DESIGN AND OPERATION OF REACTIVE DISTILLATION FOR BIODIESEL PRODUCTION
CASE STUDY: *JATROPHA CURCAS*

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SUPERVISOR DECLARATION

“I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Bachelor of Chemical Engineering”.

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STUDENT'S DECLARATION

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

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To my beloved parents,
family, lecturers and friends.

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ABSTRACT

Nowadays, the demand for the diesel fuel increase rapidly due to the increase of vehicles all over the world. Experts believed that the diesel fuel sources will be lasted for several decades only. Biodiesel has been discovered as potential fuel since biodiesel oil has some similarities to replace diesel fuel. There are many of the oil-bearing crops identified to be sources for biodiesel fuel but only soybean, palm, sunflower, cotton seed, peanut oil and safflower considered as well (Goering et al., 1982; Pryor et al., 1982). However, recently *Jatropha Curcas* oil was found to be potential source of biodiesel since it is non-edible oil and contains a high percentage of oil in the seed compared to the other non-edible oil. There are three methods to produce biodiesel, which are (1) base catalyzed trans-esterification, (2) acid catalyzed esterification, and (3) enzymatic catalysis (Kiss, 2009). The commonly used in industry is the base catalyst trans-esterification due to lower cost of production. However, this method will form soap as the by product and need a further step to obtain biodiesel. Therefore in the present study, esterification of oleic acid catalyzed by zinc acetate using subcritical methanol is used which taken from previous study done Song et al., 2009. In this study, reactive distillation will be used to produce the biodiesel where the reaction and separation will be taken part in the same unit operation. Since reactive distillation (RD) is a new technology, a simulation study should be carried out to predict the optimum condition to produce biodiesel by using reactive distillation. In this study, Aspen Plus simulation tool was used to investigate the optimum design and operation for RD column in biodiesel production. Equilibrium stage model was used where RADFRAC unit model used to present RD column and UNIQUAC as the property method. This study investigated the optimum value for distillate to feed ratio (F/D), molar ratio and reboiler duty which can affected the biodiesel yield in the process. From the simulation, the high of yield of biodiesel can be produced at distillate to feed ratio 0.5, acid to alcohol ratio (molar ratio) 1:4 and reboiler duty at 6000kW which achieved conversion of 99.99%.

ABSTRAK

Pada masa kini, permintaan bagi bahan api diesel meningkat dengan pesat disebabkan oleh peningkatan kenderaan di seluruh dunia. Pakar percaya bahawa sumber bahan api diesel akan berkekalan selama beberapa dekad sahaja. Biodiesel ditemui sebagai bahan api berpotensi kerana biodiesel mempunyai beberapa persamaan untuk menggantikan bahan api diesel. Terdapat banyak tanaman minyak yang dikenal pasti untuk menjadi sumber bagi bahan bakar biodiesel tetapi hanya kacang soya, kelapa sawit, bunga matahari, biji kapas, kacang tanah dan *Carthamus tinctorius* yang diaggap berpotensi untuk menjadi sumber biodiesel (Goering et al, 1982; Pryor et al, 1982). Walau bagaimanapun, baru-baru ini *Jatropha Curcas* minyak dikatakan berpotensi menjadi sumber biodiesel kerana ia adalah tanaman tidak boleh dimakan dan mengandungi peratusan minyak yang tinggi di dalam biji buah berbanding minyak tanaman yang lain yang tidak boleh dimakan. Terdapat tiga kaedah untuk menghasilkan biodiesel, yang (1) *trans*-esterifikasi pemangkin alkali, (2) esterifikasi pemangkin asid, dan (3) pemangkinan enzim (Kiss, 2009). Biasa digunakan dalam industri *trans*-esterifikasi pemangkin alkali disebabkan oleh kos pengeluaran yang lebih rendah. Walau bagaimanapun, kaedah ini akan menghasilkan sabun sebagai produk sampingan dan memerlukan langkah selanjutnya untuk mendapatkan biodiesel. Oleh yang demikian, dalam kajian ini, esterifikasi asid oleik menggunakan pemangkin zink asetat yang mana metanol sebagai subgenting digunakan diadaptasi daripada kajian yang dijalankan oleh Song et al, 2009.. Dalam kajian ini, penyulingan reaktif akan digunakan untuk menghasilkan biodiesel di mana tindak balas dan pengasingan berlaku dalam operasi unit yang sama. Oleh kerana penyulingan reaktif (RD) adalah teknologi yang baru, kajian simulasi perlu dijalankan untuk mengkaji keadaan optimum untuk menghasilkan biodiesel dengan menggunakan penyulingan reaktif. Dalam kajian ini, perisian simulasi Aspen Plus digunakan untuk mengkaji reka bentuk dan operasi yang optimum untuk ruangan RD dalam penghasilan biodiesel. Model keseimbangan peringkat telah digunakan di mana model unit RADFRAC digunakan untuk membentangkan ruangan RD dan UNIQUAC sebagai cirri-ciri kaedah. Kajian ini menyiasat nilai optimum untuk nisbah sulingan kepada jumlah masuk bahan (D/ F), nisbah molar dan duti pendidihan semula yang boleh menjejaskan hasil biodiesel dalam proses. Sebagai penemuan daripada simulasi, hasil biodiesel yang tinggi diperoleh pada nisbah sulingan kepada jumlah masuk 0.5, asid kepada nisbah alkohol (nisbah molar) 1:4 dan kuasa pendidih pada 6000kW yang mana mencapai penukaran asid oleic sehingga 99.99%.

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A	Pre-exponential factor
C_A	Concentration of methanol, mol.dm^{-1}
C_B	Concentration of oleic acid, mol.dm^{-1}
C_C	Concentration of methyl oleate, mol.dm^{-1}
C_D	Concentration of water, mol.dm^{-1}
D	Distillate molar flow rate, kmol/hr
Ea	Activation energy
F	Feed molar flow rate, kmol/hr
k	Forward reaction rate constant
k'	Backward reaction rate constant
n	Order of the esterification reaction
R	Gas constant, J.mol^{-1}.K^{-1}
T	Reaction temperature, K
α	Reaction order for methanol
β	Reaction order for oleic acid
γ	Reaction order for water
λ	Reaction order for methyl oleate
x_F	Composition of feed
x_D	Composition of distillate
x_W	Composition of bottom product

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND OF THE STUDY

Recently as a result from the rising costs of fuel, and the negative impact of petroleum based fuels in the environment, biodiesel was found as an alternative fuel. Since biodiesel have similar properties as diesel, biodiesel have it potential to replace diesel fuel in the future (Kiss, 2009). Biodiesel is found as a renewable, biodegradable, and environmental friendly (Janaun et al., 2010). There are three basic methods to produce biodiesel from oils or fats: (1) base catalyzed trans-esterification, (2) acid catalyzed esterification, and (3) enzymatic catalysis (Kiss, 2009). The first method is frequently used in large scale production in industry since it is 4000 times faster than the other method at the same amount of catalyst but it suffers from the side product formation which is soap formation. In this case, the soap produced will consume the catalyst used and greatly increase the viscosity and result in difficulty to separate the glycerol. Therefore, to solve this problem, the second method is used although it is much slower than the first method (Fukuda et al., 2001). However, the former method is still under development (Kiss, 2009). These fatty esters (biodiesel) are produced by transesterification method which is vegetables oil and animal’s fats are used as sources of this transesterification. The vegetables oil and animals fats are basically have higher viscosity and are not suitable to be used as a fuel (Fukuda et al., 2001, Fazal et al., 2011).Therefore, by using transesterification reaction, the triglycerides contain in the oil and fats which cause them high in viscosity can be converted to esters. The transesterification reaction consists of three sequence reversible reaction. The triglycerides are converted step by step in diglycerides, monoglycerides and finally in glycerol. Methanol is used for transesterification producing methyl esters and glycerin as a side product (Fukuda et al., 2001). There are various forms of catalyst that can be used in the transesterification reaction but so far in industrial only chemical homogeneous catalyst are used in large scale production (Sotoft et al., 2010). In this study, the transesterification reaction and hydrolysis process will be used to product biodiesel since it produce directly biodiesel and water without side product. There are more than 350 oil-bearing crops identified to be sources for biodiesel fuel but only soybean, palm, sunflower, cottonseed, peanut oil and safflower has been identified as potential sources (Goering et al., 1982; Pryor et al., 1982). However some producers using the waste oil to produce biodiesel. Although it is more economical in the cost of feedstock but it requires complicated treatment to remove the impurities and at the same time the cost will increase (Lu et al., 2009). Therefore in the present study, non-edible oils like *Jatropha Curcas* oil are use as a feedstock's. However, *Jatropha Curcas* oil with high content of free fatty acids (FFAs) which cannot be directly used in an alkali catalyzed transesterification process because FFAs react with alkali catalyst to form soaps, resulting in serious emulsification and separation problems. Pre-esterification catalyzed by homogeneous acids, such as sulfuric acid, phosphorous acid, or sulfonic acid, is a conventional and useful method to reduce the content of FFAs, which can turn the raw oils transesterificable by an alkali catalyst and convert FFAs to valuable fatty acid methyl esters (FAME) (Lu et al,. 2008). The performance of the transesterification process is affected by multiple parameters such as molar feed ratio of alcohol: vegetable or fats oil, type and quantity of catalyst that been used, reaction time, temperature of the reaction and also feedstock properties. In the present study, biodiesel is produce by using reactive distillation (RD). Reactive distillation (RD) is the process in which chemical reaction and separation are carried out simultaneously within a fractional distillation apparatus. Therefore, for producing an economical biodiesel, reactive distillation is potential equipment as it reduces the cost of equipments. The most important part in using RD for this transesterification process, it will improve the conversion of the reactant approaching to 100% improved selectivity, reduce the catalyst requirement and reduce by product formation(Taylor et. al, 2000 & Ind. Eng. Chem. Res., 2000). If the exothermic reaction taken place in this column, heat released from the reaction can be used for separation process. Therefore, by this way, the heat requirement for the separation task is reduce, result reducing the boiler duty (Gomez-Castro et al, 2010). In this study, Aspen Plus software is utilized for simulating biodiesel production by reactive distillation with the aim of obtaining good understanding about the process and finding the optimum conditions to produce a large amount of biodiesel.

1.2 PROBLEM STATEMENT

Nowadays, the demand of the diesel fuel increase rapidly since the number of vehicle and other equipment which is depend on the fuel increase. However, diesel fuel can cause certain problems which contributed to global warming and pollutions. In addition, according to some experts the sources of diesel fuel will be lasting for several decades only. Therefore, several researchers have discovered an alternative fuel to replace diesel, and one of them is biodiesel. There are many sources of biodiesel which can be derived from vegetable oils and animal's fat. However, the production cost of the biodiesel is very high than the petroleum based fuel. Therefore reactive distillation column can be considered as an alternative in order to reduce the cost of biodiesel production. A simulation process should be carried out to predict the most suitable conditions before it can be realized to a full scale plant. In the present study, the optimal performance of the esterification reaction of *Jatropha Curcas* by using acid catalyst will be determined. Aspen plus is software that act as a tool for the simulation and predict the optimum parameter (i.e. reactant ratio, pressure, distillate to feed ratio, temperature, reboiler duty) for any process. In this study, several parameters will be predicted to determine the optimum condition to produce high yield of biodiesel. The software is very useful in predicting the optimum condition compared to the cost and risk in carrying out similar study through experimental work.

1.3 OBJECTIVES

1.2.1 To study the preliminary feasibility of biodiesel production using reactive distillation.

1.2.2 To identify the design and operation parameters that can be adjusted in producing high yield of biodiesel.

1.2.3 To determine the interaction between the design and operation parameters in producing biodiesel.

1.4 SCOPE OF STUDY

To achieve the objective of this study will cover:

1.3.1 The reaction, thermodynamic model and kinetics model of selected previous experimental run for production of biodiesel will be simulated.

1.3.2 The parameter in RD will be determined by using various parameters such as the distillate to feed ratio, molar ratio, and reboiler duty.

1.3.3 Aspen Plus version 12.1 will be utilized to run the simulation. The results from the simulation will be used to verify the reliability of producing biodiesel in pilot plant and commercial plant.

1.5 RATIONALE & SIGNIFICANCE

Reactive distillation column is a new technology and has more advantages than the conventional process. In order to reduce the cost of biodiesel production many plants face nowadays, reactive distillation is regarded an alternative to solve the problem. However, in order to produce high of yield of biodiesel in product, there are several conditions need to be established. Since the reactive distillation is still new in industry and there is limited reference on this subject, a simulation study needs to be done to predict the behavior of the process. This simulation will determine the optimum condition to maximize percentage yield of biodiesel and determine the design and operation parameters that influence the production of biodiesel by using reactive distillation.

CHAPTER 2

LITERATURE REVIEW

2.1 BIODIESEL OVERVIEW

Biodiesel has recently experienced a major surge worldwide. Biodiesel production capacity is being monitored closely in developed countries such as Germany, Italy, France, and the United States, Brazil, Argentina, Indonesia, and Malaysia. However, biodiesel in Malaysia is still under the development since the diesel fuel remains as the main fuel sources. Interest and expansion of the production of the renewable fuel has been fostered by mandates and financial incentives offered by government. This interest is due to several advantages of biodiesel such as reduction of the emission of gases responsible for global warming, promote rural development, contribute toward the goal of energy security, renewable, and reduce pollution. Another feature that proponents of biodiesel put forward is that the fuel can be used without modification in engines currently in use. The replacement of this new alternative source or energy can generate higher foreign exchange savings, even more for the major oil exporting countries. As the result of this development the project not only solves their ecological problems but also to improve its economy. In view of the several advantages, vegetable oils has the potential to replace petroleum-based fuels in the long run as the petroleum fuels today can be lasted for few more decades more only (Ramadhas et al., 2005). Biodiesel have its own excellent characteristics than the diesel fuel and have potential to replace the current diesel fuel as following reason.

a) Biodiesel is derived from biomass resources; carbon dioxide generated by the use of biodiesel fuel does not have any impact to the amount of carbon dioxide in the global environment (Ueki et al, 2010).

b) Biodiesel does not containing sulfur ingredient where the sulfur oxide (SOx) is nearly zero (Ueki et al, 2010).
c) Biodiesel fuel has high ignition point and contains oxygen where complete combustion can be obtained. Therefore, the emission of the dark smoke can be reduced compared to current diesel fuel (Ueki et al., 2010).
d) Biodiesel can be readily used in any diesel engine without modification. Therefore, the cost of production is similar to the current diesel (Ueki et al., 2010).
e) As biodiesel is biodegradable fuel, it can be handled safely.

Typically biodiesel can be blended with crude petroleum oil to produce the blended fuel for vehicle use. This mixed fuel is widely used in Europe and United states (Ueki et al., 2010). Commonly, the B factor use to represent the amount of biodiesel mix with any fuel mix. Biodiesel can be used alone known as B100 (100% of biodiesel). There are others mixture of biodiesel which are B20 (20% biodiesel with 80% petro diesel), B5 (5% biodiesel with 95% petro diesel), and B2 (2% biodiesel with 98% petro diesel) (Woods et al., 2008).

2.1.1 PROPERTIES OF BIODIESEL

Biodiesel have several physical and chemical properties which are different from the current diesel and these differences contribute some significant benefits. Biodiesel has lower sulfur than today's diesel fuel and give higher lubricity. Biodiesel also contains 11% oxygen by weight, as well as a slightly higher cetane number, which provides for more complete combustion and a reduction in most emissions. Table 2.1 below shows the differences between diesel and biodiesel. The similarities between diesel and biodiesel enable the biodiesel a suitable fuel to replace the diesel fuel in the future.

Table 2.1: Properties of diesel and biodiesel

Fuel property	Diesel	Biodiesel
Fuel standard	ASTM D975	ASTM D6751
Lower heating value, Btu/gal	~129,050	~118,170
Kinematic viscosity@ 40 °C	1.3 - 1.4	4.0 - 6.0
Specific Gravity kg/l @60°F	0.87	0.88
Density.lb/gal @15°C	7.097	7.328
Water and sediment, vol%	0.005 max	0.05 max
Carbon, wt%	87	77
Hydrogen ,wt%	13	12
Oxygen, by dif. Wt%	0	11
Sulfur, wt%	0.05 max	0.0 to 0.0024
Boiling point, °C	180 to 340	315 to 350
Flash point, °C	60 to 80	100 to 170
Cloud point, °C	-15 to 5	13 to 12
Pour point, °C	-35 to -15	-15 to 10
Cetane Number	40-55	48-65
Lubricity HFRR, microns	300-600	<300

(Adapted from: article on www.utahbiodieselsupply.com)

2.1.2 BIODIESEL SOURCES

Biodiesel is a mixture of methyl esters with long-chain fatty acids and made from nontoxic, biological resources such as vegetable oils (Abreu FR et al., 2004), animal fats or even used cooking oils (Dennis et al., 2009). Biodiesel can be produced on large scale and environmental friendly since it can be produced by vegetables oils. Vegetables oils include the edible oils and non-edible oils. More than 95% of biodiesel produced by edible oils since in large scale at many places around the world (Gui et al., 2008). However as the production arise rapidly, some problem may occur. Some researchers said that the production of biodiesel from the edible oils will cause the imbalance to the food supply and market demand. In other words, biodiesel is competing limited land availability with food industry for plantation of oil crop. In addition, some environmentalist found that biodiesel production from edible oil will cause a lot of deforestation and destruction of ecosystem. Therefore, another alternative to solve this problem is by using non- edible oil. In this way, the issue on food versus fuel can be solve since non-edible oils also potentially to be the main sources of biodiesel production. A studied have been done on the prospects of fatty acid methyl esters (FAME) of some 26 non-traditional plant seed oils including Jatropha to use as potential biodiesel in India. Some of the plants are *Azadirachta indica*, *Calophyllum inophyllum, J. curcas* and *Pongamia pinnata* which are found as suitable plant to replace diesel fuel. In addition, they meet the major specification of biodiesel for use in diesel engine (Azam et al, .2005).

Table 2.2: Oil yield for major non-edible oil and edible oils sources

Type of oil	Oil yield (kg oil/hectare)	Oil yield (Wt %)	Sources
Non edible oil:			
Jatropha Curcas	1590	Kernel:50–60	Gui et al., 2008
Rubber seed	80-120	40-50	Ramadhas et al., 2005
Castor	1188	53	Karmee ., 2005
Pongamia pinnata	225-2250	30-40	Saka, 2005
Sea mango	N/A	54	Saka, 2005
Edible oil:			
Soybean	375	20	USDA, 2007
Palm	5000	20	MPOB, 2007
Rapeseed	1000	37-50	Canola Canada, 2007

(Adapted from: Gui et. al., 2008, Ramadhas et al., 2005)

Table 2.2 shows that the non-edible oil and edible oil found to be main sources of biodiesel production. The non-edible plant, *Jatropha Curcas* is the one of plant can produce a large amount of oil. Other than that, *Pongamia pinnata* plant has its own potential to produce biodiesel since the high oil contain. However, *pongamia pinnata* flowering start in general after 3 until 4 years compared to *Jatropha Curcas. Jatropha Curcas* starts yielding from 9–12 months time; the best yields are obtained only after 2 until 3 year's time. Besides the time constraint for plantation, Jatropha is potentially to be the main non-edible sources for biodiesel due to easily grown in many type of soil. The issue of food versus fuel is solving if *Jatropha Curcas* can be used as the main source of biodiesel production. However, most non-edible oils contain high free fatty acids (FFAs). Therefore they may need some addition step in the production which increase the cost of production of the biodiesel and may lower the ester yield of biodiesel below the standards.

2.2 ***JATROPHA CURCAS***

Jatropha Curcas is a species of flowering plant in the spurge family, Euphorbiaceous that is native to the American tropics, most likely Mexico and Central America. The seeds contain 35-40% oil (average: 34.4%) that can be processed to produce a high-quality biodiesel fuel and usable in a standard diesel engine (Gui et al., 2008). Furthermore, the quality of oil in its seeds is suitable for production of biodiesel as they contain more than 75% unsaturated fatty acids. However the seeds are also a source of the highly poisonous toxalbumin curcin which can cause diarrhea to human. Therefore this plant is not suitable to be consumed by human. *Jatropha Curcas* is an alternative plant instead of using food plant because *Jatropha Curcas* is a kind of non edible oil plant that can be used commercially to produce biodiesel instead of using the other edible oil plant. *Jatropha Curcas* may yield more than four times as much as fuel per hectare as soybean as and more than ten times than maize. A hectare of Jatropha has been claimed to produce more than 1 liters of fuel (Fitzgerald, 2007). In addition, plantation of Jatropha would not be a waste because the byproduct of the transesterification to produce biodiesel can be utilized to produce wide range of product including high quality of paper, cough medicine, energy pellets, cosmetics, toothpaste, pipe joint cement, moistening agent in tobacco. In addition, Jatropha seed cake which is the waste by-product of biodiesel transesterification process can be used as a rich of organic fertilizer used as biomass feedstock to power electricity plants. Table 2 shows the composition on several of non-edible oil. From the observation, Jatropha is the third ranked which is 43.1% of unsaturated fatty acid compare to sea mango and *pongamia pinnata*. Oil with higher unsaturated fatty acid will be useful since it can be used in cold flow properties. However, Jatropha is potentially to be produced in every country because it was reported that *Jatropha Curcas* plant can grow almost anywhere, even on gravely, sandy and saline soils. Due to its characteristic, Jatropha can be easily cultivated without intensive care and very minimal efforts are required to sustain its growth. It has a healthy life cycle of 30–50 years, which eliminates the need for yearly re-plantation but yet can still sustain reasonably high yield even with minimum irrigation (Gui et. al., 2008). One of the most important characteristics of biodiesel is the viscosity which determine by the amount and the type of fatty acid (FA) contain in the plant. *Jatropha Curcas* has similar viscosity to other edible oil such as peanut oil, corn oil, palm oil and sunflower oil (Arjun et.al, 2008). Since the characteristics of biodiesel produce from *Jatropha Curcas* is similar to the petroleum diesel, it is shown that Jatropha oil is a strong alternative for diesel replacement (Arjun et.al, 2008). Jatropha usually grows below 1400 meters of elevation from sea level and requires a minimum rainfall of 250mm, with an optimum rainfall between 900-1200mm (Bosswell, 2003). This plant is not even browsed by animals for its leaves. The Jatropha seed is particularly suitable for biodiesel production because it can be harvested in the third year of plantation five or six times annually Recently *Jatropha Curcas* is being considered as one of the most promising potential oil source to produce biodiesel in Asia, Europe and Africa (Arjun et al., 2008). The new and large markets for biodiesel demand are expected to emerge in China, India and Brazil (Hanna et al., 2005).

Table 2.3: Oil composition in non-edible plant

Fatty acid Composition (%)	Molecular formula	Non-edible oil				
		Jatropha	Rubber seed	Castor	Pongamia pinnata	Sea mango
Oleic	$C_{18}H_{34}O_2$	43.1	24.6	3.0	44.5–71.3	54.2
Linoleic	$C_{18}H_{32}O_2$	34.3	39.6	4.2	10.8–18.3	16.3
Palimitic	$C_{16}H_{32}O_2$	14.2	10.2	1.0	3.7–7.9	20.2
Steraric	$C_{18}H_{36}O_2$	6.9	8.7	1.0	2.4–8.9	6.9
Linoleic	$C_{18}H_{30}O_2$	-	16.3	0.3	-	-
Eicosenoic	$C_{20}H_{38}O_2$	-	-	0.3	9.5–12.4	-
Ricinoleic	$C_{18}H_{34}O_3$	-	-	89.5	-	-
Dihydroxystearic	$C_{18}H_{36}O_4$	-	-	0.7	-	-
Palmitoleic	$C_{16}H_{30}O_2$	-	-	-	-	-
Others		1.4	-	-	-	2.4

(Adapted from:Gui et al., 2008)

2.2.1 REACTION IN TRANSESTERIFICATION OF *JATROPHA CURCAS* FOR PRODUCING BIODIESEL

In conventional process, biodiesel is produce by transesterification of oils with methanol in the presence of catalysts such as alkalis (KOH, NaOH) or their alkoxides.

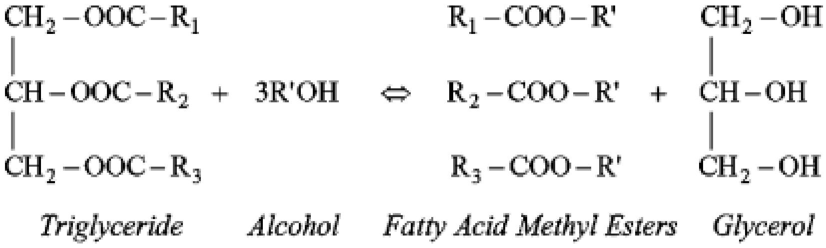


Figure 2.1: Transesterification reaction (Song et al., 2007)

Figure 2.1 show the transesterification reaction of biodiesel production. The process to produce biodiesel depends on the raw material. Since Jatropha oil is high in free fatty acids (FFAs) and cannot be used directly in an alkali catalyzed transesterification process because the FFAs can react with alkali catalyst to form soaps. The forming of soap will be a serious problem in separating the product. Therefore pre-esterification catalyzed by homogeneous acids, such as sulfuric acid, phosphorous acid, or sulfonic acid, is a conventional and useful method to reduce the content of FFAs, which turn the raw oils transesterificable by an alkali catalyst and convert FFAs to valuable fatty acid methyl esters (FAME) (Lu et al.,2009). In order to overcome the problem, a two-step process consisting of a pre-esterification and transesterification was developed to produce biodiesel from crude *Jatropha Curcas* oil. The free fatty acids (FFAs) in the oil were converted to methyl esters in the pre-esterification step using sulfuric acid or solid acid prepared by calcining metatitanic acid as catalysts. Below is the flow of the process in transesterification reaction.

Pre-Esterification → Purification → Transesterification → Phase Separation

(Source: Lu et al., 2009)

2.3 KINETIC LAW OF ESTERIFICATION

Esterification of reaction to produce biodiesel can be present as follow:

$$\text{Methanol (A)} + \text{Oleic acid (B)} \xrightarrow{\text{Catalyst}} \text{Methyl Oleate (C)} + \text{Water (D)}$$

From song et al., 2009, the rate expression for the reaction described as:

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

Figure 2.2: Oleic acid esterification reaction (Song et al., 2009; Mohd Junaidi, 2010)

Where C_{A}, C_{B}, C_{C}, and C_{D} represent the concentrations of methanol, oleic acid, methyl oleate and water respectively where α, β, λ and γ refer to their reaction orders. k and k' are the kinetic constants for the forward and reverse reactions respectively.

In this study, the kinetic model was taken from Song et al., 2009. The result from the research will be used in the stimulation.

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

$$\ln k_2 = -\frac{E_a}{RT} + \ln A$$

Figure 2.3: Arrhenius equation (Song et al., 2009)

The reaction order ***n* = 2.2**, pre-exponential factor, **A= 120.0** and activation energy, **Ea = 32.62 KJ/mol** obtained from the study esterification of oleic acid with methanol and using zinc acetate as catalyst. (Song et al., 2009)

2.4 REACTIVE DISTILLATION

Reactive distillation (RD) is the simultaneous implementation of reaction and separation within a single unit of column. Reactants are converted to products in a reaction zone in the presence of catalyst with simultaneous separation of the products and recycle of unused reactants to this zone. This combined operation is especially suited for the chemical reaction limited by equilibrium constraints, since one or more of the products of the reaction are continuously separated from the reactants. (Chin et al., 2006). The reactive distillation is a hybrid process that combines the reaction and separation in single equipment. When the reaction and separation take place in a single shell, the heat release from exothermic reaction can be used in separation task. Therefore by using reactive distillation column the heat require for the separation will be reduced and also the cost production of biodiesel (Gomez-Castro et al., 2010). The other benefits in using RD are speeding up the process, high conversion, and reduce the cost used since the number of equipment used will be less. This RD is very useful for equilibrium-limited reactions such as esterification and ester hydrolysis reactions. Being a relatively new field, research on various aspects such as modeling and simulation, process synthesis, column hardware design, non-linear dynamics and control is in progress. The suitability of RD for a particular reaction depends on various factors such as volatilities of reactants and products along with the feasible reaction and distillation temperature. Hence, the use of RD for every reaction may not be feasible. Exploring the candidate reactions for RD, it is an area that needs considerable attention to expand the domain of RD processes. However some reaction take place in RD will have some problem since the conditions in the reactive column are suboptimal both as a chemical reactor and as a distillation column, since the reactive column combines these. The introduction of an in situ separation process in the reaction zone or vice versa leads to complex interactions between vapor-liquid equilibrium, mass transfer rates, diffusion and chemical kinetics, which poses a great challenge for design and synthesis of these systems. However, using side reactors, where a separate column feeds a reactor and vice versa, is better for some reactions, if the optimal conditions of distillation and reaction differ too significantly.

2.5 SIMULATION BY USING ASPEN PLUS SOFTWARE

The purpose of simulation is to determine the optimal parameter that can contribute to the best performance of a process. It involves the decomposition of the process into its constituent units for individual study of performance. The process characteristics (flow rates, compositions, temperatures, pressures, properties, equipment sizes, etc.) are predicted using several analysis techniques. These techniques include mathematical models, empirical correlations and computer-aided process simulation tools (*ASPEN Plus* software). In addition, process analysis may involve the use of experimental means to predict and validate performance. Therefore, in process simulation, the process inputs and flow sheet are required to predict process outputs. *ASPEN Plus* is a computer-aided software which uses the underlying physical relationships (e.g., material and energy balances, thermodynamic equilibrium, rate equations) to predict process performance (e.g., stream properties, operating conditions, and equipment sizes). Since to conduct a trial plant is very costly and many tests needed to predict the optimal condition for maximizing the yield of biodiesel, *ASPEN Plus* will become a beneficial tool to determine the parameter that can affect the biodiesel production.

CHAPTER 3

METHODOLOGY

3.1 INTRODUCTION

The purpose of simulation is to model the process and predict the optimum design for the process. In this study, Aspen Plus Software version 12.1 was used as computer-aided simulation software to predict the optimum design parameter for reactive distillation column in producing biodiesel. Before starting the simulation, the base simulation case should be investigated. In the present study, the simulation was carried out by using equilibrium stage model and RADFRAC model was used to model the reactive distillation column. RADFRAC model is the steady state simulator based on rigorous equilibrium stage model for solving mass balance, phase equilibrium, summation and energy balance. Equilibrium stage model was used as the vapor and liquid assumed to be equilibrium in each stage of the reactive distillation column. In the previous study, there is lack information on methyl oleate (biodiesel) such as pressure and critical temperature. Therefore, all the information were estimated by using Aspen Plus estimation parameter and UNIQUAC thermodynamic property method was used to estimate all the missing parameters (Mohd Junaidi, 2010).

3.1 REACTION KINETIC MODEL

In this simulation, the reaction kinetic model was taken from Song et al, 2009. An experiment of producing biodiesel from oleic acid has been done in laboratory scale. The kinetic model of esterification oleic acid in subcritical methanol catalyzed by zinc acetate was investigated.

The esterification of oleic acid and methanol can be described as:

$$-\frac{dC_A}{dt} = kC_A^{\alpha} C_B^{\beta} - k' C_C^{\gamma} C_D^{\delta}$$

Where C_A, C_B, C_C and C_D represent the concentration of oleic acid, methanol, methyl oleate and water respectively; $\alpha, \beta, \gamma,$ and δ refer to their reaction orders. k and k' denote the kinetic constants for forward and reverse reaction involve in the esterification. In the experiment, since the reverse reaction is too small, then the reverse reaction is negligible. Arrhenius equation was used to calculate the pre-exponential factor, *A* and activation energy, *Ea* (song et al., 2009). As result, a kinetic model for esterification was established.

In present study, the kinetic model was taken from the result obtained in Song et al., 2009. The kinetic model obtained as stated in the Table 3.1:

Table 3.1: List of parameter used in power law kinetic expression in the simulation

Parameter	Value
Pre-exponential factor, A	120
Activation energy, Ea	32.62 kJ/mol
Reaction order, n	2.2

(Adapted from: Song et al., 2009 ; Mohd Junaidi, 2010)

3.2 REACTIVE DISTILLATION (RD) COLUMN DESIGN SPECIFICATIONS

In this study, there are several parameters have been investigated which were feed to distillate ratio, molar ratio and reboiler duty. From the previous study done by Mohd Junaidi, 2010, there are some other parameters have been stimulate and found to be optimum design for reactive distillation for biodiesel production. As a base case simulation in this study, the optimum parameters found by Mohd Junaidi, 2010 was used. The optimum design parameters taken from Mohd Junaidi, 2010 as shown in the Table 3.2.

Table 3.2: Optimum design parameter for reactive distillation for biodiesel production

Parameters	Value
Reflux ratio	0.01
Feed temperature	363.15 K
Column pressure	100 kPa
No. of stages	14
Reactive zone stages	6 (6-12)
Feed stages location	2-13

(Adapted from: Mohd Junaidi , 2010)

Esterification of oleic acid and methanol is a reversible reaction. Oleic acid reacts with methanol to produce methyl oleate (biodiesel) and water as by product. The equation for the reaction is as follow:

$$C_{18}H_{34}O_2 + CH_3OH \leftrightarrow C_{19}H_{36}O_2 + H_2\ O$$

In the simulation, the reverse and forward reactions need to be included in the reaction setup since esterification of oleic acid with methanol is a reversible reaction.

For the base case simulation, the reactive distillation specifications are as follow:

Table 3.3: Base case simulation for methyl oleate production

Category	Parameters	Value
Methanol stream	Flow rate (kmol/hr)	100
	Temperature (K)	363.15
	Feed stage	2
Oleic acid stream	Flow rate (kmol/hr)	100
	Temperature (K)	363.15
	Feed stage	13
RD column	Pressure (kPa)	100
	Liquid hold up (kg)	6
	Feed to distillate ratio	0.1

Since oleic acid have higher boiling point than methanol, methanol will be more volatile than oleic acid (Mohd Junaidi, 2010). Therefore, methanol is introduced at the top of the column where oleic acid feed at the bottom. As a result from this condition, the reaction will occur in counter current way and maximize the contact between both reactants. The flow sheet for this simulation study is as presented in the Figure 3.1.

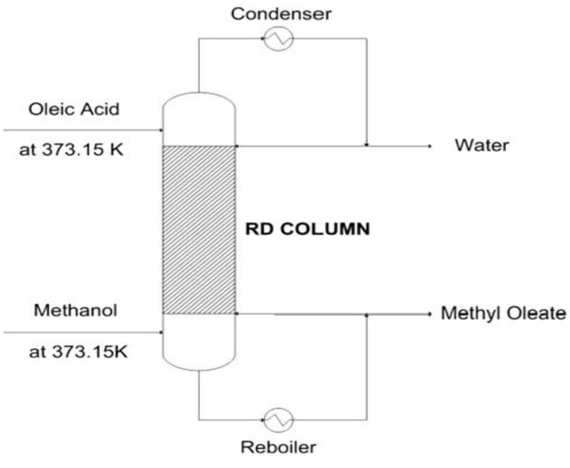


Figure 3.1: Flow sheet for simulation of methyl oleate (biodiesel) production

Table 3.4: Trial parameters for this present study

Parameters	Value
Distillate to feed ratio	0.1 – 0.5
Reboiler duty	1000kW- 6000kW
Molar ratio: Acid oleic: Methanol	1:1 – 1:4

The following steps are the simulation procedures for the simulation of methyl oleate production by using Aspen Plus 12.1 software.

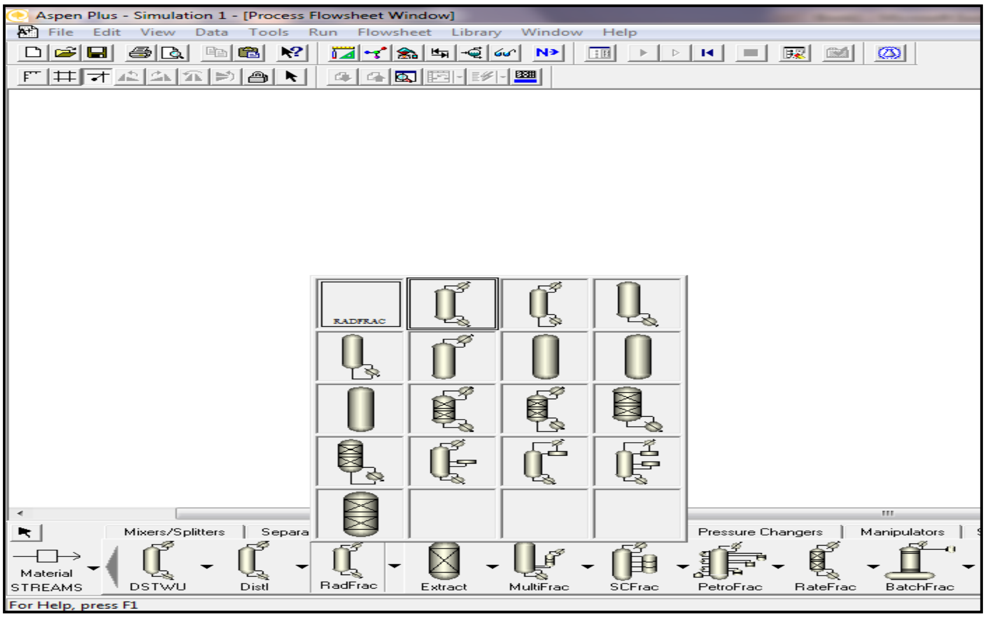


Figure 3.2: Selection of RADRFAC as the reactive distillation column

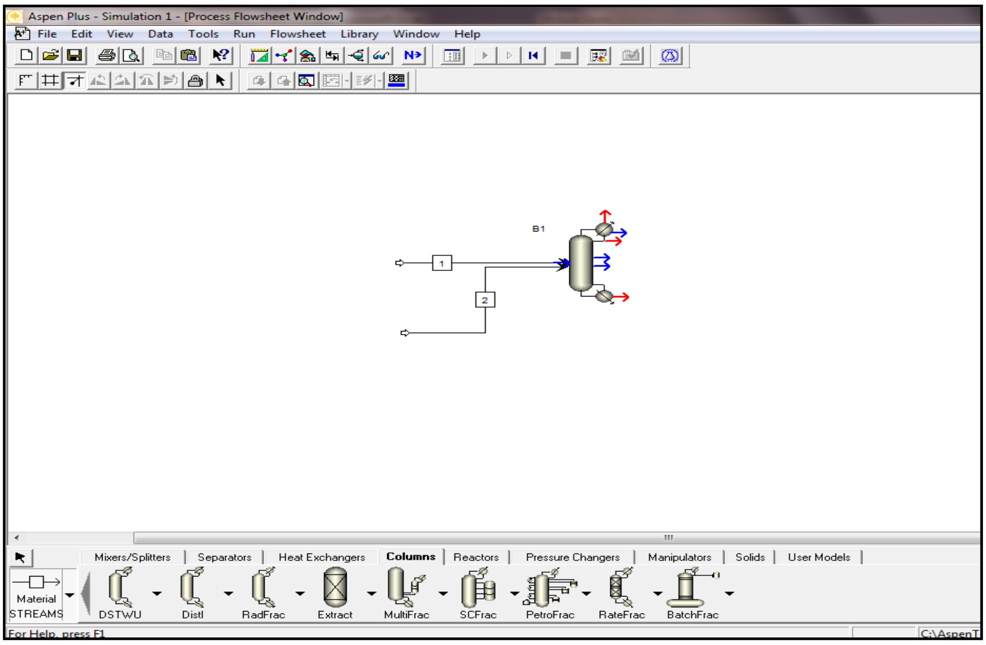
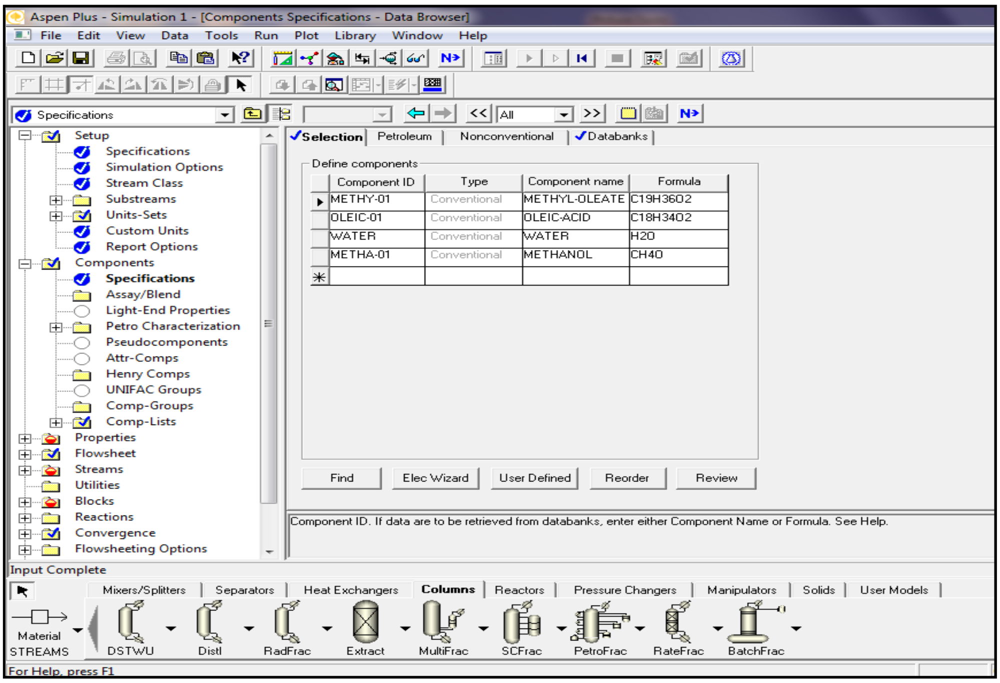


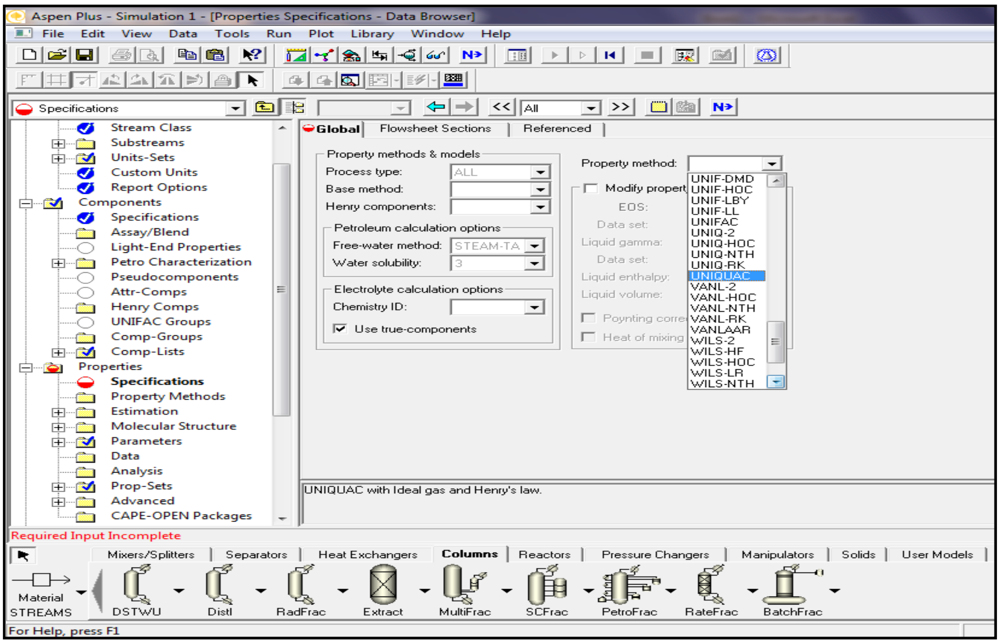
Figure 3.3: Stream added to RADFRAC block



Component ID	Type	Component name	Formula
METHY-01	Conventional	METHYL-OLEATE	C19H36O2
OLEIC-01	Conventional	OLEIC-ACID	C18H34O2
WATER	Conventional	WATER	H2O
METHA-01	Conventional	METHANOL	CH4O

Component ID. If data are to be retrieved from databanks, enter either Component Name or Formula. See Help.

Figure 3.4: Selection of component involved in the simulation



Process type: ALL

Base method:

Henry components:

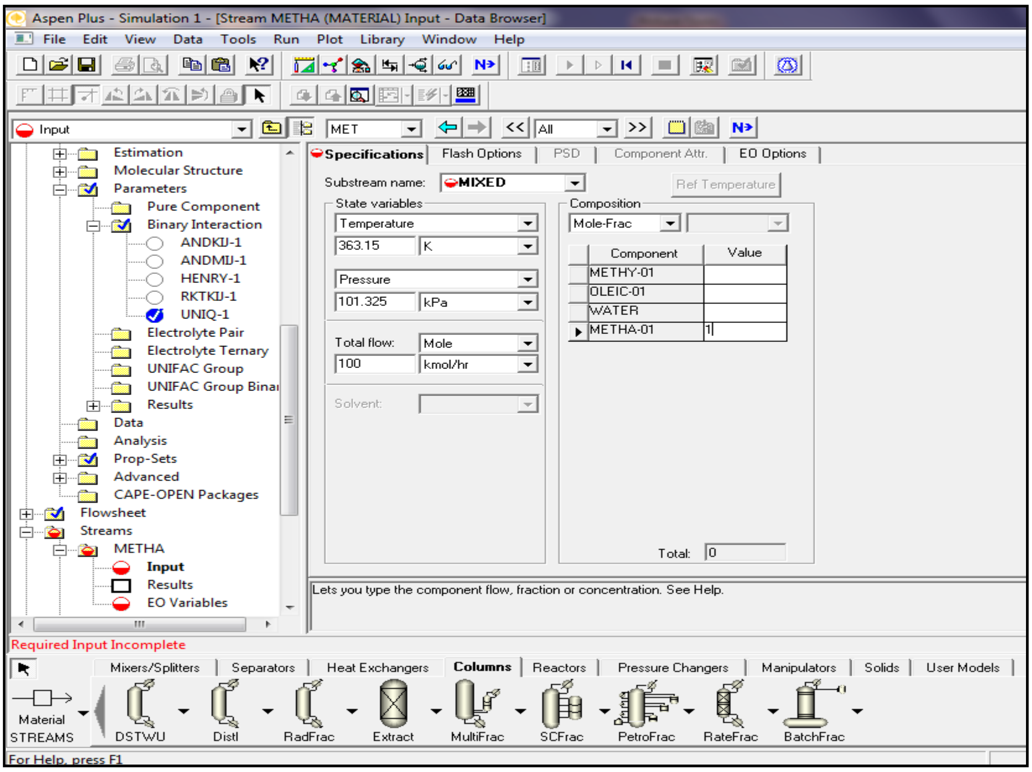
Free-water method: STEAM-TA

Water solubility: 3

☑ Use true-components

UNIQUAC with Ideal gas and Henry's law.

Figure 3.5: Property method added to the simulation



Substream name: MIXED

Temperature: 363.15 K

Pressure: 101.325 kPa

Total flow: Mole 100 kmol/hr

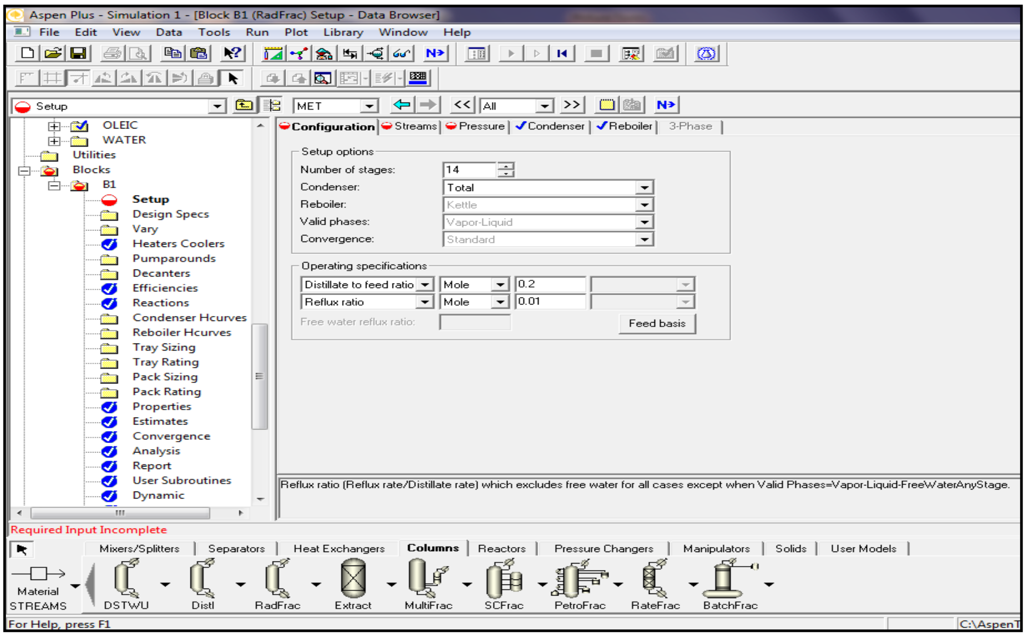
Composition: Mole-Frac

Component	Value
METHY-01	
OLEIC-01	
WATER	
METHA-01	1

Total: 0

Lets you type the component flow, fraction or concentration. See Help.

Figure 3.6: Specification for stream properties



Setup options

Number of stages: 14

Condenser: Total

Reboiler: Kettle

Valid phases: Vapor-Liquid

Convergence: Standard

Operating specifications

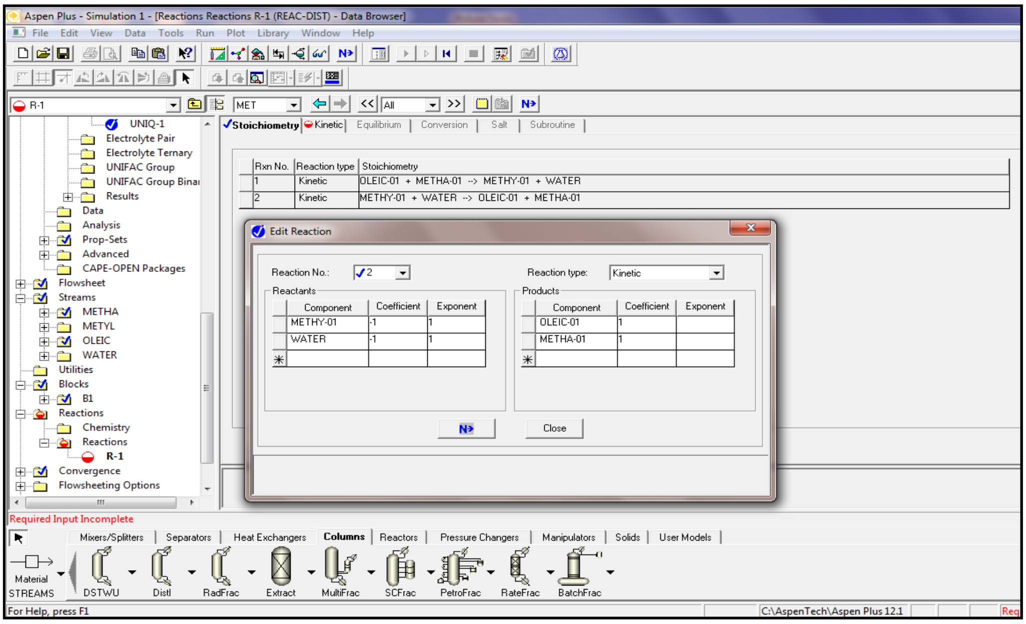
Distillate to feed ratio	Mole	0.2
Reflux ratio	Mole	0.01

Free water reflux ratio:

Reflux ratio (Reflux rate/Distillate rate) which excludes free water for all cases except when Valid Phases=Vapor-Liquid-FreeWaterAnyStage.

Required Input Incomplete

Figure 3.7: Specification for RADFRAC equipment



Rxn No.	Reaction type	Stoichiometry
1	Kinetic	OLEIC-01 + METHA-01 --> METHY-01 + WATER
2	Kinetic	METHY-01 + WATER --> OLEIC-01 + METHA-01

Reaction No.: 2

Reaction type: Kinetic

Reactants

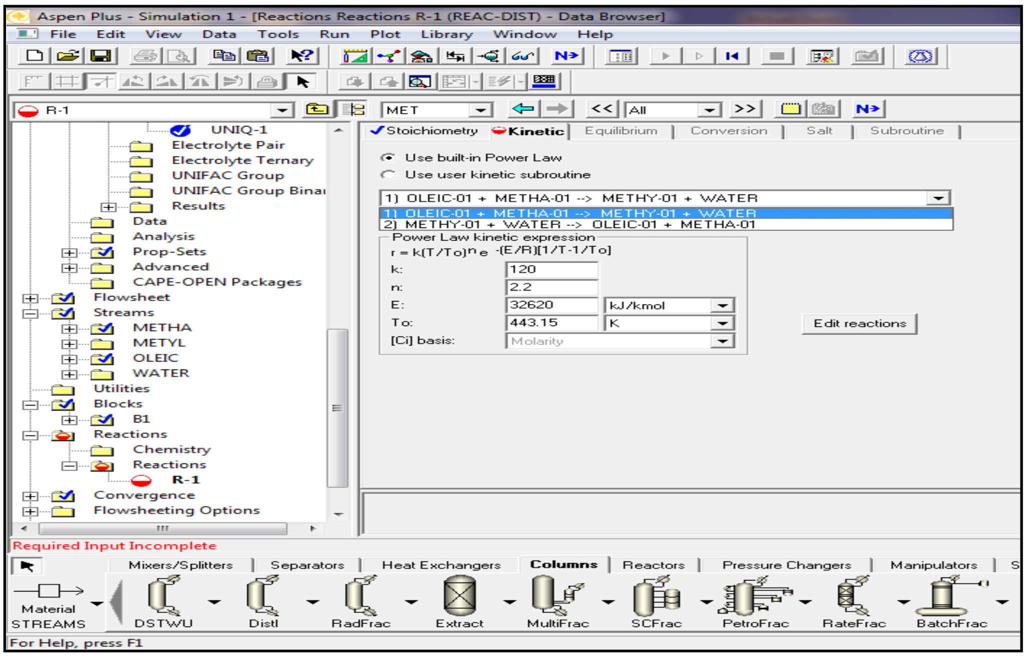
Component	Coefficient	Exponent
METHY-01	-1	1
WATER	-1	1

Products

Component	Coefficient	Exponent
OLEIC-01	1	
METHA-01	1	

Required Input Incomplete

Figure 3.8: Reaction for simulation process.



Aspen Plus - Simulation 1 - [Reactions Reactions R-1 (REAC-DIST) - Data Browser]

● Use built-in Power Law
○ Use user kinetic subroutine

1) OLEIC-01 + METHA-01 --> METHY-01 + WATER
2) METHY-01 + WATER --> OLEIC-01 + METHA-01

Power Law kinetic expression

$r = k(T/To)^n e^{-(E/R)[1/T-1/To]}$

k: 120
n: 2.2
E: 32620 kJ/kmol
To: 443.15 K
[Ci] basis: Molarity

Required Input Incomplete

For Help, press F1

Figure 3.9: Reaction kinetic expression for reaction involved

Summary of methodology in methyl oleate production simulation using reactive distillation column:

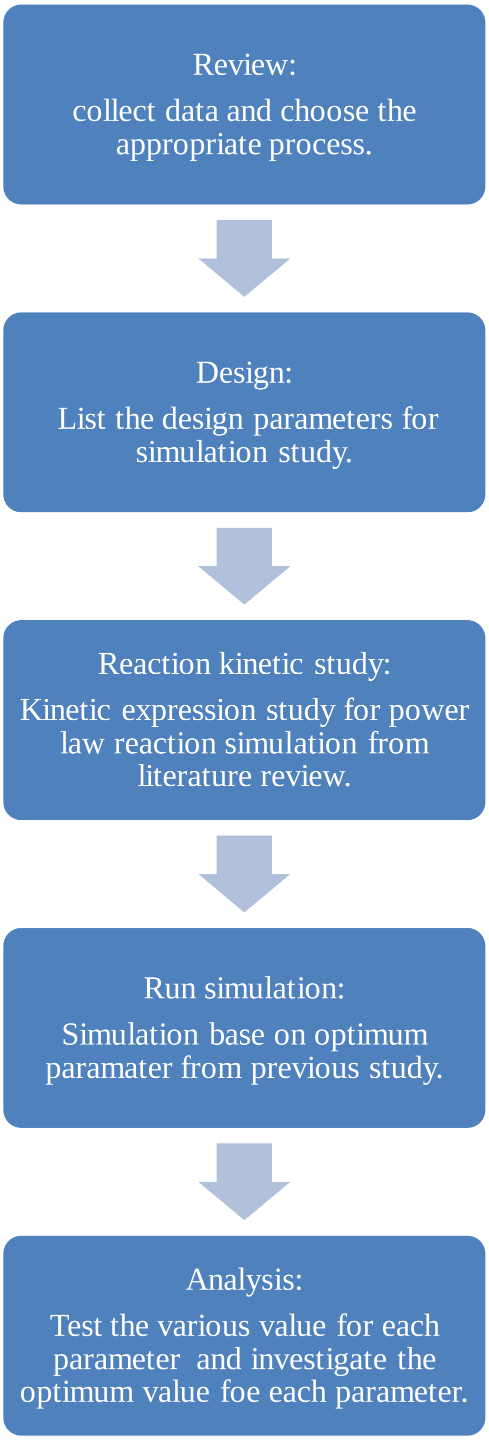


Figure 3.10: Summary of methodology

CHAPTER 4

RESULT AND DISCUSSION

4.1 INTRODUCTION

The optimum design parameters were obtained from the simulation using Aspen plus 12.1 Software. In this simulation, there are three parameters involved which are distillate to feed ratio, reboiler duty and molar ratio. Oleic acid conversion will be observed to determine the optimum value for each parameter. Oleic acid conversion represent in percentage value as shown in the table of each parameter tested. The highest oleic acid conversion on each trial parameters will be determined as optimum design value. These three parameters have been stimulated in Aspen Plus software and the effect of each parameter on oleic acid conversion will be discussed later in this chapter. The entire table obtained from the Aspen plus simulation given in the Appendix A, B, C and D.

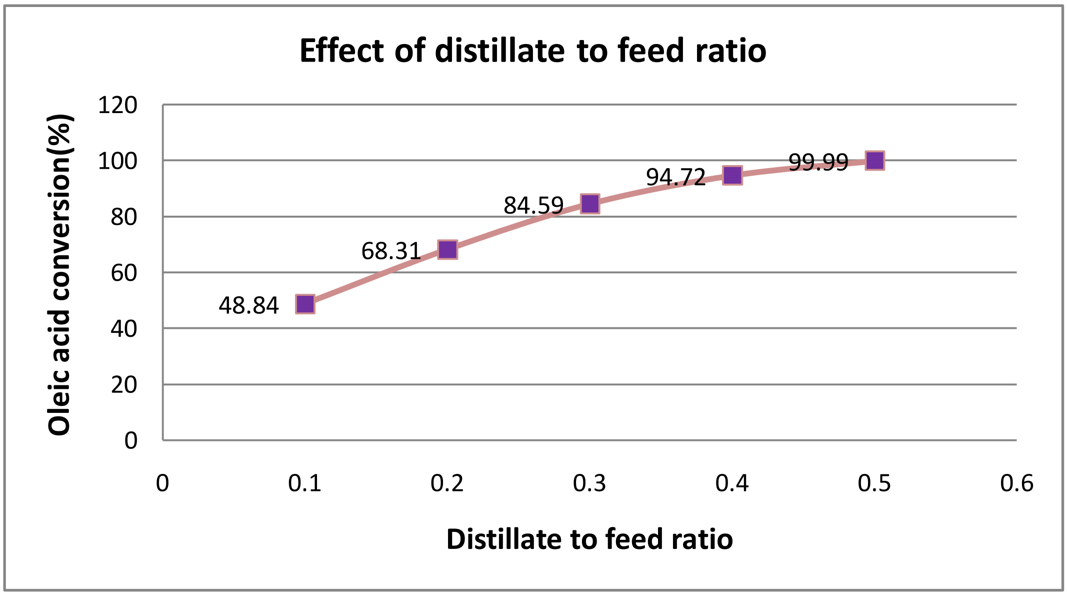
4.2 RESULT ANALYSIS AND DISCUSSION

4.2.1 DISTILLATE TO FEED RATIO.

In this simulation, the value for distillate to feed (D/F) ratio was varied from 0.1 until 0.5. In order to observe the effect of distillate to feed ratio, the molar flow rate for the feed of the column kept as 100kmol/hr for all trial simulation. The other parameters such as pressure, feed temperature and molar ratio kept as constant like stated in the methodology. The result from the trial simulation represent in the Table 4.1.

Table 4.1: Effect of distillate to feed ratio on biodiesel production

Distillate to feed ratio	Biodiesel yield (kmol/hr)	Oleic acid conversion (%)
0.1	48.84194	48.84
0.2	68.30910	68.31
0.3	84.59194	84.59
0.4	94.71691	94.72
0.5	99.99492	99.99



Graph 4.1: Effect of distillate to feed ratio

As represents in the Graph 4.1, by increasing the distillate to feed ratio, the biodiesel yield will be high. The distillate was varied from 0.1 until 0.5 while resulting in increasing the oleic acid conversion from 48.84% to 99.99%.

The feed to distillate ratio can be estimated from resolving the overall material balance of the reactive distillation column. According to Geankoplis., 2003 , an overall material balance around the entire column means that the entering feed of F (mol/hr) must equal the distillate D (mol/hr) plus the bottom W (mol/hr) as states in Figure 4.1.

$$F = D + W \qquad (4.1)$$

Figure 4.1: Total material balance for RD column.

Then the total material balance for a component gives,

$$Fx_F = Dx_D + Wx_W \qquad (4.2)$$

Figure 4.2: Material balance for a component.

Where x_F , x_D , and x_W represent the component composition of the feed, distillate and bottom respectively. By solving these two equations (Figure 4.1 & Figure 4.2), the distillate to feed ratio will be in the following equation in Figure 4.3.

$$\frac{D}{F} = \frac{(x_F - x_W)}{(x_D - x_W)} \qquad (4.3)$$

Figure 4.3: Distillate to feed ratio equation.

In this study, the feed flow rate, F kept as 100kmol/hr where the distillate flow rate D, is manipulated. From the result obtained, by increasing one of the outlet streams, the biodiesel recovered will be high. By increasing distillate flow rate, the yield of biodiesel is increase until reach the maximum conversion which is 99.99%.

Esterification of fatty acid is a reversible reaction and water is formed. In RD column, water found as distillate since the boiling point of water is lower than methyl oleate. Therefore, by increasing the D/F ration means increase the water removal. By removing water as by-product, the equilibrium is shifted towards ester formation. The methyl ester (biodiesel) will always separated in the bottom of the reactive distillation column. In this condition, higher reflux ratio is actually not beneficial as it brings back water into the column and cause decreasing of oleic acid conversion by shifting the equilibrium towards ester hydrolysis. Hence, biodiesel production can be increase if the distillate to feed ratio of the column increase and the optimum value of distillate to feed ratio is 0.5.

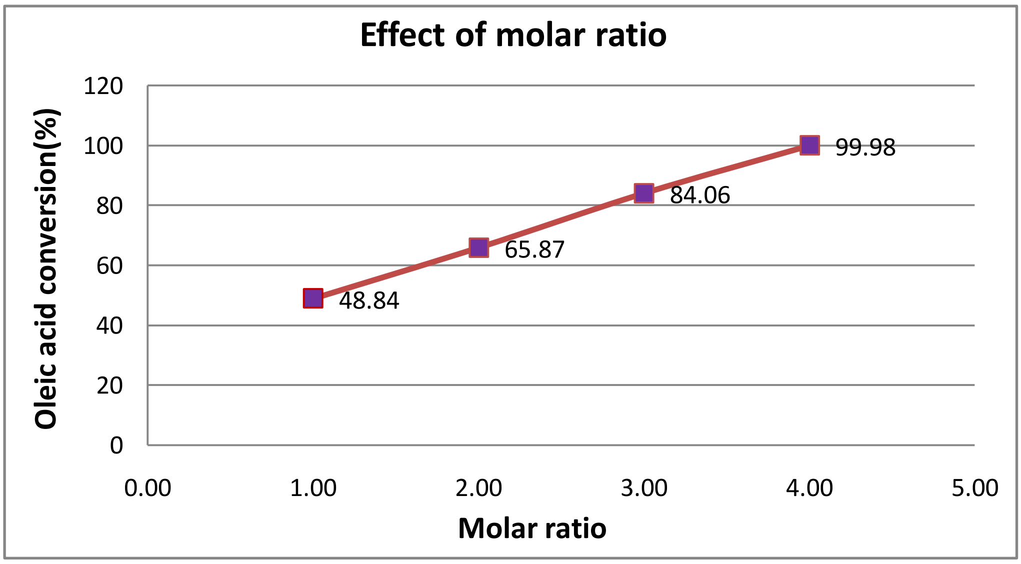
4.2.2 MOLAR RATIO

Methanol is generally used because it is cheaper and easier to recover although the other alcohol such as ethanol can be used. Hariyadi et al., 2007 said that, the molar ratio is the one of the factor influences the transesterification process in producing biodiesel. In this study; methanol is used to convert oleic acid to methyl oleate (biodiesel). Esterification is an equilibrium reaction. In order to make the reaction moves to the right, excessive alcohol is used. In this study, the molar ratio (oleic acid: methanol) was varied from 1:1 to 1:4 to investigate the effect of molar ration on biodiesel production.

Table 4.2: Effect of molar ratio on biodiesel production

Molar ratio (oleic acid: methanol)	Biodiesel yield (kmol/hr)	Oleic acid conversion (%)
1:1	48.84632	48.84
1:2	65.86899	65.87
1:3	84.06164	84.06
1:4	99.97747	99.98

Other parameters such as temperature, distillate to feed ratio and pressure kept at constant as stated in the methodology. The result obtained from the simulation as shown in Table 4.2. In this study, in order to observe the effect of molar ratio in biodiesel production, the amount of 100 kmol/hr of oleic acid maintained as constant for the four trials and amount of methanol was varied from 100kmol/hr to 400kmol/hr.



Graph 4.2: Effect of molar ratio

The result obtained have been plotted as represents in Graph 4.2, the oleic acid conversion increase steadily by increasing the amount of methanol involved in the reaction from 48.84% to 99.98%. In term of biodiesel yield, it is increases from 48.84kmol/hr to 99.98kmol/hr if the alcohol excess in amount from 100kmol/hr to 400kmol/hr accordingly. Theoretically, the excessive amount of methanol is employed to shift the equilibrium reaction towards producing more biodiesel. Therefore, if more alcohol involved, the methyl oleate produced will be higher than less alcohol involved. In the nutshell, the optimum value molar ratio investigated in this simulation is 1:4. However, in the simulation when the methanol involve exceed the optimum value (400kmol/hr) the yield of biodiesel obtain slightly drop. Although the excessive amount of the alcohol can enhanced the reaction and produce high yield of biodiesel, the excessive concentration of alcohol can inhibits the transesterification reaction. In addition, the purification of biodiesel product will be difficult and increase the cost of the production due to extreme amount of alcohol in the product stream. Therefore, the optimum molar ratio of alcohol should be keep at value 1:4.

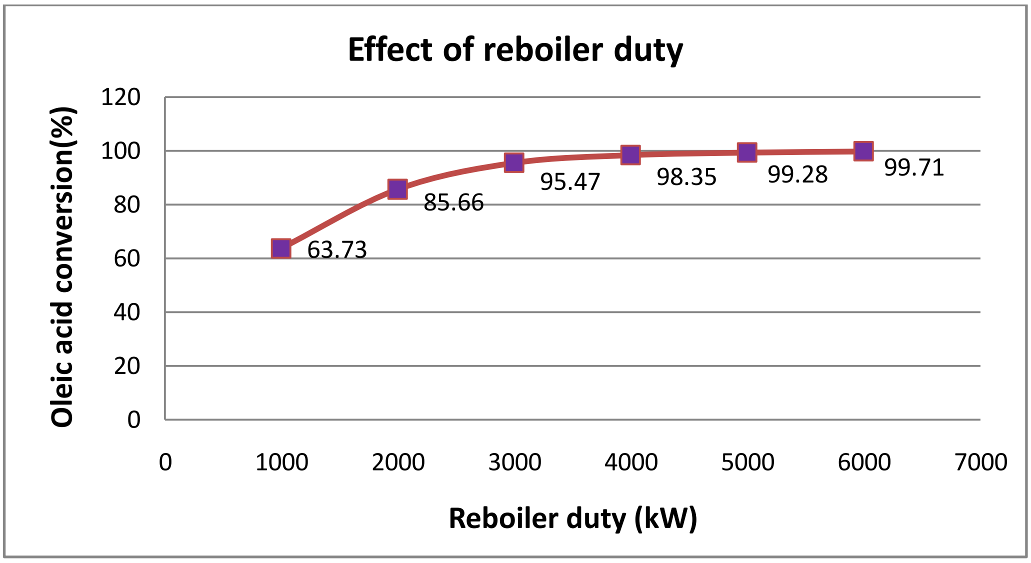
4.2.3 REBOILER DUTY

Another parameters that will be effected the biodiesel production by using reactive distillation is reboiler duty. In this study, the value of reboiler duty was varied from 1000kW to 6000kW. The total of 6 trials was done to investigate the effect of reboiler duty to the biodiesel yield by using reactive distillation column. As the previous simulation, the other parameter keep to be constant such as pressure, temperature of the column, feed to distillate ratio and also molar ratio 1:1 used as shown in the Appendix C.

Table 4.3: Effect of reboiler duty on biodiesel production

Reboiler duty (kW)	Biodiesel yield (kmol/hr)	Oleic acid conversion (%)
1000	63.72657	63.73
2000	85.66203	85.66
3000	95.47315	95.47
4000	98.34666	98.35
5000	99.28351	99.28
6000	99.70807	99.71

From the Graph 4.2, as the reboiler duty increase, high biodiesel yield obtain. The oleic acid conversion increase from 63.73% to 99.71% which is almost complete conversion obtained. In reactive distillation column, the function of reboiler is to vaporize the residual liquid methanol reaching the bottom of the column. At steady state, the boiling-up rate depend on the reboiler duty, heat transfer efficiency and amount of methanol present in the reboiler. Biodiesel yield is increased as the temperature increases due to increased increasing reboiler duty.



Graph 4.3: Effect of reboiler duty

Maximum reaction occurs when reactants present in vapor state. Therefore, by increasing the reboiler duty, higher amount of unreacts liquid methanol will vaporize to the reactive zone of the column and react with the oleic acid. Methanol start to vaporize at temperature 64.7°C. However, when the reboiler duty exceed the 6000kW, the biodiesel obtained will be slightly drop because all of the liquid methanol in the bottom vaporize and less methanol remain to be react with oleic acid. Hence, the optimum reboiler duty is 6000kW.

4.2.4 OPTIMIZED RD COLUMN

There are three optimum design parameter investigated in this study which is distillate to feed ratio (D/F), molar ratio and reboiler duty. All the optimum parameters obtained in this study will be gather and combined with the previous study done by Mohd Junaidi, 2010, for optimum column design in this section.

Table 4.4: Optimum design parameters for RD column

Parameter	Value
Reflux ratio	0.01
Feed temperature	363.15K
Column pressure	100kPa
No. of stages	14
Reactive stages	6
Feed location	At the end of the stages
Molar ratio	1:4 (acid: alcohol)
Reboiler duty	6000kW
Distillate to feed ratio	0.5

Summary of the optimum design parameter can be found in the Appendix D. As a result, in this study the conversion of the oleic can be reach until 99.99% compared to the previous study done by Mohd Junaidi., 2010 which is 99.65% oleic acid conversion.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 CONCLUSION

Biodiesel production has been seen as the new alternative fuel nowadays. In this study, *Jataropha curcas* was used as new sources of biodiesel oil since it can grown almost anywhere and has some advantages than the other non-edible oil plant. In this simulation, the esterification of oleic acid with methanol has been studied by using zinc acetate as catalyst. All the kinetic reaction involved is taken from the previous study done by Song et al., 2009 using zinc acetate as catalyst. In order to investigate the optimum condition for RD column, three parameters were observed which distillates to feed ratio, reboiler duty and molar ratio. The other parameters were taken from the optimum parameters found by Mohd Junaidi, 2010. In present study, Aspen Plus 12.1 software was used using RADFRAC as reactive distillation column and UNIQUAC as property method. As a conclusion of the present study, the optimum design parameters for RD column was found at molar ratio 1:4, reboiler duty at 6000kW and distillate to feed ratio for 0.5.

5.2 RECOMMENDATION

5.2.1 PROPERTY METHOD

In the present study, the property method used is UNIQUAC. UNIQUAC is an activity coefficient model used in description of phase equilibra. However, there are other property method can be used instead of UNIQUAC model which is UNIFAC. In UNIFAC model, it eliminates the use of experimental data to calculate in UNIQUAC parameters. If the different property method is used, the result of the simulation may be different from each other. Therefore, in the future study, we can compare the result of each property method and investigate the most effective model.

5.2.2 DESIGN PARAMETERS

In the present study and the previous study, most of the optimum design parameters have been discovered. However, there are some others parameters left which are weight of catalyst, liquid hold up, condenser duty and etc. these parameters can also effect production of biodiesel. Since Aspen Plus can also estimate the retention time for the process. Therefore, retention time can be investigated in the future by manipulating the design parameters and find the optimum retention time.

5.2.3 STIMULATION SOFTWARE

In this study, Aspen Plus software was used as the simulation tool. However, there are others simulation tool can be used in order to investigate the optimum design parameters for reactive distillation column such as HYSYS, CHEMCAD and MATLAB.

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APPENDIX A

DISTILLATE TO FEED RATIO

Molar ratio: 1:1 Feed temperature: 363.15K

No. of stages: 14 Column pressure: 100kPa

Table A.1: Summary table for simulation distillate to feed ratio 0.1

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	1.07690E-3	51.15699
METHA-01		100.0000	0.0	0.0	51.15806
METHY-01		0.0	0.0	2.0824E-26	48.84194
WATER		0.0	0.0	19.99892	28.84301
Total Flow	kmol/hr	100.0000	100.0000	20.00000	180.0000
Total Flow	kg/hr	3204.216	28246.68	360.5904	31090.30
Total Flow	l/min	49664.43	560.3078	6.547179	645.2060
Temperature	K	363.1500	363.1500	372.8006	390.4525
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66909.03	-1.2187E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.082	-705.5550
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-3.7172E+5	-6.0933E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93389	-241.7611
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937594	-1.399697
Density	mol/cc	3.35586E-5	2.97456E-3	.0509125	4.64968E-3
Density	gm/cc	1.07529E-3	.8402130	.9179281	.8031105
Average MW		32.04216	282.4668	18.02952	172.7239
Liq Vol 60F	l/min	67.22433	532.7933	6.022080	592.9775

DISTILLATE TO FEED RATIO

Molar ratio: 1:1 Feed temperature: 363.15K

No. of stages: 14 Column pressure: 100kPa

Table A.2: Summary table for simulation distillate to feed ratio 0.2.

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	2.14417E-3	31.68875
METHA-01		100.0000	0.0	3.4135E-20	31.69090
METHY-01		0.0	0.0	6.6658E-25	68.30910
WATER		0.0	0.0	39.99786	28.31125
Total Flow	kmol/hr	100.0000	100.0000	40.00000	160.0000
Total Flow	kg/hr	3204.216	28246.68	721.1782	30729.71
Total Flow	l/min	49664.43	560.3078	13.09429	645.2240
Temperature	K	363.1500	363.1500	372.8006	401.5381
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66909.00	-1.2626E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.094	-657.4215
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-7.4343E+5	-5.6118E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93381	-265.3627
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937596	-1.381660
Density	mol/cc	3.35586E-5	2.97456E-3	.0509127	4.13293E-3
Density	gm/cc	1.07529E-3	.8402130	.9179296	.7937738
Average MW		32.04216	282.4668	18.02946	192.0607
Liq Vol 60F	l/min	67.22433	532.7933	12.04411	586.5498

DISTILLATE TO FEED RATIO

Molar ratio: 1:1	Feed temperature: 363.15K
No. of stages: 14	Column pressure: 100kPa

Table A.3: Summary table for simulation distillate to feed ratio 0.3

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	3.20188E-3	15.40486
METHA-01		100.0000	0.0	1.1536E-16	15.40806
METHY-01		0.0	0.0	2.0075E-24	84.59194
WATER		0.0	0.0	59.99680	24.59514
Total Flow	kmol/hr	100.0000	100.0000	60.00000	140.0000
Total Flow	kg/hr	3204.216	28246.68	1081.764	30369.13
Total Flow	l/min	49664.43	560.3078	19.64134	648.2480
Temperature	K	363.1500	363.1500	372.8006	418.2710
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.97	-1.3153E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.105	-606.3320
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.1152E+6	-5.1149E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93372	-294.5473
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937599	-1.357847
Density	mol/cc	3.35586E-5	2.97456E-3	.0509130	3.59945E-3
Density	gm/cc	1.07529E-3	.8402130	.9179311	.7808001
Average MW		32.04216	282.4668	18.02939	216.9223
Liq Vol 60F	l/min	67.22433	532.7933	18.06610	580.1884

DISTILLATE TO FEED RATIO

Molar ratio: 1:1	Feed temperature: 363.15K
No. of stages: 14	Column pressure: 100kPa

Table A.4: Summary table for simulation distillate to feed ratio 0.4

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	4.25010E-3	5.278839
METHA-01		100.0000	0.0	1.7951E-22	5.283089
METHY-01		0.0	0.0	1.7143E-23	94.71691
WATER		0.0	0.0	79.99575	14.72116
Total Flow	kmol/hr	100.0000	100.0000	80.00000	120.0000
Total Flow	kg/hr	3204.216	28246.68	1442.346	30008.55
Total Flow	l/min	49664.43	560.3078	26.18831	658.2120
Temperature	K	363.1500	363.1500	372.8006	447.5774
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.94	-1.3733E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.117	-549.1651
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.4869E+6	-4.5777E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93364	-329.8094
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937601	-1.318862
Density	mol/cc	3.35586E-5	2.97456E-3	.0509132	3.03854E-3
Density	gm/cc	1.07529E-3	.8402130	.9179326	.7598501
Average MW		32.04216	282.4668	18.02933	250.0712
Liq Vol 60F	l/min	67.22433	532.7933	24.08803	573.9554

DISTILLATE TO FEED RATIO

Molar ratio: 1:1	Feed temperature: 363.15K
No. of stages: 14	Column pressure: 100kPa

Table A.5: Summary table for simulation distillate to feed ratio 0.5

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	5.07807E-3	0.0
METHA-01		100.0000	0.0	2.69570E-3	2.38237E-3
METHY-01		0.0	0.0	8.85769E-7	99.99492
WATER		0.0	0.0	99.99223	2.69659E-3
Total Flow	kmol/hr	100.0000	100.0000	100.0000	100.0000
Total Flow	kg/hr	3204.216	28246.68	1802.909	29647.98
Total Flow	l/min	49664.43	560.3078	32.73475	805.2490
Temperature	K	363.1500	363.1500	372.7955	616.6196
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.45	-1.1796E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.139	-397.8848
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.8586E+6	-3.2768E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93298	-329.0471
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937590	-1.109847
Density	mol/cc	3.35586E-5	2.97456E-3	.0509142	2.06975E-3
Density	gm/cc	1.07529E-3	.8402130	.9179383	.6136401
Average MW		32.04216	282.4668	18.02909	296.4798
Liq Vol 60F	l/min	67.22433	532.7933	30.10987	567.8236

APPENDIX B

MOLAR RATIO

Distillate to feed ratio: 0.1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Table B.1: Summary table for simulation molar ratio 1:1

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	1.07686E-3	51.15260
METHA-01		100.0000	0.0	3.4286E-18	51.15368
METHY-01		0.0	0.0	2.8856E-26	48.84632
WATER		0.0	0.0	19.99892	28.84740
Total Flow	kmol/hr	100.0000	100.0000	20.00000	180.0000
Total Flow	kg/hr	3204.216	28246.68	360.5904	31090.30
Total Flow	l/min	49664.43	560.3078	6.547179	645.2067
Temperature	K	363.1500	363.1500	372.8006	390.4525
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66909.03	-1.2187E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.082	-705.5535
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-3.7172E+5	-6.0933E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93389	-241.7611
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937594	-1.399697
Density	mol/cc	3.35586E-5	2.97456E-3	.0509125	4.64967E-3
Density	gm/cc	1.07529E-3	.8402130	.9179281	.8031095
Average MW		32.04216	282.4668	18.02952	172.7239
Liq Vol 60F	l/min	67.22433	532.7933	6.022080	592.9775

MOLAR RATIO

Distillate to feed ratio: 0.1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Table B.2: Summary table for simulation molar ratio 1:2

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	6.02348E-4	34.13041
METHA-01		200.0000	0.0	2.1324E-22	134.1310
METHY-01		0.0	0.0	5.4455E-27	65.86899
WATER		0.0	0.0	29.99940	35.86959
Total Flow	kmol/hr	200.0000	100.0000	30.00000	270.0000
Total Flow	kg/hr	6408.432	28246.68	540.6177	34114.49
Total Flow	l/min	99328.86	560.3078	9.813811	703.7206
Temperature	K	363.1500	363.1500	372.8118	369.0647
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66904.79	-99817.16
Enthalpy	cal/gm	-1475.396	-663.9853	-3712.686	-790.0055
Enthalpy	cal/sec	-2.6264E+6	-5.2098E+6	-5.5754E+5	-7.4863E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.92140	-181.6505
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937861	-1.437677
Density	mol/cc	3.35586E-5	2.97456E-3	.0509486	6.39458E-3
Density	gm/cc	1.07529E-3	.8402130	.9181240	.8079554
Average MW		32.04216	282.4668	18.02059	126.3500
Liq Vol 60F	l/min	134.4487	532.7933	9.028028	656.8410

MOLAR RATIO

Distillate to feed ratio: 0.1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Table B.3: Summary table simulation of molar ratio 1:3

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	2.14171E-3	15.93621
METHA-01		300.0000	0.0	0.0	215.9384
METHY-01		0.0	0.0	0.0	84.06164
WATER		0.0	0.0	39.99786	44.06379
Total Flow	kmol/hr	300.0000	100.0000	40.00000	360.0000
Total Flow	kg/hr	9612.648	28246.68	721.1776	37138.15
Total Flow	l/min	1.48993E+5	560.3078	13.09427	769.8697
Temperature	K	363.1500	363.1500	372.8006	360.3286
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.99	-88276.64
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.097	-855.7129
Enthalpy	cal/sec	-3.9396E+6	-5.2098E+6	-7.4343E+5	-8.8277E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93379	-150.6771
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937597	-1.460594
Density	mol/cc	3.35586E-5	2.97456E-3	.0509128	7.79353E-3
Density	gm/cc	1.07529E-3	.8402130	.9179300	.8039920
Average MW		32.04216	282.4668	18.02944	103.1615
Liq Vol 60F	l/min	201.6730	532.7933	12.04410	720.6701

MOLAR RATIO

Distillate to feed ratio: 0.1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Table B.4: Summary table simulation of molar ratio 1:4

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	2.67432E-3	.0198531
METHA-01		400.0000	0.0	1.17323E-8	300.0225
METHY-01		0.0	0.0	1.17780E-8	99.97747
WATER		0.0	0.0	49.99733	49.98015
Total Flow	kmol/hr	400.0000	100.0000	50.00000	450.0000
Total Flow	kg/hr	12816.86	28246.68	901.4712	40162.07
Total Flow	l/min	1.98658E+5	560.3078	16.36782	838.1234
Temperature	K	363.1500	363.1500	372.8006	355.2487
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.99	-81309.08
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.099	-911.0359
Enthalpy	cal/sec	-5.2528E+6	-5.2098E+6	-9.2929E+5	-1.0164E+7
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93377	-132.0377
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937597	-1.479429
Density	mol/cc	3.35586E-5	2.97456E-3	.0509129	8.94856E-3
Density	gm/cc	1.07529E-3	.8402130	.9179303	.7986507
Average MW		32.04216	282.4668	18.02942	89.24904
Liq Vol 60F	l/min	268.8973	532.7933	15.05511	784.5517

APPENDIX C

REBOILER DUTY

Molar ratio: 1:1	Feed temperatures: 363.15K
No. of stages: 14	Column pressure: 100kPa
Distillate to feed ratio: 0.1	

Table C.1: Summary table simulation of reboiler duty at 1000kW

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	1.88628E-3	36.27154
METHA-01		100.0000	0.0	0.0	36.27343
METHY-01		0.0	0.0	1.6295E-25	63.72657
WATER		0.0	0.0	35.14886	28.57771
Total Flow	kmol/hr	100.0000	100.0000	35.15075	164.8492
Total Flow	kg/hr	3204.216	28246.68	633.7494	30817.14
Total Flow	l/min	49664.43	560.3078	11.50687	644.9792
Temperature	K	363.1500	363.1500	372.8006	398.4349
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66909.01	-1.2513E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.091	-669.3579
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-6.5331E+5	-5.7299E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93383	-259.1803
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937596	-1.386426
Density	mol/cc	3.35586E-5	2.97456E-3	.0509127	4.25981E-3
Density	gm/cc	1.07529E-3	.8402130	.9179293	.7963343
Average MW		32.04216	282.4668	18.02947	186.9414
Liq Vol 60F	l/min	67.22433	532.7933	10.58400	588.1054

REBOILER DUTY

Molar ratio: 1:1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Distillate to feed ratio: 0.1

Table C.2: Summary table simulation of reboiler duty at 2000kW

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	3.28763E-3	14.33469
METHA-01		100.0000	0.0	2.9935E-21	14.33797
METHY-01		0.0	0.0	2.3725E-24	85.66203
WATER		0.0	0.0	61.62624	24.03578
Total Flow	kmol/hr	100.0000	100.0000	61.62953	138.3705
Total Flow	kg/hr	3204.216	28246.68	1111.143	30339.75
Total Flow	l/min	49664.43	560.3078	20.17476	648.6802
Temperature	K	363.1500	363.1500	372.8006	420.0049
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.97	-1.3200E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.106	-602.0081
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.1454E+6	-5.0735E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93372	-297.2091
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937599	-1.355481
Density	mol/cc	3.35586E-5	2.97456E-3	.0509130	3.55518E-3
Density	gm/cc	1.07529E-3	.8402130	.9179312	.7795251
Average MW		32.04216	282.4668	18.02939	219.2646
Liq Vol 60F	l/min	67.22433	532.7933	18.55674	579.6754

REBOILER DUTY

Molar ratio: 1:1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Distillate to feed ratio: 0.1

Table C.3: Summary table simulation of reboiler duty at 3000kW

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	4.36494E-3	4.522480
METHA-01		100.0000	0.0	0.0	4.526845
METHY-01		0.0	0.0	2.2286E-23	95.47315
WATER		0.0	0.0	82.19769	13.27547
Total Flow	kmol/hr	100.0000	100.0000	82.20205	117.7979
Total Flow	kg/hr	3204.216	28246.68	1482.047	29968.84
Total Flow	l/min	49664.43	560.3078	26.90915	660.5340
Temperature	K	363.1500	363.1500	372.8006	452.6961
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.94	-1.3784E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.118	-541.7989
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.5278E+6	-4.5103E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93363	-333.8359
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937601	-1.312202
Density	mol/cc	3.35586E-5	2.97456E-3	.0509133	2.97229E-3
Density	gm/cc	1.07529E-3	.8402130	.9179327	.7561771
Average MW		32.04216	282.4668	18.02932	254.4089
Liq Vol 60F	l/min	67.22433	532.7933	24.75106	573.2766

REBOILER DUTY

Molar ratio: 1:1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Distillate to feed ratio: 0.1

Table C.4: Summary table simulation of reboiler duty at 4000kW

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream : MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	4.90873E-3	1.648433
METHA-01		100.0000	0.0	3.3314E-15	1.653342
METHY-01		0.0	0.0	9.9004E-23	98.34666
WATER		0.0	0.0	92.51979	5.826870
Total Flow	kmol/hr	100.0000	100.0000	92.52470	107.4753
Total Flow	kg/hr	3204.216	28246.68	1668.156	29782.74
Total Flow	l/min	49664.43	560.3078	30.28827	684.3508
Temperature	K	363.1500	363.1500	372.8006	493.6054
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.93	-1.3762E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.120	-496.6390
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.7196E+6	-4.1087E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93361	-349.1454
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937601	-1.259942
Density	mol/cc	3.35586E-5	2.97456E-3	.0509133	2.61745E-3
Density	gm/cc	1.07529E-3	.8402130	.9179330	.7253282
Average MW		32.04216	282.4668	18.02931	277.1124
Liq Vol 60F	l/min	67.22433	532.7933	27.85919	570.1086

REBOILER DUTY

Molar ratio: 1:1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Distillate to feed ratio: 0.1

Table C.5: Summary table simulation of reboiler duty at 5000kW

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	5.11891E-3	.7113672
METHA-01		100.0000	0.0	2.3185E-19	.7164861
METHY-01		0.0	0.0	2.7538E-22	99.28351
WATER		0.0	0.0	96.77493	2.508585
Total Flow	kmol/hr	100.0000	100.0000	96.78005	103.2200
Total Flow	kg/hr	3204.216	28246.68	1744.873	29706.02
Total Flow	l/min	49664.43	560.3078	31.68117	717.3369
Temperature	K	363.1500	363.1500	372.8006	536.1327
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.92	-1.3263E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.128	-460.8442
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.7987E+6	-3.8027E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93356	-347.3518
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937603	-1.206949
Density	mol/cc	3.35586E-5	2.97456E-3	.0509135	2.39822E-3
Density	gm/cc	1.07529E-3	.8402130	.9179340	.6901922
Average MW		32.04216	282.4668	18.02927	287.7934
Liq Vol 60F	l/min	67.22433	532.7933	29.14040	568.8079

REBOILER DUTY

Molar ratio: 1:1 Feed temperatures: 363.15K

No. of stages: 14 Column pressure: 100kPa

Distillate to feed ratio: 0.1

Table C.6: Summary table simulation of reboiler duty at 6000kW

Methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	5.22688E-3	.2867070
METHA-01		100.0000	0.0	1.0518E-22	.2919339
METHY-01		0.0	0.0	7.3058E-22	99.70807
WATER		0.0	0.0	98.79780	.9102613
Total Flow	kmol/hr	100.0000	100.0000	98.80303	101.1970
Total Flow	kg/hr	3204.216	28246.68	1781.347	29669.55
Total Flow	l/min	49664.43	560.3078	32.34340	757.6164
Temperature	K	363.1500	363.1500	372.8006	577.5719
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-66908.92	-1.2565E+5
Enthalpy	cal/gm	-1475.396	-663.9853	-3711.127	-428.5594
Enthalpy	cal/sec	-1.3132E+6	-5.2098E+6	-1.8363E+6	-3.5320E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-34.93356	-339.0832
Entropy	cal/gm-K	-.8975962	-1.444938	-1.937603	-1.156546
Density	mol/cc	3.35586E-5	2.97456E-3	.0509135	2.22621E-3
Density	gm/cc	1.07529E-3	.8402130	.9179339	.6526950
Average MW		32.04216	282.4668	18.02927	293.1861
Liq Vol 60F	l/min	67.22433	532.7933	29.74952	568.1899

OPTIMIZED DESIGN

Molar ratio: 1:4	Feed temperatures: 363.15K
No. of stages: 14	Column pressure: 100kPa
Distillate to feed ratio: 0.5	Reboiler duty: 6000kW

Table C.7: Optimized design and operation parameters for RD column

methyl oleate (biodiesel) production					
Stream ID		MEOH-1	OLEIC-1	WATER	B-DIESEL
From				B1	B1
To		B1	B1		
Phase		VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED					
Mole Flow	kmol/hr				
OLEIC-01		0.0	100.0000	1.51034E-3	1.81453E-4
METHA-01		400.0000	0.0	211.3564	88.64497
METHY-01		0.0	0.0	2.70893E-7	99.99846
WATER		0.0	0.0	38.64205	61.35639
Total Flow	kmol/hr	400.0000	100.0000	250.0000	250.0000
Total Flow	kg/hr	12816.86	28246.68	7468.891	33594.69
Total Flow	l/min	1.98658E+5	560.3078	164.9413	809.1864
Temperature	K	363.1500	363.1500	339.8710	500.5345
Pressure	atm	1.000000	1.000000	.9869233	.9869233
Vapor Frac		1.000000	0.0	0.0	0.0
Liquid Frac		0.0	1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-47274.89	-1.8755E+5	-57769.46	-89707.46
Enthalpy	cal/gm	-1475.396	-663.9853	-1933.669	-667.5718
Enthalpy	cal/sec	-5.2528E+6	-5.2098E+6	-4.0118E+6	-6.2297E+6
Entropy	cal/mol-K	-28.76092	-408.1470	-51.05750	-166.7873
Entropy	cal/gm-K	-.8975962	-1.444938	-1.709005	-1.241173
Density	mol/cc	3.35586E-5	2.97456E-3	.0252615	5.14921E-3
Density	gm/cc	1.07529E-3	.8402130	.7547017	.6919437
Average MW		32.04216	282.4668	29.87556	134.3787
Liq Vol 60F	l/min	268.8973	532.7933	153.7158	645.8912