SIMULATION OF REACTIVE DISTILLATION FOR BIODIESEL PRODUCTION FROM JATROPHA CURCAS SEED OIL

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SIMULATION OF REACTIVE DISTILLATION FOR BIODIESEL PRODUCTION FROM JATROPHA CURCAS SEED OIL

MOHD USMAN BIN MOHD JUNAIDI

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

Faculty of Chemical & Natural Resources Engineering
Universiti Malaysia Pahang

NOVEMBER 2010

"I hereby declare that I have read this thesis and in my/our opinion this thesis has fulfilled the qualities and requirements for the award of Degree of Bachelor of Chemical Engineering"

Signature	:	……
Name of Supervisor	:	Prof. Dr. Badhrulhisham Bin Abdul Aziz
Date	:	2 December 2010

I declare that this thesis entitled "***Simulation of Reactive Distillation for Biodiesel Production from Jatropha Curcas Seed Oil***" is the result of my own research except as cited in references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree."

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To my beloved parents,
family, lecturers, and friends.

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ABSTRACT

Reactive distillation column (RD column) is a hybrid equipment that combines two of major equipment, i.e. reactor and distillation column. RD column brings many advantages to the chemical industries especially in reducing the cost of building plant, and energy consumption. Biodiesel is an excellent substitute for conventional diesel fuel because of being renewable, nontoxic and biodegradable. In the biodiesel industry, mainly for the biodiesel production from Jatropha Curcas seed oil (JCO oil); the reactive distillation is still being a new technology. The JCO oil contains high percentage of triolein and oleic acid which are really useful for engine performance. This study is mainly based on simulation method by using Aspen Plus 12.1 software. The biodiesel routes process used is triglyceride hydrolysis and fatty acid esterification process. This study will focus on oleic acid esterification with methanol in the reactive distillation column to produce methyl oleate. The simulation was done in equilibrium stage model incorporate with kinetic of reaction model using RADFRAC unit as the RD column model. The purpose of the simulation carried out is to determine the effect of important parameters, i.e. reflux ratio, column pressure, feed temperature, etc, that affect the RD column performance and design the optimized RD column condition to achieve highest product conversion. In the nutshell, the optimum parameters for simulated RD column are; reflux ratio 0.01, feed temperature at 363.15K @ 90^0C, column pressure at 100 kPa, 14 stages with 6 reactive stages, and oleic acid and methanol feed locations, accordingly, at 3nd stage and 8th stage, to achieve 99.65% of oleic acid conversion to biodiesel.

ABSTRAK

Kolum penyulingan bertindakbalas (Kolum RD) adalah satu peralatan gabungan antara dua peralatan yang berbeza cirinya, iaitu rector dan kolum penyulingan. Kolum RD column memberi banyak kelebihan kepada industi kimia terutamanya di dalam mengurangkan kos pembinaan kilang and penggunaan tenaga. Biodiesel adalah pilihan terbaik untuk menggantikan konvensional diesel kerana boleh diperbaharui, tiada toksik and biodegrasi. Di dalam industry biodiesel, terutamanya penghasilan biodiesel daripada minyak mentah dari biji Jatropha Curcas (minyak JCO), Kolum RD masih menjadi teknologi yang baru diperkenalkan. Minyak JCO mempunyai peratusan triolein dan asid oleic yang tinggi dan berguna untuk kemampuan enjin. Kajian ini dijalankan berasaskan kaedah simulasi menggunakan perisian simulasi Aspen Plus versi 12.1. Kaedah pemprosesan biodiesel yang diguankan di dalam kajian ini adalah hidrolisis triglicerin dan pengesteran asid lemak. Kajian ini akn memberi focus kepada pengesteran asid oleic dengan methanol di dalam kolum RD untuk menghasilkan oleate ester. Simulasi telah dijalankan di dalam model keseimbangan bersama dengan model untuk reaksi kinetic menggunakan unit RADFRAC sebagai model kolum RD. Tujuan simulasi ini dijalankan adalah untuk mengenalpasti kesan beberapa parameter yang penting, seperti; nisbah refluk, tekanan kolum, suhu kemasukan bahan mentah, dll, yang memberi kesan kepada kemampuan kolum RD dan merekabentuk kolum RD yang mempunyai keadaan yang optimum untuk mencapai penghasilan produk yang maksimum. Kesimpulannya, optimum parameter untuk simulasi kolum RD adalah; nisbah refluk 0.01, suhu kemasukan bahan mentah pada 363.15K @ 90^0C, tekanan kolum pada 100 kPa, 14 tingkat dengan 6 tingkat reaksi, dan tempat kemasukan asid oleic dan metanol masing-masing pada tingkat 3 dan 8, untuk mecapai 99.65% pertukaran asid oleic kepada biodiesel.

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NOMENCLATURE

cA	-	Oleic acid concentration, mol dm^{-1}
cB	-	Methanol concentration, mol dm^{-1}
cC	-	Methyl Oleate concentration, mol dm^{-1}
cD	-	Water concentration, mol dm^{-1}
α, β, γ, λ	-	Reaction order
k	-	Forward rate constant
k’	-	Backward rate constant
A	-	Pre-exponential factor
Ea	-	Activation energy, kJ mol^{-1}
R	-	Rate constant
T	-	Reaction temperature, K

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND OF STUDY

Demand of fuel and energy sources for daily activities are increasing recently because of the huge development of industries, agriculture, cities, and transportation. However, the fuel from fossil fuel or petroleum today is nearly depleted. Therefore, many researchers from all over the world are seeking alternative sources replacing petrol fuel. One of the solutions is biodiesel.

The usage of vegetable oils in diesel engine could be dated back to the year of 1900 when Rudolf Diesel, the inventor of the engine that bearded his name, demonstrated peanut oil as fuel in Paris World Fair. Their usage continued until 1920's before petroleum derived diesel almost completely eliminated vegetable oils in the market due to cheaper price, higher availability and government subsidies (Li *et al.*, 2010).

However, the altered diesel engine is no longer suitable for high viscosity and low volatility vegetable oils to be applied directly. Refinement has to be made in order to turn those vegetable oils into quality fuel. Several methods have been investigated such as pyrolysis, blending and micro-emulsification to lower the viscosity of vegetable oils (Berchman & Hirata, 2007). Therefore, transesterification process and

esterification process has became the most viable process to transform the vegetable oils to be used in transportation engine.

Nowadays, the new reactive distillation technology has been a major interest to replace the conventional method for biodiesel production. Reactive distillation column is a combination of two major chemical equipments, reactor and distillation column. Thus, in reactive distillation system, the reaction and separation process will be occurring simultaneously. Typically, research has been done on this new technology because of its advantages. A major advantage of reactive distillation is the breakaway azeotropic mixture equilibrium to achieve high conversion of product. (Sahapatsombud et el., 2005)

1.2 PROBLEM STATEMENT

Petroleum product mainly gasoline and diesel have played important role in the world nowadays not only in economics, also in the industrial development. However, it is not a renewable source and contributes to the unwanted effect to the world environment.

Thus, biodiesel are the best replacement for it, which did not cause sulfur contaminant and can be renewed. Although the initial cost to produce is high, the overall cost will be reduced due to a large scale of economies and agricultural subsidies in the future.

Recently, the biodiesel production from various sources especially Jatropha Curcas seed oil is produced using common reactor and distillation system. However, this conventional system in making biodiesel leads to higher cost, maintenance, byproduct production and energy consumption.

Reactive distillation can substitute the conventional reactor and distillation system, which not only potentially reduce the space and cost for equipment and maintenance, but will be able to overcome or breaking the reaction thermodynamic equilibrium (VLE) to obtain higher conversion of desired product.

1.3 OBJECTIVE

a. To develop a reactive distillation model for biodiesel process from Jatropha seed oil.
b. To simulate the reactive distillation model by using Aspen Plus for steady state and dynamic state condition.
c. To determine the optimum parameters (operation and design) to achieve highest conversion of product.

1.4 SCOPE OF STUDY

This research is mainly based on simulation method by using Aspen Plus 12.1 Software. There are three main scopes of research that will be covered to achieve the research objective;

a. Learn and simulate in general for reactive distillation column using Aspen Plus 12.1 Software.
b. Apply the simulation model for common biodiesel data.
c. Validate the simulation model with biodiesel from Jatropha Curcas seed oil experimental data if available.

1.5 SIGNIFICANT OF STUDY

Reactive distillation column is a new technology which could provide more advantages than the conventional reactor and distillation system. A common knowledge in chemical industry is that good equipment leads to high efficiency, produce less unwanted products and energy consumption; which can be found in reactive distillation. This research is intended to improve conventional system for biodiesel production with new development reactive distillation column and to reduce waste and energy consumption which are common issues that biodiesel companies face recently.

CHAPTER 2

LITERATURE REVIEW

2.1 BIODIESEL OVERVIEW

Biodiesel chemically named as fatty acid methyl ester (FAME) and have chemical formula range C_{14}-C_{24} methyl esters. It have been produced from biological sources such as soy bean, palm oil, jatropha, etc; and have chemical and physical properties similar with common diesel fuel.(Kiss, 2009) According to Demirbas, 2009, the biodiesel has boiling point range more than 475K (>202^{0}C), flash point range about 420K – 450K (147^{0}C – 177^{0}C), insoluble in water, and biodegradable.

Recently, biodiesel has attracted worldwide attention to be an alternative fuel sources for replacement of petroleum diesel, which is in the category of non-renewable fuel and will be depleted in limited period of time. (Demirbas, 2009) It also has been a major contribution of air pollution by emission of sulfur oxides, nitrogen oxides, lead, hydrocarbons, etc. By choosing biodiesel an alternative source, not only it renewable, it also free of sulfur, thus making biodiesel a environmental friendly fuel.

Nowadays, the price of biodiesel production is often more expensive than petroleum diesel, but in the future, the price is expected to be reduced due to the agriculture subsidies, and large scale economies. (Kiss, 2009)

2.2 BIODIESEL PRODUCTION

There are many methods to produce biodiesel from various sources. The very basic method is reacting sources with methanol in a batch stirred tank reactor, (Vyas et el., 2009) but recently, there are three methods to produce biodiesel from its sources, oil or fats; that are base catalyzed trans-esterification, solid acid catalyzed esterification and enzymatic catalysis. (Kiss, 2009) From three methods above, the solid acid catalyzed esterification is the most efficient method in biodiesel production because it can operate in a low temperature and pressure environment and yields high conversion with minimal side reaction. (Biodiesel Production, 2007)

Biodiesel from various sources is processed by using common reaction and separation system. There are six systems or processes that currently use at pilot and industrial scale; batch processes using trans-esterification, continuous processes that combine esterification and trans-esterification steps, supercritical processes that required high operating temperature and pressure, hydrolysis and esterification processes that produced high purity of glycerol, enzymatic processes that have low energy consumption, and hydro-pyrolysis processes that required more complex equipment and implies the availability of a low-cost hydrogen course. (Kiss, 2009)

Nowadays, most of the biodiesel processes in industrial scale are using liquid acid or base homogenous catalysts to produce high quality products. However, the uses of homogenous catalyst will lead to major economical and environmental penalties. (Knothe, Gerpen, & Krahl, 2005) Therefore, heterogeneous catalyst (solid acid) was invented to overcome the problems.

2.3 HYDROLYSIS AND ESTERIFICATION PROCESS

For this research, the hydrolysis and esterification process have been taken as the biodiesel production process. In hydrolysis and esterification process plant, there are 2 reactions occurs in the 2 different types of reactors. The first reaction is to hydrolyze triglycerides in the oil feedstock with water to form fatty acid and byproduct, glycerol. The chemical equation for hydrolysis process is stated below;

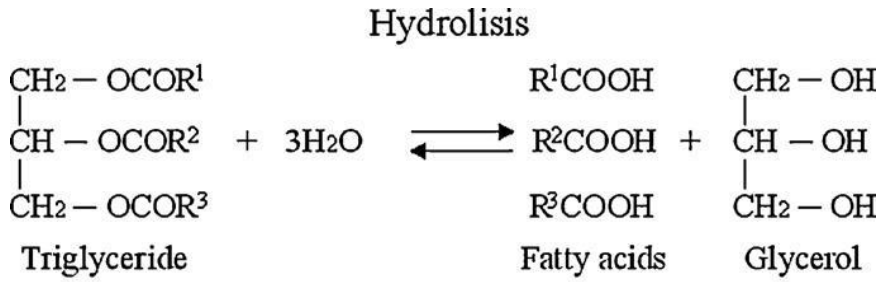

Figure 2.1: Hydrolysis reaction of Triglyceride

Esterification reaction process occurs after the separation of byproduct glycerol form fatty acid in the decanter. The conventional esterification process occurs in the plug flow the reactive distillation column. In esterification reaction, fatty acid will react with methanol with the present of heterogeneous catalyst to form methyl ester (biodiesel) and water as a byproduct. The chemical equation for esterification is stated below;

$$\underset{\text{Fatty acid}}{R^4COOH} + CH_3OH \xrightleftharpoons{\text{Esterification}} \underset{\text{Biodiesel}}{R^4COOCH_3} + H_2O$$

Figure 2.2: Esterification reaction of Fatty Acid

2.4 BIODIESEL PRODUCTION FROM JATROPHA SEED OIL

Jatropha Curcas is a non food plant that grows in arid, semiarid and wasteland. (Lu et el. 2009) This plant has various advantages. Jatropha fruit can be applied to minor wound when it is added with sulfur. Jatropha leaves have anti-malaria properties. The Jatropha roots can treat rheumatism. (For biodiesel production, Jatropha seed can be process to obtain biological oil. From this biological oil, the biodiesel is produce. Jatropha seed oil is categorized as non-edible biological oil sources and has a high-seed yield and high oil content (Wood, 2005).

Recently, the demand for Jatropha oil is increasing tremendously because of the worldwide growing interest for renewable energy sources. (Acten et el., 2008) Plantation of Jatropha plant for biodiesel has become more reasonable rather than other biological source because of the highest amount of biodiesel produce form jatropha plant.

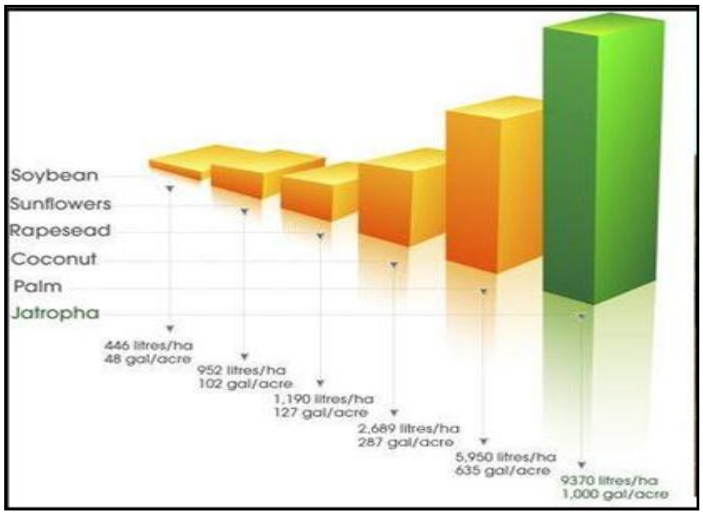

Figure 2.3 Biodiesel production in 1 acre of land for various source (Jatropha Blog, 2009)

Jatropha curcas has been scientifically developed to give better yield and productivity of oil. Jatropha oil has higher cetane number (51) compared to other oils, which is compared to diesel (46–50) and make it an ideal alternative fuel and requires no modification in the engine (Jain *et al.*, 2009). Table 2.1 show the physical n chemical properties for Jatropha Curcas seed crude oil.

From table 2.1, fatty acid compositions in the Jatropha Curcas crude oil have high mass composition of oleic acid (43.1 %) and linoleic acid (34.3%). However, linoleic acid has almost similar physical and chemical properties with oleic acid such as boiling point temperature difference is about 4-5 ^{0}C, and molecular weight different is about 2-3 kg/mol. Therefore, for this simulation study, it is assumed that all the fatty acid composition in the Jatropha Curcas crude oil will consist only oleic acid.

Table 2.1 Physical and chemical properties for Jatropha crude oil taken from http://www.plantoils.in/portal/jatropha/jao/pro/pro.html

PROPERTIES	**VALUE**
Flash point	240/110 °C
Cetane value	51.0
Distillation point (°C)	295 °C
Sulphur %	0.13 %
Viscosity (cp) (30 °C)	52.6 (5.51)2
Speciflc gravity (15 °C/4 °C)	0.917/ 0.923(0.881)
Iodine Value	390.8 -112.5
Acid value	1.0 - 38.2
Palmitic acid %	4.2
Stearic acid %	6.9
Oleic acid %	43.1
Linoleic acid %	34.3
Other acids %	1.4

2.5 ESTERIFICATION KINETIC MODEL

By assumption on the composition in the Jatropha made earlier, for the esterification reaction, only oleic acid will be react with methanol to produce methyl oleate (biodiesel) and water. According to Song et al., 2009, for the esterification of oleic acid and methanol, the reaction rate can be described as:

$$-\frac{dc_A}{dt} = kc_A^{\alpha}c_B^{\beta} - k'c_C^{\gamma}c_D^{\lambda}$$

Figure 2.4 Oleic acid esterification reaction rate (Song et al., 2009)

where c_A, c_B, c_C and c_D denote the concentrations of oleic acid, methanol, methyl oleate and water, respectively; α, β, γ and λ refer to their reaction orders. k and k' are the kinetic constants for the forward and reverse reactions, respectively. However, the value for the rate for reverse reaction is far too small than forward, thus, it assumed neglected.

The rate constants can be used to get the pre-exponential factor, A and activation energy, Ea with the Arrhenius equation,

$$\ln k = -\frac{E_a}{RT} + \ln A$$

Figure 2.5 Arrhenius equation (Song et al., 2009)

Table below shows the values for Arrhenius equation for esterification reaction between oleic acid and methanol using Zinc Acetate catalyst were taken from Song et al., 2009.

Table 2.2. List of parameters and values for rate constant calculation

Parameter	Value
Pre-exponential factor, A	120
Activation energy, Ea	32.62 kJ/mol
Reaction order, n	2.22

2.6 REACTIVE DISTILLATION SIMULATION MODEL

Reactive distillation is a new developed technology for chemical industries especially in biodiesel production. Many researches have been carried out related to this technology to improve the common reactor and distillation system. There are four advantages that make researchers are more interested in studying this new technology, (i) shifting an equilibrium conversion, (ii) improve product selectivity, (iii) breaking azeotropic mixtures, and (iv) saving energy due to the use of reaction heat for separation process (Baur et al., 2000).

One of successful research done by Kiss et el., 2008, making biodiesel suitable to process in reactive distillation column by present of metal oxides catalysts using trans-esterification process. The research is done by using Aspen Plus simulation software. Simulation is an alternative tool to be use in develops or constructs new equipment or technology for new and old process without having risk of lost life, investments, and time to build pilot plant for experiment.

CHAPTER 3

METHODOLOGY

3.1 OVERVIEW

In present study, the simulation was conducted to obtain useful information needed for the design of real plant. Thus, simulation was carried out using Aspen Plus Simulator version 12.1 software package. Radfrac Model with equilibrium stage model is available to be use along this simulation. Moreover, there are kinetic model in the Radfrac system that can be used along the simulation if the required data is available. Before start with any simulation, the base case study simulation is done to ensure the references case for simulation is done within the range. Therefore, in the base case study for the simulation of reactive distillation column, five parameters need to be considered to define all five optimum parameters needed in the design for esterification of oleic acid process; - pressure column, feed temperature, reflux ratio, reactive zone height and feed location.

3.2. ASPEN PLUS 12.1 SOFTWARE

3.2.1 EQULIBRIUM STAGE MODEL

In the simulation of reactive distillation column for esterification of oleic acid with methanol, the chemical reaction equation for esterification process to produce methyl oleate and water is as below;

$$\underset{\text{Fatty acid}}{R^4COOH} + CH_3OH \xrightleftharpoons{\text{Esterification}} \underset{\text{Biodiesel}}{R^4COOCH_3} + H_2O$$

Figure 3.1: Esterification reaction

From previous literature study, there are lack of information on methyl oleate such as vapour pressure and critical temperature. However, all the information ware estimated by the Aspen estimation. For the simulation, the vapour phase was assumed to be ideal and the thermodynamics property method used is UNIQUAC model with the estimation for all missing parameters to represent the concentration coefficient in rate expression.

In the simulation, Radfrac model unit will be use as reactive distillation model. Radfrac model is based on rigorous equilibrium stage model and operate by solving mass balance, energy balance, phase equilibrium, and summation equation. For the Radfrac simulation, assumption of each stage in Radfrac unit is in vapour-liquid equilibrium (VLE) was made.

3.2.2 KINETICS MODEL

In the reaction kinetics model, the key requirement for the simulation to run accordingly to the thermodynamics properties is the accurate reaction kinetics data. In the previous study, the reaction kinetics for oleic acid esterification process was taken from Song et al., 2009. Accordingly, the reaction rate for the esterification of oleic acid and methanol can be described as below;

$$-\frac{dc_A}{dt} = kc_A^{\alpha}c_B^{\beta} - k'c_C^{\gamma}c_D^{\lambda}$$

For the activation energy of esterification reaction between oleic acid and methanol using Zinc Acetate catalyst were taken from Song et al., 2009. The kinetics model will be added in the Aspen Plus Power Law Kinetic Expression.

3.3. BASE CASE STUDY SIMULATION

Base case study simulation has to be done before start with any simulation, as reference data in the simulation to ensure the simulation is run within the base case study range. The flow sheet design for the reactive distillation column equipment process is presented as shown in **Figure 3.2**. The design consist 10 reactive stages from 15 stages used and was characterized by catalyst loading. Oleic acid has high boiling point than methanol. Thus, methanol will be more volatile than oleic acid. Due to that matter, oleic acid is introduced to feed at the top of the column and methanol, on the other hand, will be fed at bottom. By using this feed flows arrangement, the reaction will be occur in counter current ways, which increase effectiveness of reaction. For the molar ratio in the column, both of reactants will fed to the column in 1:1 ratio.

The design specification of the reactive distillation column for base case study simulation is presented **Table 3.1**. The specification of the column are then implemented in the simulation, and varies the simulation by changed several trial parameters to determine the optimum parameters conditions that give the highest conversion for methyl oleate production and operate at lowest energy consumption for the column. All the trial parameters has been tabulated in **Table 3.2**

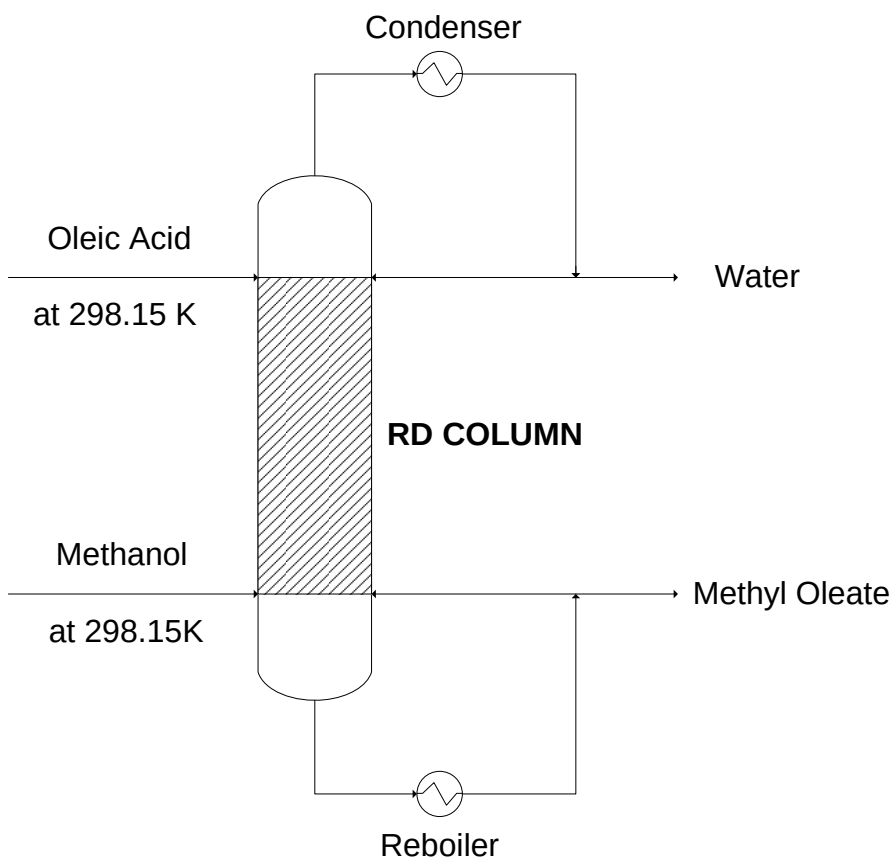

Figure 3.2 Reactive distillation column diagram

Table 3.1 Design specification parameters of column

Category	**Parameter**	**Value**
Oleic acid feed	Flow rate (kmol/h)	100
	Temperature (K)	298.15
Methanol feed	Flow rate (kmol/h)	100
	Temperature (K)	298.15
RD Column	Pressure (kPa)	80
	Reflux ratio	0.1
	Distillate to feed ratio	0.5
	No. of stages	15
	Liquid hold up (kg)	6

Table 3.2 Trial parameters for base case simulation study

Parameter	Value
Reflux ratio	0.01 – 0.2
Feed temperature (K)	298.15 – 363.15
Column pressure (kPa)	30 - 100
No. of Stages	14 - 20
Reaction zone stages	6 - 12
Feed stages location	2-13, 3-12, 5-10, both at 7

List of **Figure 3.3** until **3.11** shows the sequence of procedure for simulate the reactive distillation column using Aspen Plus 12.1 simulator for the methyl oleate (biodiesel) production.

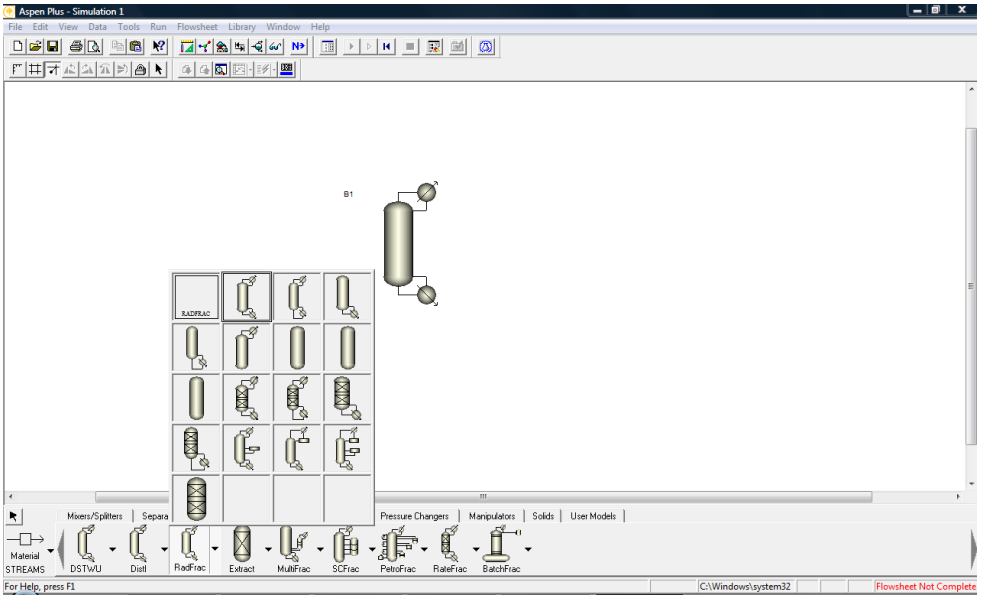

Figure 3.3 Selection of equipment unit

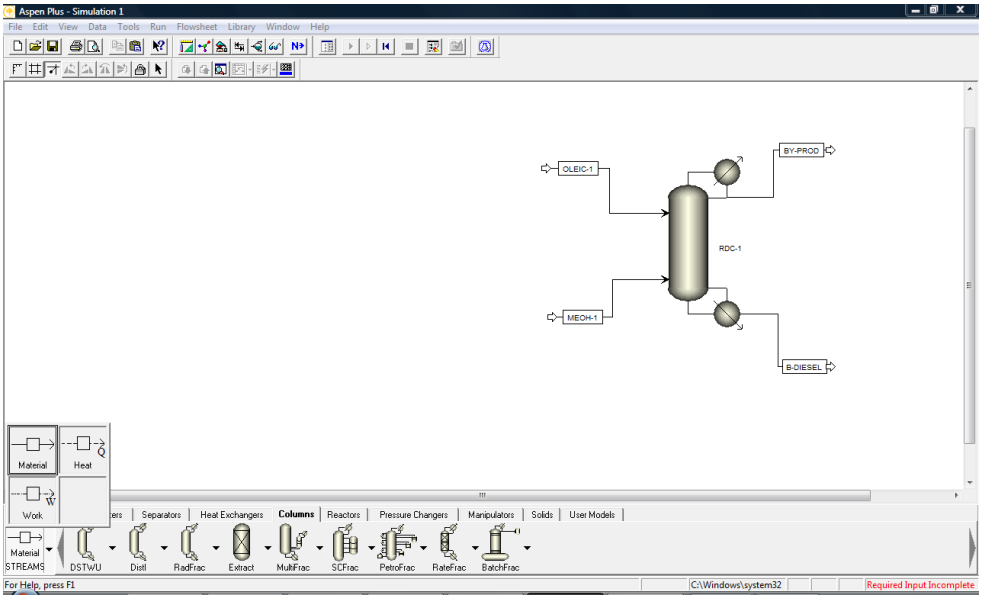

Figure 3.4 Stream added to equipment unit

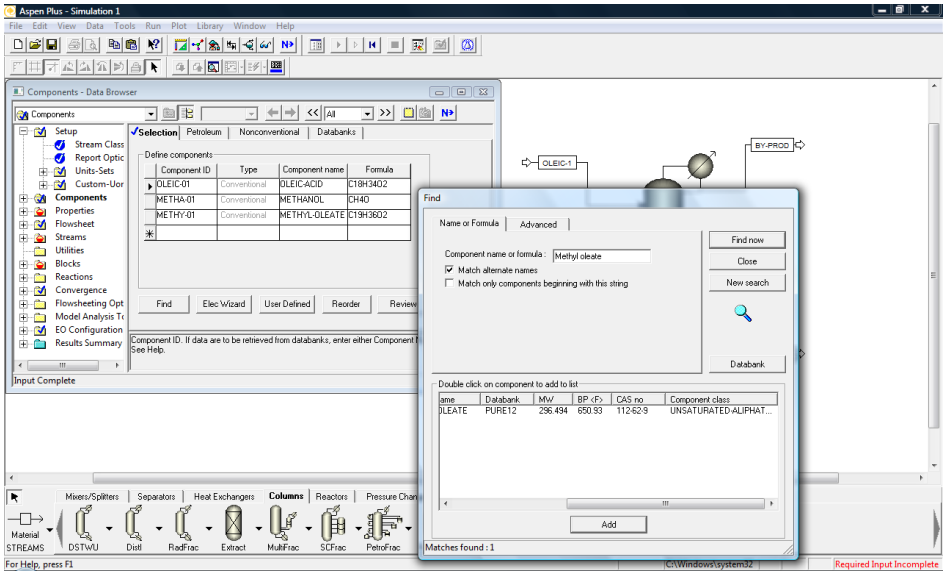

Figure 3.5 Components selection for simulation process

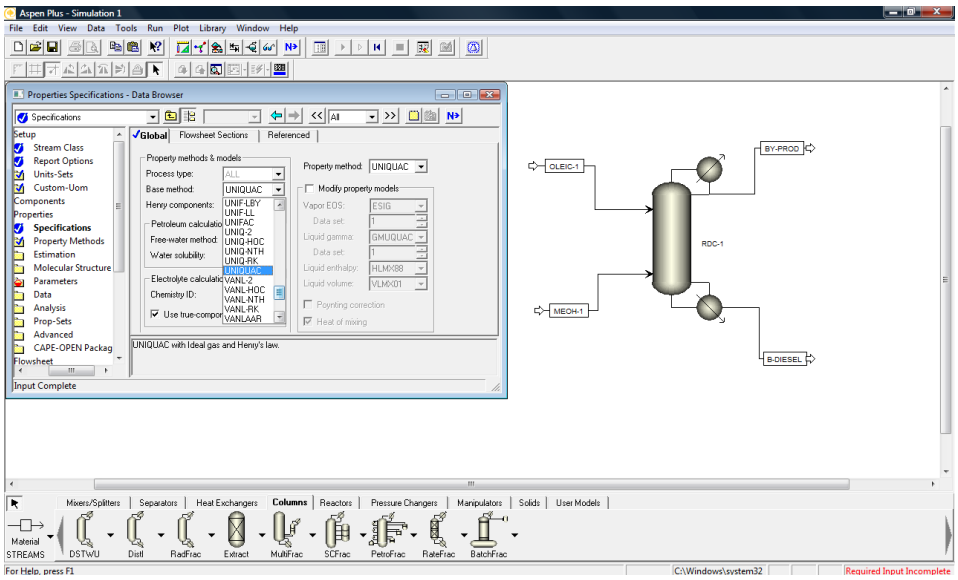

Figure 3.6 Properties specification for simulation process

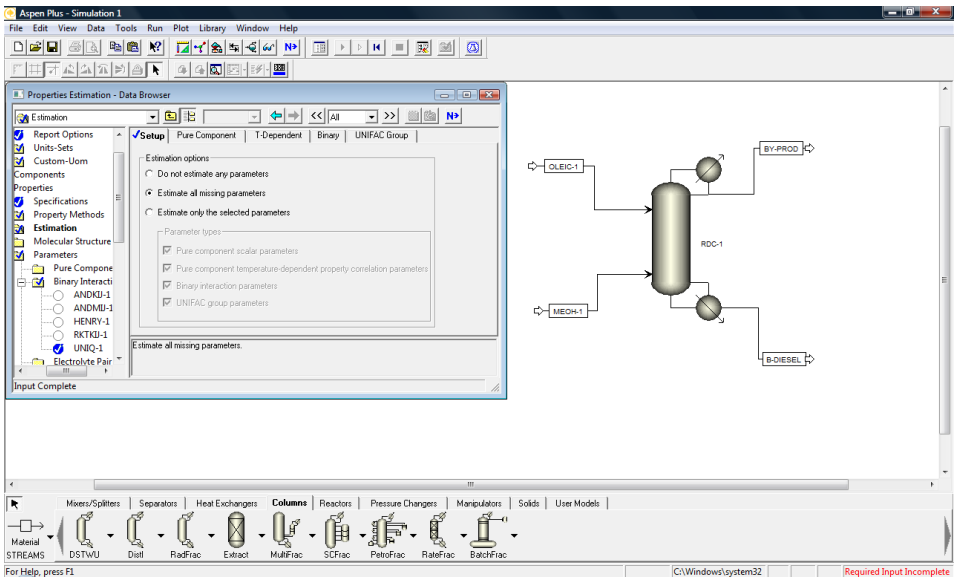

Figure 3.7 Properties estimation for simulation process

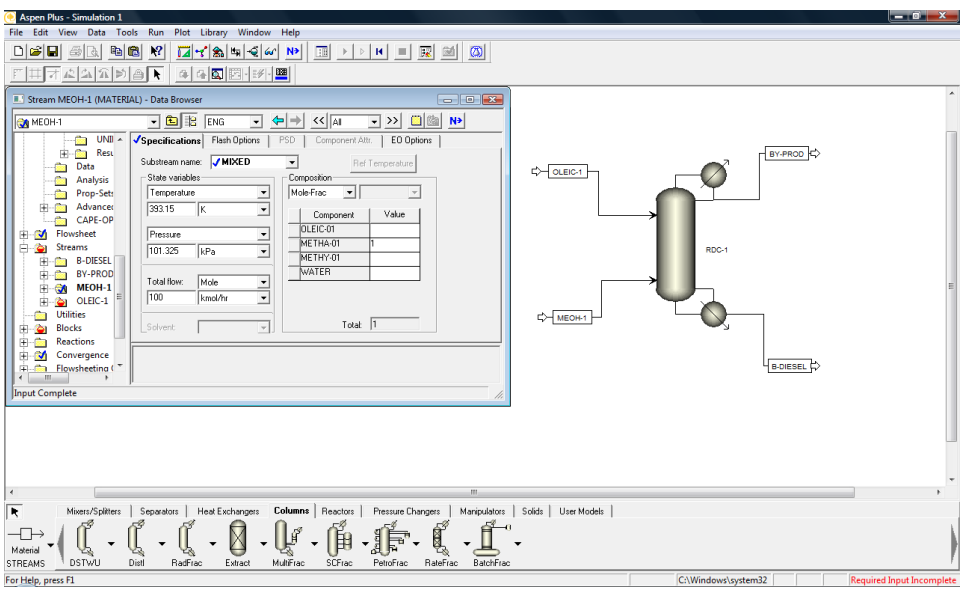

Figure 3.8 Stream properties parameter add to the simulation

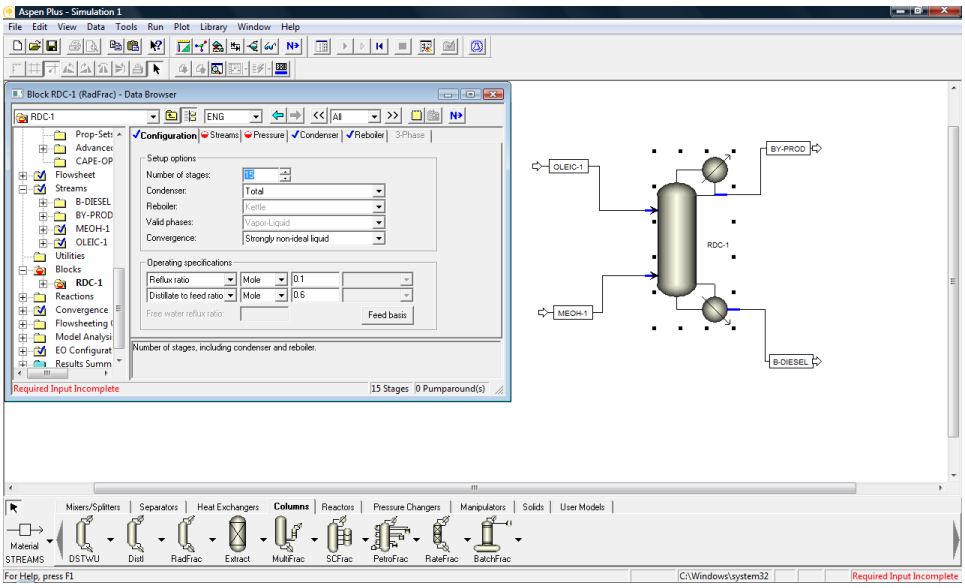

Figure 3.9 Design equipment parameters add to the simulation

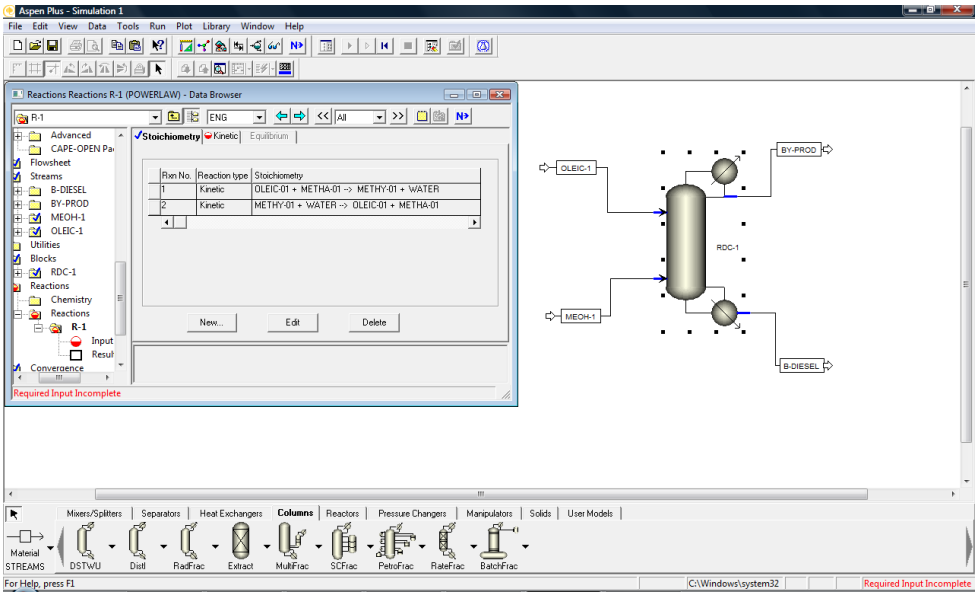

Figure 3.10 Reaction equation add to the simulation

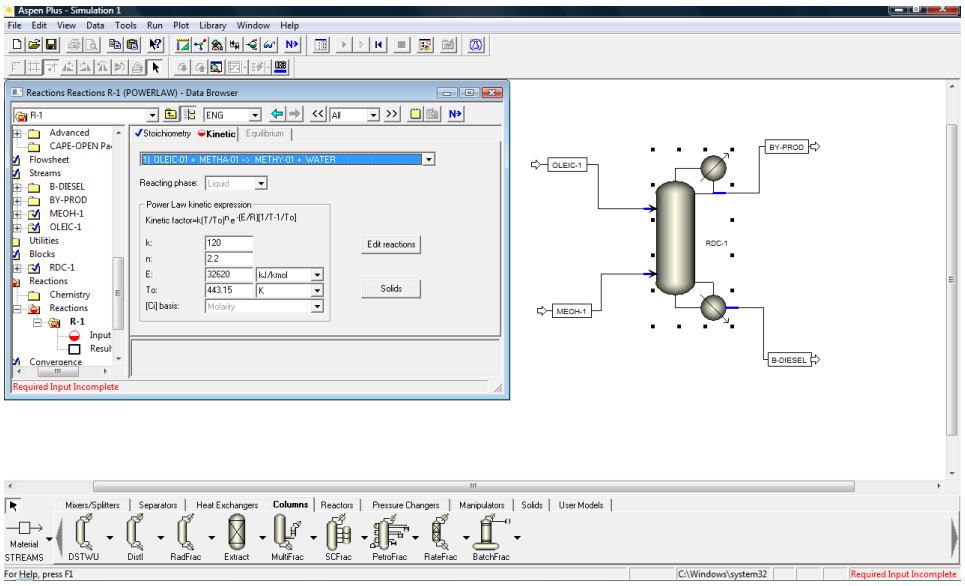

Figure 3.11 Kinetics parameters added in Built-in Power Law

3.3 SUMMARY OF METHODOLOGY

Figure 3.12 below shows the working flow procedure to do the research simulation for RD column design.

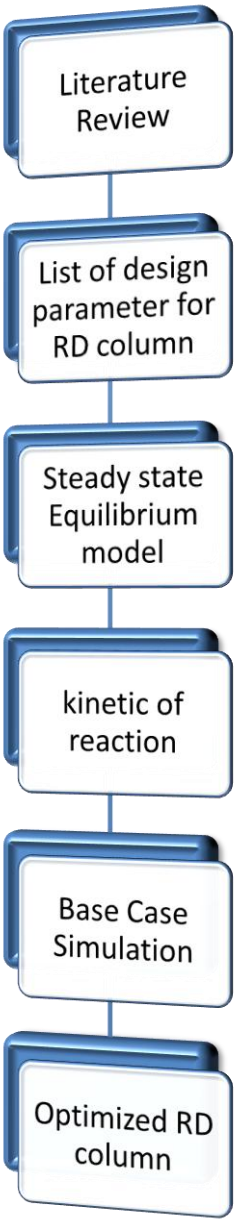

Figure 3.12 Summary of methodology

CHAPTER 4

RESULT AND DISCUSSION

4.1 INTRODUCTION

In this chapter, the result and analysis from the entire study and simulation was carried out. The result obtained from this study is based on the simulation done in Aspen Plus 12.1 software. A total 28 simulations trial have been done to study the effect of design parameters to the RD column performance and to find the optimum value for every trial design parameters to determine the highest oleic acid conversion.

4.2 RESULT ANALYSIS AND DISCUSSION

4.2.1 REFLUX RATIO

In study on reflux ratio, this parameter will be analyzed from 0.01 to 0.2. The function of reflux ratio is to maintain the process in the column. The reflux ratio is always can be attribute to water distillation, which otherwise would accumulate in the bottom column. The amount of water flow at distillate and enter back to the column will be analyzed to study its effect to the column performance, as well as the methyl oleate production, bottom composition and methyl oleate purity.

The data on table 4.1 shows by increasing the amount of water flown back to the column will reduce the oleic acid conversion. Thus, by reducing the reflux ratio value, the methyl oleate production will be increase. Moreover, with increasing the reflux ratio, the water flown back to the column is tending to reduce the product purity. Therefore, reflux ration is inversely proportional to the acid conversion.

Table 4.1 Effect on reflux ratio on oleic acid conversion

REFLUX RATIO	OLEIC ACID CONVERSION
0.01	99.37
0.03	99.31
0.05	99.26
0.10	99.15
0.20	98.98

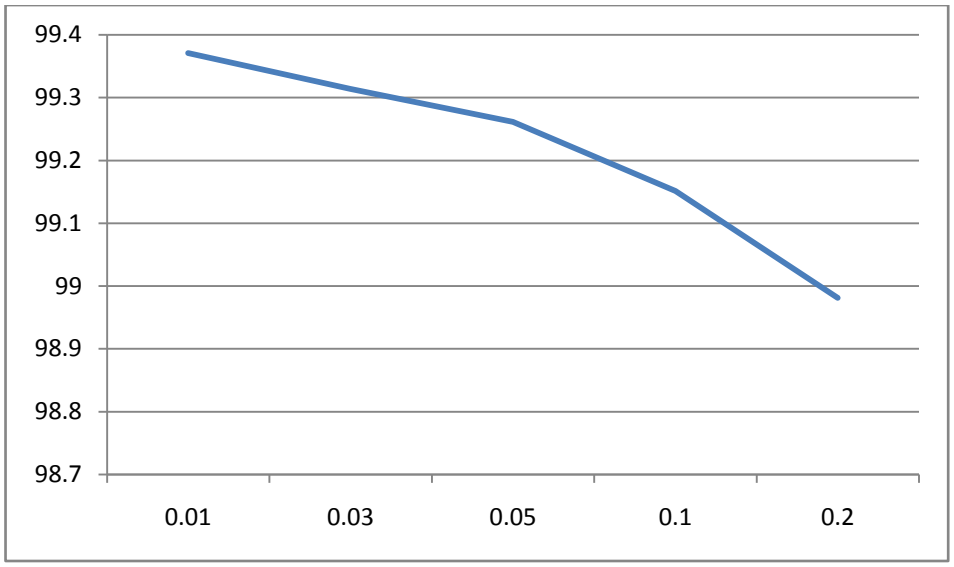

Figure 4.1 Graph of oleic acid conversion versus reflux ratio

Figure 4.1 shows the graph of acid conversion versus reflux ratio. From the graph, as reflux ration increase, amount of water enters back the column from the distillate will increased. Thus, it will affect the RD column performance by reducing the amount of methyl oleate production needed at the bottom of column. From the analysis, the reflux ratio value, 0.01 will be accepted as the optimum reflux ratio value.

4.2.2 FEED TEMPERATURE

In the temperature analysis, there are about five trials for temperature parameter to find the optimum feed temperature to be fitted into RD column condition. The temperature was varies from 298.15K to 363.15K. Table 4.2 shows the result data of feed temperature condition and oleic acid conversion.

Table 4.2 Effect on feed temperature to oleic acid conversion

FEED TEMPERATURE, K	OLEIC ACID CONVERSION
298.15	99.15
303.15	99.16
323.15	99.21
343.15	99.27
363.15	99.33

From table above, by increasing the feed temperature, the oleic acid conversion will be increase. Thus, feed temperature condition is directly proportional with the oleic acid conversion and RD column performance. Figure 4.2 shows the graph of feed temperature condition versus oleic acid conversion. From the graph, the optimum feed temperature to get the highest conversion of oleic acid is 363.15K and the optimum temperature is taken for further analysis for optimized RD column performance.

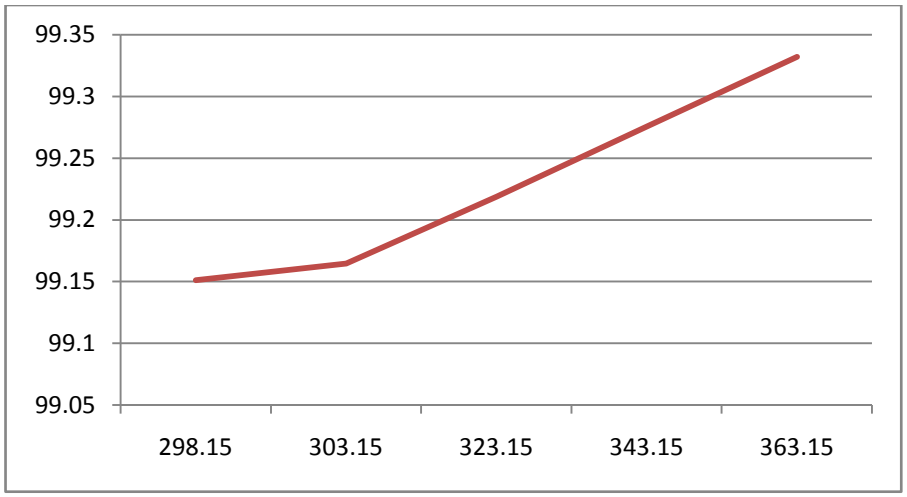

Figure 4.2 Graph of oleic acid conversion versus feed temperature

4.2.3 COLUMN PRESSURE

In RD column, the choice of operating temperature is justified by the effect of pressure condition on the reaction equilibrium and reaction rate. For this design parameter, the column pressure is analyzed from 30kPa to 100kPa. The RD column was operated under vacuum and adiabatic condition to minimize the use of energy in the column. Through the analysis, by increasing the operating pressure, the oleic acid conversion also increased. This is due to the increasing of temperature inside the column that will increase the bottom and distillate temperature and tend to increase the reaction rate. Thus, the oleic acid conversion will also increase. Table 4.3 shows the pressure column profile data with oleic acid conversion.

Table 4.3 Effect on feed temperature to oleic acid conversion

PRESSURE, kPa	OLEIC ACID CONVERSION
30	92.66
50	97.53
70	98.84
90	99.35
100	99.49

Data above shows the acid conversion was increased about 5% when column pressures increase. Figure 4.3 shows the graph of oleic acid conversion versus column pressure. From the graph shows when elevating the pressure will tend to increase the rate of reaction that caused the increasing of oleic acid conversion. From the data, column pressure value, 100 kPa is taken to be optimum column pressure. The summary for the simulation can be found in Appendix C.

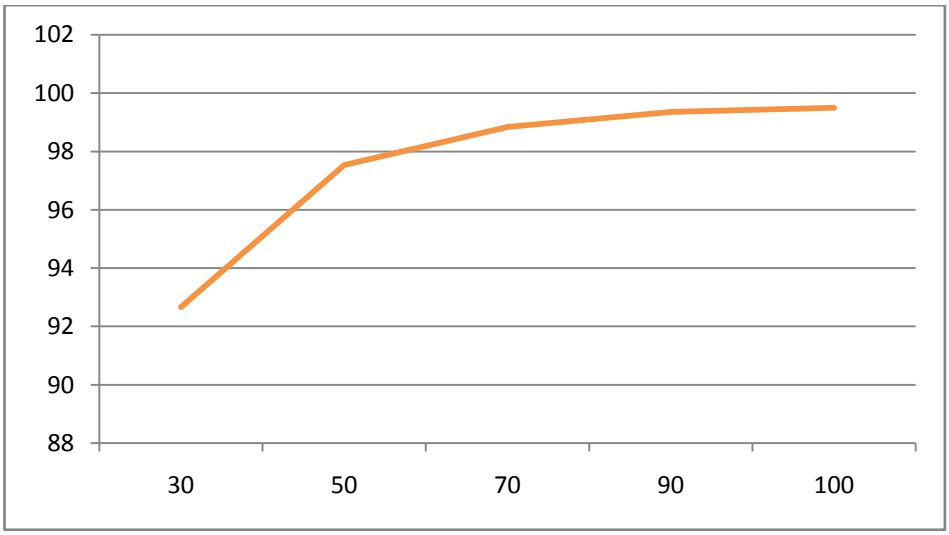

Figure 4.3 Graph of oleic acid conversion versus column pressure

4.2.4 NUMBER OF STAGES

In this part of analysis, number of stages will be effect the efficiency of separation. The number of stages varies is stripping section of the column. The reaction zone will be keep at 10 stages. The number of stages will be varies from 14 to 20 stages. Table 4.4 shows the number of stages affecting the acid conversion.

Table 4.4 Effect on number of stages to oleic acid conversion

NO. OF STAGES	OLEIC ACID CONVERSION
14	99.157
15	99.154
16	99.153
18	99.150
20	99.149

Table above shows the conversion of oleic acid decreased as the number of stages increase. This is due to the reactive zone is put in constant number of stages and location. The reactive zone is on the 3rd to 12th stages. Due to that, the separation zone for water at the distillate is remains the same through the analysis. If the water separation zone is changing for this analysis, the efficiency for water to remove at the distillate will be increase. In the other hand, by increasing the separation or stripping zone at the bottom column, the purity of product, methyl oleate is increased. However, by increasing the bottom separation zone, the stages temperature at reactive zone will decrease and due to that, reaction rate will decrease. Thus, to increase the reaction rate, the reboiler duty and bottom temperature has to be increased. The optimum number of stages for this analysis is 14 stages and the summary for the simulation can be found in Appendix D. Figure 4.4 shows the graph of oleic acid conversion versus number of column stages.

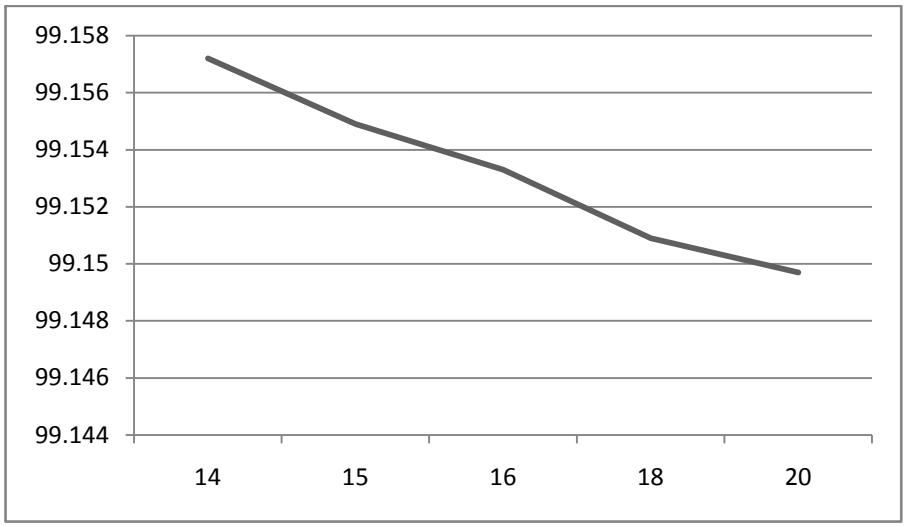

Figure 4.4 Graph of oleic acid conversion versus number of column stages

4.2.5 REACTIVE ZONE STAGES

The amount of reactive zone stages is dependable with the catalyst characteristic, such as, catalyst bed, catalyst density, and catalyst volume fraction of the packing. The amount of catalyst weight that can accommodate per unit volume of column is being limit by pressure drop in the catalytic bed. In order to avoid this problem and residence time limitation, by increasing either column diameter of reactive zone stages, the additional places is available to accommodate sufficient weight of catalyst. However, the increasing amount of reactive stages will tend to interrupt separation efficient and thus, affect the product purity. In the other hand, by increasing the reactive stage also will contribute to higher cost of catalyst used due to the increasing mass of catalyst. Therefore, the analysis for number of reactive stages parameter is being done. The reactive zone is varied from 6 reactive stages to 12 reactive stages.

Table 4.5 Effect on number of reactive stages to oleic acid conversion

REACTIVE STAGES	OLEIC ACID CONVERSION
6	99.155
8	99.155
10	99.155
12	99.155

Table 4.5 shows that oleic acid conversion is remain the same for 6 reactive stages until 12 reactive stages. Form the table, clearly stated that reactive stage do not affect the rate of reaction. This is due to the adiabatic condition applied to the column makes the pressure drop limitation avoided. Therefore, the optimum reactive stage for oleic acid esterification process is 6 stages. Figure 4.5 shows the graph of oleic acid conversion versus reactive stages number. The summary for simulation trial can be found in Appendix E.

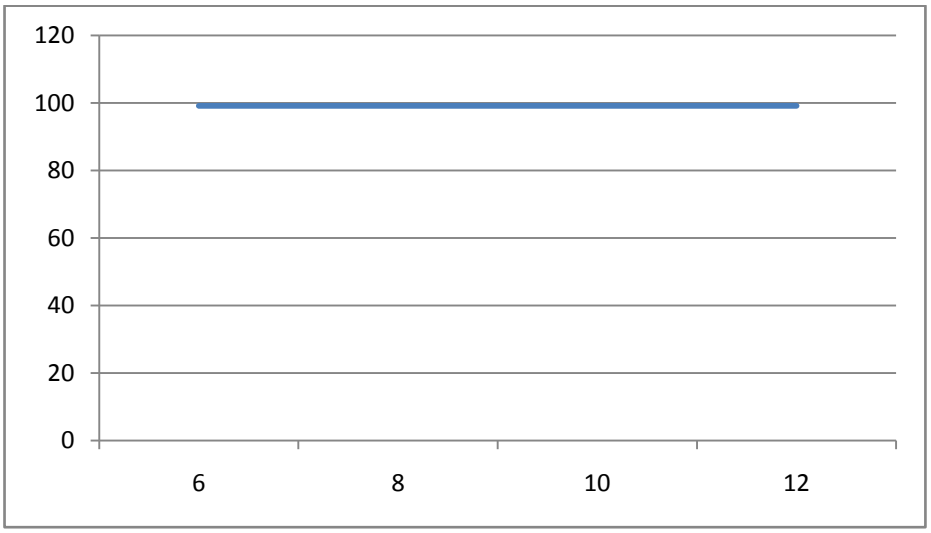

Figure 4.5 Graph of oleic acid conversion versus number of reactive stages

4.2.6 REACTANT FEED LOCATION

In this analysis, the feed tray locations appear to be one of the most important variables for the RD column design. The right choice of feed location can be affect the oleic acid conversion in the reactive zone. For the analysis, there are 4 RD column design with different feed trays location. The RD columns were evaluated by comparing the oleic acid conversion. Figure 4.6 below shows the diagram for 4 RD columns.

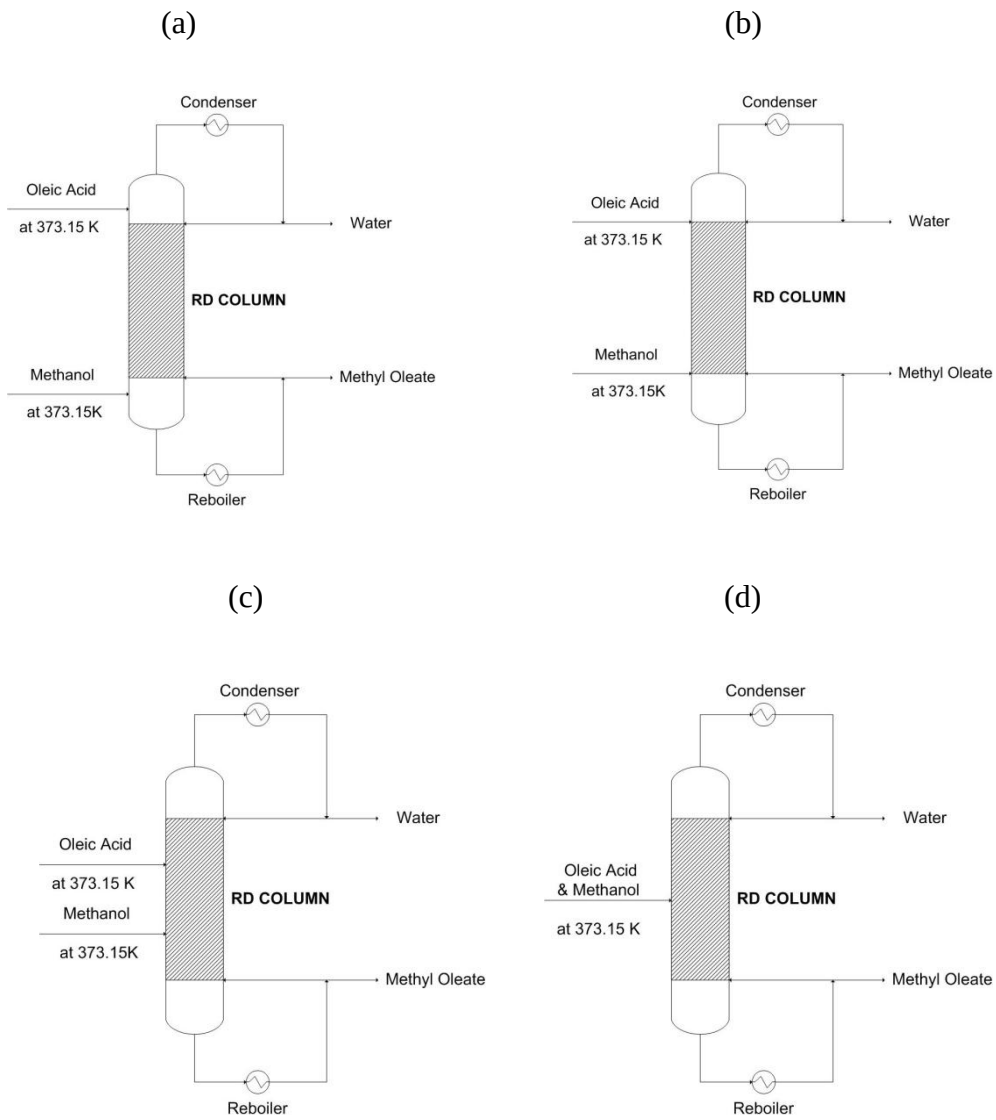

Figure 4.6 RD column diagrams with different feed locations

Figure 4.6(a) shows the oleic acid enters higher from the reactive zone and methanol enters lower than reactive zone. In figure 4.6(b), the feeds enter relatively right at the end of each reactive zone. For figure 4.9(c), the feeds enter between the reactive zone. Finally, both of feed will be enter at 7th stage is shown in figure 4.6(d). The result data for the analysis is tabulated at Table 4.6.

Table 4.5 Effect on number of reactive stages to oleic acid conversion

FEED LOCATION	OLEIC ACID CONVERSION
2 and 13	97.93
3 and 12	99.68
5 and 10	99.15
Both at 7	0.02

From the table above, 3 and 12 stages feed locations give the highest oleic acid conversion. 2 and 13 stages feed location is not favourable because of oleic acid conversion is lower than 2 and 12 stages feed location. For the 5 and 10 stages, this location arrangement can be accepted and used due to the oleic conversion is almost similar with 3 and 12 stages feed location. For the feed locations both at 7th stages is not suitable due to the feed location is not make the esterification reaction occurs effectively.

Therefore, the optimum feed location chosen to apply in the optimized RD column is the feeds enter right at the end of each reactive stage. The summary of the simulation for this parameter can be found in Appendix F.

4.3 OPTIMIZED RD COLUMN

In this section, all the optimum trial parameters will be gather for optimized RD column design analysis. Table 4.7 shows the optimum trial parameters from base case study simulation analysis.

Table 4.7 Optimum trial parameters for optimized RD column

PARAMETER	VALUE
Reflux Ratio	0.01
Feed Temperature	363.15 K
Column Pressure	100 kPa
No. of Stages	14
Reactive Stages	6
Feed Location	At end of each reactive stages

Summary of the optimized RD column simulation can be found in the Appendix F. For the result, the optimized RD column gives the highest oleic acid conversion, 99.65%. Figure 4.7 shows the optimized RD column diagram.

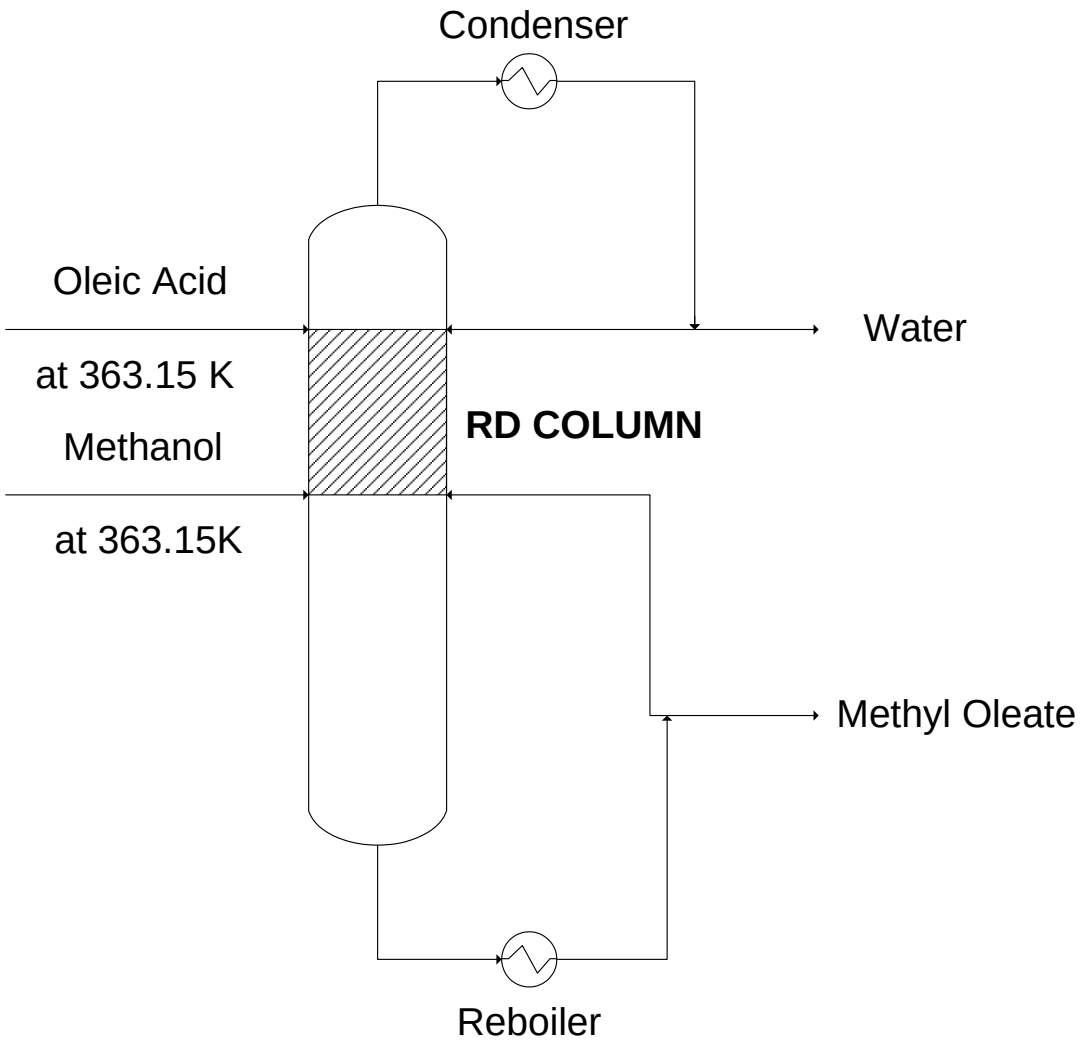

Figure 4.7 Optimized RD column diagram

CHAPTER 5

CONCLUSION

5.1 CONCLUSION

The simulation of RD column for oleic acid esterification with methanol to produce methyl oleate (biodiesel) was studied. The Zinc acetate catalyst was used in the process and kinetic data for the simulation is taken from previous study based on the type of catalyst use. For the Jatropha crude oil composition, oleic acid is assumed to be the overall fatty acid exist in the crude oil because of its highest mass percentage in the crude oil and its physical and chemical properties is almost similar with linoleic acid, which also have high mass percentage in the crude oil.

The simulation was conducted under different design and operating conditions. There are 6 parameters that need to be analyzed for this simulation; reflux ratio, feed temperature, column pressure, number of stages, reactive stages, and feeds location. The simulation is done in Aspen Plus 12.1 software using RADFRAC model and UNIQUAC thermodynamic properties.

In the nutshell, the optimum parameters for simulated RD column are; reflux ratio 0.01, feed temperature at 363.15K @ 90^0C, column pressure at 100 kPa, 14 stages with 6 reactive stages, and oleic acid and methanol feed locations, accordingly, at 3nd stage and 8th stage, to achieve 99.65% of oleic acid conversion to biodiesel.

5.2 RECOMMENDATION

5.2.1 DESIGN AND OPERATING PARAMETERS

In the parameters study, instead of analyzed 6 parameters in this simulation, there are variety of design and operating parameters that can be studied such as catalyst weight, feed ratio, boiler duty, etc. In the catalyst weight parameter analysis, inadequate amount of catalyst can affect the acid conversion and give poor RD column performance.

5.2.2 HYSYS

HYSYS is a powerful engineering simulation tool and has been uniquely created with respect to the program architecture, interface design and interactive operation. The package combines comprehensive data regression, thermodynamic database access, and Mayflower distillation technology to enable the design and analysis of separation system, including azeotropic, non-ideal, multiple liquid phase system, etc. HYSYS can be one of the alternative ways to complete process simulation with accurate value for the estimated chemical data.

5.2.3 MATLAB

In Matlab software, there are collection of functions to constant and solve ODEs for deterministic simulations and to implement realisations of CMEs for stochastic simulation using advance Matlab coding.

5.2.4 NON-EQULIBRIUM STAGE MODEL

This simulation study used equilibrium stage model which is RADFRAC to obtain the experiment data and result. Therefore, it is proposed that further study on reaction process using the non-equilibrium stage model is required to study the effect on operating parameters and conversion value.

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APPENDIX A

REFLUX RATIO

Molar Ratio: 1:1

Pressure: 80 kPa

Feed to Distillate Ratio: 0.5

No. of Stages: 15

Reflux Ratio: 0.01

Reactive stages: 10

Table A.1: Result summary for reflux ratio analysis at 0.01

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.6226375	6.87865E-3
METHY-01		0.0	0.0	99.27736	.0931213
METHA-01		0.0	100.0000	3.0036E-17	.6295161
WATER		0.0	0.0	5.5912E-27	99.37048
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29610.98	1839.911
Total Flow	l/min	532.6892	67.35048	790.9738	32.84306
Temperature	K	298.1500	298.1500	606.9342	348.7863
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2026E+5	-67376.73
Enthalpy	cal/gm	-694.1225	-1778.430	-405.7212	-3665.618
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3372E+6	-1.8734E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3682	-36.59557
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121327	-1.990975
Density	mol/cc	3.12878E-3	.0247461	2.10500E-3	.0507971
Density	gm/cc	.8837759	.7929208	.6239351	.9336885
Average MW		282.4668	32.04216	296.4062	18.38073
Liq Vol 60F	l/min	532.7933	67.22433	567.0639	30.88258

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.03

Pressure: 80 kPa

No. of Stages: 15

Reactive stages: 10

Table A.2: Result summary for reflux ratio analysis at 0.03

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.6813751	4.87990E-3
METHY-01		0.0	0.0	99.21862	.0951201
METHA-01		0.0	100.0000	2.9891E-17	.6862550
WATER		0.0	0.0	1.0353E-21	99.31374
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29610.16	1840.735
Total Flow	l/min	532.6892	67.35048	790.9409	32.86539
Temperature	K	298.1500	298.1500	606.9370	348.7188
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2027E+5	-67371.20
Enthalpy	cal/gm	-694.1225	-1778.430	-405.7788	-3663.677
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3375E+6	-1.8733E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3537	-36.60562
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121309	-1.990630
Density	mol/cc	3.12878E-3	.0247461	2.10509E-3	.0507626
Density	gm/cc	.8837759	.7929208	.6239437	.9334718
Average MW		282.4668	32.04216	296.3980	18.38896
Liq Vol 60F	l/min	532.7933	67.22433	567.0433	30.90435

Molar Ratio: 1:1

Pressure: 80 kPa

Feed to Distillate Ratio: 0.5

No. of Stages: 15

Reflux Ratio: 0.05

Reactive stages: 10

Table A.3: Result summary for reflux ratio analysis at 0.05

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.7348484	4.27102E-3
METHY-01		0.0	0.0	99.16515	.0957289
METHA-01		0.0	100.0000	2.9739E-17	.7391195
WATER		0.0	0.0	2.1083E-23	99.26088
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29609.41	1841.485
Total Flow	l/min	532.6892	67.35048	790.9109	32.88991
Temperature	K	298.1500	298.1500	606.9395	348.7754
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2028E+5	-67364.13
Enthalpy	cal/gm	-694.1225	-1778.430	-405.8312	-3661.800
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3379E+6	-1.8731E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3405	-36.60842
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121293	-1.989972
Density	mol/cc	3.12878E-3	.0247461	2.10517E-3	.0507247
Density	gm/cc	.8837759	.7929208	.6239516	.9331561
Average MW		282.4668	32.04216	296.3905	18.39645
Liq Vol 60F	l/min	532.7933	67.22433	567.0245	30.92420

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 80 kPa

No. of Stages: 15

Reactive stages: 10

Table A.4: Result summary for reflux ratio analysis at 0.1

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8453184	3.64603E-3
METHY-01		0.0	0.0	99.05468	.0963539
METHA-01		0.0	100.0000	2.9353E-17	.8489645
WATER		0.0	0.0	0.0	99.15104
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.86	1843.035
Total Flow	l/min	532.6892	67.35048	790.8493	32.94262
Temperature	K	298.1500	298.1500	606.9450	348.9500
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67348.51
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9394	-3657.873
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3135	-36.61129
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121260	-1.988455
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506436
Density	gm/cc	.8837759	.7929208	.6239675	.9324468
Average MW		282.4668	32.04216	296.3750	18.41193
Liq Vol 60F	l/min	532.7933	67.22433	566.9858	30.96522

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.2

Pressure: 80 kPa

No. of Stages: 15

Reactive stages: 10

Table A.5: Result summary for reflux ratio analysis at 0.2

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	1.015866	3.13853E-3
METHY-01		0.0	0.0	98.88413	.0968614
METHA-01		0.0	100.0000	2.8530E-17	1.019005
WATER		0.0	0.0	0.0	98.98100
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29605.47	1845.427
Total Flow	l/min	532.6892	67.35048	790.7534	33.02518
Temperature	K	298.1500	298.1500	606.9529	349.2508
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2035E+5	-67323.86
Enthalpy	cal/gm	-694.1225	-1778.430	-406.1068	-3651.794
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3397E+6	-1.8720E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.2726	-36.61450
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121213	-1.986051
Density	mol/cc	3.12878E-3	.0247461	2.10559E-3	.0505170
Density	gm/cc	.8837759	.7929208	.6239928	.9313231
Average MW		282.4668	32.04216	296.3510	18.43583
Liq Vol 60F	l/min	532.7933	67.22433	566.9260	31.02855

APPENDIX B

FEED TEMPERATURE

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table B.1: Result summary for feed temperature analysis at 298.15K

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8453184	3.64603E-3
METHY-01		0.0	0.0	99.05468	.0963539
METHA-01		0.0	100.0000	2.9353E-17	.8489645
WATER		0.0	0.0	0.0	99.15104
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.86	1843.035
Total Flow	l/min	532.6892	67.35048	790.8493	32.94262
Temperature	K	298.1500	298.1500	606.9450	348.9500
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67348.51
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9394	-3657.873
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3135	-36.61129
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121260	-1.988455
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506436
Density	gm/cc	.8837759	.7929208	.6239675	.9324468
Average MW		282.4668	32.04216	296.3750	18.41193
Liq Vol 60F	l/min	532.7933	67.22433	566.9858	30.96522

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 80 kPa

No. of Stages: 15

Reactive stages: 10

Table B.2: Result summary for feed temperature analysis at 303.15K

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8317279	3.69071E-3
METHY-01		0.0	0.0	99.06827	.0963092
METHA-01		0.0	100.0000	2.9921E-17	.8354186
WATER		0.0	0.0	0.0	99.16458
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29608.05	1842.844
Total Flow	l/min	534.6688	67.86168	790.8566	32.93604
Temperature	K	303.1500	303.1500	606.9441	348.9259
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9546E+5	-56860.99	-1.2031E+5	-67350.48
Enthalpy	cal/gm	-691.9602	-1774.568	-405.9262	-3658.358
Enthalpy	cal/sec	-5.4293E+6	-1.5795E+6	-3.3385E+6	-1.8727E+6
Entropy	cal/mol-K	-431.7407	-57.13225	-332.3169	-36.61107
Entropy	cal/gm-K	-1.528466	-1.783034	-1.121265	-1.988648
Density	mol/cc	3.11719E-3	.0245597	2.10531E-3	.0506537
Density	gm/cc	.8805038	.7869477	.6239658	.9325366
Average MW		282.4668	32.04216	296.3769	18.41003
Liq Vol 60F	l/min	532.7933	67.22433	566.9906	30.96017

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table B.3: Result summary for feed temperature analysis at 323.15K

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.7772361	3.88665E-3
METHY-01		0.0	0.0	99.12276	.0961133
METHA-01		0.0	100.0000	3.2472E-17	.7811227
WATER		0.0	0.0	0.0	99.21888
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29608.81	1842.080
Total Flow	l/min	542.8148	70.04065	790.8871	32.90967
Temperature	K	323.1500	323.1500	606.9415	348.8295
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9294E+5	-56350.09	-1.2029E+5	-67358.36
Enthalpy	cal/gm	-683.0553	-1758.623	-405.8728	-3660.304
Enthalpy	cal/sec	-5.3595E+6	-1.5653E+6	-3.3382E+6	-1.8729E+6
Entropy	cal/mol-K	-423.7967	-55.56939	-332.3302	-36.61020
Entropy	cal/gm-K	-1.500342	-1.734259	-1.121280	-1.989426
Density	mol/cc	3.07042E-3	.0237957	2.10523E-3	.0506943
Density	gm/cc	.8672901	.7624658	.6239578	.9328967
Average MW		282.4668	32.04216	296.3845	18.40239
Liq Vol 60F	l/min	532.7933	67.22433	567.0097	30.93994

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table B.4: Result summary for feed temperature analysis at 343.15K

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	VAPOR	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.7203433	4.11758E-3
METHY-01		0.0	0.0	99.17966	.0958824
METHA-01		0.0	100.0000	1.1587E-19	.7244609
WATER		0.0	0.0	3.0011E-21	99.27554
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29609.61	1841.282
Total Flow	l/min	551.3493	46929.23	790.9190	32.88223
Temperature	K	343.1500	343.1500	606.9388	348.7309
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	1.000000	0.0	0.0
Liquid Frac		1.000000	0.0	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9031E+5	-47504.03	-1.2028E+5	-67366.55
Enthalpy	cal/gm	-673.7324	-1482.548	-405.8170	-3662.336
Enthalpy	cal/sec	-5.2863E+6	-1.3196E+6	-3.3378E+6	-1.8732E+6
Entropy	cal/mol-K	-415.9341	-29.40986	-332.3441	-36.60925
Entropy	cal/gm-K	-1.472506	-.9178488	-1.121297	-1.990237
Density	mol/cc	3.02289E-3	3.55145E-5	2.10515E-3	.0507366
Density	gm/cc	.8538652	1.13796E-3	.6239495	.9332709
Average MW		282.4668	32.04216	296.3925	18.39442
Liq Vol 60F	l/min	532.7933	67.22433	567.0296	30.91881

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table B.5: Result summary for feed temperature analysis at 363.15K

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	VAPOR	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.6635311	4.38256E-3
METHY-01		0.0	0.0	99.23647	.0956174
METHA-01		0.0	100.0000	1.5885E-19	.6679137
WATER		0.0	0.0	7.2047E-21	99.33209
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29610.41	1840.485
Total Flow	l/min	560.3078	49664.43	790.9509	32.85490
Temperature	K	363.1500	363.1500	606.9361	348.6346
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	1.000000	0.0	0.0
Liquid Frac		1.000000	0.0	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.8755E+5	-47274.89	-1.2027E+5	-67374.69
Enthalpy	cal/gm	-663.9853	-1475.396	-405.7613	-3664.364
Enthalpy	cal/sec	-5.2098E+6	-1.3132E+6	-3.3374E+6	-1.8734E+6
Entropy	cal/mol-K	-408.1470	-28.76092	-332.3581	-36.60826
Entropy	cal/gm-K	-1.444938	-.8975962	-1.121314	-1.991045
Density	mol/cc	2.97456E-3	3.35586E-5	2.10506E-3	.0507788
Density	gm/cc	.8402130	1.07529E-3	.6239411	.9336428
Average MW		282.4668	32.04216	296.4005	18.38646
Liq Vol 60F	l/min	532.7933	67.22433	567.0495	30.89772

APPENDIX C

COLUMN PRESSURE

Molar Ratio: 1:1 Pressure: 30 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table C.1: Result summary for column pressure analysis at 30 kPa

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	7.335468	3.27821E-3
METHY-01		0.0	0.0	92.56453	.0967217
METHA-01		0.0	100.0000	1.3758E-18	7.338746
WATER		0.0	0.0	1.6289E-18	92.66125
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29516.82	1934.071
Total Flow	l/min	532.6892	67.35048	741.7326	34.98941
Temperature	K	298.1500	298.1500	568.2106	332.3864
Pressure	atm	1.000000	1.000000	.2960770	.2960770
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.3012E+5	-66940.80
Enthalpy	cal/gm	-694.1225	-1778.430	-440.3957	-3464.595
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.6109E+6	-1.8613E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-344.9569	-38.41810
Entropy	cal/gm-K	-1.535546	-1.795414	-1.167510	-1.988372
Density	mol/cc	3.12878E-3	.0247461	2.24474E-3	.0476811
Density	gm/cc	.8837759	.7929208	.6632404	.9212651
Average MW		282.4668	32.04216	295.4637	19.32139
Liq Vol 60F	l/min	532.7933	67.22433	564.7106	33.37572

Molar Ratio: 1:1 Pressure: 50 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table C.2: Result summary for column pressure analysis at 50 kPa

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	2.464067	3.34080E-3
METHY-01		0.0	0.0	97.43593	.0966592
METHA-01		0.0	100.0000	5.9861E-18	2.467408
WATER		0.0	0.0	0.0	97.53259
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29585.15	1865.741
Total Flow	l/min	532.6892	67.35048	765.7197	33.37315
Temperature	K	298.1500	298.1500	587.4106	342.3438
Pressure	atm	1.000000	1.000000	.4934616	.4934616
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2492E+5	-67291.35
Enthalpy	cal/gm	-694.1225	-1778.430	-421.8160	-3610.290
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.4665E+6	-1.8711E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-338.9744	-37.16149
Entropy	cal/gm-K	-1.535546	-1.795414	-1.144613	-1.993774
Density	mol/cc	3.12878E-3	.0247461	2.17443E-3	.0499902
Density	gm/cc	.8837759	.7929208	.6439509	.9317572
Average MW		282.4668	32.04216	296.1477	18.63877
Liq Vol 60F	l/min	532.7933	67.22433	566.4183	31.56643

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 70 kPa

No. of Stages: 15

Reactive stages: 10

Table C.3: Result summary for column pressure analysis at 70 kPa

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	1.152242	3.53848E-3
METHY-01		0.0	0.0	98.74776	.0964615
METHA-01		0.0	100.0000	1.8439E-17	1.155780
WATER		0.0	0.0	0.0	98.84422
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29603.55	1847.340
Total Flow	l/min	532.6892	67.35048	783.2773	32.99997
Temperature	K	298.1500	298.1500	601.2154	347.0117
Pressure	atm	1.000000	1.000000	.6908463	.6908463
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2163E+5	-67350.29
Enthalpy	cal/gm	-694.1225	-1778.430	-410.4680	-3649.445
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3754E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-334.2964	-36.74837
Entropy	cal/gm-K	-1.535546	-1.795414	-1.128115	-1.991248
Density	mol/cc	3.12878E-3	.0247461	2.12568E-3	.0505556
Density	gm/cc	.8837759	.7929208	.6299079	.9330008
Average MW		282.4668	32.04216	296.3319	18.45494
Liq Vol 60F	l/min	532.7933	67.22433	566.8782	31.07921

Molar Ratio: 1:1 Pressure: 90 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table C.4: Result summary for column pressure analysis at 90 kPa

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.6403824	3.75410E-3
METHY-01		0.0	0.0	99.25962	.0962459
METHA-01		0.0	100.0000	4.4535E-17	.6441365
WATER		0.0	0.0	0.0	99.35586
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29610.73	1840.160
Total Flow	l/min	532.6892	67.35048	797.8761	32.92234
Temperature	K	298.1500	298.1500	612.1187	350.7426
Pressure	atm	1.000000	1.000000	.8882309	.8882309
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.1912E+5	-67338.08
Enthalpy	cal/gm	-694.1225	-1778.430	-401.8921	-3663.020
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3056E+6	-1.8724E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-330.5108	-36.49510
Entropy	cal/gm-K	-1.535546	-1.795414	-1.115070	-1.985240
Density	mol/cc	3.12878E-3	.0247461	2.08679E-3	.0506748
Density	gm/cc	.8837759	.7929208	.6185324	.9315659
Average MW		282.4668	32.04216	296.4037	18.38322
Liq Vol 60F	l/min	532.7933	67.22433	567.0576	30.88911

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 100 kPa

No. of Stages: 15

Reactive stages: 10

Table C.5: Result summary for column pressure analysis at 100 kPa

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.4977438	3.86309E-3
METHY-01		0.0	0.0	99.40226	.0961369
METHA-01		0.0	100.0000	6.4616E-17	.5016069
WATER		0.0	0.0	2.7126E-20	99.49839
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29612.73	1838.159
Total Flow	l/min	532.6892	67.35048	804.4720	32.92374
Temperature	K	298.1500	298.1500	616.8442	352.4151
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.1804E+5	-67322.90
Enthalpy	cal/gm	-694.1225	-1778.430	-398.2140	-3666.180
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.2756E+6	-1.8720E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-328.8569	-36.39296
Entropy	cal/gm-K	-1.535546	-1.795414	-1.109415	-1.981839
Density	mol/cc	3.12878E-3	.0247461	2.06968E-3	.0506726
Density	gm/cc	.8837759	.7929208	.6135025	.9305135
Average MW		282.4668	32.04216	296.4238	18.36323
Liq Vol 60F	l/min	532.7933	67.22433	567.1077	30.83613

APPENDIX D

NO. OF STAGES

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 14

Reflux Ratio: 0.1 Reactive stages: 10

Table D.1: Result summary for number of stages analysis (14 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8390771	3.66256E-3
METHY-01		0.0	0.0	99.06092	.0963378
METHA-01		0.0	100.0000	4.46488E-7	.8427392
WATER		0.0	0.0	1.2679E-20	99.15726
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.94	1842.947
Total Flow	l/min	532.6892	67.35048	790.8523	32.93955
Temperature	K	298.1500	298.1500	606.9444	348.9375
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67349.44
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9335	-3658.097
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3151	-36.61127
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121263	-1.988547
Density	mol/cc	3.12878E-3	.0247461	2.10532E-3	.0506483
Density	gm/cc	.8837759	.7929208	.6239670	.9324895
Average MW		282.4668	32.04216	296.3758	18.41106
Liq Vol 60F	l/min	532.7933	67.22433	566.9880	30.96290

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table D.2: Result summary for number of stages analysis (15 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8413558	3.65624E-3
METHY-01		0.0	0.0	99.05864	.0963437
METHA-01		0.0	100.0000	1.27152E-9	.8450121
WATER		0.0	0.0	7.7173E-22	99.15499
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.91	1842.979
Total Flow	l/min	532.6892	67.35048	790.8512	32.94067
Temperature	K	298.1500	298.1500	606.9446	348.9421
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67349.10
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9357	-3658.015
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3146	-36.61127
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121262	-1.988514
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506466
Density	gm/cc	.8837759	.7929208	.6239672	.9324739
Average MW		282.4668	32.04216	296.3755	18.41138
Liq Vol 60F	l/min	532.7933	67.22433	566.9872	30.96375

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 80 kPa

No. of Stages: 16

Reactive stages: 10

Table D.3: Result summary for number of stages analysis (16 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8430307	3.65155E-3
METHY-01		0.0	0.0	99.05697	.0963484
METHA-01		0.0	100.0000	3.6207E-12	.8466823
WATER		0.0	0.0	7.6610E-20	99.15332
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.89	1843.002
Total Flow	l/min	532.6892	67.35048	790.8502	32.94148
Temperature	K	298.1500	298.1500	606.9447	348.9451
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67348.86
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9373	-3657.955
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3142	-36.61130
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121261	-1.988490
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506453
Density	gm/cc	.8837759	.7929208	.6239675	.9324628
Average MW		282.4668	32.04216	296.3753	18.41161
Liq Vol 60F	l/min	532.7933	67.22433	566.9866	30.96437

Molar Ratio: 1:1

Pressure: 80 kPa

Feed to Distillate Ratio: 0.5

No. of Stages: 18

Reflux Ratio: 0.1

Reactive stages: 10

Table D.4: Result summary for number of stages analysis (18 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8453936	3.64509E-3
METHY-01		0.0	0.0	99.05461	.0963549
METHA-01		0.0	100.0000	2.9280E-17	.8490387
WATER		0.0	0.0	2.8357E-19	99.15096
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.86	1843.036
Total Flow	l/min	532.6892	67.35048	790.8489	32.94261
Temperature	K	298.1500	298.1500	606.9448	348.9489
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67348.53
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9396	-3657.872
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3136	-36.61136
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121261	-1.988457
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506436
Density	gm/cc	.8837759	.7929208	.6239678	.9324476
Average MW		282.4668	32.04216	296.3749	18.41194
Liq Vol 60F	l/min	532.7933	67.22433	566.9858	30.96525

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 80 kPa

No. of Stages: 20

Reactive stages: 10

Table D.5: Result summary for number of stages analysis (20 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8466542	3.64173E-3
METHY-01		0.0	0.0	99.05335	.0963582
METHA-01		0.0	100.0000	3.4320E-19	.8502959
WATER		0.0	0.0	0.0	99.14970
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.84	1843.053
Total Flow	l/min	532.6892	67.35048	790.8482	32.94322
Temperature	K	298.1500	298.1500	606.9448	348.9511
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67348.34
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9409	-3657.827
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3133	-36.61138
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121260	-1.988439
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506426
Density	gm/cc	.8837759	.7929208	.6239680	.9324393
Average MW		282.4668	32.04216	296.3748	18.41212
Liq Vol 60F	l/min	532.7933	67.22433	566.9853	30.96571

APPENDIX E

REACTIVE STAGES

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 6

Table E.1: Result summary for reactive stages analysis (6 stages)

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIO L-01		100.0000	0.0	.8413664	3.65621E-3
METHY -01		0.0	0.0	99.05863	.0963437
METHA -01		0.0	100.0000	1.27152E-9	.8450226
WATER		0.0	0.0	0.0	99.15498
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.91	1842.979
Total Flow	l/min	532.6892	67.35048	790.8512	32.94067
Temperature	K	298.1500	298.1500	606.9446	348.9420
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67349.10
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9357	-3658.015
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3146	-36.61128
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121262	-1.988514
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506466
Density	gm/cc	.8837759	.7929208	.6239672	.9324739
Average MW		282.4668	32.04216	296.3755	18.41138
Liq Vol 60F	l/min	532.7933	67.22433	566.9872	30.96375

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 8

Table E.2: Result summary for reactive stages analysis (8 stages)

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8413124	3.65634E-3
METHY-01		0.0	0.0	99.05869	.0963436
METHA-01		0.0	100.0000	1.27152E-9	.8449687
WATER		0.0	0.0	0.0	99.15503
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.91	1842.978
Total Flow	l/min	532.6892	67.35048	790.8512	32.94066
Temperature	K	298.1500	298.1500	606.9446	348.9422
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67349.11
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9356	-3658.017
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3146	-36.61126
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121262	-1.988514
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506466
Density	gm/cc	.8837759	.7929208	.6239672	.9324740
Average MW		282.4668	32.04216	296.3755	18.41137
Liq Vol 60F	l/min	532.7933	67.22433	566.9872	30.96373

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table E.3: Result summary for reactive stages analysis (10 stages)

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8413551	3.65624E-3
METHY-01		0.0	0.0	99.05864	.0963437
METHA-01		0.0	100.0000	1.27152E-9	.8450114
WATER		0.0	0.0	4.3944E-24	99.15499
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.91	1842.979
Total Flow	l/min	532.6892	67.35048	790.8512	32.94067
Temperature	K	298.1500	298.1500	606.9446	348.9421
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67349.10
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9357	-3658.015
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3146	-36.61128
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121262	-1.988514
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506466
Density	gm/cc	.8837759	.7929208	.6239672	.9324739
Average MW		282.4668	32.04216	296.3755	18.41138
Liq Vol 60F	l/min	532.7933	67.22433	566.9872	30.96375

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 12

Table E.4: Result summary for reactive stages analysis (12 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8421861	3.66079E-3
METHY-01		0.0	0.0	99.05766	.0964959
METHA-01		0.0	100.0000	1.56751E-4	.8456902
WATER		0.0	0.0	0.0	99.15415
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.86	1843.032
Total Flow	l/min	532.6892	67.35048	790.8120	32.94180
Temperature	K	298.1500	298.1500	606.9159	348.9346
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2032E+5	-67349.31
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9579	-3657.921
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3388E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3241	-36.61236
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121296	-1.988515
Density	mol/cc	3.12878E-3	.0247461	2.10543E-3	.0506448
Density	gm/cc	.8837759	.7929208	.6239970	.9324687
Average MW		282.4668	32.04216	296.3750	18.41191
Liq Vol 60F	l/min	532.7933	67.22433	566.9861	30.96484

APPENDIX F

FEED LOCATION

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table F.1: Result summary for feed location analysis (2 and 13 stages)

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIO L-01		100.0000	0.0	2.023315	.0400393
METHY -01		0.0	0.0	97.87668	.0599611
METHA -01		0.0	100.0000	4.51705E-7	2.063353
WATER		0.0	0.0	0.0	97.93665
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29591.33	1859.558
Total Flow	l/min	532.6892	67.35048	790.1907	33.63808
Temperature	K	298.1500	298.1500	607.0024	354.3698
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2059E+5	-67119.47
Enthalpy	cal/gm	-694.1225	-1778.430	-407.0944	-3613.040
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3462E+6	-1.8663E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.0394	-36.45961
Entropy	cal/gm-K	-1.535546	-1.795414	-1.120961	-1.962620
Density	mol/cc	3.12878E-3	.0247461	2.10709E-3	.0495965
Density	gm/cc	.8837759	.7929208	.6241391	.9213558
Average MW		282.4668	32.04216	296.2095	18.57701
Liq Vol 60F	l/min	532.7933	67.22433	566.5728	31.40350

Molar Ratio: 1:1

Feed to Distillate Ratio: 0.5

Reflux Ratio: 0.1

Pressure: 80 kPa

No. of Stages: 15

Reactive stages: 10

Table F.2: Result summary for feed location analysis (3 and 12 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIO L-01		100.0000	0.0	.8413739	3.65618E-3
METHY -01		0.0	0.0	99.05863	.0963438
METHA -01		0.0	100.0000	1.27151E-9	.8450301
WA TER		0.0	0.0	6.9503E-21	99.15497
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.91	1842.979
Total Flow	l/min	532.6892	67.35048	790.8512	32.94067
Temperature	K	298.1500	298.1500	606.9446	348.9419
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67349.10
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9357	-3658.015
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8727E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3146	-36.61129
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121262	-1.988514
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506466
Density	gm/cc	.8837759	.7929208	.6239672	.9324740
Average MW		282.4668	32.04216	296.3755	18.41138
Liq Vol 60F	l/min	532.7933	67.22433	566.9872	30.96375

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table F.3: Result summary for feed location analysis (5 and 10 stages)

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.8467495	4.47073E-8
METHY-01		0.0	0.0	99.05325	.0999999
METHA-01		0.0	100.0000	1.0318E-14	.8467495
WATER		0.0	0.0	0.0	99.15325
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29607.84	1843.055
Total Flow	l/min	532.6892	67.35048	790.8482	32.93156
Temperature	K	298.1500	298.1500	606.9449	348.6213
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.2031E+5	-67354.02
Enthalpy	cal/gm	-694.1225	-1778.430	-405.9410	-3658.132
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.3386E+6	-1.8728E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-332.3133	-36.62951
Entropy	cal/gm-K	-1.535546	-1.795414	-1.121260	-1.989423
Density	mol/cc	3.12878E-3	.0247461	2.10533E-3	.0506606
Density	gm/cc	.8837759	.7929208	.6239680	.9327701
Average MW		282.4668	32.04216	296.3747	18.41213
Liq Vol 60F	l/min	532.7933	67.22433	566.9853	30.96567

Molar Ratio: 1:1 Pressure: 80 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 15

Reflux Ratio: 0.1 Reactive stages: 10

Table F.4: Result summary for feed location analysis (both at 7 stages)

Heat and Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	99.75991	4.00124E-7
METHY-01		0.0	0.0	.1400882	.0999996
METHA-01		0.0	100.0000	3.5288E-19	99.75991
WATER		0.0	0.0	0.0	.2400878
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	28220.39	3230.498
Total Flow	l/min	532.6892	67.35048	748.7811	71.64018
Temperature	K	298.1500	298.1500	623.0450	331.8589
Pressure	atm	1.000000	1.000000	.7895386	.7895386
Vapor Frac		0.0	0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.9607E+5	-56984.75	-1.4123E+5	-56259.15
Enthalpy	cal/gm	-694.1225	-1778.430	-499.9599	-1743.242
Enthalpy	cal/sec	-5.4463E+6	-1.5829E+6	-3.9192E+6	-1.5643E+6
Entropy	cal/mol-K	-433.7407	-57.52893	-313.7285	-55.19696
Entropy	cal/gm-K	-1.535546	-1.795414	-1.110597	-1.710330
Density	mol/cc	3.12878E-3	.0247461	2.22361E-3	.0232876
Density	gm/cc	.8837759	.7929208	.6281407	.7515562
Average MW		282.4668	32.04216	282.4864	32.27270
Liq Vol 60F	l/min	532.7933	67.22433	532.3096	67.70301

APPENDIX G

OPTIMUM RD DESIGN

Molar Ratio: 1:1 Pressure: 100 kPa

Feed to Distillate Ratio: 0.5 No. of Stages: 14

Reflux Ratio: 0.01 Reactive stages: 6

Table G.1: Summary result for optimum design parameter for RD column

Heatand Material Balance Table					
Stream ID		1	2	3	4
From				B1	B1
To		B1	B1		
Phase		LIQUID	VAPOR	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
TRIOL-01		100.0000	0.0	.2634439	7.14810E-3
METHY-01		0.0	0.0	99.63656	.0928519
METHA-01		0.0	100.0000	1.0357E-16	.2705920
WATER		0.0	0.0	0.0	99.72941
Total Flow	kmol/hr	100.0000	100.0000	99.90000	100.1000
Total Flow	kg/hr	28246.68	3204.216	29616.02	1834.873
Total Flow	l/min	560.3078	49664.43	804.6103	32.81620
Temperature	K	363.1500	363.1500	616.8352	352.1852
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		0.0	1.000000	0.0	0.0
Liquid Frac		1.000000	0.0	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-1.8755E+5	-47274.89	-1.1798E+5	-67353.77
Enthalpy	cal/gm	-663.9853	-1475.396	-397.9830	-3674.431
Enthalpy	cal/sec	-5.2098E+6	-1.3132E+6	-3.2741E+6	-1.8728E+6
Entropy	cal/mol-K	-408.1470	-28.76092	-328.9164	-36.38270
Entropy	cal/gm-K	-1.444938	-.8975962	-1.109492	-1.984829
Density	mol/cc	2.97456E-3	3.35586E-5	2.06933E-3	.0508387
Density	gm/cc	.8402130	1.07529E-3	.6134650	.9318936
Average MW		282.4668	32.04216	296.4567	18.33040
Liq Vol 60F	l/min	532.7933	67.22433	567.1898	30.74918