SIMULATION OF HETEROGENOUSLY CATALYZED ESTERIFICATION FOR THE PRODUCTION OF BIODIESEL USING REACTIVE DISTILLATION COLUMN

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BORANG PENGESAHAN STATUS TESIS

JUDUL : **SIMULATION OF HETEROGENEOUSLY CATALYZED ESTERIFICATIONFOR THE PRODUCTION OF BIODIESEL USING REACTIVE DISTILLATION COLUMN**

SESI PENGAJIAN: **2008/2009**

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SIMULATION OF HETEROGENOUSLY CATALYZED ESTERIFICATION FOR THE PRODUCTION OF BIODIESEL USING REACTIVE DISTILLATION COLUMN

AHMAD ATIQURRAHMAN BIN HASAN

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

APRIL 2009

I declare that this thesis entitled “simulation of heterogenously catalyzed esterification for the production of biodiesel using reactive distillation column ” 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.”

Signature :……..

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Date : 30 April 2009

Special Dedication to my mother, Rus Binti Omar and
my father Dr. Hasan Bin Bahrom,my brothers and sister and
all my family members,my girlfriend Fatimawati Binti Mat Isa
my friends, my fellow colleague and all faculty members

For all your care, support and believe in me, Thank You.

ACKNOWLEDGEMENT

Praise be to God for bestowing His mercy and give me good health upon doing this thesis.

I would like to forward my appreciation to my thesis supervisor, Dr. Chin Shim Yee for her endless guidance and support in making this thesis a success. I am also thankful to all my lecturers for their knowledge and guidance to during my studies in University Malaysia Pahang.

I'm very thankful to Universiti Malaysia Pahang (UMP) for providing good facilities in the campus. To all the staff in Faculty of Chemical & Natural Resources Engineering, a very big thank you to all.

My sincere appreciation also extends to all my fellow colleagues and others who have provided assistance at various occasions. Their views and tips are useful indeed. Thank you for the time sacrificed to accompany me. And last but not least, I am grateful to all my family members and my girlfriend for their support and love.

ABSTRACT

Fatty acid esters serve as feedstock for production of cosmetic, detergents, and as a fuel for production of biodiesel. They were produced by the reaction between fatty acids and the alcohols to produced fatty acid ester and water. The reactive distillation column performance for the production of 2-ethylhexyl dodecanoate by esterification of dodecanoic acid with 2-ethylhexanol has been studied in present research. Simulation on esterification process was done in equilibrium stage model using RADFRAC model. Kinetic model and thermodynamic model based on concentration is incorporate into RD equilibrium stage model. The simulation was carried out to determine the effect of the important parameter and design factor such as column operating pressure, reflux ratio, feed location arrangement, height of reactive zone and also the temperature of reactant feed enters to the column. A technically optimized RD process for production of 2-ethylhexyl dodecanoate has been proposed based on the simulated data. As a result, the optimum operating parameters are, reflux ratio at 0.1, temperature of feed enters to the column both are at 303.15 right on the reactive zone at stage five and stage 10, Height of reactive zone is six stages, whereby the operating column pressure is 30kpa in order to have an acid conversion about 99.3%.

ABSTRAK

Ester asid lemak digunakan sebagai bahan mentah untuk penghasilan kosmetik, detergen dan bahan api untuk penghasilan biodiesel. Ianya dihasilkan melalui tindak balas antara asid lemak dan alkohol untuk menghasilkan ester asid lemak dan air. Perlaksanaan kolum penyulingan reaktif untuk penghasilan 2-ethylhexyl dodecanoate melalui proses esterifikasi dodecanoic acid dengan 2-ethylhexanol telah dikaji ketika ini. Simulasi terhadap proses esterifikasi telah dilakukan pada model tahap persamaan menggunakan RADFRAC model. Model kinetic dan thermodinamik berdasarkan kepekatan digabungkan kepada model tahap persamaan RD. Simulasi yang dilakukan adalah untuk mengenal pasti kesan parameter yang penting dan faktor reka bentuk seperti tekanan operasi kolum, kadar refluk, susunan lokasi bahan kemasukan, ketinggian zon reaktif dan juga suhu bahan tindak balas yang masuk kedalam kolum. Secara teknikal, pengoptimaan proses RD untuk penghasilan 2-ethylhexyl dodecanoate telah dicadangkan berdasarkan kepada data yang disimulasi. Keputusannya, parameter operasi yang optima adalah, kadar reflux 0.1, suhu bahan tindak balas yang masuk kedalam kolum adalah 303.15 pada zon reaktif pada peringkat ke lima dan peringkatan, ketinggian zon reaktif ialah enam peringkat, di mana tekanan operasi kolum adalah 30kPa untuk mendapatkan penukaran asid sehingga mencapai 99.3%.

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LIST OF SYMBOLS/ABBREVIATIONS

E_a	activation energy, kJ mol^{-1}
K_c	rate constant for catalysed reactio, m^6 s^{-1} $mol^{-1}kg^{-1}$
K_u	rate constant for non-catalysed reactio, m^6 s^{-1} $mol^{-1}kg^{-1}$
K_x	activity-based reaction equilibrium constant
P	pressure, kPa
r	reaction rate per unit volume, mol $s^{-1}m^{-3}$
T	temperature, K

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CHAPTER 1

INTRODUCTION

1.1 Background of study

Fatty acid esters serve as feedstock for production of cosmetic, detergents, and surfactant and as a fuel for production of biodiesel. They were produced by the reaction between fatty acids and the alcohols to produced fatty acid ester and water. Fatty acid or derivatives fatty acid are used in a wide varieties of applications. The demands of fatty acid are even increasing for the past 10 years. Fatty acids are typically present in the raw material used for production of biodiesel. Esterifications, transesterifications and etherifications are the reaction to produced fatty acid ester. Transesterification reaction of triolein with alcohol for a production of biodiesel carried out by (Tanguy F. Dossin et al., 2006) to produce methyl oleate from rapeseed oil and also the direct esterification of fatty acid with alcohol and catalyzed by acid catalyzed as homogenously (F. Omota et al., 2003)

Since biodiesel has become increasingly attractive because it is made from renewable sources and combines high performance with environmental benefits. The idea of using vegetable oil as fuel for diesel engines is over a century old. In fact, Rudolph Diesel himself demonstrated the performances of his engine using peanut oil as fuel. Unlike petroleum diesel that contains hydrocarbons, biodiesel consists of a mixture of monoalkyl esters of long-chain fatty acids. These are typically produced by (Trans) esterification. Biodiesel has several advantages over petroleum diesel: it is safe, renewable, nontoxic, and biodegradable; it contains no sulfur and is a better

lubricant. The investigations for esterification reactions also have been carried out. They are and heterogeneously catalyzed using solid catalyst such as zinc acetate (Bhatia et al., 2006), Amberlyst 15 (Guido et al. 2006), magnesium oxide (Tanguy, 2006). However there are problem occur in this homogenously catalyzed process whereby it requires neutralization and separation from the reaction mixture, leading to a series of environmental problem that related to large amounts of solvent and energy.

Because of homogenous problem, heterogeneously catalyzed esterification process is presented. This is because esterification of alkyl ester can be easily separated from the reaction mixture without requiring the use of a solvent, show easily regeneration and have less corrosive character that leading to safer, cheaper, and more environmental-friendly operation. In addition heterogeneously catalyzed reactive distillation offers advantages over the homogenously catalyzed process alternative e.g. sulfuric acid. Size and location of the reactive section can be chosen regardless of the thermodynamic constrain and at the same time corrosion problem will be minimized. Furthermore, the separation of the homogenous catalyst from the product (ester) that is obtained as bottom product can be avoided.

Esterification of heterogeneously catalyzed in fact brings to the used of reactive distillation column (RD). Reactive distillation column has become an interesting alternative to some conventional process processes, especially for equilibrium-limited reaction as esterification and etherification. RD is cheapest method than the traditional method that consists of reactor followed by trains of distillation column shows in the flow sheet; see figure 1.1.

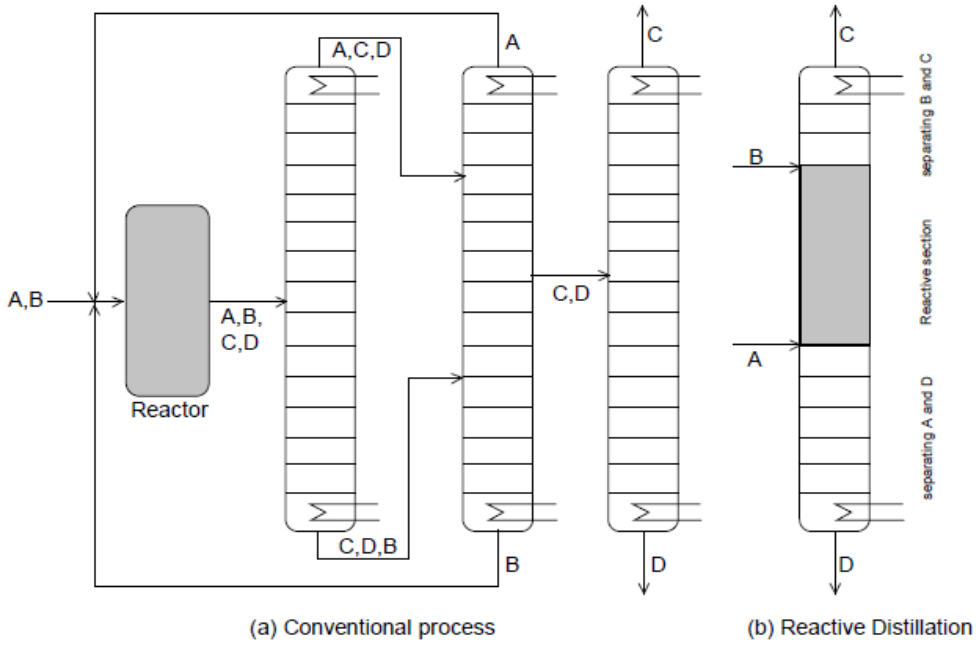

Figure 1.1: Processing scheme for processing A and B to produce C and D where (a) typical configuration of a conventional process consisting of a reactor followed by a distillation train (b) the reactive distillation configuration

The reactive distillation is featured with merits not only in reducing both capital and operational cost as its multifunctional nature, but also in promoting the reaction conversion. Not only that, the commercial success of RD for production of methyl tert-butyl ether (MTBE) and methyl acetate demonstrate its ability to render cost-effectiveness and compactness to the chemical plant (Sharma & Mahajani, 2003). So, as a consequence, RD has been explored as potentially alternative for several chemical production and reactions.

1.2 Problem statement

The needs and demands for fuel has been sky rocketing for the past years as a result to increment price of world's crude oil. Fossil fuel that has been the major contributor to global economy is unsustainable but yet the demand for the energy is increasing year by year, as well as increases of environmental and human health

impact. This contributes to the high productions of biodiesel fuel as an alternative fuel that costless and environmentally harmless. However, the combination of reaction and distillation within one unit operation is called reactive distillation can contribute to costless operation while producing these demands. The direct removal of the products or intermediates results in higher conversions and selectivity in comparison with the classical, sequential approach.

In recent years RD have been used as one of the important simultaneous implementation of reaction separation within a single unit of column. It also been used as a production of biodiesel. The natural multiple function of RD become more popular to be explored in several other chemical production and reactions. In several systems such as methyl acetate system serves as a model esterification system in a reactive distillation (Steigeneweget al., 2001). To generate the experimental data, RD pilot plant should be build first. However, to build a pilot plant, the feasibility and operating parameters need to be studied so that a suitable configuration can be proposed to build the RD column.

In fact, the previous study by (Steinigeweg & Gmehling, 2003) has done to determine the influence of important operating and design factor of reactive distillation for esterification of fatty acid decanoic acid with methanol to produce decanoic acid methyl esters. Simulations on RD need to be running in order to attain the result for feasibility and configuration for production of biodiesel. Therefore in, the use and design of RD is still developing to produce suitable RD and use less cost of production.

1.3 Objectives of Study

The specific objectives of this study are:

i. To propose a suitable configuration for reactive distillation
ii. To identify the important parameter that affect the process in reactive distillation

iii. To study feasibility of producing biodiesel, esterification of lauric acid and 2-ethylhexanol using super acidic sulfate zirconia catalyst in reactive distillation

1.4 Scope of studies

This study consists of three main scopes namely:

i. Setup base case RD using existed reactive reaction and using suitable thermodynamic model in the ASPEN Plus 12.1

ii. Find the important parameter of RD by changing the reflux ratio, feed location, pressure, height or reactive section and also the temperature of the reactant.

1.5 Rational and significant

Rationally, in this present study, simulation should be considered before setting up the biodiesel plant, this will cost of preventing from building not appropriate plant. The simulation study also can bring forward toward reducing the cost of building the plant. Significantly, the main purpose of this study can be archived by finding the important parameters that can be cooperating into RD column before building up the plant to produce biodiesel.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

2.1.1 Production of Biodiesel

Recent concern over diminishing fossil fuel supplies and the unsustainable price of oil, as well as adverse environmental and human health impact from the use of petroleum fuel have prompted considerable interest in research and development of fuel from renewable resources such as biodiesel. Biodiesel is a very attractive alternative fuel, as it is derive from a renewable, domestic resource and can, therefore, reduce reliance on foreign petroleum imports (Alex et al., 2007). Biodiesel reduces net carbon dioxide emissions by 78% on a life-cycle basis when compared to traditional diesel fuel (Tyson, 2001). In addition biodiesel is also been shown to have dramatic improvements on engine exhaust emission. For instance, combustion of neat biodiesel decreases carbon monoxide (CO) emission 46.7% , particulate matter emission by 66.7% and unburned hydrocarbons by 45.2% (Schumacher et al., 2001). Biodiesel also biodegradable and non-toxic, making it useful for transportation application in highly sensitive environments, such as marine ecosystem and mining enclosure.

Biodiesel is usually produced by the transesterification of a lipid feedstock. Transesterification are mainly performed using acid or base homogenous catalyst: sulfuric, sulfonic, phosphoric and hydrochloric acid as acid catalyst (Otera, 1993;

Corma, 1998) and alkaline hydroxide, metal alkoxide or acetates as based catalyst. However, the use of homogenous catalyst required neutralization and separation from the reaction mixture. As this matter occurs, heterogeneous catalyst is used instead of homogenous catalyst that leads to environmental problem. Furthermore, study on heterogeneously catalyzed transesterification for production of biodiesel industrial production by (Tanguy et al., 2006). In addition esterification of fatty acid is also a common practice in producing biodiesel and also in chemical industry. Because of this matter, the uses of reactive distillation (RD) currently develop for chemical and biodiesel production.

An experimental study have also been done using either in stirred batch reactor and also fixed bed-reactor to investigate the promising method esterification of free fatty acid (FFA) found in vegetable oil with methanol using solid catalyst to convert FFA into valuable fatty acid methyl ester (FAME) or biodiesel (Ni & Meunier, 2007). Kinetic behavior for the esterification of acetic acid with isoamyl alcohol in the temperature and molar feed ratios was investigated experimentally in a stirred batch reactor using Purolite C-175 calatlyst and resulting the equilibrium conversion of acetic acid was found to increase slightly with an increase in temperature and also it increases appreciably with an excess of isoamyl alcohol in the reacting system (Teo & Saha, 2004).

2.2 Reactive Distillation (RD) Column

2.2.1 Why RD?

The combination of reaction and distillation within one unit operation is called distillation column. RD has become interesting alternative to some conventional processes, especially for equilibrium-limited reaction as esterification and etherification. RD gives a direct removal of the product and intermediates results in higher conversion and selectivity compare to conventional processes. Conceptually, a RD column consists of there basic elements: rectifying section on the

top, reactive section in the middle and stripping section at the bottom (I-Kuan Lai et al., 2008). The reactive distillation is featured with its merits not only in promoting the reaction conversion, but also reducing both capital and operational cost as its multifunctional nature.

Since the RD process is first appeared in 1932 (Keyes, 1932) for production of ethyl acetate and lately become new focus in 1980's, since Eastman Chemical Company owned commercial RD process for production of methyl acetate. Later on, extensive researches on RD process appeared in the literature. At the same time, successful commercial processes that applied reactive distillation are installed for producing various chemicals such as methyl *tert*-butyl ether, (MTBE), cumene, ethyl-benzene and 3-methyl-1-butene, etc. In fact, practices of using RD for production methyl acetate and MTBE demonstrate its ability to render cost-effectiveness and compactness to chemical plant (Sharma & Mahajani, 2003).

Reactive distillation (RD) is widely used in many processes where a reversible reaction takes place (Malone and Doberty, 2000; Taylor and Krishna, 2000). RD process has shown great economical and environmental benefits in many existing applications (Jakobsson and Pyhalahti, 2002; Andreas and Franz, 2002; Wang and Shen, 2000; Kening et al., 2001), e.g., production of MTBE, methyl acetate, and so on. A comprehensive review article on RD has been published recently (Halpern, 2003). By using a solid super-acid catalysts fixed inside a catalytic zone of a distillation column, RD brings new possibilities of simplification to the ethyl lactate technology, making the process more environmental friendly compared with common homogeneous processes.In general, reactive distillation seems to be a simple, energy-saving process with lower investment and operation costs (Doherty and Buzad, 1992; Sundmacher and Homann, 1994).

2.2.2 Simulation of the RD Process

2.2.2.1 What is Process Simulation/Analysis?

The purpose of analysis/simulation is to model and predict the performance of a process. It involves the decomposition of the process into its constituent elements (units) for individual study of performance. The process characteristics (flowrates, compositions, temperatures, pressures, properties, equipment sizes, etc.) are predicted using analysis techniques. These techniques include mathematical models, empirical correlations and computer-aided process simulation tools (*ASPEN Plus*). In addition, process analysis may involve the use of experimental means to predict and validate performance. Therefore, in process simulation, we are given the process inputs and flowsheet and are required to predict process outputs (Fig. 2.2). The lab will focus on ASPEN Plus. It 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.

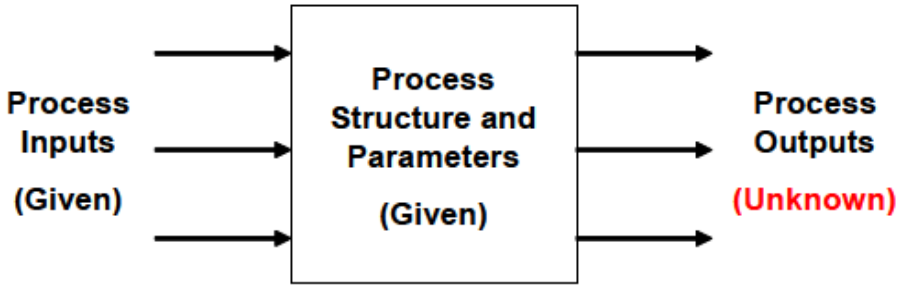

Figure 2.1 process simulation problems

2.2.2.2 Reactor Column

Usually, reactive distillation process requires several experimental data for the evaluation of its performance and deign. In order to reduce the experimental work, reliable and accurate process simulation tool can be used for obtaining useful information needed for the design (S. Bahtia et al., 2007). In the present study all simulation has been carried out using equilibrium stage model available in aspen plus

version 12.1 to simulate the process in reactive distillation column. Five parameters have been carried out to determine the important parameters that affect the process in RD distillation.

RADFRAC module is the steady state simulator Aspen Plus version 12.1 is based on rigorous equilibrium stage model for solving mass balance, phase equilibrium, summation and energy balance (MESH) equations. The equilibrium stage model assumes vapor liquid equilibrium at each stage. The departure from equilibrium is accounted at each stage for by tray efficiency or height equivalent to theoretical plate (HETP) (Bahtia et al., 2007). Besides that (Steinigeweg et al., 2003; Bhatia et al. 2007) practiced the used of RADFRAC module in RD column.

2.2.3 Phase equilibrium model

Vapor phase was assumed to be ideal and the UNIQUAC model was used to represent the activity coefficients in the rate expression. The UNIQUAC model has been reported to predict the non ideality in liquid phase satisfactorily for the esterification reaction system (Bhatia et al.,, 2006). The values of two activity-based kinetic parameters, was estimated from experimental data on initial reaction rates and liquid activity coefficients as assessed from UNIQUAC (Omota et al., 2003).

2.2.4 Reaction kinetics model

In process of 2-ethylhexanol and dodecanoic acid the reaction order was found to be linear regression by (Omota et al., 2003) using Eq (2.1), in logaritmatic form.

$$r_{0,u} = k_u C_{acid,0}^{n1} C_{alcohol,0}^{n2} \qquad \textbf{(2.1)}$$

First order regard to 2-ethylhexanol and catalyst concentration, respectively. Accordingly, the initial reaction rate r_0 is the sum of non-catalyzed and catalyzed rate:

$$r_{0,u} = k_u C_{acid,0}^2 C_{alcohol,0} + k_c C_{acid,0} C_{alcohol,0} C_{catalyst,0} \quad \textbf{(2.2)}$$

The initial reaction rates r_0 were estimated measurements of conversion versus time in temperature of 333 to 453 K. The rate constants k_u and k_c were calculated from initial reaction rates and initial concentration. All this information was gained by (Omota et al., 2003). The activation energies of esterification of 2-ethylhexanol and dodecanoate acid using sulfated zirconia and being plotted into graph of Arrhenius is 55.5kJ mol^{-1}. Concentration-based constant Eqn. (2.3), K_x already presented earlier (Omota, Dimian, & Bliek, 2003)

$$K_x = \frac{C_{ester}^{eq} C_{water}^{eq}}{C_{acid}^{eq} C_{alcohol}^{eq}} \quad \textbf{(2.3)}$$

Hence, the following expression can be formulated for the overall reaction rate which is consistent over whole concentration interval between zero and equilibrium as in Eqn (2.4).

$$r = \left(k_u C_{acid} + k_c C_{catalyst}\right)\left(C_{acid} C_{alcohol} - \frac{C_{ester} C_{water}}{K_x}\right) \quad \textbf{(2.4)}$$

The regressed values for concentration-based equilibrium constant for forward reaction were taken from (Omota et al., 2003). The values of K_x which varies for each temperature then used to find rate constant of backward reaction K_b using Arrhenius equation. Kinetic parameter need to be included to find the values of K_b are shown in the table 2.1

Table 2.1 Kinetic parameter for esterification of dodecanoic acid with 2-ethylhexanol

Parameter	Value
$A_{Forward}$ (m^6 $kmol^{-1}kg^{-1}$ s^{-1})	**3277.00**
$A_{Backward}$ (m^6 $kmol^{-1}kg^{-1}$ s^{-1})	**2660.24**
$Ea_{forward}$ (kJ mol^{-1})	**55.5**
$Ea_{backward}$ (kJ mol^{-1})	**3.25**

However, K_x in Eqn. (2.3) is merely regression parameter than a true thermodynamic equilibrium constant. Mixtures of dodecanoic acid, 2-ethylhexyl dodecanoate, 2-ethylhexanol and water behave in strongly non-ideal manner. Therefore concentration-based equilibrium constant K_x depends on the liquid composition. A kinetic model based on liquid is required for non-ideal system was modified by replacing molar concentration

2.2.5 Esterification

Esterification process to produce fatty acid ester have been already studied by (Omota et al., 2003; Steinigeweg et al., 2003; Bhatia et al., 2007; N. Calvar, 2006) for different production. Esterification of fatty acid is a common practice in chemical industry whereby fatty acid ester is important intermediates, surfactants, lubricants or tendencies (Steinigeweg et al., 2003). But it was still hard to find in literature about esterification of long carboxylic acid by reactive distillation.

An innovative esterification process of fatty acids based on reactive distillation was proposed (Omota et al., 2003), which makes use of super-acid solid catalyst, more specifically sulfated zirconia (SZr), capable of working at higher temperatures from 130 to 200 ◦C. More details about the equipment design can be found in a recent book (Dimian & Bildea, 2008). When using a solid catalyst, a generic problem is the removal of water, necessary for shifting the chemical

equilibrium to high conversion and consequently high ester purity, but also necessary for preserving the catalyst activity. Several methods for enhancing the water removal have been developed by the authors.

In previous study by (Omota et al., 2003), was investigated that the chemical and phase equilibrium (CPE) for the esterification of dodecanoic acid and 2-ethylhexanol has shown that a strong interaction exist in liquid phase, leading to highly non-ideal behavior, and potentially to liquid segregation into an aqueous and an organic phase at temperature below 373K and atmospheric pressure. Furthermore, it was demonstrate that RD unit to alcohol-to-acid ratio might very three orders of magnitude, a condition not likely to be encountered in conventional process.

2.2.5.1 Homogeneously catalyzed esterification

Esterification fatty acid can be in homogenously or heterogeneously catalyzed. Homogeneous and heterogeneous reaction have been investigated and been described using model proposed by (Popken et al., Gmehling et al., 2003; Brehlin 2007). A homogeneous catalyst Alkali resin is most commonly used to produce biodiesel. Although homogeneous alkali catalysts (e.g., NaOH) are commonly used to produce biodiesel by transesterification of triglycerides (vegetable oils and animal fats) and methanol, solid acid catalysts, such as acidic resins, are attractive alternatives because they are easy to separate and recover from the product mixture and also show significant activity in the presence of fatty acid impurities, which are common in low-cost feed stocks (Lopez et al. 2006). Sulfuric acid, methane sulfonic acid, *p*-toluene sulfonic acid, and sodium hydrogen sulfate are the most conventional homogeneous used catalysts. Titanium alkylates and organo tin compounds are also used as amphoteric catalysts at elevated temperatures (200 ◦C). The applications of these catalysts cause some problems such as corrosion, loss of catalyst, and environment problems.

2.2.5.2 Heterogeneously catalyzed esterification

Information about heterogeneously catalyzed esterification of fatty acid by reactive distillation is hardly being found in open literature. In addition heterogeneously catalyzed were too many credits differ to homogeneously catalyze. The usage of homogenous catalyst will constrain the developing of the yield as the catalyst is sensitive to free fatty acid (FFAs) and water content. In fact the homogenous catalyst will need separation after production and since it causes a formation of soap with high free fatty acid feedstock. But Heterogeneous catalyst is preferred because it beneficial as the catalyst can be regenerated and thus reduces the catalyst cost. Since it was a solid catalyst, it would be needed another separation to separate product with catalyst and bring toward environmental friendly issue. (Lotero et al., 2005) reported that the ability of the acid functionality to process low cost, high free fatty acid feedstock will yield the most economical biodiesel method.

A solid catalyst has been used due to its benefits not only on the purity of the secondary product, glycerin, but also because it will make a much simpler down streaming separation process, since it does not need any washing or neutralizing equipment (Marchetti et al., 2006).

CHAPTER III

METHODOLOGY

3.1 Introduction

In earlier work by (Omota et al. 2003), a RD column was designed according to chemical equilibrium and heterogeneous phase equilibrium. This approach enables the identification of key elements of design, i.e. the flow sheet configuration, the feasible reaction region and the corresponding temperature and composition profiles. In the present study the simulation was conducted for obtaining useful information needed for the design. So the simulation was carried out using Aspen Plus software package. The equilibrium stage model, RADFRAC that already available in Aspen Plus 12.1 are being used along this simulation. Before start any simulation, the base case simulation, acts as reference case are done, this because to ensure the simulation done within the range. Thus, during the simulations, there are five parameters need to be considered to find its optimum value of fatty acid ester production are reflux ratio, height of reactive zone, feed location, pressure of column and also the feed (reactant) temperature.

3.2 Simulation Method

3.2.1 Equilibrium Stage Model

In simulation of 2-ethylhexyl dodecanoate process, the reaction required to produce fatty acid ester is by, 2-ethylhexanol + Dodecanoic Acid ⇆ water + 2-ethylhexyl dodecanoate. From studies, there is lack of information on fatty acid ester such as temperature of critical boiling point, vapor pressure. This is because the information is not available in open literature. The only available information for this fatty acid ester was it molecular weight, and temperature of its normal boiling point. Since it was lack of information this fatty acid ester, pressure, critical boiling point were estimated using Gani's method. In present work, the vapor phase was assumed to be ideal and UNIQUAC model used to represent the concentration coefficients in the rate expression.

RADFRAC module is the steady state simulator Asper Plus version 12.1 is based on rigorous equilibrium stage model for solving mass balance, phase equilibrium, summation and energy balance (MESH) equations. The equilibrium stage model assumes vapor liquid equilibrium at each stage. The departure from equilibrium is accounted at each stage for by tray efficiency or height equivalent to theoretical plate (HETP) (Bahtia et al., 2007). Besides that (Steinigeweg et al., 2003; Bhatia et al. 2007) practiced the used of RADFRAC module in RD column.

3.2.2 Reaction Kinetics

In present study, kinetic model used was from (Omota et al., 2003). 2-ethylhexanol and dodecanoic acid process using sulfated zirconia was to have an activation energies 55.5kJ mol^{-1}. With the same catalyst also (Thorat et al., 1992) was found to be E_a= 52 kJ mol^{-1} for esterification of mono 2-ethylhexyl phathalate with 2-ethtlhexanol. A concentration-based equilibrium constant K_x can be calculated from concentration measurement as presented earlier by (Omota et al., 2003).

Reaction kinetic used were taken form Omota's previous research. Accordingly, the initial reaction rate r_0 is the sum of non-catalyzed and catalyzed rate:

$$r_{0,u} = k_u C_{acid,0}^2 C_{alcohol,0} + k_c C_{acid,0} C_{alcohol,0} C_{catalyst,0}$$

Hence, the following expression can be formulated for the overall reaction rate which is consistent over whole concentration interval between zero and equilibrium as in Eqn (2.4).

$$r = \left(k_u C_{acid} + k_c C_{catalyst}\right)\left(C_{acid} C_{alcohol} - \frac{C_{ester} C_{water}}{K_x}\right)$$

3.2.3 Base case simulation

Simulation was done on a base case simulation. Base case simulation was been setup, and figured out before any simulation done. The process then was presented as shown in figure 3.1. The RD are consists of 13 reactive stages of 14 stages used and was characterized by a liquid hold up and catalyst loading. Dodecanoic acid has high boiling point than 2-ethylhexanol so 2-ethylhexanol will be more volatile than dodecanoic acid. Because of that matter dodecanoic acid was the one to introduce at the top and the 2-ethylhexanol was introduced at the bottom of the RD column. Feed ratio of two reactants is 1:1. Operating pressure of the column was about 32 kPa.

The specification of RD column is presented for the base case design in the table 3.1. Most of this specification was taken from (Omota et al., 2003). The specification of RD then implemented into a simulation then varies the simulation by changed the temperature, pressure, reflux ratio, reactive zone, and feed location, to determine the important parameter that would effect the process in RD. All the trials done has been summarized into table 3.2.

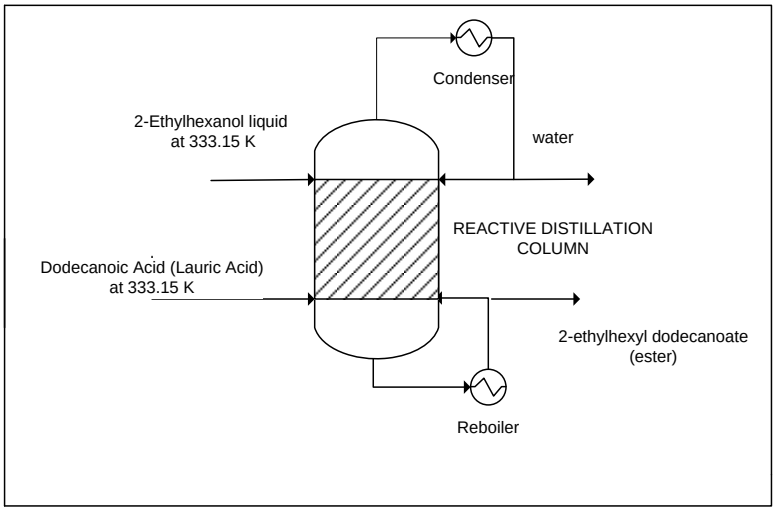

Figure 3.1 Flowsheet for esterification of dodecanoic acid with 2-ethylhexanol in catalytic for RD column

Table 3.1 Specification for base case design as presented in figure 3.1

Category	**Variable**	**Value**
Feed 1 (Dodecanoic Acid)	Flow rate (kmol/h)	100
	Temperature (K)	333.15
Feed 2 (2-Ethylhexanol)	Flow rate (kmol/h)	100
	Temperature (K)	333.15
RD Column	Pressure (kPa)	32
	Number of stages	14
	Reactive stages	6
	Reflux ratio	0.5
	Distillate to feed ratio	0.6
	Liquid hold up (kg)	5

Table 3.2 Trial parameters study

Parameter	**Value**
Temperature (K)	303.15 to 373.15
Reflux ratio	0.1 to 0.8
Pressure (kPa)	10 to 90
Feed location (Stage)	2 &13, 3 to 11, 5 to 10, 4 to 9, both 6
Reactive zone (stages)	12, 10, 8, 6, 4

List of figure 3.2 to figure 3.11, shows the sequence of Aspen Plus working sheets have that been define to produce fatty acid ester. The unavailable component data which is not available in Aspen Plus simulator, was define by using user define method. The minimum data required is Normal boiling point and also molecular weight of the fatty acid, and also the structure of the of fatty acid ester.

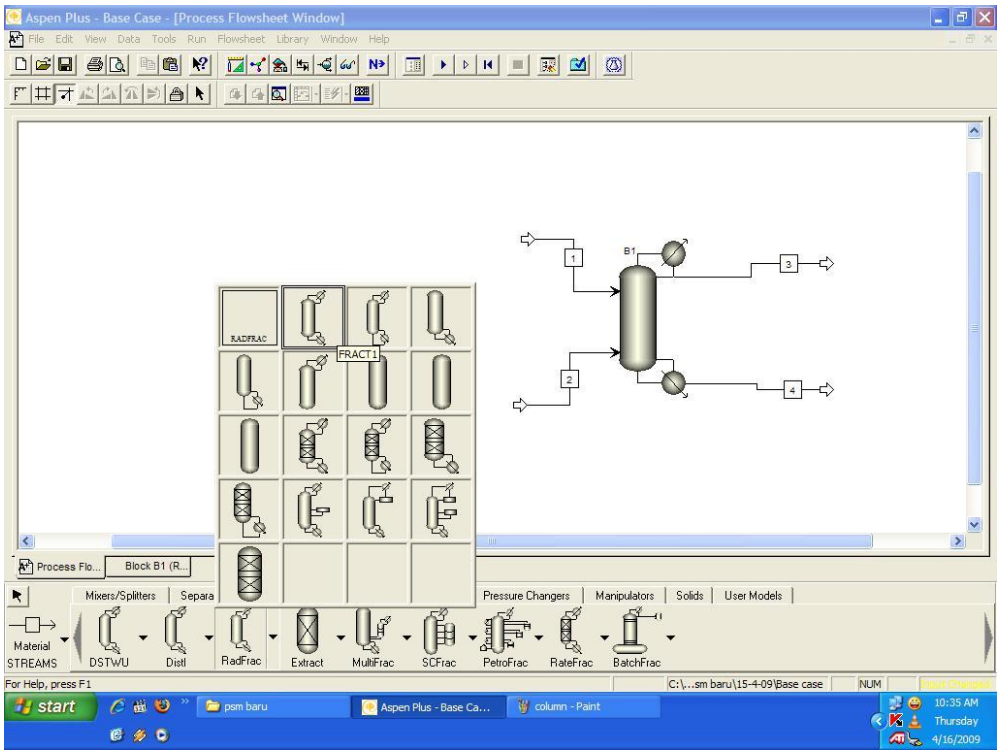

Figure 3.2 Column selections for reactive distillation, using RADFRAC module.

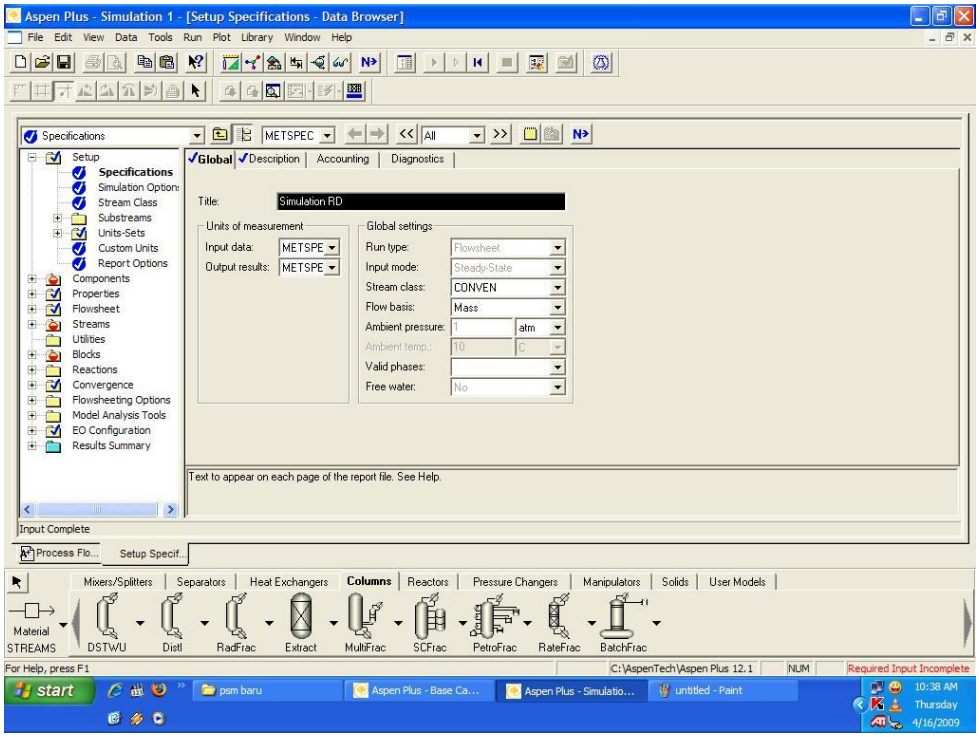

Figure 3.3 Process title to incorporated into Aspen. Plus simulator

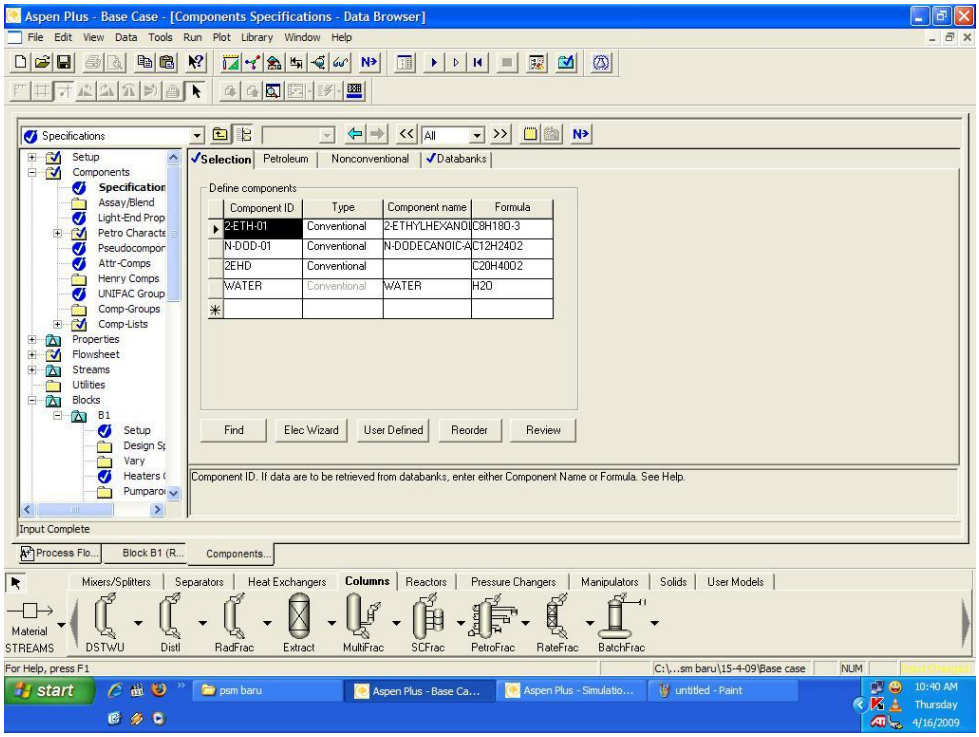

Figure 3.4 List of component selection

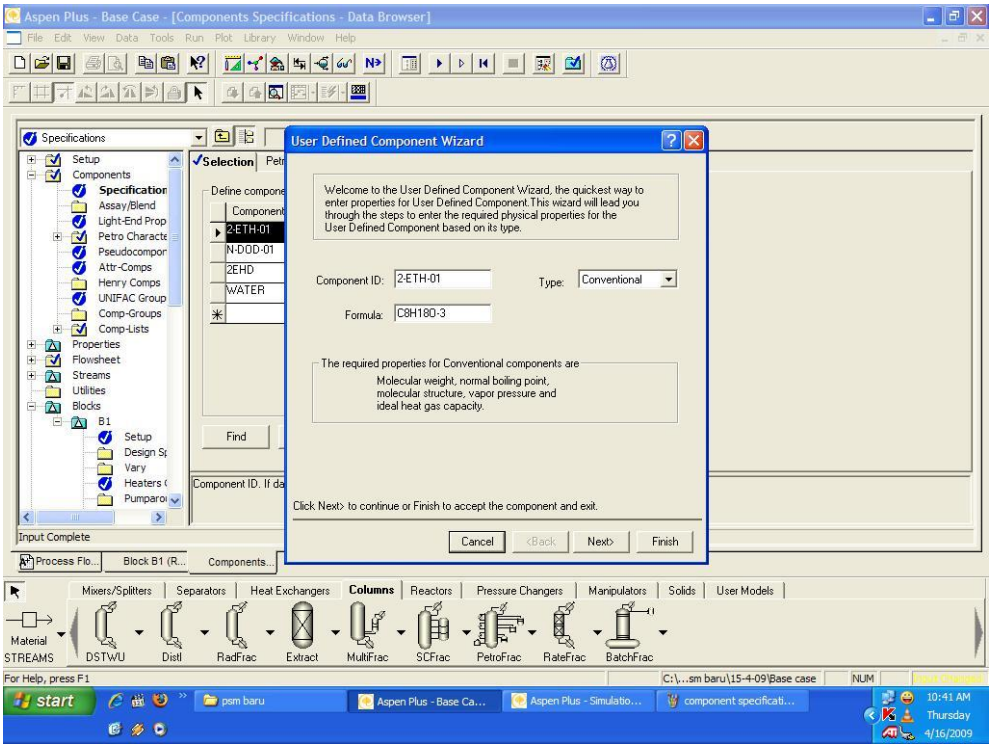

Figure 3.5 User define method to define the unavailable data in Aspen Plus databanks

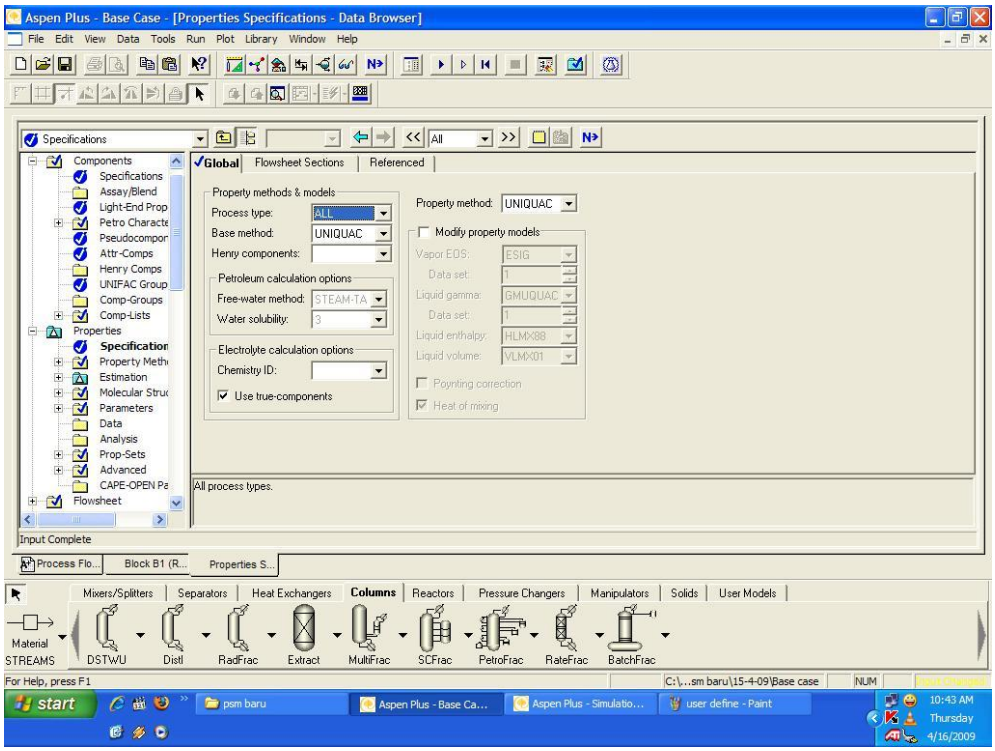

Figure 3.6 Phase equilibrium stage to incorporate into aspen plus

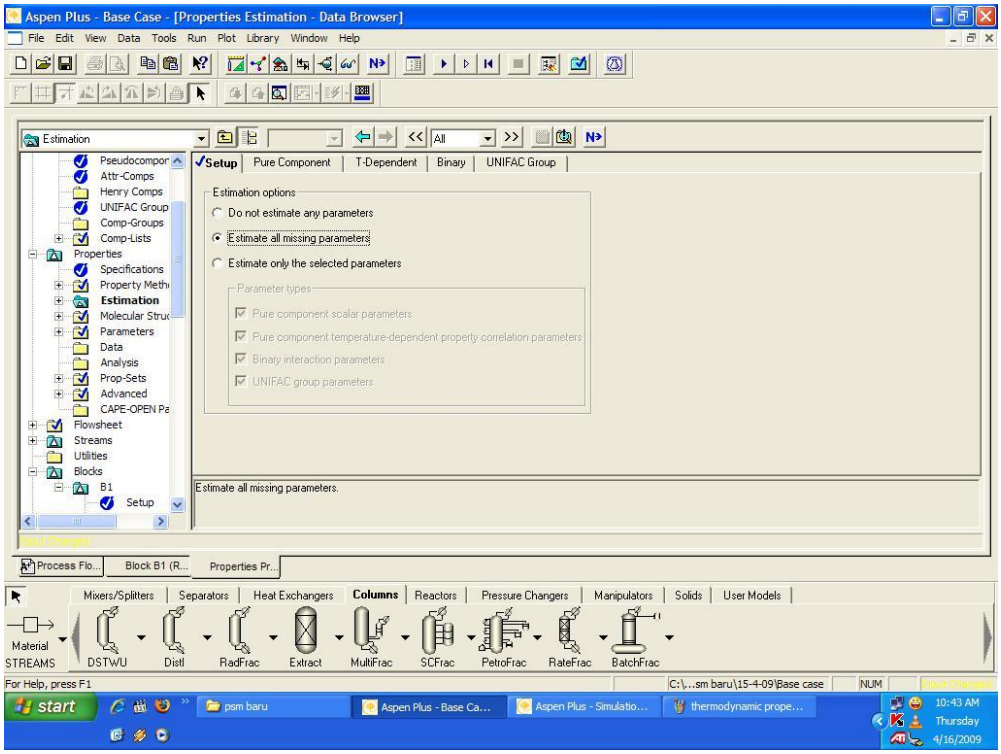

Figure 3.7 Estimation part for Aspen define the parameters for the unavailable component.

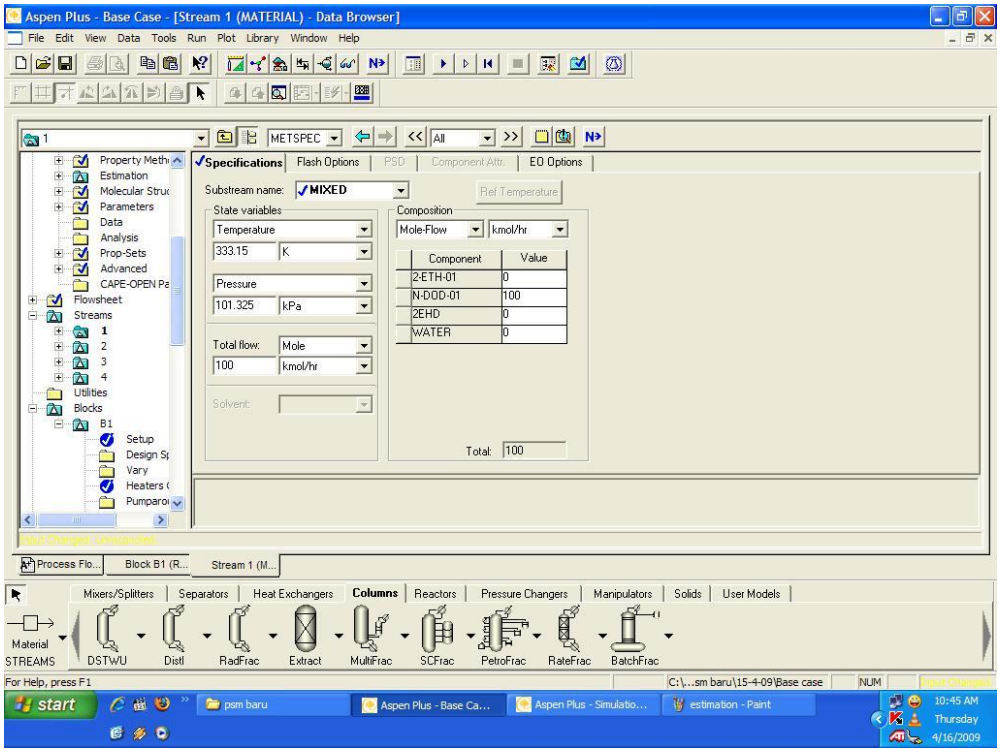

Figure 3.8 Feed streams 1 of the reactant enters to the column

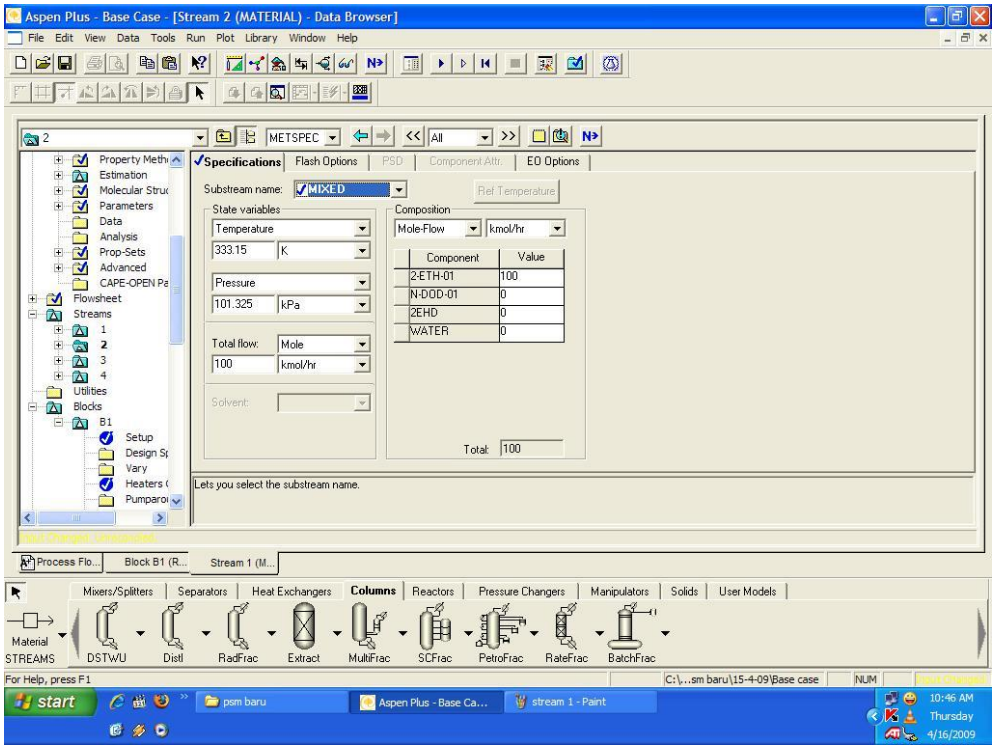

Figure 3.9 Feed stream to enters to the column

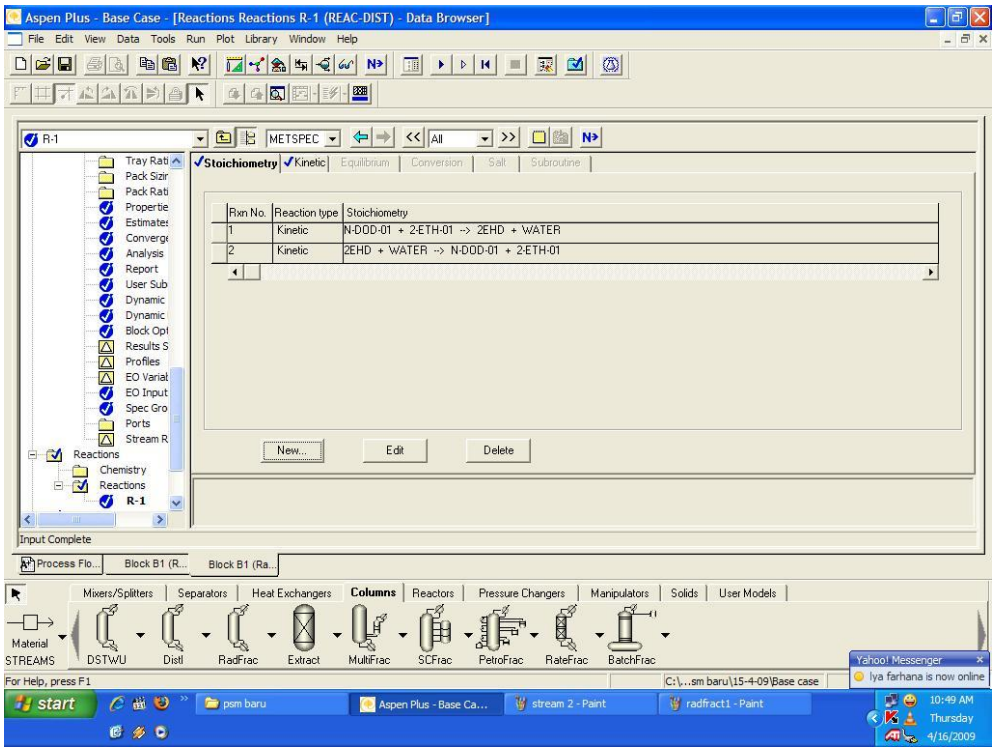

Figure 3.10 Forward and backward reaction stoichiometry

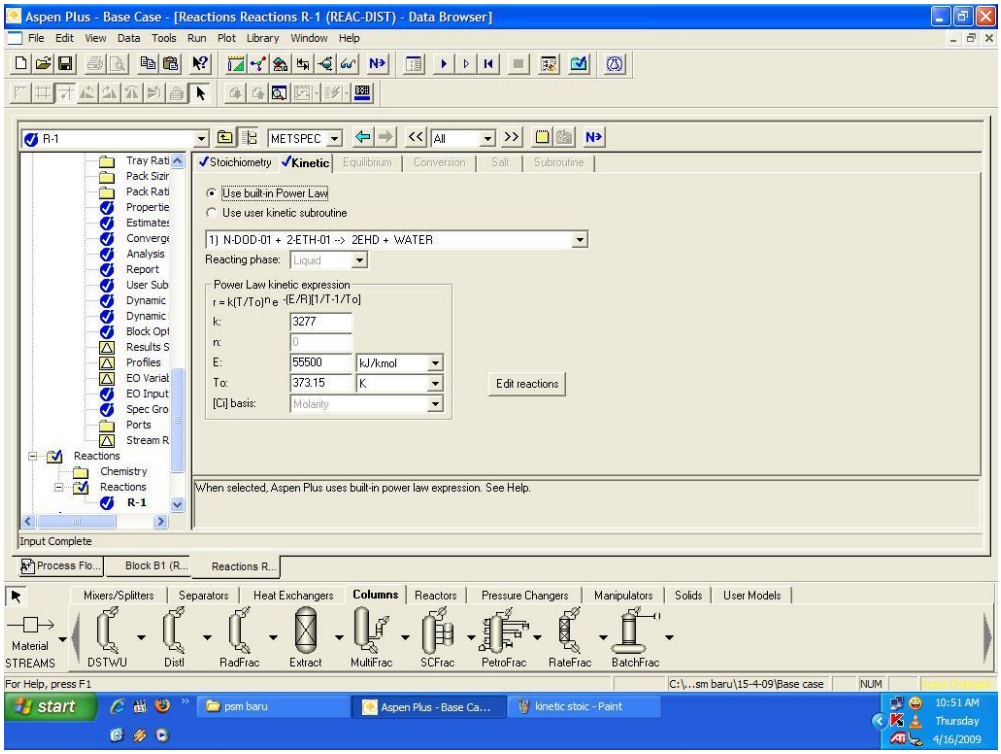

Figure 3.11 Entering value in the build in Power Law

3.3 Summary of methodology

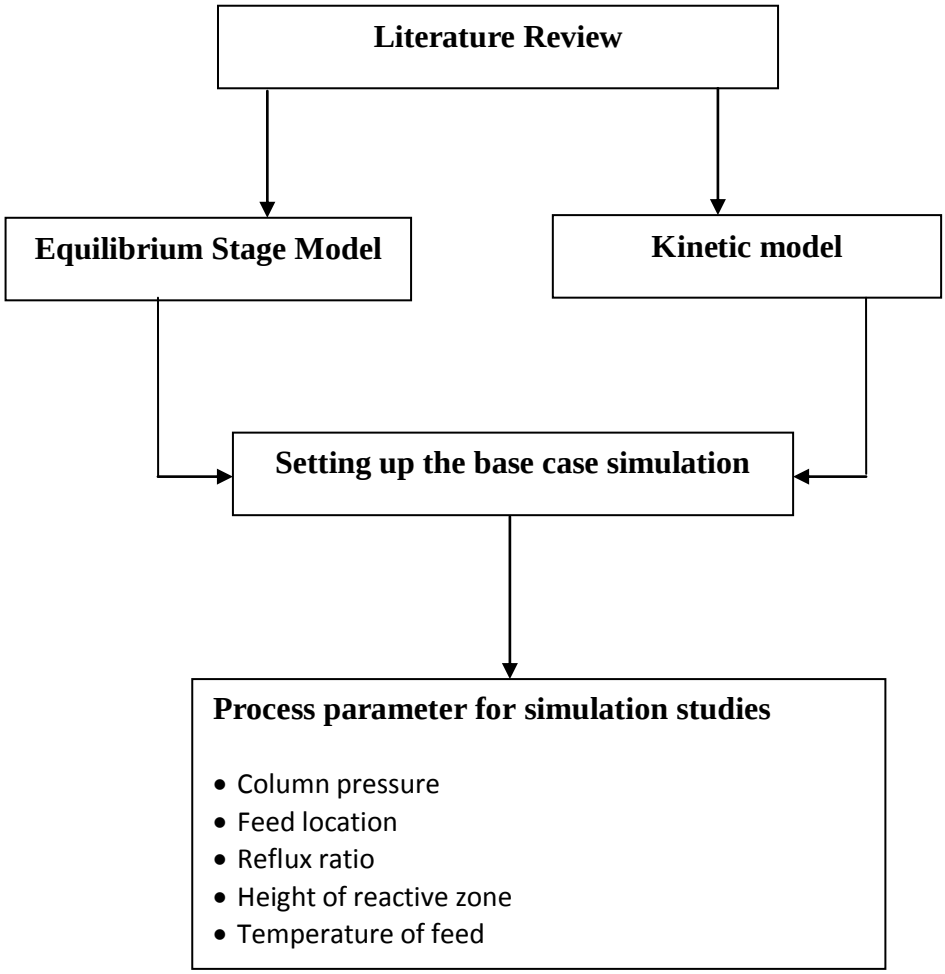

Figure 3.12 Summary of methodology

CHAPTER IV

RESULT AND DISCUSSION

4.1 INTRODUCTION

This chapter depicts the results and analysis from the entire study that have been carried out. Results obtained from this study are based on simulation done using Aspen Plus 12.1. Throughout span of this study, a total of thirty two trials have been carried out to determine which is the most important parameters that would affect the process in RD column. Only the values near to optimum that give higher acid conversion are taken to be fitted into final RD configuration

4.2 Result and Discussion

4.2.1 Temperature

There are about seven trials for temperature parameters to determine the best temperature to be fitted into RD column. All the temperatures are temperature of feed reactant enters to the column. And these temperature was varies from 303.15 K to 372.15 K. Table 4.1 states the result data of temperature profile of RD and acid conversion in the column.

Table 4.1 Effect of temperature and acid conversion (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature varies from 303.15 K to 373.15K, feed location at stage 5 and 10)

Temperature	Acid Conversion %
303.15	0.96245629
313.15	0.96245629
323.15	0.96245628
343.15	0.96245628
353.15	0.96245628
363.15	0.96245628
373.15	0.96245628

From the results, it shows there is no significant difference in acid conversion for each of temperature trials. The difference is about $1x10^{-8}$ and it can be neglected since the difference was too small. This is because of the temperature of reactant enters to the column not effect the process in the column since the operating pressure of the column was conducted under vacuum in order pressure to low down the boiling point of reactant. The column is dependent to the operating pressure column but not dependent to reactant temperature.

4.2.2 Column Pressure

In conventional distillation, the operating pressure of a column was set through an economic rationalization of heat-transfer costs and the value of improved separation (via increasing relative volatility with reducing pressure) (Kister, 1992). However in reactive distillation, the choice of operating pressure is governed by the effect of pressure on the reaction rate and the reaction equilibrium. The column pressure was increased from 10 kPa to 90 kPa. Column was conducted under vacuum condition to minimized the used of energy in the column. The increases of operating pressure column raised the reactive zone temperature and subsequently increased the

reaction rate as well as the reaction equilibrium constant and result to a higher conversion. Table 4.2 below shows the data of pressure column profile and the dodecanoic acid conversion.

Table 4.2 Effect of temperature and acid conversion (Pressure varies from 10kpa to 90kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

Pressure	**Acid conversion %**
10	0.940
20	0.954
32	0.962
40	0.965
50	0.968
60	0.970
70	0.972
80	0.974
90	0.975

The data values shows the acid conversion was increased about 4% when pressure increase from 10kPa to 90kPa. Figure 4.2 shows in elevating the pressure column will leads to higher reaction rates and caused in higher of dodecanoic acid conversion. Since this process was conducted under vacuum condition, the maximum operating pressure up to 90 kPa. As mentioned before, RD column was dependent to operating pressure, whenever the pressure increase would give a higher of acid conversion and increasing the boiler duty and temperature of the boiler also increased.

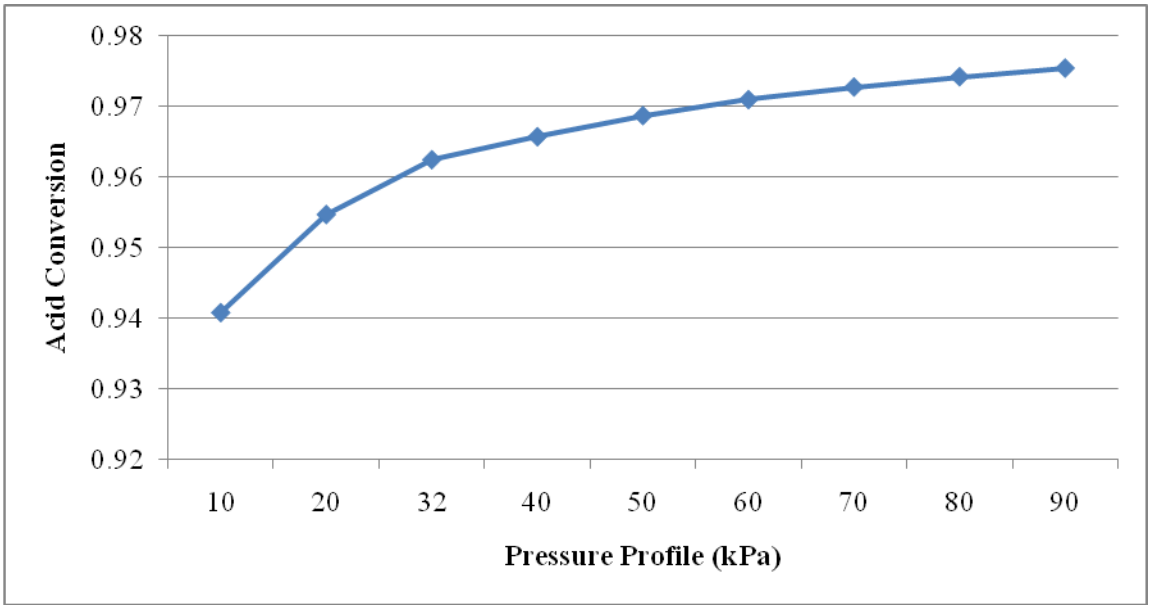

Figure 4.2 Effect of elevating the pressure on acid conversion (Pressure varies from 10kpa to 90kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

4.2.3 Result and Discussion on Reflux Ratio Profile

Reflux ratio used to maintain the process in the column. This always can attribute to water distillation, which otherwise would accumulate in the bottom. Amount of liquid or water was entered back to the column to study the effect reflux ratio to the process in the column. This will contribute to the effect of acid conversion, and product purity and thus brings to product quality. The reflux ratio increased from 0.1 to 0.7. The data in table 4.3 shows in increasing the reflux ratio will reduce the acid conversion. Low reflux ratio will give higher dodecanoic acid conversion. In other hand an excessive reflux ratio will result the in reduced product purity and reduced acid conversion. In this case acid conversion of 99.9 % would be archived when reflux ratio reached to a minimum value.

Table 4.3 Effect of reflux ratio profile and the acid conversion (P=32kpa, reflux ratio varies from0.1 to 0.7 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

Reflux ratio	Acid conversion %
0.1	0.978
0.2	0.966
0.3	0.965
0.4	0.963
0.5	0.962
0.6	0.961
0.7	0.959

Figure 4.3 below shows reflux ratio on acid conversion, at reflux ratio of 0.1 will give almost 97% of acid conversion but at 0.7 give about 96% of acid conversion. As the reflux ratio increased amount of liquid or water at the top of the column enters back to the column would also increased. This brings toward reduced the amount of end product or ester needed in the simulation. As mentioned before, the lesser amount of reflux ratio is the higher acid conversion.

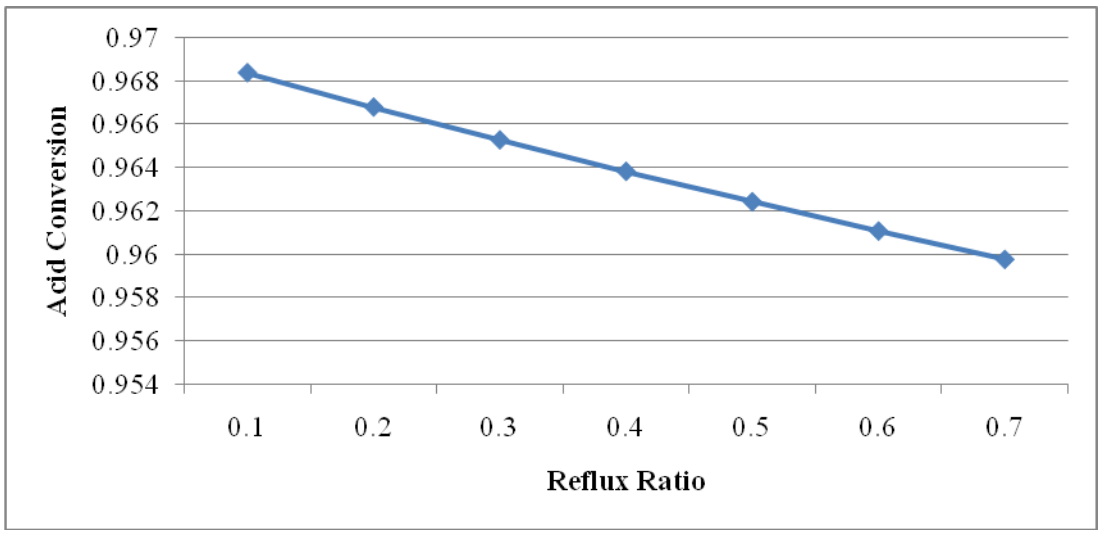

Figure 4.3 Effect of reflux ratio on acid conversion (P=32kpa, reflux ratio varies from0.1 to 0.7 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

4.2.4 Height of Reactive Zone

Height of reactive zone depends on catalyst weight, catalyst volume fraction of the packing, catalyst density and column diameter. Pressure drop in catalytic bed limits the amount of catalyst can be accommodate per unit volume of column. In order to avoid the residence time limitation (in adequate catalyst weight), either column diameter or reactive zone height should be increased, to accommodate the additional catalyst weight. Increasing in reactive zone height is not an always better option, because changes in the packing height could affect column separation performance. Hence, it still needs to study the effect of changing the height of reactive zone. Thereby height of reactive zone was increased from 4 stages height to 12 stages height. The data result shows that in increasing the height of reactive zone, will give a high of dodecanoic acid conversion. The 12 stages conversion gives about 97% of acid conversion differs to 4 stages height give 88% of acid conversion. Since, in increasing the height of reactive zone will contribute to higher cost catalyst used. The most cheapest but higher in conversion is 6 stages of height reactive zone

Table 4.4 Effect height of reactive zone profile and acid conversion (P=32kpa, reflux ratio =0.5, Distillate to feed ratio=0.6, reactive zone varies from 4 to 12 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

Stages	acid conversion%
4	0.833
6	0.962
8	0.962
10	0.966
12	0.970

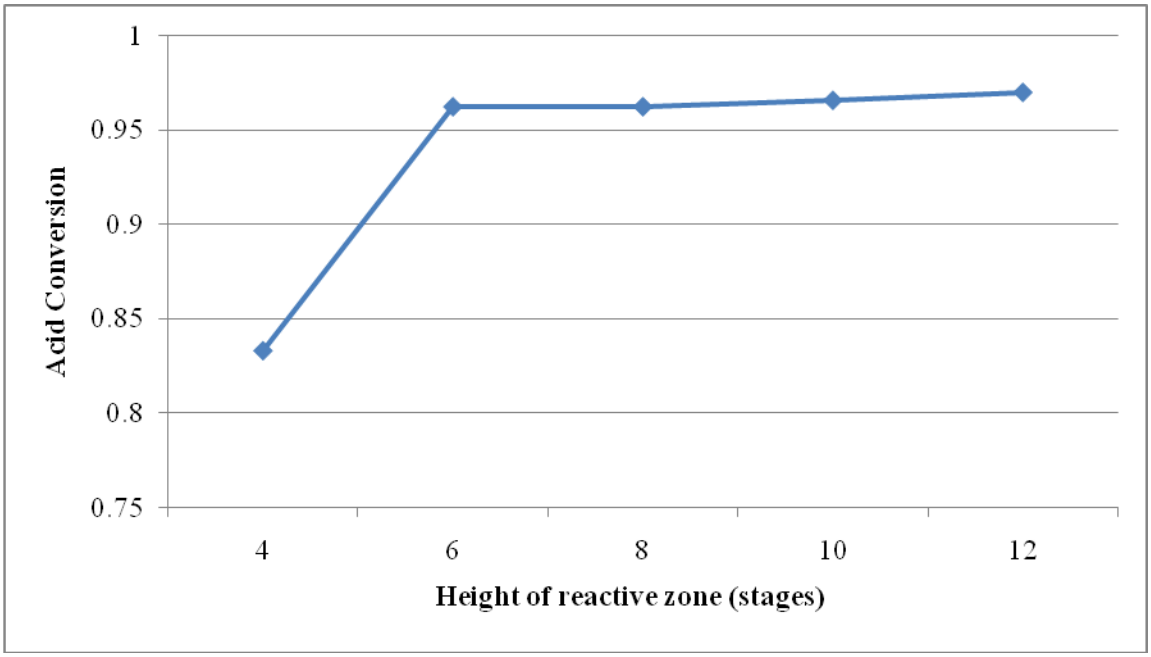

Figure 4.4 Effect of reflux ratio on acid conversion (P=32kpa, reflux ratio =0.5, Distillate to feed ratio=0.6, reactive zone varies from 4 to 12 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

Figure 4.4 shows effect of height reactive zone give higher conversion. Different conversion in 6 stages to 12 stages height is about $1x10^{-2}$. It is better to use 6 stages height rather than 12 stages height because if will effect the cost of production, since RD are used to minimized the capital cost of production. The 6 stages height of reactive zone was used in further simulation.

4.2.5 Feed point location

The reactive distillation column could be treated as a tubular reactor cascade with separation units while reactive zone of reactive distillation column can be viewed as cascade-type two-phase reactor with the reactor temperature determined from the bubble-point temperature of the tray liquid phase composition (Doherty & Malone, 2001) The composition and temperature profile could affect the performance of reactive zone, and the feed tray locations appear to be one of the most important variable for these profile redistribution. The right choice of feed

location ensures high concentrations of reactant in reactive zone. Present study there are 4 reactive distillation columns with different feed tray locations were investigated. The distillation column was evaluated by comparing the acid conversion. From figure 4.5(a) feed enters at relatively at top of the column which is above reactive zone and at the bottom which is below the reactive distillation column. Meanwhile figure 4.5(b) is location for base case design which is the location of feed enters in right on the reactive zone whereby at stage 5 and stage 10. Feed location was in between the reactive zone was introduce at figure 4.5(c) and last is location of both feed was introduced at the middle of RD figure 4.5(d). Result of these different locations arrangement was detailed up in table 4.5.

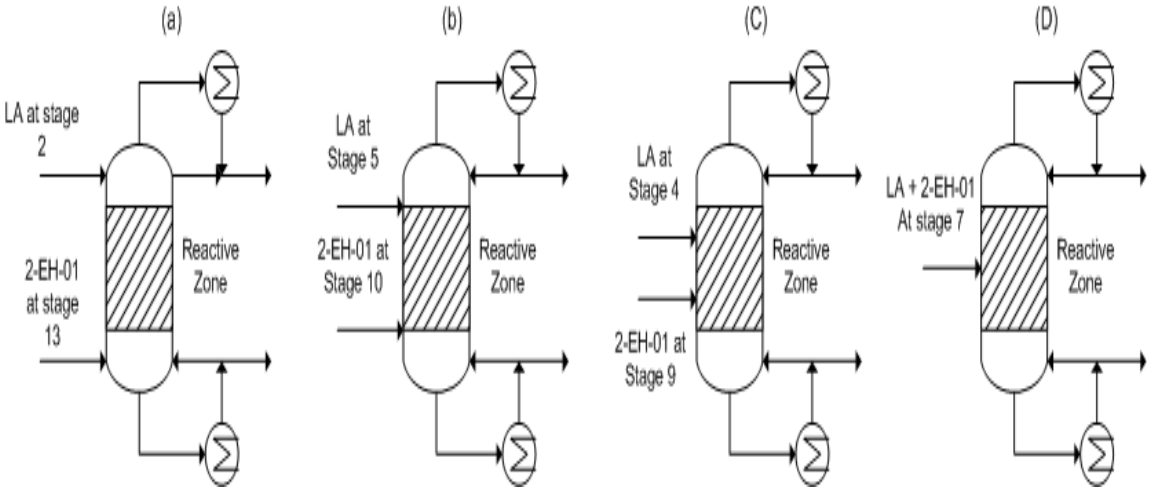

Figure 4.5 Reactive Distillation with different feed point location arrangement (P=32kpa, reflux ratio =0.5, Distillate to feed ratio=0.6, reactive zone varies from 4 to 12 stages, reactant temperature 333.15K, feed location as shown in figure)

Table 4.5 Location arrangement and acid conversion (P=32kpa, reflux ratio =0.5, Distillate to feed ratio=0.6, reactive zone varies from 4 to 12 stages, reactant temperature 333.15K)

Reactor	**A (stage 2 and 13)**	**B (stage 5 and 10)**	**C (stage 4 and 9)**	**D (both stage 7)**
Conversion	**0.833**	**0.962**	**0.833**	**0.962**

Location arrangement for feed location above and below the reactive distillation (a) and also location arrangement in between of reactive distillation give low of acid conversion. So the location for both (a) and (b) is not preferable. Location arrangement for (b) and (d) gives a bit higher acid conversion than both (a) and (c) about 13% higher. Since (b) is a base case design, so it the most preferable feed location to be use for further simulation.

4.3 Final process

The simulations studies indicate that temperature of feed or reactant enters to the column are will not give any effect to the process in the column. Therefore, the process comprised of a column consisting 6 stages height of reactive zone. Dodecanoic acid is enters at stage 5 right on above of reactive zone with feed temperature of 303.15 K and 2-ethylhexanol was entered the column at stage 10 right on bottom of the reactive zone with feed temperature of 303.15 K. The column operating pressure was set to be 30 kPa, the reflux ratio was 0.1, distillate to feed ratio was meant to be 0.6. Figure 4.6 shows the proposed flowsheet for esterification of dodecanoic acid and 2-ethylhexanol reactive distillation column with the above configuration entered into the simulation. The distillate will produce from RD column contained water. Fatty acid ester of 2-ethylhexyl dodecanoate or product will get at the bottom of the column with acid conversion 99.3%.

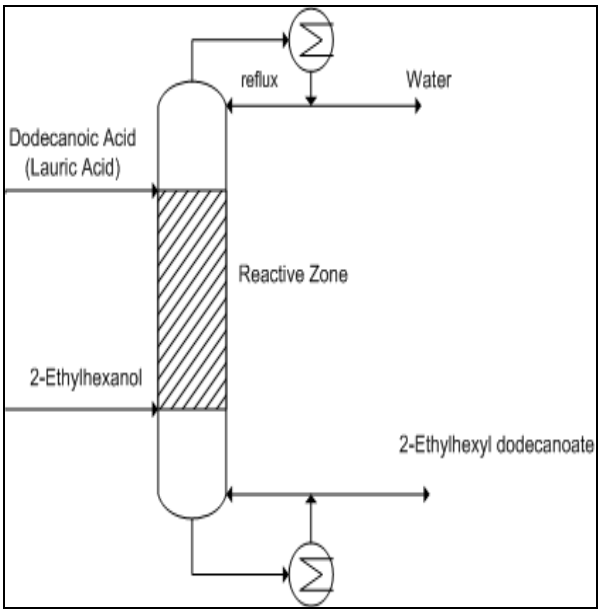

Figure 4.6 Proposed flowsheet for esterification of dodecanoic acid and 2-ethylhexanol reactive distillation column (P=30kpa, reflux ratio =0.1, Distillate to feed ratio=0.6, reactive zone varies from 4 to 12 stages, reactant temperature 303.15K)

CHAPTER V

CONCLUSION AND RECOMMENDATION

5.1 CONCLUSION

The simulation of esterification process of dodecanoic acid and 2-ethylhexanol was studied in reactive distillation column using sulfated zirconia (SZ) catalyst. The simulation was conducted under different operating conditions. The operating parameters include height of reactive zone, reflux ratio, operating pressure column, temperature and location arrangement of feed enters to the column. The simulation indicates the important parameter were all the parameter investigated but only temperature not give any changes to the process in the column. Furthermore, kinetic constant for heterogeneously catalyzed model based on concentration has been fitted and incorporated into process simulator Aspen-Plus 12.1 using RADFRAC module with thermodynamic equilibrium model of UNIQUAC.

As a result, the optimum operating parameters are, reflux ratio at 0.1, temperature of feed enters to the column both are at 303.15 right on the reactive zone at stage five and stage 10, Height of reactive zone is six stages, whereby the operating column pressure is 30kpa in order to have an acid conversion about 99.3%.

5.2 Recommendation

5.2.1 Process simulator

The present simulation study was using Aspen-Plus 12.1 simulator. Instead of using Aspen-Plus those are limited to some data available in simulator data bank, HYSYS can be one of the alternative way to complete the process simulation. This will give a accurate value for the estimated chemical data to be fit into Aspen Plus user define method.

5.2.2 Parameter study

There are more parameter can be studied other than on top of the five parameters that have been used in present study. Parameters to be considered in the study are like distillate to feed ratio because there are some quantities of 2-ethylhexanol are stripped out at upper column with water. Second is catalyst weight because inadequate amount of catalyst weight will cause in poor acid conversion. Feed ratio enters to the column also can be further studied in the future.

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APPENDIX A

This appendix A shows the results for condenser duty and boiler duty for temperature, pressure, reflux ratio, height of reactive zone and the location of feed arrangement using Aspen Plus 12.1 simulator

Base Case

Table A 1 Base case on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7193215	kcal/hr
bottom rate	80	kmol/hr
boiler rate	397.9813	kmol/hr
boilup ratio	4.974766	

Temperature

Table A 2 Temperature of reactant 303 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7749446	kcal/hr
bottom rate	80	kmol/hr
boiler rate	428.7563	kmol/hr
boilup ratio	5.359454	

Table A 3 Temperature of reactant 313 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7567682	kcal/hr
bottom rate	80	kmol/hr
boiler rate	418.6997	kmol/hr
boilup ratio	5.233746	

Table A 4 Temperature of reactant 323 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7382357	kcal/hr
bottom rate	80	kmol/hr
boiler rate	408.4461	kmol/hr
boilup ratio	5.105576	

Table A 5 Temperature of reactant 343 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7000216	kcal/hr
bottom rate	80	kmol/hr
boiler rate	387.3031	kmol/hr
boilup ratio	4.841289	

Table A 6 Temperature of reactant 353 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6803353	kcal/hr
bottom rate	80	kmol/hr
boiler rate	376.411	kmol/hr
boilup ratio	4.705138	

Table A 7 Temperature of reactant 363 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6602623	kcal/hr
bottom rate	80	kmol/hr
boiler rate	365.3051	kmol/hr
boilup ratio	4.566314	

Table A 8 Temperature of reactant 373 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605185	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6398015	kcal/hr
bottom rate	80	kmol/hr
boiler rate	353.9846	kmol/hr
boilup ratio	4.424807	

Pressure

Table A 9 Pressure of column 10kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	48.06132	c
heat duty	-3559268	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	301.0448	c
heat duty	6209363	kcal/hr
bottom rate	80	kmol/hr
boiler rate	304.407	kmol/hr
boilup ratio	3.805087	

Table A 10 Pressure of column 20kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	62.74666	c
heat duty	-3587785	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	325.2621	c
heat duty	6763602	kcal/hr
bottom rate	80	kmol/hr
boiler rate	354.1824	kmol/hr
boilup ratio	4.427281	

Table A 11 Pressure of column 40kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	79.01913	c
heat duty	-3613045	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	352.9857	c
heat duty	7415022	kcal/hr
bottom rate	80	kmol/hr
boiler rate	422.7225	kmol/hr
boilup ratio	5.284032	

Table A 12 Pressure of column 50kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	84.64245	c
heat duty	-3620727	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	362.7772	c
heat duty	7649625	kcal/hr
bottom rate	80	kmol/hr
boiler rate	450.6862	kmol/hr
boilup ratio	5.633578	

Table A 13 Pressure of column 60kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	89.38955	c
heat duty	-3626874	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	371.1184	c
heat duty	7851430	kcal/hr
bottom rate	80	kmol/hr
boiler rate	476.3976	kmol/hr
boilup ratio	5.95497	

Table A 14 Pressure of column 70kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	93.51547	c
heat duty	-3631880	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	378.4194	c
heat duty	8029464	kcal/hr
bottom rate	80	kmol/hr
boiler rate	500.5026	kmol/hr
boilup ratio	6.256282	

Table A 15 Pressure of column 80kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	97.17611	c
heat duty	-3636184	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	384.9337	c
heat duty	8189539	kcal/hr
bottom rate	80	kmol/hr
boiler rate	523.4169	kmol/hr
boilup ratio	6.542712	

Table A 16 Pressure of column 90kpa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	100.4742	c
heat duty	-3640029	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	390.8267	c
heat duty	8335470	kcal/hr
bottom rate	80	kmol/hr
boiler rate	545.431	kmol/hr
boilup ratio	6.817888	

Reflux Ratio

Table A 17 Reflux ratio of 0.1 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.67113	c
heat duty	-2652584	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	12	kmol/hr
reflux rate	0.1	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6231074	kcal/hr
bottom rate	80	kmol/hr
boiler rate	344.7477	kmol/hr
boilup ratio	4.309347	

Table A 18 Reflux ratio of 0.2 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.64954	c
heat duty	-2891154	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	24	kmol/hr
reflux rate	0.2	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6472181	kcal/hr
bottom rate	80	kmol/hr
boiler rate	358.0878	kmol/hr
boilup ratio	4.476097	

Table A 19 Reflux ratio of 0.3 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.629	c
heat duty	-3129514	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	36	kmol/hr
reflux rate	0.3	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6712967	kcal/hr
bottom rate	80	kmol/hr
boiler rate	371.4101	kmol/hr
boilup ratio	4.642626	

Table A 20 Reflux ratio of 0.4 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.60935	c
heat duty	-3367498	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	48	kmol/hr
reflux rate	0.4	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6953282	kcal/hr
bottom rate	80	kmol/hr
boiler rate	384.7063	kmol/hr
boilup ratio	4.808828	

Table A 21 Reflux ratio of 0.6 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages,)

condenser/ top stage		
Temperature	73.57235	c
heat duty	-3842600	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	72	kmol/hr
reflux rate	0.6	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7432799	kcal/hr
bottom rate	80	kmol/hr
boiler rate	411.2369	kmol/hr
boilup ratio	5.140462	

Table A 22 Reflux ratio of 0.7 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.55486	c
heat duty	-4079706	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	84	kmol/hr
reflux rate	0.7	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7672004	kcal/hr
bottom rate	80	kmol/hr
boiler rate	424.4717	kmol/hr
boilup ratio	5.305896	

Height of Reactive zone

Table A 23 Reactive zone of 12 stages from stage 2-13 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.69385	c
heat duty	-3620431	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7196262	kcal/hr
bottom rate	80	kmol/hr
boiler rate	398.1498	kmol/hr
boilup ratio	4.976873	

Table A 24 Reactive zone of 10 stages from stage 3 to 12 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.63674	c
heat duty	-3612082	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7194615	kcal/hr
bottom rate	80	kmol/hr
boiler rate	398.0587	kmol/hr
boilup ratio	4.975734	

Table A 25 Reactive zone of 8 stages from stage 4 to 11 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.59855	c
heat duty	-3606394	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7193460	kcal/hr
bottom rate	80	kmol/hr
boiler rate	397.9948	kmol/hr
boilup ratio	4.974935	

Table A 26 Reactive zone of 4 stages from stage 6 to9 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	72.13166	c
heat duty	-3054995	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6850307	kcal/hr
bottom rate	80	kmol/hr
boiler rate	379.0088	kmol/hr
boilup ratio	4.737611	

Feed Location of feed

Table A 27 Feed location at 2 and 13 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	72.14143	c
heat duty	-3056072	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.1057	c
heat duty	6840389	kcal/hr
bottom rate	80	kmol/hr
boiler rate	289.2984	kmol/hr
boilup ratio	3.61623	

Table A 28 Feed location at 5 and 10 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.59047	c
heat duty	-3605231	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7193260	kcal/hr
bottom rate	80	kmol/hr
boiler rate	397.9839	kmol/hr
boilup ratio	4.974799	

Table A 29 Feed location at 4 and 9 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	72.13191	c
heat duty	-3055825	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	6851094	kcal/hr
bottom rate	80	kmol/hr
boiler rate	379.0544	kmol/hr
boilup ratio	4.738179	

Table A 30 Feed location both at 6 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

condenser/ top stage		
Temperature	73.5905	c
heat duty	-3605190	kcal/hr
ditillate rate	120	kmol/hr
reflux rate	60	kmol/hr
reflux rate	0.5	
Boiler/bottom stage		
Temperature	343.6353	c
heat duty	7193218	kcal/hr
bottom rate	80	kmol/hr
boiler rate	397.9833	kmol/hr
boilup ratio	4.974791	

APPENDIX B

Appendix B shows the result of liquid composition in every stage in reactor and the data was use to find percent of acid conversion for temperature, pressure, reflux ratio, height of reactive zone, location of feed arrangement in reactor using Aspen Plus 12.1 simulator

Base case

Table B 1 Base case on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages, reactant temperature 333.15K, feed location at stage 5 and 10)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.037544	0.037544	0.129123	0.79579
2	0.002195	0.02293	0.966223	0.008652
3	0.001055	0.010298	0.984352	0.004295
4	0.000926	0.008203	0.987056	0.003815
5	0.000906	0.007856	0.987499	0.003739
6	0.011255	7.68E-06	0.988679	5.87E-05
7	0.0099	4.66E-08	0.990099	3.29E-07
8	0.009532	2.69E-10	0.990468	1.85E-09
9	0.009448	1.53E-12	0.990552	1.04E-11
10	0.009429	8.61E-15	0.990571	5.85E-14
11	0.000247	1.49E-15	0.999753	3.19E-16
12	6.15E-06	2.43E-16	0.999994	1.65E-18
13	1.53E-07	3.96E-17	1	8.54E-21
14	3.78E-09	6.31E-18	1	4.41E-23

Temperature

Table B 2 Temperature of reactant 303 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01054	7.95E-06	0.9894	5.81E-05
7	0.00916	4.85E-08	0.99084	3.23E-07
8	0.00881	2.80E-10	0.99119	1.81E-09
9	0.00874	1.58E-12	0.99126	1.02E-11
10	0.00872	8.88E-15	0.99128	5.70E-14
11	0.00022	1.50E-15	0.99978	3.05E-16
12	5.51E-06	2.43E-16	0.99999	1.56E-18
13	1.35E-07	3.91E-17	1	7.99E-21
14	3.31E-09	6.17E-18	1	4.01E-23

Table B.3 Temperature of reactant 313 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01076	7.86E-06	0.98917	5.83E-05
7	0.00939	4.79E-08	0.99061	3.25E-07
8	0.00903	2.76E-10	0.99097	1.82E-09
9	0.00896	1.56E-12	0.99104	1.02E-11
10	0.00894	8.78E-15	0.99106	5.74E-14
11	0.00023	1.50E-15	0.99977	3.09E-16
12	5.70E-06	2.43E-16	0.99999	1.59E-18
13	1.40E-07	3.92E-17	1	8.16E-21
14	3.45E-09	6.20E-18	1	4.21E-23

Table B.4 Temperature of reactant 323 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.011	7.77E-06	0.98893	5.85E-05
7	0.00964	4.73E-08	0.99036	3.27E-07
8	0.00927	2.73E-10	0.99073	1.83E-09
9	0.00919	1.54E-12	0.99081	1.03E-11
10	0.00917	8.69E-15	0.99083	5.80E-14
11	0.00024	1.49E-15	0.99976	3.14E-16
12	5.91E-06	2.43E-16	0.99999	1.62E-18
13	1.46E-07	3.94E-17	1	8.32E-21
14	3.60E-09	6.25E-18	1	4.28E-23

Table B.5 Temperature of reactant 343 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01153	7.59E-06	0.98841	5.90E-05
7	0.01019	4.60E-08	0.98981	3.31E-07
8	0.00981	2.66E-10	0.99019	1.86E-09
9	0.00972	1.51E-12	0.99028	1.05E-11
10	0.0097	8.53E-15	0.9903	5.92E-14
11	0.00026	1.48E-15	0.99974	3.25E-16
12	6.40E-06	2.44E-16	0.99999	1.69E-18
13	1.60E-07	3.99E-17	1	8.78E-21
14	3.97E-09	6.38E-18	1	4.56E-23

Table B.6 Temperature of reactant 353 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01182	7.49E-06	0.98811	5.93E-05
7	0.0105	4.53E-08	0.9895	3.33E-07
8	0.01012	2.62E-10	0.98988	1.88E-09
9	0.01002	1.49E-12	0.98998	1.06E-11
10	0.01	8.45E-15	0.99	6.00E-14
11	0.00027	1.48E-15	0.99973	3.32E-16
12	6.69E-06	2.45E-16	0.99999	1.74E-18
13	1.68E-07	4.03E-17	1	9.07E-21
14	4.19E-09	6.46E-18	1	4.73E-23

Table B.7 Temperature of reactant 363 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01214	7.39E-06	0.9878	5.95E-05
7	0.01083	4.47E-08	0.98917	3.36E-07
8	0.01045	2.59E-10	0.98955	1.90E-09
9	0.01035	1.48E-12	0.98965	1.07E-11
10	0.01033	8.38E-15	0.98967	6.09E-14
11	0.00028	1.48E-15	0.99972	3.40E-16
12	7.00E-06	2.47E-16	0.99999	1.79E-18
13	1.77E-07	4.07E-17	1	9.38E-21
14	4.43E-09	6.57E-18	1	4.92E-23

Table B.8 Temperature of reactant 373 K on condenser and boiler duty with (P=32kpa, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	0.12912	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01248	7.30E-06	0.98746	5.98E-05
7	0.0112	4.41E-08	0.9888	3.39E-07
8	0.01081	2.56E-10	0.98919	1.92E-09
9	0.01071	1.46E-12	0.98929	1.09E-11
10	0.01068	8.32E-15	0.98932	6.19E-14
11	0.00029	1.49E-15	0.99971	3.49E-16
12	7.36E-06	2.49E-16	0.99999	1.84E-18
13	1.87E-07	4.13E-17	1	9.72E-21
14	4.71E-09	6.69E-18	1	5.13E-23

Pressure

Table B.9 Pressure of the column 10kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.05922	0.05922	0.10745	0.77411
2	0.00203	0.03043	0.96291	0.00462
3	0.00096	0.01237	0.98439	0.00228
4	0.00086	0.01006	0.98702	0.00206
5	0.00085	0.00976	0.98736	0.00204
6	0.00769	1.40E-05	0.99226	3.30E-05
7	0.00708	5.75E-08	0.99292	1.29E-07
8	0.00692	2.31E-10	0.99308	5.12E-10
9	0.00688	9.19E-13	0.99312	2.03E-12
10	0.00688	3.62E-15	0.99312	8.01E-15
11	0.00011	4.97E-16	0.99989	2.52E-17
12	1.71E-06	6.42E-17	1	7.11E-20
13	2.63E-08	8.27E-18	1	2.00E-21
14	4.02E-10	1.05E-18	1	1.45E-23

Table B.10 Pressure of the column 20kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.04531	0.04531	0.12136	0.78802
2	0.00213	0.0256	0.96554	0.00672
3	0.00102	0.01109	0.98455	0.00334
4	0.00091	0.00893	0.98717	0.00299
5	0.00089	0.0086	0.98756	0.00295
6	0.00975	9.72E-06	0.99019	4.64E-05
7	0.00877	4.93E-08	0.99123	2.20E-07
8	0.0085	2.41E-10	0.9915	1.05E-09
9	0.00845	1.16E-12	0.99155	5.06E-12
10	0.00844	5.58E-15	0.99156	2.43E-14
11	0.00018	8.81E-16	0.99982	1.07E-16
12	3.80E-06	1.32E-16	1	4.46E-19
13	7.85E-08	1.95E-17	1	1.86E-21
14	1.61E-09	2.84E-18	1	7.73E-24

Table B.11 Pressure of the column 40kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03429	0.03429	0.13238	0.79905
2	0.00222	0.02179	0.96626	0.00974
3	0.00107	0.00994	0.98416	0.00483
4	0.00093	0.00787	0.98693	0.00427
5	0.00091	0.00751	0.98741	0.00417
6	0.01197	6.90E-06	0.98796	6.59E-05
7	0.0104	4.59E-08	0.9896	4.00E-07
8	0.00997	2.89E-10	0.99003	2.44E-09
9	0.00986	1.78E-12	0.99014	1.49E-11
10	0.00984	1.09E-14	0.99016	9.09E-14
11	0.00028	1.95E-15	0.99972	5.46E-16
12	7.55E-06	3.33E-16	0.99999	3.12E-18
13	2.04E-07	5.66E-17	1	1.78E-20
14	5.47E-09	9.40E-18	1	1.02E-22

Table B.12 Pressure of the column 50kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03129	0.03129	0.13537	0.80204
2	0.00224	0.02071	0.96611	0.01094
3	0.00108	0.00959	0.98391	0.00542
4	0.00093	0.00755	0.98676	0.00476
5	0.00091	0.00717	0.98728	0.00464
6	0.01266	6.22E-06	0.98726	7.39E-05
7	0.01085	4.56E-08	0.98915	4.89E-07
8	0.01034	3.13E-10	0.98966	3.23E-09
9	0.01022	2.09E-12	0.98978	2.14E-11
10	0.01019	1.39E-14	0.98981	1.42E-13
11	0.00031	2.60E-15	0.99969	9.39E-16
12	9.12E-06	4.61E-16	0.99999	5.92E-18
13	2.66E-07	8.15E-17	1	3.77E-20
14	7.72E-09	1.41E-17	1	2.29E-22

Table B.13 Pressure of the column 60kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.02903	0.02903	0.13764	0.8043
2	0.00226	0.01988	0.96584	0.01203
3	0.00108	0.00931	0.98366	0.00594
4	0.00093	0.00729	0.98659	0.00519
5	0.0009	0.0069	0.98714	0.00505
6	0.0132	5.73E-06	0.98672	8.13E-05
7	0.01117	4.55E-08	0.98883	5.76E-07
8	0.01059	3.36E-10	0.98941	4.08E-09
9	0.01045	2.41E-12	0.98955	2.90E-11
10	0.01042	1.71E-14	0.98958	2.06E-13
11	0.00034	3.30E-15	0.99966	1.47E-15
12	1.05E-05	6.04E-16	0.99999	9.98E-18
13	3.25E-07	1.10E-16	1	6.78E-20
14	1.00E-08	1.96E-17	1	4.60E-22

Table B.14 Pressure of the column 70kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.02724	0.02724	0.13942	0.80609
2	0.00227	0.01921	0.9655	0.01302
3	0.00109	0.00909	0.98341	0.00642
4	0.00093	0.00707	0.98642	0.00558
5	0.0009	0.00667	0.98701	0.00542
6	0.01362	5.36E-06	0.98628	8.82E-05
7	0.01139	4.56E-08	0.98861	6.63E-07
8	0.01076	3.58E-10	0.98924	4.98E-09
9	0.0106	2.72E-12	0.9894	3.75E-11
10	0.01056	2.06E-14	0.98944	2.82E-13
11	0.00036	4.05E-15	0.99964	2.14E-15
12	1.17E-05	7.61E-16	0.99999	1.55E-17
13	3.82E-07	1.42E-16	1	1.12E-19
14	1.24E-08	2.60E-17	1	8.12E-22

Table B.15 Pressure of the column 80kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.02578	0.02578	0.14088	0.80755
2	0.00228	0.01865	0.96513	0.01394
3	0.00109	0.00889	0.98316	0.00686
4	0.00092	0.00689	0.98625	0.00594
5	0.00089	0.00648	0.98687	0.00576
6	0.01397	5.07E-06	0.98593	9.46E-05
7	0.01155	4.58E-08	0.98845	7.48E-07
8	0.01085	3.80E-10	0.98915	5.91E-09
9	0.01068	3.04E-12	0.98932	4.67E-11
10	0.01063	2.41E-14	0.98937	3.70E-13
11	0.00038	4.85E-15	0.99962	2.96E-15
12	1.28E-05	9.30E-16	0.99999	2.27E-17
13	4.36E-07	1.77E-16	1	1.73E-19
14	1.47E-08	3.31E-17	1	1.33E-21

Table B.16 Pressure of the column 90kPa on condenser and boiler duty with (T=333.15K, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.02456	0.02456	0.1421	0.80877
2	0.00228	0.01818	0.96475	0.01479
3	0.00109	0.00872	0.98292	0.00727
4	0.00092	0.00673	0.98609	0.00626
5	0.00089	0.00631	0.98675	0.00606
6	0.01425	4.83E-06	0.98564	1.01E-04
7	0.01166	4.61E-08	0.98834	8.32E-07
8	0.01092	4.01E-10	0.98908	6.88E-09
9	0.01073	3.36E-12	0.98927	5.68E-11
10	0.01068	2.79E-14	0.98932	4.70E-13
11	0.00039	5.69E-15	0.99961	3.94E-15
12	1.39E-05	1.11E-15	0.99999	3.17E-17
13	4.88E-07	2.15E-16	1	2.55E-19
14	1.71E-08	4.09E-17	1	2.05E-21

Reflux ratio

Table B.17 Reflux ratio of 0.1 on condenser and boiler duty with (T=333.15K, P=32, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03161	0.03161	0.13506	0.80173
2	0.00181	0.01875	0.97085	0.00858
3	0.00145	0.01425	0.97737	0.00694
4	0.00142	0.01383	0.97792	0.00683
5	0.00142	0.0138	0.97796	0.00682
6	0.01822	1.14E-05	0.98165	1.17E-04
7	0.0144	7.49E-08	0.9856	6.79E-07
8	0.01315	4.58E-10	0.98685	3.92E-09
9	0.01279	2.69E-12	0.98721	2.26E-11
10	0.01269	1.56E-14	0.98731	1.31E-13
11	0.00035	2.85E-15	0.99965	7.49E-16
12	8.95E-06	4.78E-16	0.99999	3.98E-18
13	2.28E-07	7.98E-17	1	2.11E-20
14	5.79E-09	1.30E-17	1	1.12E-22

Table B.18 Reflux ratio of 0.2 on condenser and boiler duty with (T=333.15K, P=32, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03319	0.03319	0.13348	0.80015
2	0.00191	0.01984	0.96964	0.0086
3	0.00129	0.01252	0.98025	0.00594
4	0.00124	0.01156	0.98152	0.00569
5	0.00123	0.01144	0.98167	0.00566
6	0.01567	9.87E-06	0.98423	9.29E-05
7	0.01283	6.31E-08	0.98717	5.32E-07
8	0.01196	3.78E-10	0.98804	3.04E-09
9	0.01172	2.19E-12	0.98828	1.74E-11
10	0.01166	1.26E-14	0.98834	9.94E-14
11	0.00032	2.26E-15	0.99968	5.61E-16
12	8.03E-06	3.76E-16	0.99999	2.96E-18
13	2.03E-07	6.24E-17	1	1.56E-20
14	5.12E-09	1.01E-17	1	8.21E-23

Table B.19 Reflux ratio of 0.3 on condenser and boiler duty with (T=333.15K, P=32, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.0347	0.0347	0.13197	0.79864
2	0.00201	0.02089	0.96848	0.00862
3	0.00119	0.01147	0.9821	0.00524
4	0.0011	0.01006	0.98395	0.00489
5	0.00109	0.00985	0.98422	0.00484
6	0.0138	8.87E-06	0.98611	7.74E-05
7	0.01163	5.56E-08	0.98836	4.39E-07
8	0.011	3.27E-10	0.989	2.49E-09
9	0.01084	1.88E-12	0.98916	1.41E-11
10	0.01079	1.07E-14	0.98921	8.02E-14
11	0.00029	1.89E-15	0.99971	4.47E-16
12	7.29E-06	3.14E-16	0.99999	2.34E-18
13	1.83E-07	5.17E-17	1	1.23E-20
14	4.59E-09	8.31E-18	1	6.41E-23

Table B.20 Reflux ratio of 0.4 on condenser and boiler duty with (T=333.15K, P=32, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03615	0.03615	0.13052	0.79719
2	0.0021	0.02192	0.96734	0.00863
3	0.00111	0.01078	0.9834	0.00471
4	0.001	0.009	0.98572	0.00428
5	0.00099	0.00871	0.98608	0.00422
6	0.01238	8.18E-06	0.98754	6.67E-05
7	0.01068	5.04E-08	0.98932	3.75E-07
8	0.0102	2.93E-10	0.9898	2.11E-09
9	0.01009	1.67E-12	0.98991	1.19E-11
10	0.01006	9.47E-15	0.98994	6.75E-14
11	0.00027	1.65E-15	0.99973	3.72E-16
12	6.67E-06	2.72E-16	0.99999	1.94E-18
13	1.67E-07	4.46E-17	1	1.01E-20
14	4.15E-09	7.13E-18	1	5.23E-23

Table B.21 Reflux ratio of 0.6 on condenser and boiler duty with (T=333.15K, P=32, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03889	0.03889	0.12777	0.79444
2	0.00228	0.02392	0.96513	0.00867
3	0.00101	0.00995	0.98509	0.00396
4	0.00086	0.00759	0.98811	0.00344
5	0.00084	0.00719	0.98862	0.00336
6	0.01034	7.30E-06	0.9896	5.26E-05
7	0.00924	4.38E-08	0.99076	2.94E-07
8	0.00895	2.51E-10	0.99105	1.65E-09
9	0.00889	1.42E-12	0.99111	9.24E-12
10	0.00888	7.98E-15	0.99112	5.19E-14
11	0.00023	1.36E-15	0.99977	2.80E-16
12	5.70E-06	2.22E-16	0.99999	1.44E-18
13	1.41E-07	3.60E-17	1	7.41E-21
14	3.46E-09	5.70E-18	1	3.81E-23

Table B.22 Reflux ratio of 0.7 on condenser and boiler duty with (T=333.15K, P=32, reflux ratio=0.5 Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.0402	0.0402	0.12647	0.79313
2	0.00237	0.02488	0.96406	0.00869
3	0.00097	0.00969	0.98567	0.00367
4	0.00081	0.00709	0.98897	0.00313
5	0.00079	0.00665	0.98952	0.00304
6	0.00957	7.00E-06	0.99037	4.78E-05
7	0.00868	4.16E-08	0.99132	2.66E-07
8	0.00845	2.38E-10	0.99155	1.49E-09
9	0.0084	1.34E-12	0.9916	8.35E-12
10	0.00839	7.51E-15	0.99161	4.68E-14
11	0.00022	1.27E-15	0.99978	2.50E-16
12	5.31E-06	2.06E-16	0.99999	1.28E-18
13	1.30E-07	3.32E-17	1	6.56E-21
14	3.20E-09	5.25E-18	1	3.36E-23

Table B.23 Reactive zone of 12 stages from stage 2-13 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages,)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.00374	7.88E-07	2.85E-09	0.99626
2	0.02995	0.02995	0.13671	0.80338
3	0.02632	0.03034	0.3439	0.59944
4	0.02642	0.02884	0.38395	0.56078
5	0.02644	0.02859	0.39037	0.5546
6	0.40577	3.78E-05	0.58362	1.06E-02
7	0.37135	2.42E-07	0.62859	6.12E-05
8	0.36077	1.42E-09	0.63923	3.47E-07
9	0.35832	8.05E-12	0.64168	1.95E-09
10	0.35775	4.54E-14	0.64225	1.10E-11
11	0.01185	1.00E-14	0.98815	7.42E-14
12	2.97E-04	1.65E-15	0.9997	3.86E-16
13	7.37E-06	2.69E-16	0.99999	2.00E-18
14	1.82E-07	4.28E-17	1	1.03E-20

Table B.24 Reactive zone of 10 stages from stage 3-12 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages,)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03412	0.03412	0.13254	0.79921
2	0.00197	0.02049	0.96892	0.00861
3	0.00095	0.00925	0.98551	0.00429
4	0.00091	0.00801	0.98727	0.00381
5	0.00091	0.00784	0.98752	0.00373
6	0.01125	7.67E-06	0.98869	5.86E-05
7	0.0099	4.66E-08	0.9901	3.28E-07
8	0.00953	2.69E-10	0.99047	1.84E-09
9	0.00944	1.52E-12	0.99056	1.04E-11
10	0.00943	8.59E-15	0.99057	5.84E-14
11	0.00025	1.38E-15	0.99975	3.22E-16
12	6.14E-06	2.25E-16	0.99999	1.67E-18
13	1.53E-07	3.67E-17	1	8.61E-21
14	3.78E-09	5.84E-18	1	4.45E-23

Table B 25 Reactive zone of 8 stages from stage 4 to11 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03694	0.03694	0.12972	0.79639
2	0.00216	0.0225	0.9667	0.00864
3	0.00104	0.01011	0.98456	0.00429
4	0.00091	0.00806	0.98722	0.00381
5	0.00091	0.00785	0.98751	0.00374
6	0.01125	7.67E-06	0.98868	5.87E-05
7	0.0099	4.66E-08	0.9901	3.28E-07
8	0.00953	2.69E-10	0.99047	1.84E-09
9	0.00945	1.52E-12	0.99055	1.04E-11
10	0.00943	8.60E-15	0.99057	5.85E-14
11	0.00025	1.38E-15	0.99975	3.22E-16
12	6.14E-06	2.25E-16	0.99999	1.67E-18
13	1.53E-07	3.67E-17	1	8.62E-21
14	3.78E-09	5.84E-18	1	4.45E-23

Table B 26 Reactive zone of 4 stages from stage 6 to 9 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.16667	0.16667	1.55E-06	0.66667
2	0.03339	0.94914	0.00031	0.01716
3	0.01597	0.96995	0.00573	0.00835
4	0.01393	0.88856	0.08974	0.00777
5	0.0112	0.45512	0.52646	0.00722
6	0.00345	1.24E-03	0.99278	2.53E-03
7	0.01151	2.45E-06	0.98847	1.91E-05
8	0.01066	1.45E-08	0.98934	1.08E-07
9	0.01043	8.36E-11	0.98957	6.11E-10
10	0.01037	1.51E-11	0.98963	3.06E-12
11	0.00028	2.65E-12	0.99972	1.69E-14
12	6.93E-06	4.37E-13	0.99999	8.83E-17
13	1.74E-07	7.17E-14	1	4.60E-19
14	4.33E-09	1.15E-14	1	2.40E-21

Feed Location of feed

Table B 27 Feed location at 2 and 13 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages,)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.16666	0.16684	8.44E-06	0.66649
2	0.03335	0.94783	0.00168	0.01714
3	0.0109	0.92654	0.05772	0.00485
4	0.00544	0.4176	0.57359	0.00337
5	0.00291	0.00122	0.99365	0.00222
6	0.01103	2.28E-06	0.98896	1.73E-05
7	0.01053	1.33E-08	0.98947	9.79E-08
8	0.01039	7.59E-11	0.98961	5.54E-10
9	0.01036	4.31E-13	0.98964	3.14E-12
10	0.01035	2.44E-15	0.98965	1.78E-14
11	0.01035	4.40E-16	0.98965	8.89E-17
12	1.03E-02	7.93E-17	0.98965	4.44E-19
13	1.03E-02	1.42E-17	0.98965	2.22E-21
14	2.74E-04	2.39E-18	0.99973	1.23E-23

Table B 28 Feed location at 5 and 10 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages,)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	1.29E-01	0.79579
2	0.00219	0.02293	0.96623	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.01125	7.68E-06	0.98868	5.87E-05
7	0.0099	4.66E-08	0.9901	3.29E-07
8	0.00953	2.69E-10	0.99047	1.85E-09
9	0.00945	1.53E-12	0.99055	1.04E-11
10	0.00943	8.60E-15	0.99057	5.85E-14
11	0.00025	1.49E-15	0.99975	3.19E-16
12	6.14E-06	2.43E-16	0.99999	1.65E-18
13	1.53E-07	3.96E-17	1	8.53E-21
14	3.78E-09	6.31E-18	1	4.41E-23

Table B 29 Feed location at 4 and 9 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.16664	0.16664	2.84E-05	0.6667
2	0.03331	0.94391	0.00562	0.01716
3	0.01553	0.88661	0.08948	0.00838
4	0.01131	0.45548	0.52594	0.00727
5	0.00346	0.00124	0.99277	0.00253
6	0.01151	2.45E-06	0.98847	1.92E-05
7	0.01066	1.46E-08	0.98934	1.08E-07
8	0.01042	8.36E-11	0.98958	6.12E-10
9	0.01037	4.76E-13	0.98963	3.46E-12
10	0.00028	7.46E-14	0.99972	1.95E-14
11	6.92E-06	1.23E-14	0.99999	1.02E-16
12	1.74E-07	2.03E-15	1	5.30E-19
13	4.35E-09	3.33E-16	1	1.70E-21
14	1.08E-10	5.35E-17	1	1.24E-23

Table A 30 Feed location both at 6 on condenser and boiler duty with (T=333.15K, reflux P=32kpa, Distillate to feed ratio=0.6, reactive zone 6 stages)

Stage	2-ETH-01	N-DOD-01	2EHD	WATER
1	0.03754	0.03754	1.29E-01	0.79579
2	0.0022	0.02293	0.96622	0.00865
3	0.00106	0.0103	0.98435	0.00429
4	0.00093	0.0082	0.98706	0.00381
5	0.00091	0.00786	0.9875	0.00374
6	0.00091	7.82E-03	0.98755	3.73E-03
7	1.76E-05	1.38E-03	0.99858	2.29E-05
8	4.96E-07	2.26E-04	0.99977	1.07E-07
9	1.28E-08	3.70E-05	0.99996	4.52E-10
10	3.21E-10	6.05E-06	0.99999	1.85E-12
11	7.97E-12	9.90E-07	1	9.58E-15
12	1.98E-13	1.62E-07	1	4.95E-17
13	4.92E-15	2.63E-08	1	2.56E-19
14	1.22E-16	4.19E-09	1	1.32E-21