the early stages can reap enormous economic benefits later in the project in term of rapid, trouble-free startups, reduced product-quality variability, less-frequent emergency shutdowns, reduced environmental contamination and safer operation.

The purpose with the dynamic simulations is to make a comparison with the real experiments. This comparison can only be made if the simulation and real experiments experience the same condition. Dynamic plant simulation is a powerful tool that helps engineers and managers link business operations to process operations and faces the challenging as state above.

Process engineers routinely address difficult manufacturing and production issues. Unfortunately, experience alone is not always sufficient to answer the questions that continually arise and 'trial and error' efforts to provide meaningful insight are usually cost-prohibitive if not occasionally risky.

For most companies the benefits of using simulation go beyond simply providing take a look into the future. These benefits are mentioned by many authors (Banks *et al.*, 1996; Law and Kelton, 1991; Pegden *et al.*, 1995 and Schriber, 1991).

#### 2.4 Aspen Software

Lots of different digital simulation software packages are available on the market. Modern tools are numerically powerful, highly interactive and allow complicated types of graphically and numerical output. Many packages also allow optimization and parameter estimation. Table 2.1 below listed some of the available software that can be used for simulation process. This software were discussed by Banks (1998).

SOFTWARE	COMPANY
AspenPlus/AspenDynamics	Aspen Technology
HYSIS	Hyprotech Inc.
Dymola	Dynasim
GPSS/H	Wolvrine Software Corporation
SLX	Wolvrine Software Corporation
SIMSCRIPT II.5	CACI Products Company
AweSim	Symix (formerly Pritsker Corporation)
SIMPLE++	AESOP Corporation
Extend	Imagine That Inc.

**Table 2.1:** List of Available Software for Simulation

There are several commercial software packages that have dynamic capability. The two most widely used are "HYSIS" from Hyprotech Inc. and "AspenPlus /AspenDynamic" from Aspen Technology. But justAspenPlus /AspenDynamic simulator will be used in this project.

For the dynamic simulation using Aspen software, dynamics products enable comprehensive dynamic plant modeling to evaluate design for profitability, operability, safety, and to improve existing plant operation over their lifecycle. By linking dynamic modeling, fast start-ups, optimum feed switch strategies, detailed unit and plant wide performance improvements, and optimal safety of the plant, can be accomplished. Although these simulators are far from perfect, they do provide a reasonably effective tool for studying process dynamics (Luyben, 2002).

#### 2.4.1 Aspen Dynamics

Aspen Dynamics complements the steady-state simulation capabilities of Aspen Plus and delivers the benefits of dynamic modeling to the Petrochemicals, Chemicals, and Specialty Chemicals industries throughout plant operation and engineering organizations.

In the chemical process industries, operational efficiencies, production economies, product quality and, ultimately, bottom line performance can be adversely affected by a multitude of factors. Many of these factors are extremely complex and subject to varying degrees of unpredictability. To avoid production delays, downtime or off-spec product, process manufacturers require cost-effective tools that help identify and correct anticipated problems before they occur.

To understand the dynamic behavior of a complex chemical process, process manufacturers require a dynamic process simulator. Aspen Dynamics is a state-ofthe-art solution designed specifically for dynamic process simulation. Aspen Dynamics is tightly integrated with Aspen Plus AspenTech steady-state simulator for the chemical process industries. This integration enables users to use an existing Aspen Plus steady-state simulation and quickly create a dynamic simulation. This enables users to fully leverage their existing investments in steady-state Aspen Plus models and ensures consistency with their steady-state simulation results. Aspen Dynamics is built upon proven technologies, with more than 20 years experience supplying dynamic simulation tools to the chemical process industries and provides the following features (AspenTech, 1994):

- 1. 3-phase and reactive distillation, including user-specified reaction kinetics.
- 2. Rigorous modeling of distillation column hydraulics and pressure drop for both tray and packed columns.
- 3. Vapor holdup modeling that ensures accurate results for high-pressure processes (including processes with high-pressure distillation columns) and applications such as pressure relief.
- 4. Option to choose simpler flow-driven simulations or more rigorous pressuredriven simulations. Pressure-driven simulations relate the flows around the flowsheet to the pressures in each unit operations. This capability is essential for simulation of pressure relief, steam networks, compressor systems and many other applications.
- 5. Usage of the physical property models and data available in Aspen Properties "AspenTech<sup>TM</sup>s physical property system" to facilitate consistent use of properties across the enterprise. Dynamic simulations use continuously updated local property correlations to deliver high performance without loss of accuracy.
- Support for polymer processes via Polymers Plus<sup>®</sup> "AspenTech<sup>™</sup>s generalpurpose polymer process modeling system.
- Open models created using Aspen Custom Modeler® "AspenTech™s model authoring technology " to enable companies to capture their specific expertise and proprietary knowledge.
- 8. Several models and other features for simulation of pressure relief systems, including pipe, bursting disk and pressure safety valve models. The stirred tank reactor can model frothing and liquid carryover in the relief.
- 9. Advanced, equation-based solution techniques and state-of-the-art numerical methods to ensure fast, reliable and accurate simulation solutions. The implicit integrator ensures stable solution of the dynamic simulation and varies the integration step to ensure accuracy while maximizing performance.
- 10. A dynamic optimizer for quick and easy dynamic optimization of conventional unit operations and processes.

With applications across the chemical process manufacturing lifecycle, Aspen Dynamics helps companies improve productivity and profitability. Its dynamic models are useful throughout the operational life of the plant, thus extending the value of engineering completed during the design phase. Aspen Dynamics supports concurrent process and control design, which helps reduce capital costs, lower operating costs, improve plant safety and prevent control problems.

#### 2.5 PID Control Systems

PID is an enhanced feedback system designed to determine the overall system behavior. A simple feedback system comprises a single feedback path and is proportional only as shown in Figure 2.3.



Figure 2.3: A simple feedback system

Feedback systems are used to reduce or eliminate errors. In a typical PID installation, a set point and the PID feedback systems works to keep the output value equal to the setpoint value. It is possible for the setpoint value to be a changing value, but this can add complication. An ideal system would have a linear transfer function, zero phase shift and zero delay. Under these conditions, a proportional control is all that is needed. A real world system commonly has a non linear transfer function (pumping is a classic case) and there can be a considerable delay between the "action" and the "reaction" (measured value). If a purely proportional control is

applied under these conditions, there will be overshoot and oscillations and it will not be possible to achieve a stable output over the whole control range.

The PID controller is a three term controller incorporating a Proportional feedback element (P), an Integral feedback Element (I) and a Derivative feedback element (D). The Integral element is added to the proportional element to provide a means for eliminating a changing offset in a non linear system, and to slow down the reaction to allow for the time delays in the system. This will reduce the overshoot experienced in the practical proportional control system. The derivative element is added to provide a means of reducing sudden changes in the output and will provide a faster response to step functions and transients (Seborg, *et al.*, 2004).

Setting up a PID system is a balancing act with all terms interacting. Excessive Integral gain will slow the response rate excessively and may result in the output moving with load changes. Insufficient integral gain will cause the output to overshoot and oscillate around the set point. Excessive derivative gain will result in instability with severe oscillation around the set point. The derivative gain should be used sparingly to improve transient performance, and is best added in only after the proportional and integral gains have been set for best performance. The derivative gain can then be slowly increased to the point of best stability of the output.

In theory, a controller can be used to control any process which has a measurable output, process variables (PV), a known ideal value for that output, set point (SP) and an input to the process, manipulated variable (MV) that will affect the relevant PV. Controllers are used in industry to regulate <u>temperature</u>, <u>pressure</u>, <u>flow rate</u>, <u>chemical</u> composition, level in a tank containing fluid, <u>speed</u> and practically every other variable for which a measurement exists. Due to their long history, simplicity well grounded theory and simple setup and maintenance requirements, PID controllers are the controller of choice for many of these applications (Seborg *et al.*, 2004).

#### 2.5.1 PID Controller Theory

The PID control scheme is named after its three correcting terms, whose sum constitutes the output. Hence:

$$Output(t) = Pout + I out + D out$$
  
(2.1)

Where  $P_{out}$ ,  $I_{out}$ , and  $D_{out}$  are the contributions to the output from the PID controller from each of the three terms, as defined in the next section (Seborg *et al.*, 2004).

#### 2.5.1.1 Proportional Term

The proportional term makes a change to the output that is proportional to the current error value. The proportional response can be adjusted by multiplying the error by a constant  $K_p$ , called the proportional gain.

The proportional term is given by:

$$P out = K_p e(t)$$
(2.2)

Where

- *P*<sub>out</sub>: **Proportional output**
- *K<sub>p</sub>*: **Proportional Gain**, a tuning parameter
- $e: \mathbf{Error} = SP PV$
- *t*: **Time** or instantaneous time (the present)
A high proportional gain results in a large change in the output for a given change in the error. If the proportional gain is too high, the system can become unstable (See the section on Loop Tuning). In contrast, a small gain results in a small output response to a large input error, and a less responsive (or sensitive) controller. If the proportional gain is too low, the control action may be too small when responding to system disturbances.

In the absence of disturbances pure proportional control will not settle at its target value, but will rather move towards the setpoint, but will retain a steady state error that is a function of the proportional gain and the process gain. Despite the steady-state offset, both tuning theory and industrial practice indicate that it is the proportional term that should contribute the bulk of the output change (Seborg *et al.*, 2004).

### 2.5.1.2 Integral Term

The contribution from the integral term is proportional to both the magnitude of the error and the duration of the error. Summing the instantaneous error over time (integrating the error) gives the accumulated offset that should have been corrected previously. The accumulated error is then multiplied by the integral gain and added to the controller output. The magnitude of the contribution of the integral term to the overall control action is determined the integral gain,  $K_i$ .

The integral term is given by:

$$I_{\text{out}} = K_i \int_0^t e(\tau) \, d\tau \tag{2.3}$$

Where

- *I*<sub>out</sub>: **Integral output**
- *K<sub>i</sub>*: Integral Gain, a tuning parameter
- $e: \mathbf{Error} = SP PV$
- τ: **Time** in the past contributing to the integral response

The integral term (when added to the proportional term) accelerates the movement of the process towards setpoint and eliminates the residual steady-state error that occurs with a proportional only controller. However, since the integral term is responding to accumulated errors from the past, it can cause the present value to overshoot the setpoint value (cross over the setpoint and then create a deviation in the other direction). For further notes regarding integral gain tuning and controller stability, see the section on Loop Tuning (Seborg *et al.*, 2004).

### 2.5.1.3 Derivative Term

The rate of change of the process error is calculated by determining the slope of the error over time (i.e. its first derivative with respect to time) and multiplying this rate of change by the derivative gain  $K_d$ . The magnitude of the contribution of the derivative term to the overall control action is determined the derivative gain,  $K_d$ .

The derivative term is given by:

$$D_{\text{out}} = K_d \frac{de}{dt}$$
(2.4)

Where

- *D*<sub>out</sub>: **Derivative output**
- *K<sub>d</sub>*: **Derivative Gain**, a tuning parameter
- $e: \mathbf{Error} = SP PV$
- *t*: **Time** or instantaneous time (the present)

The derivative term slows the rate of change of the controller output and this effect is most noticeable close to the controller setpoint. Hence, derivative control is used to reduce the magnitude of the overshoot produced by the integral component and improve the combined controller-process stability. However, differentiation of a signal amplifies noise in the signal and thus this term in the controller is highly sensitive to noise in the error term, and can cause a process to become unstable if the noise and the derivative gain are sufficiently large (Seborg *et al.*, 2004).

### 2.5.1.4 Summary

The output from the three terms, the proportional, the integral and the derivative terms are summed to calculate the output of the PID controller. Then defining u(t) as the controller output, the final form of the PID algorithm is:

$$u(t) = K_p e(t) + K_i \int_0^t e(\tau) \, d\tau + K_d \frac{de}{dt}$$
(2.5)

and the tuning parameters are

- 1.  $K_p$ : *Proportional Gain* Larger  $K_p$  typically means faster response since the larger the error, the larger the feedback to compensate. An excessively large proportional gain will lead to process instability.
- 2.  $K_i$ : *Integral Gain* Larger  $K_i$  implies steady state errors are eliminated quicker. The trade-off is larger overshoot: any negative error integrated during transient response must be integrated away by positive error before we reach steady state.
- 3.  $K_d$ : **Derivative Gain** Larger  $K_d$  decreases overshoot, but slows down transient response and may lead to instability.

#### 2.6 Sensitivity Analysis

Fatty acids production important process in the Palm Oil Fractionation Plant, whose process flowsheets consist of a Precut column followed by a sequence of fractionation columns. In general, Pre Cut column has a complex behavior, such as high non-linearity due to complex kinetics and thermodynamic models, strong inputoutput interactions, steady state multiplicity, high potential to instability, sensitivity to disturbances, etc. However, the complexity of the Pre Cut column process is known to create unusual responses to changes in operating variables.

Many of these effects are related to the phenomenon of multiplicity of steady states (which occurs as either input or output multiplicity) and have significant implications on the effectiveness of operability and control schemes. On the other hand, from a thermodynamic point of view, as the driving force is increased, the separation becomes easier, the energy consumption is reduced and the control requirement becomes easier. Moreover from a control point of view, it is reported that passive systems are easy to control and a passive state, in chemical processes, is related to state of minimum entropy production (Coffey *et al.*, 2000). Thus, analyses of both steady state and dynamic behavior, together with thermodynamics concepts, facilitate the studies related to process operation, control, monitoring and optimization of the plant.

Young and Yan (1991) present a preliminary study of the sensitivity analysis for dynamic systems with emphasis on its applications to structural control. Definitions are first given for different sensitivity functions in the time and the frequency domains. Since most physical quantities of dynamic systems cannot be expressed in analytical forms, he introduces an indirect approach to determine their sensitivity derivatives from the sensitivity equations derived from governing equations. A direct application of the sensitivity analysis can be found in the integrated control and optimization in which design variables and control variables are treated equally as the system parameters active in optimization. An extensive review and evaluation of the existing techniques in this area are given to identify a feasible algorithm for future improvements. Finally, a new control algorithm, called optimization based instant control, is proposed for those systems subjected to general deterministic or random excitations. Unlike the conventional algorithm, the optimal control is designed and implemented according to instant information of the excitations. The important feature of this approach is that the original optimal control becomes a problem of static parameter optimization. **CHAPTER 3** 

## METHODOLOGY

### 3.1 Introduction

Every simulation study begins with a statement of the problem. The task is recognizing, which is to develop a dynamic simulation of Pre Cut Column. The first step of simulation process is gathering or collecting data for each of the equipment and operation condition that will be used in the simulation. These data are very important, because it will be filled in the dialog box during the simulation process. This simulation will be run in Aspen Software. Later the control system is installed into distillation column model. Figure 3.1 is the summary of the methodology of the project. Finally, all the process and the achievement results will be recorded in a report.



Figure 3.1: Flow chart for Simulated Pre Cut Column

## **3.2 Data Collection**

Firstly, data will be collected from a manufacturing company from Palm Oil Industry and has the information that will be needed for the input parameters to the model. These raw data will provide a basis for establishing the model's input parameters and will help identify those input parameters requiring more precise data collection. The data that needed here is one that related to the equipment that we used in the simulation process. This information data is the variables that use in the Pre Cut Column such as plate spacing, number of actual tray, actual feed position and etc.

# 3.2.1 The Information of Pre Cut Column

The summaries of the specification of the precut column, components composition and condition are presented in Table 3.1 and 3.2 respectively.

Variables	Specification		
Number of actual tray	28		
Actual feed position	Tray 14 from the top		
Plate spacing	50 cm		
Plate diameter	120 cm		
Plate type	Sieve tray		
Type of reboiler	Total		
Reflux rate	10 kmol/hr		
Pumparound rate	49.6 kmol/hr		
Sidedraw rate	63.6 kmol/hr		
Reboiler duty	2.158 x 10 <sup>6</sup> kJ/hr		
Weir length	0.912 m		
Weir height	0.076 m		

 Table 3.1: Specification of the precut column

Component	Composition (kmol/kmol)			
	Feed stream	Distillate stream	Bottom stream	
Hexanoic acid, C-6	0.002	0.023	0	
(Caproic acid)				
Octanoic acid, C-8	0.051	0.528	0	
(Caprylic acid)				
Decanoic acid, C-10	0.043	0.438	0.001	
(Capric acid)				
Dodecanoic acid, C-12	0.518	0.006	0.574	
(Lauric acid)				
Tetradecanoic acid, C-14	0.156	0	0.173	
(Myristic acid)				
Hexadecanoic acid, C-16	0.068	0	0.075	
(Palmitic acid)				
Stearic acid, C-18	0.014	0	0.013	
Oleic acid, C-18-1	0.121	0	0.134	
Linoleic acid, C-18-2	0.020	0	0.023	
Tempeture	483.15 K	442.55 K	509.55 K	
Pressure	2.5 bar	0.11 bar	0.13 bar	

 Table 3.2: Components composition and condition of the precut column

#### 3.3 Simulation Process

The goal of dynamic simulation is to be able to relate the dynamic output response of a system to the form of the input disturbances, in such a way that an improved knowledge and understanding of the dynamic characteristics of the system obtained. Figure 3.2 shows the relation of a process input disturbance to a process output response based on discussed by Ingham *et al.*, (2000).



Figure 3.2: Relation of process input to process output

The block will interact through its 'dialog box'. The dialog box is a window shown by clicking twice on the graphic or 'Icon' of the block. The dialog box can contain variables, buttons, checkboxes, control buttons, data tables, as well as text. These variables, buttons, and others can be changed by us by typing in new values or by pointing and clicking with the mouse. A third layer, which normally would be invisible to us, is the source code. Variables in the dialog box as well as variables received from other blocks are all available to the source code. A simulation can also write variables to a report file and or debugging file. So that, the input can be modify, insert new model blocks and view results dynamically all without having to enter or even see a line of code. Actually, there is another stage before doing a dynamic simulation. The stage here is steady-state simulation.

### 3.3.1 Steady-state Simulation

First thing that need to do in simulation is by opening up a blank flowsheet by going to Start and Programs and then clicking sequentially on Aspen Tech, Aspen Engineering Suite, Aspen Plus 12.1, and Aspen Plus User Interface.

## **3.3.1.1** New Simulation Configuration

Selecting the Blank Simulation button and clicking OK opens up the blank flowsheet shown in Figure 3.3. The page tabs along the bottom let us choose which unit operation to place on the flowsheet. We are going to need a distillation column, pumps, and control valves.



Figure 3.3: Aspen Plus startup

#### **3.3.1.2 Chemical Components Specifications**

Feedstock to the process consists of caproic acid (C6), caprylic acid (C8), capric acid (C10), lauric acid (C12), myristic acid (C14), palmitic acid (C16), stearic acid (C18), oleic acid (C18-1), linoleic acid (C18-2) and residue. Due to the non-conventional nature of the fatty acid distillation system, the development of the required flowsheet for plant simulation requires some modifications. But by using the updated version of Aspen Plus (Aspen Plus 12.1) the long-chained fatty acid, caprylic acid (C8) is available within the Aspen Component Properties Library. The residue of the feedstock is ignored in this simulation and considered as heavy component by replacing it by oleic and linoleic acid. Moreover, only a little amount of residue is contained in the feedstock.

To start specifying chemical components, go to the toolbar at the top of the window and click the fourth item from the left *Data*. This opens the *Data Browser* window that is used to look all aspects of the simulation. It is used to define components, set physical properties, and specify the parameters of the equipment.

### **3.3.1.3 Stream Properties and Physical Properties Specifications**

The input streams of the process must be specified. Here, MW is the molecular weight, Tb is the boiling point temperature,  $\rho$  is density,  $\delta$  is surface tension, and  $\eta$  is viscosity as shown in Table 3.3. Clicking Streams and then Input opens the windows shown in Figure 3.4.

Component	MW	T <sub>b</sub> (°C)	$\rho(kg/m^3)$	$\delta(mN/m)$	η(cP)
Caproic Acid, C6	116.16	202.00	923.80	26.60	2.53
Caprylic Acid, C8	144.22	237.50	906.40	27.70	5.16
Capric Acid, C10	172.27	268.40	1017.60	28.40	5.37
Laurie Aeid, C12	200.32	299.20	1009.90	28.10	7.30
Myristic Acid, C14	228.38	318.00	1002.00	28.40	7.48
Palmitic Acid, C16	256.43	353.80	1025.00	28.20	7.80
Stearic Acid, C18	284.49	370.00	1025.00	28.90	9.04
Oleic Acid, C18-1	282.47	360.00	887.00	35.20	9.41
Linoliec Acid, C18-2	280.45	355.00	902.50	-	-

 Table 3.3: Physical property of the fatty acid component



Figure 3.4: Input stream data

### **3.3.1.4 Equipment Parameters Specifications**

The parameters for all the equipment must be specified. Clicking on Blocks on the left side of the Data Browser windows produces a list of all the blocks that must be handled. The equipments that must be specified are Column Precut, valves and pumps.

#### 3.3.1.5 Running the Simulation

The blue N button ("next") at the top of the Data Browser window on the far right is clicked to run the simulation. If everything is ready to calculate, the message shown in Figure 3.5 will appear, and should click OK. The Control Panel window shown in Figure 3.6 opens and indicates that the column was successfully converged.



Figure 3.5: Ready-to-run messages

iii Control Panel	the second s	-12
> I H E Solve	1 1 1	
E-D Calculation Sequence	->Calculations begin	4
-B P12	Bincks V1 Bodel: VALVE	
- B P11	Blocke CT Robell RADFRAC	
- II VII	Convergnment iterationed : 06 ML TL KryfTol 2 1 3 20,225 2 1 5 5,9405 4 1 3 0,820515-01 Binchs F13 Rodel: FIMP Binchs F13 Rodel: FIMP Binchs F13 Rodel: FIMP	
	Dinck: Vii Bodwi: VALVE	
	Diocks Fil Rodel: FIRP	
	Diock: 712 Rodel: FURP	
	-s8imulation calmulations completes	
Xome¥]		

Figure 3.6: Control Panel

### 3.3.2 Dynamic Simulation

The steady-state simulation does not need information that has no effect on steady-state results such as sizes of control valves and others. However, the dynamic simulation does need this information because the dynamic response of a process unit depends on size of the equipment. The time constant of the system is dictated by its size, relative to the flowrate, volume or mass, etc.

There are two types of dynamic simulations that are "Flow Driven Dyn Simulation" and "Pressure Driven Dyn Simulation". In this project it will only consider Flow Driven Dyn Simulation. When first starting Aspen Dynamics, there is no simulation information and will start with a blank simulation. The following diagram shows the three windows of Aspen Dynamics as shown in Figure 3.7.



Figure 3.7: Aspen Dynamics flowsheet

There are several steps that must be done in order to do dynamic simulation. So those, the first step that need to do by exporting the steady-state into dynamic simulation. Below are the steps to save into Flow Driven Dyn Simulation file:

- 1. Click Export from file tab.
- Type the file name for example "filename.dynf" and save it as "F Driven Dyn Simulation".

The "export" is successful, and ready to go to Aspen Dynamics.

After that, to run this dynamic simulation, the Process Flowsheet Window will be developed. The Simulation Message window where the progress of the simulation is shown and simulation time is displayed. Below are the steps to run the dynamic simulation:

- 1. Make an "initialization" run to ensure that everything is running. Select Initialization and click the Run button.
- 2. Changing from Initialization back to Dynamic to make sure that the integrator is working properly. Then, click the Run button again.

Then, the dynamic simulation now can be run.

### 3.3.2.1 Aspen Dynamics Control

When an Aspen Dynamics simulation is created, level, pressure and temperature controllers are automatically included where appropriate. For flowdriven dynamic simulations, these controllers are configured as shown in Table 3.4.

**Table 3.4:** Configuration of controller for flow-driven dynamic simulation

For this type of control	This type of controller is used	To directly manipulate	
Liquid level	Proportional only	Liquid flow rate	
	roportionar only	Elquid no il fato	
Pressure	Proportional integral	Vapor flow rate or duty, as	
		appropriate	
Temperature	Proportional integral	Duty	

The initial flowsheet has some default controllers already installed. The action of the controller, the range of the pressure transmitter, the maximum heat removal, and the controller tuning constants are all setup at some nominal values. But this indicates the number of items that must be specified for each new controller that added to the flowsheet. At the minimum, four additional controllers must be added to achieve effective operation in the column:

- a) Temperature indicator controller
- b) Flow indicator controller
- c) Level indicator controller
- d) Pressure indicator controller

Each automatically-generated controller has a Process variable, Operator set point, and Controller output whose values are calculated from the steady-state results of the Aspen Plus run. Each controller also has its own tuning parameters such as gain, integral time, derivative time, and so on. For each controller block, Aspen Dynamics has an associated results table that displays the values of the process variable, set point and output.

### **3.3.2.2 Performance Evaluation**

A disturbance is made and the transient response are plotted to see how well the alternative control structures developed perform in the face of disturbances, specifically how close to the desired values of temperature and composition these variables are maintained. So, the first thing to do is set up a plot or a stripchart. This will show how the variables of interest change dynamically with time.

Although these Aspen Dynamics plots are useful to see what is going on during each run, they have a fixed structure (multiple variables per plot) and do not permit comparison of results from different runs. Fortunately, this is easily handled by storing the data in a file and then producing own plots using favorite plotting software. To store the data, right click the plot and select *Show as History*.

## 3.4 Comparison of Simulation Results

In order to validate either this simulation data can represent the actual process, the comparison between simulation and industrial data will carry out. The results obtained will be suggested that the model adequately represent the selected distillation column

**CHAPTER 4** 

## **RESULTS AND DISCUSSION**

## 4.1 Steady-state Simulation Using Aspen Plus

The plant simulation was carried out using Aspen Plus, a commercial simulator having both the steady state and dynamic simulation capabilities. The flowsheet was generated based on a standard P&I Diagram of a Fatty Acid Plant and validated against typical plant data obtained from a local plant. In Chapter 3, Aspen Plus is used to tabulate the data and results of precut column flow sheet. Process simulation with Aspen Plus allows predicting the behavior of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium and reaction kinetics. Given reliable thermodynamic data, realistic operating conditions and the rigorous Aspen Plus equipment models, actual plant behavior can be simulated. Aspen Plus can help to design better plants and increase profitability in existing plants. (Luyben, 2006).

#### 4.1.1 Precut Column Description

From the methodology in previous chapter, the result that can get is the flow sheet that fully specified as shown in Figure 4.1.

Typically, the simulation process takes the following stages:

- (i) Preparation Stage
- a) Selecting the thermodynamic model
- b) Defining chemical components
- (ii) Building Stage
- a) Adding and defining streams
- b) Adding and defining unit operations
- c) Connecting streams to unit operations
- d) Installing valves and controllers
- (iii) Execution Stage
- a) Starting integration

Summarizing, the distillation of precut column is accomplished by the following steps: The fatty acid mixtures, caproic acid (C6), caprylic acid (C8), capric acid (C10), lauric acid (C12), myristic acid (C14), palmitic acid (C16), stearic acid (C18), oleic acid (C18), and linoleic acid (C18) enter the precut column in liquid form at tray 14. The light components (C6-C10) are condensed by direct contact in the pumparound section and recovered as distillate. Then, the distillate product is pumped to storage. The heavy components (C12-C18) recovered at the bottom of the precut column. These components will be passed to other system in the fractionation unit for further fractionation process. (Noorlisa, 2005).



Figure 4.1: Flow diagram steady state simulation of precut column

### Aspen Unit Operations Blocks and streams

Following is a description of each ASPEN Unit Operations Block in the simulation.

- T101 Precut column DI Distillate stream
- V101 Valve at distillate stream B Bottom stream
- V102 Valve at bottom stream V Vent stream
- V103 Valve at vent F Feed stream
- P101 Pump at distillate stream
- S101, S102, S103, S104 Connection stream to distillate, bottom and vent stream

When all the items in the Data Browser window are blue, so the simulation is ready to run. The Control Panel window opens and means that it has take 14 iterations to converge. Convergence of the Aspen simulation is accomplished through a nested Convergence Blocks, both employing the bounded Wegstein method with relative tolerances of 0.0001 as shown in Figure 4.2.

<< Loading S	Simu	ulation	n Engine 15:07:22 Wed Apr 9, 2008>>		
->Processing input specifications					
Flowsheet An	Flowsheet Analysis :				
COMPUTATION C	RDEF	FOR TH	HE FLOWSHEET:		
T101 V103 P10	1 V1	LO1 V102	2		
->Calculations	beg	jin			
Block: T10	1	Model	1: RADFRAC		
Converg	ence	e iterat	tions:		
OL	ML	IL	Err/Tol		
1	1	10	776.93		
2	1	10	4748.7		
3	1	9	2381.4		
4	1	6	2099.9		
5	1	10	2034.0		
6	1	3	1146.8		
7	1	2	373.91		
8	1	1	208.69		
9	1	2	96.778		
10	1	1	32.175		
11	1	2	7.8689		
12	1	2	2.5551		
13	1	1	1.1305		
14	1	1	0.17732		
Block: V10	3	Model	1: VALVE		
Block: P10	1	Model	1: PUMP		
Block: V10	1	Model	1: VALVE		
Block: V10	2	Model	1: VALVE		
->Generating block results					
Block: P10	1	Model	1: PUMP		
->Simulation c	alcı	lations	s completed		

Figure 4.2: Information of Control Panel

#### 4.1.2 Steady-state Simulation Results

Aspen Plus solves the critical engineering and operating problems that arise throughout the lifecycle of a chemical process, such as designing a new process, troubleshooting a process unit or optimizing operations of a full process like Fatty acids precut plant (Aspen Tech Inc, 2002).

The design basis for this case processes is a fatty acids feed stream with the volume flow rate of 649.668136 L/min. The detailed stream composition is provided in Aspen Plus as shown in Appendix A. The feed rate is 21572.1242 kg/hr (100.00 kmol/hr) and the net process yield is approximately 21089.2176 kg/hr (96.0003 kmol/hr) of liquid fatty acids at the bottom and 477.4578 kg/hr (3.6975 kmol/hr) at the top of precut column (distillate products). For the stream Vent the yield is 5.44773 kg/hr (0.3025 kmol/hr).

Figure 4.3 showed that the graph represents temperature and pressure profile of stages in precut column. The feedstock of fatty acids was entering at temperature of 483.15 K and pressure of 2.5 bar at stage 14. Starting from stage 14 until stage 1 the temperature and pressure was decreasing extremely to 248.025003 K and 0.11003 bar in distillate part of the precut column. At the bottom part, the temperature and pressure were remain constant from stage 14 until stage 25 and increasing slowly to temperature of 499.4966 K until stage 29. The pressure constantly increases up to the value of 0.0987 atm until the last stage. This performance of graph shows that the temperature and pressure were increasing from the first stage until the last stage to achieve the steady state simulation result.

Figure 4.4 and Figure 4.5 show the graph of mass flowrate and molar flowrate profile for the flow of liquid and vapor of fatty acids components products to achieve steady state simulation. At the vapor flow the mass flowrates and molar flowrates were constantly increasing until the value of 5449.455 kg/hr and 30.2481 kmol/hr from the first stage until the stage 29 respectively. The vapor flowrate product only form at the vent section on the top of precut column. At the liquid flow, the mass was constantly increasing to 2500 kg/hr and the molar flowrates was slightly increasing to 10 kmol/hr from stage 1 until stage 14 at distillate section. Starting stage 14 the mass and molar flowrates were extremely increasing until stage 28. At the last stage the mass and molar flowrates was decreasing slightly to 21089.22 kg/hr and 96.00 kmol/hr because the effects of high pressure drop in last tray at bottom section.



Figure 4.3: Graphs of Temperature and Pressure Profile



Figure 4.4: Graph of Mass Flowrate Profile





#### 4.1.3 Comparison Results by Aspen Plus and Palm Oil Fractionation Plant

Based on the mole fraction result of fatty acids obtained from Aspen Plus, the data of results will be compared with actual data results from Palm Oil Fractionation Plant. The comparison of simulation and plant results as a rough guideline and error between them preferably should be less than 10 %. The results of simulation depend on the availability and precision of input data such as material composition, geometric design targets and heat requirements (Gaiser *et. al.*, 2001).

Below is the calculation in determining the percent of error between simulated results with actual results from Palm Oil Fractionation Plant.

#### Percentage Difference

= | (Plant simulated data – Aspen Plus result) / (Plant simulated data)| x 100 % (4.1)

From the comparison shown in Table 4.2, the maximum difference is about 8.69 %. The written program is able to achieve the desired bottom and distillate compositions that are close to the simulator. The liquid and vapor flow rate profile of the Aspen Plus program were also compared to the plant simulated data. The liquid profile of the Aspen Plus program was very close to the liquid profile of the plant simulated data. The vapor profile exhibits some differences but the maximum difference is about 5% which is acceptable. This difference is caused by the different method in calculating the enthalpies between the two programs and also in the plant simulated data, the presence of neutrals and water was considered in the feed stream to the column while in the Aspen Plus program, these components were ignored as their compositions in the feed stream is very small (around 0.004 for each component). However, the developed Aspen Plus program was able to achieve the desired bottom and distillate flow rate and compositions. Therefore, the developed Aspen Plus program is capable of generating the desired data for this research.

a) Distillate stream

	Distillat		
Components of fatty	( <b>k</b> n	% Difference	
acids	Plant	Simulation	(%)
Hexanoic acid, C-6 (Caproic acid)	0.023	0.024	0.00
Octanoic acid, C-8 (Caprylic acid)	0.528	0.532	0.76
Decanoic acid, C-10 (Capric acid)	0.438	0.441	0.68
Dodecanoic acid, C-12 (Lauric acid)	0.006	0.005	0.00
Tetradecanoic acid, C-14 (Myristic acid)	0.000	0.000	0.00
Hexadecanoic acid, C-16 (Palmitic acid)	0.000	0.000	0.00
Stearic acid, C-18	0.000	0.000	0.00
Oleic acid, C-18-1	0.000	0.000	0.00
Linoleic acid, C-18-2	0.000	0.000	0.00
Temperature	442.55 K	440.03 K	0.57
Pressure	0.110 bar	0.108 bar	0.00

# b) Bottom stream

	Botto		
<b>Components of</b>	(1	% Difference	
fatty acids	Plant	Simulation	(%)
Hexanoic acid, C-6	0.000	0.000	0.00
(Caproic acid)			
Octanoic acid, C-8	0.000	0.001	0.00
(Caprylic acid)			
Decanoic acid, C-10	0.001	0.003	0.00
(Capric acid)			
Dodecanoic acid, C-12	0.574	0.539	6.09
(Lauric acid)			
Tetradecanoic acid, C-14	0.173	0.163	5.78
(Myristic acid)			
Hexadecanoic acid, C-16	0.075	0.071	5.33
(Palmitic acid)			
Stearic acid, C-18	0.013	0.015	0.00
Oleic acid, C-18-1	0.134	0.126	5.97
Linoleic acid, C-18-2	0.023	0.021	8.69
Temperature	509.55 K	499.49 K	1.97
Pressure	0.13 bar	0.10 bar	0.00

### 4.2 Dynamic Simulation Using Aspen Dynamics

The plant simulation was carried out using Aspen Plus is continued by using Aspen Dynamics. Aspen Dynamics extends Aspen Plus steady-state models into dynamic process models, enabling design and verification of process control schemes, safety studies, relief valve sizing, failure analysis, and development of startup, shutdown, rate-change, and grade transition policies. Aspen Dynamics is a core element of Aspen Tech's Process Engineering applications. Aspen Dynamics enables to gain a detailed understanding of the unique dynamics of precut column process. (Aspen Technology, Inc., 1994-2008). The flowsheet was generated based on a standard P&I Diagram of a Fatty Acid Plant as shown in Figure 4.6.



Figure 4.6: Flow Diagram Dynamic Simulation of Precut Column

#### 4.2.1 Tuning

Controller tuning problem can be viewed as a process of determining appropriate value for control parameter. For a PID controller, there are three control parameter need to be adjusted, namely proportional gain, Kc, integral time constant,  $t_I$  and derivative time constant,  $t_D$ . Among the approaches in solving controller tuning problem, process reaction curve method or better known as Cohen-Coon method is the most popular empirical technique (Stephanopoulos, 1984).

In this work, the effects of  $\pm 20$  % of control parameters need to be adjusted to construct the process reaction curves. Based on these curves, the control parameter for each scheme was calculated using the equation suggested by Cohen and Coon. However, these control parameters may not be as accurate as they are derived based on good approximation for the sigmoidal response of a process. In that case, the Cohen and Coon setting for these parameters were used as first guesses in further fine tuning. The fine tuning was done by trial and error method until it gave the best control performances to the system.

### 4.2.1.1 Tuning of Distillate Level Controller (LC1)

For distillate level controller the type of controller used is PI controller. One challenge of the PI controller is that there are two tuning parameters which are controller gain, *Kc* and integral time or reset time,  $\tau_i$  to adjust and difficulties can arise because these parameters interact with each other.

Figure 4.7 shows the response behavior of original controlled process of precut column. At Kc = 10 and  $\tau_i = 60$  when the output flowrate reached to 1050 lb/hr, the level of process variable is far away to reach the set point level at 4.921260 ft in five hours of process.



**Figure 4.7:** Distillate Level Controller Response at Kc=10;  $\tau i = 60$ 

When *Kc* is increasing to 20% from the original value while maintaining the value of  $\tau_i = 60$  the level of process variable is close to reach the set point level at 4.921260 ft but when *Kc* is decreasing to 20% from the original value, the level of process variable is become more distance to reach the set point level as shown in Figure 4.8.



**Figure 4.8:** Distillate Level Control Response: (a) Kc = 12; (b) Kc = 8

When  $\tau_i$  is increasing to 20% from the original value while maintaining the value of Kc = 10 the level of process variable is distant to reach the set point level at 4.921260 ft but when  $\tau_i$  is decreasing to 20% from the original value, the level of process variable is become close to reach the set point level as shown in Figure 4.9.



**Figure 4.9:** Distillate Level Control Response: (a)  $\tau_i = 72$ ; (b)  $\tau_i = 48$ 

These level control response have an unusual characteristic: increasing the gain of PI controller can increase stability, while reducing the gain can increase the degree of oscillation and thus reduce stability. If *Kc* becomes too large, oscillations or even instability can result. Integral control action is often used but can be omitted if small offsets in the liquid level ( $\pm 5\%$ ) can be tolerated.
#### 4.2.1.2 Tuning of Bottom Level Controller (LC2)

For bottom level controller the type of controller used is PI controller. One challenge of the PI controller is that there are two tuning parameters which are controller gain, Kc and integral time or reset time,  $\tau_i$  to adjust and difficulties can arise because these parameters interact with each other.

Figure 4.10 shows the response behavior of original controlled process of precut column at the bottom. At Kc = 10 and  $\tau_i = 60$  when the output flowrate reached to 45600 lb/hr, the level of process variable reached the set point level at 25.9501 ft in two hours of process.



**Figure 4.10:** Bottom Level Controller Response at Kc=10;  $\tau i = 60$ 

When *Kc* is increasing to 30% from the original value while maintaining the value of  $\tau_i = 60$  the level of process variable reach the set point level at 25.9501 ft in less than two hours process but when *Kc* is decreasing to 30% from the original value, the level of process variable reach the set point level in more than two hours process as shown in Figure 4.11. The key concept behind proportional control is the controller gain can be adjusted to make the controller output changes as sensitive as desired to deviations between set point and controlled variables.



**Figure 4.11:** Bottom Level Control Response: (a) Kc = 13; (b) Kc = 7

When  $\tau_i$  is increasing to 30% from the original value while maintaining the value of Kc = 10 the level of process variable is reach the set point level at 4.921260 ft in 2.5 hours but when  $\tau_i$  is decreasing to 30% from the original value, the level of process variable reach the set point level in 1.5 hours which is the fastest response to reach the set point as shown in Figure 4.12. Integral control action is used to provide an important practical advantage to eliminate the offset. Thus, the process variable automatically changes until it attains the value required to make the steady state error zero.



**Figure 4.12:** Bottom Level Control Response: (a)  $\tau_i = 78$ ; (b)  $\tau_i = 42$ 

#### 4.2.1.3 Tuning of Vent Pressure Controller (PC1)

For vent pressure controller the type of controller used is PI controller with only a small amount of integral control action. Figure 4.13 shows the response behavior of original controlled process of precut column. At Kc = 10 and  $\tau_i = 60$  when the output molar flowrate is 0.66 lbmol/hr, the pressure of process reach the set point pressure at 1.595414 psi in 4.5 hours of process.



Figure 4.13: Pressure Controller Response at Kc=20;  $\tau i = 12$ 

When *Kc* is increasing to 20% from the original value while maintaining the value of  $\tau_i = 12$  the pressure of process variable reach the set point pressure at 1.595414 psi in less than four hours process but when *Kc* is decreasing to 20% from the original value, the level of process variable reach the set point pressure in more than five hours process as shown in Figure 4.14.



**Figure 4.14:** Pressure Control Response: (a) Kc = 24; (b) Kc = 16

When  $\tau_i$  is increasing to 20% from the original value while maintaining the value of Kc = 20 the level of process variable is reach the set point level at 1.595414 psi in five hours but when  $\tau_i$  is decreasing to 20% from the original value, the level of process variable reach the set point level in four hours as shown in Figure 4.15. The control of vapor pressure is very analogous to the control of liquid level in the sense that some applications use averaging control while other requires tight control around a set point.



**Figure 4.15:** Pressure Control Response: (a)  $\tau_i = 14.4$ ; (b)  $\tau_i = 9.6$ 

## 4.2.1.4 Summary

The responses shown from Figure 4.7 to Figure 4.15 illustrate the typical behavior of controlled process before and after changing the parameter controllers which are gain and integral controller. Proportional controls speeds up the process response and reduce the offset. The addition of integral control action eliminates offset but tends to make the response more oscillatory. The use of PI controller does not always result in oscillatory process responses; the nature of the response depends on the choice of controller settings (*Kc* and  $\tau_i$ ) and the process dynamics.

### 4.3 **Performance Controller Evaluation**

Servomechanisms and regulators are used to control the process either via automatic controllers or as a self contained unit. They are physically doing the job of adjusting the manipulated variable to have the controlled variable at around set point. A controller automatically adjusts one of the inputs to the process in response to a signal fed back from the process output.

## 4.3.1 Effect of Set Point Tracking

In the following controller performance evaluation, the control system was examined on the ability to track changes in set point without impact of disturbance. Generally, the set point of product quality is normally maintained at some fixed operation. But at times, adjustments are needed in order to compensate for some error or changes in product grade. Set point is also changed to fulfill customer specifications for different market demand at different time.

Here, only  $\pm 0.20\%$  of the initial set point was changed in sequence. Larger percentage may not be appropriate since the original set point were considered high and had nearly reach its limit. This evaluation was simulated for five hours. Pressure and level control were considered in this evaluation. Their results are demonstrated in the corresponding illustration plots in Figure 4.16 until Figure 4.18





**Figure 4.16:** Control performance plots in set point tracking of PC1 a) original set point (sp); b) +20% original sp; c) -20% original sp



(c)

Figure 4.17: Control performance plots in set point tracking of LC1 a) original set point (sp); b) +20% original sp; c) -20% original sp



**Figure 4.18:** Control performance plots in set point tracking of LC2 a) original set point (sp); b) +20% original sp; c) -20% original sp

As expected, the level control strategy of LC1 and LC2 were able to follow the set point changes excellently. On the other hand, pressure control strategy used did not deviate significantly from the set point as well. If inspection was made in more detail, the response of flowrate at vent section using direct control strategy may be criticized for its larger overshoot and longer settling time.

#### 4.3.2 Disturbance Changes

Disturbance changes were carried out using Aspen simulator. The dynamic behavior of the fractionation plant for closed-loop system was considered. These analyses were carried out to provide the necessary process insights needed to guide control implementation. Step changes were imposed to various process inputs and their effects on process outputs were studied. In this work, two input variables were chosen which are feed flowrate and feed temperature as disturbances. Corresponding dynamic responses precut column were studied.

Figure 4.19 shows the dynamic response when the feed flowrate was changed. The curves on top left corner indicate that feed flowrate was changed after 30minutes and simulated for 300 minutes (5 hours). The solid line denotes result for 5% increased in feed flowrate while dotted line represent s the case when feed flowrate was decreased 5% from its steady state value. The results demonstrated that the variables in closed loops, which were top pressure, liquid level and bottom liquid level, were well controlled at their prescribed set points.



Figure 4.19: Dynamic responses for  $\pm 5$  % disturbances in feed flowrate

Figure 4.20 shows the effect of 5% increase and decrease in feed temperature. These curves are represented by solid lines and dotted lines respectively. As shown in the top right corner, the top column pressure line curves dropped dramatically when the feed temperature was increased. This revealed that if disturbance of feed temperature is large, severe impact may be induced on the system leading to ill performance of control loops. However, close loop variables were kept constant after some fluctuations.



**Figure 4.20:** Dynamic responses for  $\pm 5$  % disturbances in feed temperature

**CHAPTER 5** 

## CONCLUSION AND RECOMMENDATION

## 5.1 Conclusion

The proposed scheme was implemented in a precut column in the fatty acid fractionation plant. The simulation of the column was carried out using Aspen Plus and Aspen Dynamics, the commercial simulators, having both the steady state and dynamic simulation capabilities. Overall case study in this research presents literature review on steady state and dynamic simulation algorithm, modeling of the precut column of the fatty acids using Aspen Plus simulator and dynamic simulation program development and program performance evaluation using Aspen Dynamics. The precut column is a distillation column from literature. There are nine chemical components in this column. The variables that are fixed in this precut column are the 28 trays, pressure, the reboiler duty, reflux flow rate and pumparound flow rate.

From the comparison results between plant simulated data and Aspen calculation, the maximum difference is about 8.69 %. The Aspen program is able to

achieve the desired bottom and distillate compositions that are close to the plant simulated data. The liquid and vapor flow rate profile of the Aspen program were also compared to the plant simulated data. The developed Aspen program was able to achieve the desired bottom and distillate flow rate and compositions. A good match to actual industrial data was obtained. Therefore, the developed Aspen program is capable of generating the desired data for this research.

Understanding the dynamic behavior of a process is essential to the proper design and tuning of a PI controller. The design and tuning methodology is to:

- a) Step, pulse or otherwise perturb the controller output near the design level of operation,
- b) Use the dynamic model parameters in a correlation to compute PI with Filter
- c) Test the controller to ensure satisfactory performance.

## 5.2 **Recommendations**

In this research, chemical processes tend to change continuously and the dynamic performance developed from history data may not truly represent the relationship between process variables. Therefore, online updating of the data used to develop the performance can take account into process dynamics.

Finally, the author hopes that this research work can be a platform for future studies on the field of designing and control development of the other fractions of separating fatty acids components such as Light Cut Column, Middle Cut Column, Still and Residue Still.

## LIST OF REFERENCES

ASPEN Plus User's Manual. (2002), Calgary, Canada: Aspen Tech Ltd.,

- Banks, J. (1998). Handbook of Simulation: Principles, Methodology, Advances, Application, and Practice. New York: John-Interscience.
- Basualdo M. S. (1990) *Dynamic and Control of Distillation Columns*,: Ph. D Thesis INTEC- CONICET-UNL.
- Chen W. S. (2005). Application of Artificial Neural Network Genetic Algorithm in Inferential Estimation and Control of A Distillation Column. Universiti Teknologi Malaysia: Master Thesis.
- Coffey, D.P., Ydstie, B. E., and Farschman, C.A. (2000). *Computational Chem. Eng*: 24, 317.
- Cooper, Douglas (2004).*Practical Process Control Using Control Station*. Storrs, CT: Control Station,Inc,
- Hurowitz, S., Anderson, J., Duvall, M. and Riggs, J. B. (2003). Distillation control configuration selection: *Journal of Process Control*. 13: 357-362.
- Kaddour Najim.(1989).*Process Modeling and Control in Chemical Engineering*. Madison Avenue, New York: Marcel Dekker, Inc.
- Kister, Henry Z. (1992). *Distillation Design*, 1st Edition, USA: McGraw-Hill.
- Lausberg, Nataly. (2006). Process for obtaining fatty acids with improved odor, color and heat stability. (U.S. Patent 20060006056).

- Liptak, Bela (1995). *Instrument Engineers' Handbook: Process Control*. Radnor, Pennsylvania: Chilton Book Company, 20-29. <u>ISBN 0-8019-8242-1</u>.
- Luyben, W. L. (1990). Process Modeling, Simulation and Control for Chemical Engineers. 2nd ed. USA: McGraw-Hill.
- Luyben, W. L. (2002). *Plantwide Dynamic Simulators in Chemical Processing and Control*. Madison Avenue, New York: Marcel Dekker, Inc.
- Luyben, W. L. (2006). *Distillation Design and Control Using Aspen<sup>™</sup> Simulation*. Hoboken, New Jersey: John Wiley & Sons.
- Luyben, W. L., Björn D. Tyreus, Micheal L.Luyben (1999). *Plantwide Process Control*. USA: McGraw-Hill.
- Mohd Kamaruddin Abd Hamid (July 2004). *Multiple Faults Detection Using Artificial Neural Network*. Universiti Teknologi Malaysia: Master Thesis
- Nirwayanti binti Tajuddin (2005). *Dynamic Simulation of Shell and Tube Heat Exchanger Process.* Universiti Malaysia Pahang: Degree Thesis.
- Noorlisa binti Harun (2005). Fault Detection and Diagnosis via Improved Multivariate Statistical Process Control. Universiti Teknologi Malaysia: Master Thesis.
- Ogunnaike, B. A. and Ray, W. H. (1994). Process. *Dynamics, Modeling and Control*. New York: Oxford University Press.
- Pérez-Cisneros, E.S., Gani, R., and Michelsen, M.L. (1997). *Chemical Engineering Science* : 52, 527.
- Perry, Robert H. and Green, Don W. (1984). <u>Perry's Chemical Engineers'</u> <u>Handbook</u>, 6th Edition. USA: McGraw-Hill.
- Seborg, Edgar and Mellichamp (2004). *Process Dynamics and Control*. Second Edition. Hoboken, New Jersey: John Wiley & Sons, Inc

Stephanopoulos, G (1984). *Chemical Process Control: An Introduction to Theory and Practice*. Englewood Cliffs, NJ : Prentice Hall.

Van, Doren, Vance J. (2003). Loop Tuning Fundamentals. Control Engineering.

- Young, J. of Aspen Technology. Innovative Training Program to Increase Process Plant Skill Levels While Reducing Costs. Cambridge: Aspen Technology, Inc.
- Young and Yan (January, 1991). A Preliminary Study of Sensitivity Analysis and its Applications to Structural Control Problems. *Florida Atlantic Univ Boca Raton Dept of Ocean Engineering*. :35

# APPENDIX A

# Calculation result by Aspen Plus simulation

			DES	IGN OF PREC	UT COLUMN	1			
Stream ID		v	В	DI	F	S101	S102	S103	S104
From		B7	V102	V101		T101	P101	T101	T101
То					T101	P101	V101	V102	B7
Phase		MIXED	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	VAPOR
Substream: MIXED									
Mole Flow	kmol/hr								
N-HEX-01		4.68097E-7	9.79206E-7	.1999986	.2000000	.1999986	.1999986	9.79206E-7	4.68097E-7
N-OCT-01		1.00619E-6	2.000084	3.099915	5.100000	3.099915	3.099915	2.000084	1.00619E-6
N-DEC-01		6.7800E-12	4.299919	8.08313E-5	4.300000	8.08313E-5	8.08313E-5	4.299919	6.7800E-12
N-DOD-01		3.1415E-16	51.80000	1.66724E-8	51.80000	1.66724E-8	1.66724E-8	51.80000	3.1415E-16
N-TET-01		1.9427E-21	15.60000	3.2916E-13	15.60000	3.2916E-13	3.2916E-13	15.60000	1.9427E-21
N-HEX-02		4.6926E-25	6.800000	1.5370E-16	6.800000	1.5370E-16	1.5370E-16	6.800000	4.6926E-25
STEAR-01		7.1152E-30	1.400000	6.4467E-21	1.400000	6.4467E-21	6.4467E-21	1.400000	7.1152E-30
OLEIC-01		5.1505E-28	12.10000	6.5073E-19	12.10000	6.5073E-19	6.5073E-19	12.10000	5.1505E-28
LINOL-01		1.1758E-28	2.000000	1.6348E-19	2.000000	1.6348E-19	1.6348E-19	2.000000	1.1758E-28
WATER		.3025207	6.7207E-21	.3974793	.7000000	.3974793	.3974793	6.7207E-21	.3025207
Mole Frac									
N-HEX-01		1.54732E-6	1.02001E-8	.0540905	2.00000E-3	.0540905	.0540905	1.02001E-8	1.54732E-6
N-OCT-01		3.32599E-6	.0208342	.8383873	.0510000	.8383873	.8383873	.0208342	3.32599E-6
N-DEC-01		2.2412E-11	.0447908	2.18612E-5	.0430000	2.18612E-5	2.18612E-5	.0447908	2.2412E-11
N-DOD-01		1.0384E-15	.5395833	4.50914E-9	.5180000	4.50914E-9	4.50914E-9	.5395833	1.0384E-15
N-TET-01		6.4216E-21	.1625000	8.9024E-14	.1560000	8.9024E-14	8.9024E-14	.1625000	6.4216E-21
N-HEX-02		1.5512E-24	.0708333	4.1568E-17	.0680000	4.1568E-17	4.1568E-17	.0708333	1.5512E-24
STEAR-01		2.3519E-29	.0145833	1.7435E-21	.0140000	1.7435E-21	1.7435E-21	.0145833	2.3519E-29
OLEIC-01		1.7025E-27	.1260417	1.7599E-19	.1210000	1.7599E-19	1.7599E-19	.1260417	1.7025E-27
LINOL-01		3.8866E-28	.0208333	4.4213E-20	.0200000	4.4213E-20	4.4213E-20	.0208333	3.8866E-28
WATER		.9999951	7.0008E-23	.1075002	7.00000E-3	.1075002	.1075002	7.0008E-23	.9999951
Total Flow	kmol/hr	.3025222	96.00001	3.697474	100.0000	3.697474	3.697474	96.00001	.3025222
Total Flow	kg/hr	5.450195	21089.22	477.4571	21572.12	477.4571	477.4571	21089.22	5.450195
Total Flow	l/min	1170.901	480.2282	8.353408	649.6681	8.353408	8.353408	480.2281	943.1127
Temperature	К	318.4276	499.4977	248.0250	483.1500	248.0250	248.0250	499.4976	248.0250
Pressure	atm	.1065877	.0986923	.1085616	2.467308	.1085616	.1085616	.1085901	.1085616
Vapor Frac		.9484118	0.0	0.0	6.31686E-3	0.0	0.0	0.0	1.000000
Liquid Frac		.0515881	1.000000	1.000000	.9936831	1.000000	1.000000	1.000000	0.0
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	cal/mol	4.30612E-6	-1.5459E+5	-1.4475E+5	-1.5549E+5	-1.4475E+5	-1.4475E+5	-1.5459E+5	-4888.038
Enthalpy	cal/gm	<u>5</u> 8167.43	703.6917	1120.983	720.7800	1120.983	1120.983	703.6917	58167.43
Enthalpy	cal/sec	<u>3</u> 228.681	-4.1223E+6	-1.4867E+5	-4.3191E+6	-1.4867E+5	-1.4867E+5	-4.1223E+6	3228.681
Entropy	cal/mol-K	4888.038	-283.3461	-215.9565	-282.3848	-215.9565	-215.9565	-283.3464	-7.664251
Entropy	cal/gm-K	-4609586	1.289817	1.67238	1.309026	1.672388	1.672388	1.289818	.4254171
Density	mol/cc		3.33175E-3	7.37718E-3	2.56541E-3	7.37718E-3	7.37718E-3	3.33175E-3	5.34617E-6
Density	gm/cc	8.304562 7.75783E-5	.7319165	.9526195	.5534140	.9526195	.9526195	.7319167	9.63157E-5
Average MW		18.01585	219.6793	129.1306	215.7212	129.1306	129.1306	219.6793	18.01585
Liq Vol 60F	l/min	.0910119	403.3444	8.783020	412.2184	8.783020	8.783020	403.3444	.0910119
	-			-		-			