SIMULATION OF REACTIVE DISTILLATION COLUMN FOR n-BUTYL ACRYLATE PRODUCTION FROM DILUTE ACRYLIC ACID

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JESSLYN TAN KIM EAN

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SUPERVISOR'S DECLARATION

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

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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 and is not concurrently submitted for award of other degree.

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Dedication

To my loving and supportive parents and sister who have been encouraging me to move forward in completing my undergraduate research project, and also to my supervisor and co-supervisor, Dr. Ramesh Kanthasamy and Dr. Chin Sim Yee who taught me so much on simulation throughout the course of this project.

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ABSTRACT

The recovery of dilute acrylic acid from the wastewater stream during the production of acrylic esters in the industries has gained a significant amount of attention due to its economic and environment issues. The amounts of acrylic acid which are usually found to contain in the wastewater stream range from 4-10 % w/w. The most frequent used method to treat wastewater containing acrylic acid is by incineration which is neither economically feasible nor environment friendly. One of the promising methods is recovery of acrylic acid from wastewater through esterification. Acrylic acid could be converted to acrylic ester while wastewater could be purified. To date, study about esterification by using diluted acrylic acid has not been reported in the literature.

In this present work, a simulation study on the direct utilization of dilute acrylic acid in the production of n-butyl acrylate via esterification with n-butanol in a reactive distillation column was presented. The reaction is heterogeneously catalyzed by ion exchanged resin (Amberlyst-46). A pseudo-homogeneous kinetic model was used to describe the reaction kinetics. An equilibrium stage model was applied and the proposed model was validated with experimental data from past research study. The validated model was then used to study effect of various parameters like acrylic acid concentration, catalyst loading, reboiler duty, reflux ratio, number of trays in reactive section and number of trays in separation section. From this study, it can be seen that the best operating conditions in recovering 4% w/w acrylic acid from the wastewater stream were with a catalyst loading of 0.105 kg/m, reboiler duty of 283.133 kJ/hr, reflux ratio of 1.0 and finally with 7 trays in the reactive section and 2 trays in the rectifying and stripping section respectively. With these operating conditions, 95.245 % of AA managed to be converted into BA. The findings have proven the feasibility of the acrylic acid recovery via esterification in reactive distillation column and it serves as the groundwork for the detailed column design and experimental study in the future.

ABSTRAK

Pemulihan asid akrilik cair dari aliram air sisa semasa pengeluaran ester akrilik dalam industry telah mendapat sejumlah besar perhatian kerana isu-isu ekonomi dan alam sekitar. Jumlah asid akrilik yang biasanya didapati di dalam aliran air sisa adalah dalam lingkungan 4-10 % w/w. Kaedah yang paling kerap digunakan untuk merawat air sisa yang mengandungi asid akrilik adalah dengan kaedah pembakaran yang tidak digalakkan disebabkan oleh isu-isu ekonomi dan alam sekitar. Oleh itu, salah satu kaedah yang digalakkan untuk pemulihan asid akrilik daripada air sisa adalah melalui pengesteran.Asid akrilik boleh ditukar kepada ester akrilik manakala air sisa boleh disucikan.Setakat ini, kajian mengenai pengesteran dengan meggunakan asid akrilik dicairkan tidak pernah dilaporkan dalam kesusasteraan.

Bagi karya semasa, kajian simulasi kepada penggunaan secara langsung asid akrilik yang telah dicairkan dalam pengeluaran n-butil akrilat melalui pengesteran dengan n-butanol dalam kolum penyulingan reaktif telah dibentangkan. Selain itu, tindak balas adalah heterogen dimangkinkan oleh ion pertukaran resin (Amberlyst-46). Model kinetic berdasarkan kaedah Langmuir-Hinshelwood-Hougen-Watson (LHHW) telah diperolehi dan pemalar kinetic pendekatan ini dan model pseudohomogeneous telah digunakan. Satu model peringkat keseimbangan telah digunakan dan model yang dicadangkan telah disahkan dengan data eksperimen daripada kajian penyelidikan yang lepas.Selanjut itu, model yang telah disahkan digunakan untuk mengkaji kesan pelbagai parameter seperti kepekatan asid akrilik, pemangkin muatan, tugas pengulang didih, nisbah refluks, bilangan dulang dalam seksyen reaktif dan bilangan dulang dalam seksyen pemisahan. Daripada kajian ini, ia boleh dilihat bahawa keadaan operasi terbaik dalam memulihkan 4 % w/w asid akrilik dari aliran air sisa adalah dengan beban mangkin 0.105 kg/m, duti pengulang didih daripada 283.133 kJ/ jam, nisbah refluks 1.0 dan akhirnya dengan 7 dulang di bahagian reaktif and 2 dulang di bahagian membetulkan dan pelucutan masing-masing. Dengan keadaan operasi ini, 95.245 % AA berjaya ditukar menjadi BA. Hasil kajian ini telah membuktikan kebolehlaksanaan pemulihan asid akrilik melalui pengesteran dalam ruangan penyulingan reaktif dan ia berfungsi sebagai asas untuk reka bentuk ruang terperinci dan kajian eksperimen pada masa hadapan.

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SYMBOL	**DEFINITION**
a_i	activity of component *i* (mol/mol)
C_{act}	concentration of active sites (mol/kg^3)
C_i	concentration of component *i* (kmol/L)
E_a	activation energy (J/mol)
γ	activity coefficient
K_a	activity-based kinetic constant
k	rate constant for pseudo homogeneous model
k_o	pre-exponential factor in Arrhenius equation
K_{eq}	equilibrium constant
$m_{cat,dry}$	mass of dry catalyst per meter packing height (kg/m)
$\dot{n}_i$	mole flow rate of flow *i* (kg/hr)
R	ideal gas constant (J/ (mol K))
r_i	reaction rate of component *i* (mol/s)
T	temperature (K)
v_i	stoichiometric coefficient

LIST OF ABBREVIATION

AA	acrylic acid
BuOH	n-butanol
BA	n-butyl acrylate
CSTR	continuous stirred-tank reactor
EQ	equilibrium model
ER	Eley-Rideal
HETP	height equivalent of a theoretical plate
H_2O	water
LH	Langmuir-Hinshelwood
LHHW	Langmuir-Hinshelwood-Hougen-Watson
LLE	liquid-liquid equilibrium
MTBE	methyl tertiary butyl ether
NEQ	non-equilibrium model
NRTL	non-random two-liquid model
PH	pseudo homogeneous model
RD	reactive distillation
RDC	reactive distillation column
RR	reflux ratio
SAT	super absorbent polymer
UNIFAC	UNIQUAC Functional-group Activity Coefficient model
UNIQUAC	UNIversal QUAsiChemical model
VLE	vapour-liquid equilibrium
WAO	wet air oxidation

1 INTRODUCTION

1.1 *Background of study and motivation*

Acrylic acid (AA) and its derivatives as the basic building block in the chemical synthesis process have received overwhelming demands for the last few years (Bell, 2003). This in turn has caused the overall production of AA to rise from 3.4 million tons per year to 4.7 million tons per year from year 2003 until 2006 (Glauser *et al.,* 2007). It was reported that the global capacity demand of AA for second quarter of 2011 reached 5.32 million ton per year to cater the demand from United States, Europe, Japan and China. AA is mainly used for producing super absorbent polymer (SAT) which mainly used in baby diapers, adult protective underwear and sanitary napkins (ResearchInChina, 2012; IHS Inc., 2011).

One of the important derivatives of AA is n-Butyl Acrylate (BA), which values at about 30% of the global demand of AA according to Nexant Inc. (2006). It is widely used in the industry as a precursor for varnishes, adhesives and finishes of textiles and papers (Zeng *et al.,* 2006; Altiokka and Ödeş, 2009). Other derivatives of AA and its applications are shown in Table 1.1.

AA possesses harmful properties which could lead to health complication in living species. According to the Dow Chemical Company (2010), AA is corrosive and toxic if absorbed through the skin or inhaled. It is a strong irritant to the skins, eyes and mucous membranes in humans. Possible blindness may occur if its liquids were splashed into eyes. In a typical AA production plant, the wastewater contains 4-10% w/w of AA (Kumar *et al.,* 2010). Some other toxicant of AA family besides AA such as acrylonitrile and acetonitrile are also present in the wastewater stream which is mostly being incinerated due to its high chemical oxygen demand and total organic content. This method suffers from several drawbacks because it is neither economic feasible nor environmental friendly.

Table 1.1: Derivatives of AA and its applications (BASF> Products & Industries> Product finder > acrylic acid, 2013).

Acrylate Ester	Application
Allyl Methacrylate	Mainly used for hydrosilylation of Acrylics and as a cross linking monomer.
Butyl Acrylate	As a building block for homo- and copolymers.
Tert-Butyl Acrylate	Used in several applications, e.g. coatings, adhesives, personal care and plastics.
Tert-Butyl Methacrylate	As a co-monomer in resins for low VOC clear coats, e.g. in car refinish applications.
Tert-ButylaminoethylMethacry	Used for cationic polymers. Main application is in personal care and hair care products.
Ethyl Acrylate	Used as a building block for homo- and copolymers.
2-Ethylhexyl Acrylate	Used as a building block for homo- and copolymers.
2-Hydroxyethyl Acrylate	Used in acrylics for coatings, adhesives and UV reactive oligomers, cross linking with isocyantes or melamines.
Isobutyl Acrylate	Used in coatings, adhesives and PE plastics.
Lauryl Acrylate	Used in coatings, adhesives, plastics and textile applications.

Until today, several treatment methods have been explored which include adsorption through activated carbon, biological and wet air oxidation (Kumar *et al.*, 2010; Lin *et al.*, 1996). This also includes the conventional physical separation methods such as azeotropic distillation, simple distillation and liquid-liquid extraction (Saha *et al.*, 2000). However, these methods present some downfalls whereby adsorption is only practical for low concentration of AA, long retention time is needed for biological treatment and wet air oxidation requires high energy consumption which leads to high operating cost. In view of this, alternative methods of recovering AA have been explored. Recovery of AA from the dilute aqueous wastewater stream through esterification process in a reactive distillation column (RDC) has been identified as a potential important solution (Arpornwichanop *et al.*, 2008). This method would be favour as higher valued esters can be produced through the recovery of dilute AA in a

RDC which in turn would overcome the economic and environmental issue (Taylor and Krishna, 2000).

1.2 Statement of problem

Esterification of AA with alcohols is an equilibrium limited reaction catalyzed by acidic catalyst. To date, RDC is one of the best known examples of process intensification particularly for the equilibrium limited reaction. In an RDC, both the chemical reaction and separation by distillation is combined in one unit operation which is able to drive the reaction to the product site due to *in situ* separation of products (Taylor and Krishna, 2000). RDC has shown its potential for capital productivity improvements, selectivity improvements, reduced energy use and the reduction or elimination of solvents in the process (Malone and Doherty, 2000). Thus, it decreases the amount of equipment required which in turn will results in the reduction in terms of operating cost and investment. As a result, the combination of reaction and separation by distillation assist in overcoming limitations of both operations, such as azeotropes or reaction equilibria.

Currently, the production of acrylate ester is catalyzed by homogeneous catalyst such as sulphuric acid, hydrofluoric acid and para-toluenesulfonic acid (Altiokka and Çitak, 2003). The reaction is carried out in two reactors while the separation of acrylate ester and the recovery of the reactants require a train of three distillation columns after the reactors (Bell, 2003).

However, there are several drawbacks for the homogeneous catalysis system. According to Altiokka and Çitak (2003), homogeneous catalyst is toxic and corrosive towards the environment, it is hard to be removed from the reaction mixture and it causes the purity of the products to be lower compare to heterogeneous catalyst. Since then, heterogeneous catalyst such as solid acid ion exchange resin, zeolite, metal oxides and enzymes has been developed to be applied in the esterification process as solid acid is less toxic towards the environment and it facilitates the recovery and recycling of catalysts (Altiokka and Çitak, 2003; Okuhara *et al.*, 1998; Marchetti and Errazu, 2008; Kiss *et al.*, 2008).

Experimental investigations on the reaction kinetics and the chemical equilibrium of the heterogeneously catalyzed esterification of AA and n-butanol

(BuOH) were investigated in the previous work (Schwarzer and Hoffmann, 2002). To the best of our knowledge, RDC is not practiced for the recovery of AA from diluted aqueous wastewater and only a few publications on the production of BA in a RDC can be found in the literature (Niesbach *et al.*, 2012; Niesbach *et al.*, 2013).

In the present study, AA will be recovered by esterification of wastewater containing AA with BuOH catalyzed by heterogeneous catalyst, ion-exchange resin in a RDC. Since the presence of water in the reactant could reduce the equilibrium conversion due to the shift of reaction equilibrium to the reactant side, efficiency of the AA recovery will be examined in a reactive distillation column (RDC) through simulation study.

1.3 Objectives

This study aims to examine the efficiency of recovering AA from the wastewater containing AA. The effects of important operating parameters for the esterification of diluted AA with Butanol (BuOH) in RDC are investigated.

1.4 Scope of study

In this research, the suitable RDC models (equilibrium or non-equilibrium model), thermodynamics models (UNIFAC, UNIQUAC or NRTL) and reaction kinetics (Langmuir-Hinshelwood-Hougen-Watson, Eley-Rideal or pseudo-homogeneous) were screened before it is employed for the simulation studies. The verification for the simulation on the RDC was carried out by comparing with pilot scale data from past research. Several operating parameters such as acrylic acid concentration, catalyst loading, reflux ratio, reboiler duty and column configuration were varied during the simulation using the validated model.

1.5 Organisation of thesis

This thesis consists of 5 chapters. Chapter 1 (Introduction) provides a description on the application of acrylic acid (AA) and its derivatives in the chemical industries and the effect of its harmful properties. The conventional methods of recovering AA from the dilute aqueous wastewater are briefly described. This chapter includes the problem statements which lead to the identification of the objectives and scopes for the present study. Finally, the organization of thesis is presented.

Chapter 2 (Literature review) describes in details the conventional methods which have been applied in the recovery of AA from wastewater. Besides that, different types of esterification process and catalysts that have been investigated by past researches are also review in this chapter. Information concerning with the implementation of reactive distillation technology for the production of different types of carboxylic acid esters which were review from past researches have also lead to the consideration of catalysts, thermodynamics, modelling and simulation for the reactive distillation(RD) implementation for the current study.

The modelling and simulation procedure is illustrated in detail in Chapter 3 (Methodology). It gives a review on the procedures involved during the simulation of RDC using ASPEN PLUS V7.0 software. The selection of the suitable RD model, thermodynamics model and kinetics model are also being described in this chapter.

Chapter 4 (Results and discussion) is devoted to the simulation results obtained and discussion of the present study. Validation of the RD model for this present study is carried out by comparing with experimental results from past research papers which can be found in the literature. Besides that, the suitable ranges of operating parameters for the recovery of AA in RDC are also being determined after the model has been validated.

Chapter 5 (Conclusion and recommendation) focuses on the conclusion that can be made by the end of the study after analysis the simulation results. The best operating conditions for the recovery of dilute AA in RDC are also presented in this chapter. Lastly, several recommendations are presented in this chapter in order to be considered in future studies.

2 LITERATURE REVIEW

2.1 Overview

This chapter reviewed on the available technology in recovering carboxylic acid from diluted aqueous wastewater streams in today's world. It also describes the recovery of carboxylic acid through esterification process which has been carried out in RDC by past researchers. Besides that, the different types of process which have been investigated through RDC and hardware selections in modelling RDC are also being reviewed in the later parts of this chapter. Finally, a review on the types of RD, thermodynamic and kinetic models which have been investigated in the past for the modelling and simulation of RDC is presented in the final part of this chapter.

2.2 Introduction

Acrylic Acid (AA) is very toxic to living species and it appears as an unsaturated organic acid. During the manufacture of acrylic esters, acrylic acid is being released to the environment. It have been reported that in a typical AA plant, the concentration of AA range from 10-20 g/l in the wastewater stream (Kumar *et al.,* 2008). Thus, the recovery of dilute acrylic acid from the wastewater stream has become very important due to its economical and environmental awareness.

2.3 Wastewater treatment technology for carboxylic acid recovery

According to Cheremisinoff (2002, p.1), wastewater treatment technology can be divided into three areas: Physical Methods, Chemical Methods and Energy Intensive Methods. Physical methods for wastewater treatment are mainly represented by solid-liquid separation techniques. Filtration plays an important role in solid-liquid separation techniques as it is an integral component of wastewater treatment application. In understanding the role of filtration, it is important to make distinctions not only with other technologies applied in the purification of industrial water, but also includes the objectives of different unit processes.

Besides that, chemical methods for wastewater treatment depend upon the chemical reaction of the contaminants to be recovered from the water. It is applied as a stand-alone technologies as well as an integral part of the treatment process with physical methods.

Moreover, as for energy intensive technologies, the thermal methods have gained much attention due to its dual role in wastewater treatment applications. They can be utilized as a mean of sterilization or utilized to the processing of solid wastes or sludge. In the latter cases, thermal methods can also be applied to sterilize sludge contaminated with organic contaminants.

Several methods have been explored in recovering carboxylic acids from wastewater. In the past, the conventional method includes adsorption through activated carbon (Kumar *et al.,* 2010) and distillation and extraction (Arpornwichanop *et al.,* 2008). However, distillation approach requires high energy usage in vaporizing the water present whereas, extraction is limited by the phase separation and distribution of the component (Saha *et al.,* 2000). As for adsorption through activated carbon, it only deals with chemical wastewater with a low concentration of organic compounds (Kumar *et al.*, 2010). Wet air oxidation (WAO) treatment has also been explored as an alternative method. Due to the high energy consumption which leads to high operation cost, this method is not being favoured (Lin *et al.*, 1996).

Thus, reactive distillation has been introduced as a method in recovering acrylic acid from its dilute aqueous solution. It applies the concept of using the recovered acrylic acid as the reactant for esterification. According to Arpornwichanop *et al.* (2008), this approach is able to produce a higher valued ester, which could save raw material cost and environment issues. Table 2.1 shows the several methods for the recovery of carboxylic acids that have been investigated by past investigators.

Table 2.1: Methods which have been applied for the recovery of carboxylic acids.

Method	**Reference**	**Remarks**
Adsorption through activated carbon	Kumar *et al.* (2010)	Deals only with low concentration of organic compounds (50-500 mg/l) due to long residence time.

Method	**Reference**	**Remarks**
Distillation	Saha *et al.* (2000); Arpronwichanop *et al.* (2008)	Unable to achieve high conversion due to esterification process is reactive equilibrium limited.
Extraction	Saha *et al.* (2000); Arpronwichanop *et al.* (2008)	Unable to achieve high conversion due to esterification process is reactive equilibrium limited.
Wet air oxidation (WAO)	Lin *et al.* (1996)	High temperature of 250 ^{o}C to maintain the pressure inside the reactor. This will cause high energy consumption to occur.
Esterification process by RDC	Arpornwichanop *et al.* (2008)	Able to achieve a conversion of around 95% with 35 % w/w acetic acid.

2.4 General esterification system

Esterification process involves the reaction between a carboxylic acids and alcohols in the present of acid catalysts. The chemical structures of carboxylic acids, alcohols and the acid catalysts affect the rate of reaction. Esters have distinct fruit like smell which have led to the use in artificial flavouring and fragrances. Esterification is a reversible process where the reactions are equilibrium reactions and thus, is required to be driven to completion according to Le Chatelier's principle.

It is known that the esterification of acetic acid with different types of alcohols have been studied by several researches in the past. This goes the same for the esterification of acrylic acid with different alcohols. The aim of this several investigators was to determine the kinetic model of each of the esterification process for the reaction of different alcohols with acetic acid and acrylic acid in the present of homogeneous and heterogeneous catalysts. Some examples of esterification process which can be found in past literature are given in Table 2.2 below.

Table 2.2: Summary of esterification process that have been studied by past researchers.

Reactants	**Products**	**Type of catalyst used**	**Reference**
Acetic acid + isobutanol	isobutyl acetate + Water	Amberlyst IR-120 (Heterogeneous catalyst)	Altiokka and Çitak (2003)
Acrylic acid + 2-ethylhexan-1-ol	2-ethylhexyl acrylate + Water	Amberlyst-70 (Heterogeneous catalyst)	Komoń *et al.* (2013)
Acrylic acid + propylene glycol	Propylene glycol acrylate + Water	Amberlyst-15 (Heterogeneous catalyst)	Altiokka and Ödeş (2009)
Acetic acid + Butanol	Butyl acrylate + Water	Sulfuric acid (Homogeneous catalyst)	Leyes and Othmer (1945)
		Amberlyst-15 (Heterogeneous catalyst)	Gangadwala *et al.* (2003)
Acetic acid + 1-octanol	1-octyl acetate + Water	Amberlyst-36 (Heterogeneous catalyst)	Akyalçin and Altiokka (2012)
Acetic acid + propanol	Propyl acetate + Water	Dowx 50Wx8-400 (Heterogeneous catalyst) Amberlite IR-120 (Heterogeneous catalyst) Amberlyst-15 (Heterogeneous catalyst)	Ali and Merchant (2006)
Acetic acid + Methanol	Methyl acetate + Water	Acetic acid (Homogeneous catalyst)	Pöpken *et al.* (2000)

Reactants	Products	Type of catalyst used	Reference
Acetic acid + Methanol	Methyl acetate + Water	Amberlyst-15 (Heterogeneous catalyst)	Pöpken *et al.* (2000)

2.5 Esterification reaction to recover carboxylic acid from wastewater

According to Arpornwichanop *et al.* (2008), esterification reaction can be applied to recover carboxylic acid from wastewater by in cooperating with RDC. Through RD, the recovered carboxylic acid will be used as a reactant for the esterification process which in turn will produce a higher valued ester, save raw material cost and environmental issues concerning with the present of carboxylic acid in wastewater can be overcome. Some esterification reaction which has been applied for the recovery of carboxylic acid is shown in Table 2.3 below. Based on the table below, it can be seen that only the recovery of acetic acid through RDC has been studied by past researches up till now. Generally, it can be summarized that the overall conversion of acetic acid with different degree of dilution into acetate esters range from 67- 95 %.

Table 2.3: Summary of esterification reaction which have been applied in recovery of carboxylic acid through RDC.

Reactants	Products	Type of catalyst used	Remarks	Reference
Acetic acid + n-butanol	n-butyl acetate + Water	Amberlyst-15 (Heterogeneous catalyst)	35 % w/w Acetic acid	Arpornwichanop *et al.* (2008)
		-	30 % w/w Acetic acid	Gangadwala *et al.* (2007)
Acetic acid + 2-ethyl-1-hexanol	2-ethylhexyl acetate + Water	Amberlyst-15 (Heterogeneous catalyst)	6-15 % w/w Acetic acid	Ragaini *et al.* (2007)

Reactants	**Products**	**Type of catalyst used**	**Remarks**	**Reference**
Trifluoroacetic acid + 2-propanol	2-propyl trifluoroacetate + Water	Ion exchange resin, T-63 (Heterogeneous catalyst)	10 % w/w Trifluoroacetic acid	Mahajan *et al.* (2008)
Acetic acid + ethanol	Ethyl acetate + Water	Polystyrene-supported sulfonic acid (Heterogeneous acid)	50 % w/w Acetic acid	Yagyu *et al.* (2013)

2.6 Catalyst in esterification

2.6.1 Introduction

Basically, catalyst can be divided into homogeneous or heterogeneous. This is also applicable for reactive distillation column.

In the term of chemistry, homogeneous catalysis occurs when the catalyst is in the same phase (solid, liquid or gas) as the reactants. Homogeneous catalysis on the other hand is likely to be influenced by the changing of concentration to enhance or lower the reaction velocity (Sundmacher and Kienle, 2003, p.48). Enzymes are homogeneous catalysts which are also known as biocatalysts.

Meanwhile, heterogeneous catalysts which are practically used in the industry are in the form of solids. According to Altiokka and Çitak (2003), heterogeneous catalyst is more advantages compare to homogeneous catalyst. Heterogeneous catalyst is able to eliminate corrosive environment, can be easily remove from the reaction mixture by decantation or filtration and lastly, the purity of the products is higher compare to homogeneous catalyst since the side reactions can be completely eliminated or are less significant. Examples of heterogeneous catalysts used for esterification reaction in the recovery of carboxylic acid from wastewater are Amberlyst-15 (Arpornwichanop *et al.,* 2008; Ragaini *et al.,* 2007) and Indion 130 (Saha *et al.,* 2000).

2.6.2 Homogeneous

Strong mineral acids, such as H_2SO_4, HCl and HI, and also strong organic acids, such as HCOOH are some types of homogeneous catalysts which are being applied for the esterification of carboxylic acid (Lilja *et al.,* 2002). During the esterification reaction involving homogeneous catalyst, the slow step of the reaction involves the nucleophilic attack of the alcohol on the protonated carbonyl group of carboxylic group. According to Liu *et al.* (2006), the mechanisms route can be describe as follows:

- Firstly, protonation of the carboxylic acid takes place.
- Then, reaction with nonprotonated alcohol to yield a tetrahedral intermediate is activated.
- Finally, by decomposition, it produces the products of reaction which are ester and water.

However, there are some drawbacks towards homogeneous catalyst. According to Lilja *et al.* (2002), the miscibility of homogeneous catalyst with the reaction medium will cause difficulty in the separation between the products and reactants. Furthermore, the present of higher catalyst concentration will cause corrosion of the equipment to occur.

Even though due to the disadvantages of homogeneous catalyst which have been stated above, there are still studies being carried out by researchers on the esterification process by applying homogeneous catalyst. Lilja *et al.* (2002) have studied the esterfication of acetic, propanoic and pentanoic acid with methanol, ethanol, 1-propanol, 2-propanol, butanol and 2-butanol in the present of liquid HCl whereas Liu *et al.* (2006) have studied the esterification of acetic acid with methanol in the present of H_2SO_4.

2.6.3 Heterogeneous

Heterogeneous catalyst can be divided into three categories: solid ion exchange resins, zeolite and enzymes. According to Komoń *et al.* (2013), there are two main classes of sulfonated ion exchange resins which are popular in the industry: one is based on polystyrene/divinylbenzene matrix which includes Amberlyst and Dowex type resins and the other is based on perfluorinated sulfonic acid resins like Nafion and Aciplex.

On the other hand, as for zeolite type heterogeneous catalyst, H-ZSM-5 and NaY and VOx over USY have been stated in past literatures (Okuhara *et al.,* 1998;

Marchetti and Errazu, 2008). The NaY over USY is a base catalyst whereas the VOx over USY is an acid catalyst. Lipozyme CALB and Lipozyme T.L 100L from Novozymes are some example of enzyme based heterogeneous catalysts which have been studied by Marchetti and Errazu (2008).

Examples of heterogeneous catalysts which have been used for esterification reaction are as follows:

- Esterfication of acetic, propanoic and pentanoic acid with methanol, ethanol, 1-propanol, 2-propanol, butanol and 2-butanol in the present of fibrous polymer-supported sulphonic acid catalyst, Smopex-101 (Lilja *et al.*, 2002).
- Esterification of acetic acid with methanol on the present of Nafion/silica nanocomposite catalyst (SAC-13) (Liu *et al.*, 2006).
- Esterification of propanoic acid with n-butanol in the present of solid acid $Cs_{2.5}H_{0.5}PW_{12}O_{40}$ in the present of excess water (Okuhara *et al.*, 1998).

2.7 Reactive distillation technology

2.7.1 Introduction

Instead of carrying out the reaction and separation process separately, it is possible to combine these operations into a single unit operation. This is called reactive distillation or catalytic distillation (Luyben and Yu, 2008, p. xvii). Reactive distillation is an excellent example of process intensification which is able to provide an economically and environmentally attractive alternative to conventional multiunit flow sheets in some systems. RDC consists of a reactive section in the middle with non-reactive rectifying and stripping sections at the top and bottom of the RDC. In the reactive column, the products are separated *in situ*, which drives the equilibrium to the product side and thus, preventing any undesired side reactions between the reactants and product which could hinders the achievements of a high conversion (Taylor and Krishna, 2000; Luyben and Yu, 2008, p.2). Figure 2.1 below shows the conventional method and the RD method of carrying out a chemical process.

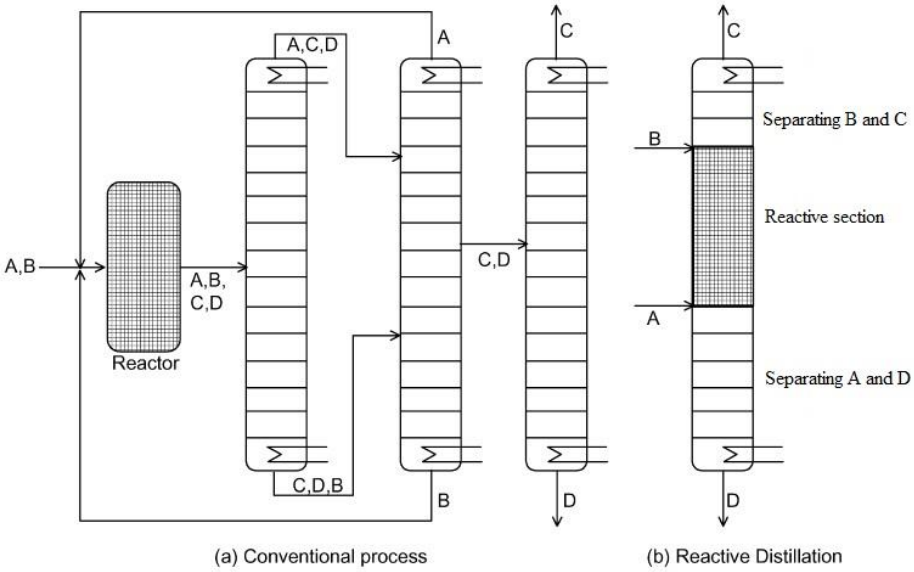


Figure 2.1: a) A conventional process consisting of a reactor followed by three distillation column for a reaction sequence A + B ↔ C + D. b) The reactive distillation configuration where the reactive sections in a) and b) are indicated by grid lines (Stichlmair and Frey, 1999).

Industrial reactive distillation comprises of homogeneous and heterogeneous catalyst and irreversible and reversible reactions. Some application processes of reactive distillation that have been used in the industries are esterification, etherification, hydrolysis, dehydration and alkylation (Harmsen, 2007).

For many decades, a small number of industrial applications of reactive distillation have been seen. The most important industrial application which has gained much attention was the production of methyl tertiary butyl ether (MTBE). Moreover, about two decades ago, engineers at Eastman Chemical published a very inspiring paper which has cause reactive distillation to gain so much interest in both industry and academia (Agreda *et al.*, 1990). The Eastman single RD column managed to keep the concentration of methyl acetate low in liquid form where reversible reaction is occurring. Therefore, the reaction is driven to the product side where high conversion can be achieved. Table 2.4 gives a comprehensive insight of different types of reactions which has been investigated as candidates for RD column.

Table 2.4: Important industrial process investigated in RDC

Reactants	**Products**	**Catalyst used**	**Reference**
Acetalization			
Methanol + Aqueous formaldehyde	Methylal + Water	Ion exchange resin, Indion 130	Kolah *et al.* (1996)
Ethanol + Aqueous formaldehyde	Ethylal + Water	Ion exchange resin, Indion 130	Chopade and Sharma (1997)
Propylene glycol + acetaldehyde	Acetal + Water	Amberlyst-15	Dhale *et al.* (2004)
Hydration			
Cyclohexane + Water	Cyclohexanol	SiO_2/Ga_2O_3	Khaledi and Bishnoi (2006)
Ethylene oxide + Water	Ethylene glycol	Cationic/anionic exchange resins	Liu *et al.* (2002)
Isoamylene + Water	*Tert*-amyl alcohol	Amberlyst-15	Gonzalez *et al.* (1997)
Isobutene + Water	*Tert*-butanol	Cationic exchange resin	Reusch *et al.* (2006)
Propylene + Water	Isopropanol	Cationic exchange resin	Sakuth and Peters (1998)
Alkylation			
Benzene + Ethylene	Ethyl benzene	Zeolite-β	Pohl (2006)
Benzene + Propylene	Cumene	Union Carbide-LZY-82	Pohl (2006)
Isobutane + Propylene/Butylene	Highly branched paraffins	Lewis acid promoted inorganic oxide catalyst	Huss and Kennedy (1990)
Hydrogenation/Dehydrogenation			
α-methyl styrene + Hydrogen	Cumene	Palladium oxide supported on alumina, carbon or silica	Hildreth and Wyckoff (1999)

Reactants	Products	Catalyst used	Reference
Benzene + Hydrogen	Cyclohexane	Alumina supported Ni catalyst	Gildert (2001)
Isophorone + Hydrogen	Trimethylcyclohexanol	-	Schmitt (1996)
Mesityl oxide + Hydrogen	Methyl isobutyl ketone (MIBK)	Bifunctional catalyst: cation exchange resin with palladium/nickel	Vandersall and Weinand (2005)
Isopropanol	Acetone + Hydrogen	-	Chung *et al.* (1997)
Etherification			
Methanol + Isobutene	Methyl *tert* butyl ether	Amberlyst-15	Ryu and Gelbein (2002)
Methanol + Isoamylene	*Tert*-amyl methyl ether	Ion exchange resin	Kolodziej *et al.* (2004)
Esterification			
30 % w/w Acetic acid + n-Butanol	n-Butyl acetate + Water	Indion 130	Saha *et al.* (2000)
10 % w/w Trifluoroacetic acid + 2-propanol	2-propyl trifluoroacetate + Water	Ion exchange resin, T-63	Mahajan *et al.* (2008)
Palmitic acid + Isopropanol	Isopropyl palmitate + Water	Zinc acetate supported silica gel catalyst	Bhatia *et al.* (2007)

On the other hand, besides its role as a reactor and distillation, RDC can function as an efficient separator to enhance the recovery rate and further purify the chemicals. Reaction such as etherification and esterification are suitable to be used in the RDC. Theoretically, the recovery of acrylic acid through esterification process by RDC as proposed in this study can be fully understands. Furthermore, due to the *in situ* separation of products, the component to be removed is allowed to react in the RDC and the resultant product can be separated simultaneously which in turn will decrease the operational cost and also overcome environmental issues.

2.7.2 Advantages of RDC

According to Taylor and Krishna, (2000), RDC has several discrete advantages. The most important advantage is seen when comes to dealing with equilibrium limited reaction as in esterification reaction. RDC is able to overcome the conversion limitation by the continuous removal of products from the reactive zone. Apart from the increased in conversion, some other advantages are as follows:

- Through RDC, significant capital savings can be achieved as the separation and reactive process is combined into one unit.
- The catalytic requirement for a RDC is significantly reduced. This is due to the use of a solid catalyst which is able to degrade more slowly compared to a homogeneous catalyst.
- RDC also improved the selectivity. This is due to the *in situ* separation of the products where the reaction is being driven to the product site.
- If RDC is carried out in an exothermic reaction, the heat of reaction can be recycled to provide the heat of vaporization which in turn will reduce the reboiler duty.
- As for the production of n-butyl arcylate being studied here, azeotropic mixture is present. Therefore, through RDC, azeoptropes can be avoided where the azeotropes will be able to “reacted away” in a single vessel.

2.8 Reactive distillation with structured packings

Sulzer Chemtech has been one of the leading provider of structured packings to the chemical industry up till today. Through the discovery of structured packings, reactive distillation technology has been made possible. As reactive distillation consists of reactive and non reactive section, KATAPAK-SP and Sulzer-BX is mostly being applied in the reactive and non reactive section respectively. Pöpken *et al.* (2001), Bhatia *et al.* (2007) and Niesbach *et al.* (2012) have used KATAPAK-SP and Sulzer-BX in their simulation studies on esterification process through RDC in their past research respectively. Table 2.5 below shows the different types of structured packings from Sulzer Chemtech.

Table 2.5: Summary of different types of structured packings available. (Sulzer Chemtech, n.d).

Types of packing	**Material used**	**Applications**	**Size and operating conditions**	**Characteristics**
Mellapak 64.X/64.Y Mellapak 125.X/125.Y Mellapak 170.X/170.Y Mellapak 2 X/2 Y Mellapak 250.X/250.Y	Stainless steels Carbon steel Hastelloy, monel, aluminium, copper-bronze, brass, titanium, nickel	Basic chemicals and petrochemicals, ethylbenzene/styrene, fatty acids, refinery operations, absorption/desorption columns	From 80 mm up to 17 m Vacuum to high pressure Liquid load 0.2 to more than 200 m^3/m^2h	Universal packing type, suitable for wide range of applications Low to very high liquid loads
BX gauze packing BXPlus gauze packing CY gauze packing	Stainless steels Copper-bronze, monel, hastelloy, nickel, titanium	Fine chemicals Isomers Fragrances Flavours Low liquid loads with aqueous solutions	40 mm to 6 m 1 mbar to atmospheric pressure, optimum: 1-100 mbar 100 mm to 4m 1 mbar to moderate pressure 80 ^oC (max. temp.)	High separation efficiency, even at small liquids loads Low pressure drop, small hold-up BXPlus: same efficiency as BX, lower pressure drop, self wetting, even with aqueous solutions Large number of transfer units per meter, even with small liquid loads

Types of packing	Material used	Applications	Size and operating conditions	Characteristics
Katapak-SP 11 Katapak-SP 12 Katapak-SP 13	Stainless steels	Acetates, methyl acetate hydrolysis, fatty acid esters Acetals MTBE, ETBE, TAME	From 50 mm Vacuum to moderate pressure	Packing for reactive distillation and trickle-bed reactors High separation efficiency and high reaction capacity Modular concept

2.9 RDC modelling and simulation

Modelling and simulation for a RDC involves the proper selection of the RD model, kinetic model and thermodynamic model for the production of acrylic ester.

RADFRAC model is being chosen due to the lack of data on the physical properties such as surface tension, diffusion coefficients and viscosities which are needed for the calculation of mass and heat transfer coefficients and interfacial areas for the synthesis of n-butyl acrylate via esterification process. This is because there is only a few investigation on reactive distillation for the production of n-butyl acrylate up till now, which is summarized in the previous research (Niesbach *et al.,* 2012). Besides that, according to Peng *et al.* (2002), RATEFRAC (rate-based model) is more complicated compare to RADFRAC (equilibrium-based model) and it is also more difficult to converge. Generally, the results obtained from RADFRAC and RATEFRAC are similar with only a few differences under every simulation conditions. Moreover, through a simulation on methyl acetate system which was researched by Peng *et al.* (2002), the simulation results predicted by both RADFRAC and RATEFRAC matches with the experimental data by Popken *et al.* (2001). With this, it shows that RADFRAC is capable in simulating a reliable data for the synthesis of n-Butyl Acrylate as RATEFRAC shows more complexity compare to RADFRAC according to the past research by Baur *et al.* (2000).

The UNIQUAC thermodynamic model was used to describe liquid-liquid equilibrium with liquid activity coefficients calculated by UNIQUAC model and vapor association of AA was assumed to be ideal. According to Bouneb *et al.* (2010), UNIQUAC is preferred over NRTL because UNIQUAC is based on group contribution method which will be an advantage when it comes to calculations for distillation column. Finally, the kinetic model used was a simple pseudohomogeneous (PH) model. It was developed based on an activity-based Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach (Hougen and Watson, 1943; Hougen and Watson, 1947; Niesbach *et al.*, 2012 & Niesbach *et al.*, 2013). The (PH) model is similar to the power law of homogeneous reaction whereby the reaction rate is described by the concentration of reactants. Table 2.6 gives the summary of RD, thermodynamic and kinetic models studied by past researches. From their findings, every researches reported that for the different models being studied by each researches, the models agrees with the experimental data which was based on.

Table 2.6: Summary of RD, thermodynamic and kinetic models.

Esterification system	**RD model**	**Thermodynamic model**	**Kinetic model**	**Reference**
Acetic acid & n-hexanol	Equilibrium model	NRTL	Pseudo homogeneous	Schmitt *et al.* (2004)
Acetic acid & methanol	Not mention	UNIQUAC	Pseudo homogeneous	Kim and Han (2012)
Acetic acid & n-butanol	Equilibrium model	UNIQUAC	LHHW	Steinigeweg and Gmehling (2002)
	Equilibrium model	UNIQUAC-HOC	LHHW	Tian *et al.* (2012)
Acrylic acid & n-butanol	Non-equilibrium	UNIQUAC-HOC	LHHW	Niesbach *et al.* (2012); Niesbach *et al.* (2013)
Decanoic acid & methanol	Equilibrium model	UNIFAC	LHHW	Steinigeweg and Gmehling (2003)

Esterification system	**RD model**	**Thermodynamic model**	**Kinetic model**	**Reference**
Palmitic acid & isopropyl	Equilibrium & non-equilibrium model	UNIFAC	LHHW	Bhatia *et al.* (2007)

2.10 Summary

Based on the review done on the different types of reactions which were investigated in RDC by past researchers, we can summarized that up to date, not a single study on the recovery of acrylic acid through esterification process in RDC has even been carried out before. On the other hand, there was only a few study was done on the esterification process between acrylic acid and n-butanol in RDC (Niesbach *et al.*, 2012; Niesbach *et al.*, 2013). Thus, the study on the recovery of acrylic through esteification process in RDC will be carried out in this research.

3 METHODOLOGY

3.1 *Overview*

This chapter describes the steps that were taken in order to carry out the simulation of RDC on the equilibrium stage model (RADFRAC) in Aspen Plus V7.0. The formulae for equilibrium model and kinetic were stated here in this chapter together with the 'selection tree' for choosing the correct thermodynamic model. Finally, a simple flow chart on the procedure to carry out RADFRAC in Aspen PlusV7.0 for the reactive process was presented.

3.2 *Introduction*

In order to obtain reliable information for the design of RDC for the production of BA, a reliable and accurate programming tool was used as it also reduces the experimental work load of the researchers. This is because reactive distillation process requires a few experimental data so that analysis procedures can be carried out to see its performance and design of RDC. All the models used in this present study were presented in this chapter. These models were used to determine a suitable reaction kinetic model and also to validate the proposed RD model for the production of n-butyl acrylate through dilute acrylic acid which will be further discussed in the next chapter.

3.3 *Process design description*

The esterification between AA and BuOH taking place in the RDC can be seen as below:

$$CH_3(CH_2)_3OH+CH_2CHCOOH \leftrightarrow CH_2CHCOOC_4H_9+H_2O \qquad (3.1)$$

(BuOH) (AA) (BA)

In order to carry out the simulation study for this present research, the scheme of the pilot-scale RDC setup taken from Zeng *et al.* (2006) which can be seen in Figure 3.1 below:

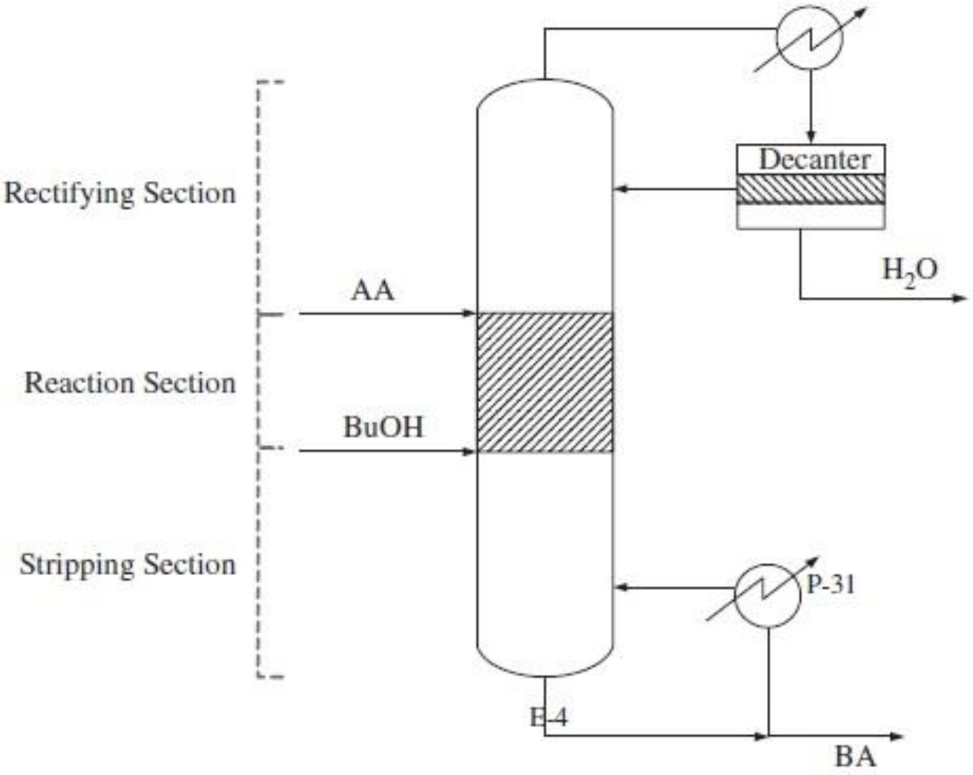


Figure 3.1: Pilot scale RDC for the production of n-Butyl Acrylate (Zeng *et al.,* 2006).

According to Niesbach *et al.* (2012), the column which was made up of glass has a diameter of 50 mm. The RDC has a total height of 12 m which 5.7 m was used for structured packing while the remaining 6.3 m was used for liquid distributors, total condenser, reboiler and other minor equipments which made up the RDC. The rectifying and stripping section was equipped with Sulzer BX packing for the separation process. Meanwhile, in the reaction section, Sulzer Katapak SP-11 reaction packing was impaired with acidic ion-exchange resin, Amberlyst 46. The sections were plugged using liquid distributors. It is to assist in the minimization of non-ideal liquid flow conditions such as wall effects and poor liquid distributions.

3.4 RDC modelling

The modelling and simulation for this esterification reaction was carried out by equilibrium stage model, RADFRAC in Aspen Plus V7.0. RADFRAC was chosen due to its ability to predict a comparable result with experimental data despite its simplicity (Peng *et al.,* 2002). RADFRAC module in the steady state simulator was based upon a rigorous equilibrium stage model. The model equations include mass and energy balances, vapor-liquid equilibrium, summation equation and enthalpy equation (MESH).

Several assumptions were made in order to carry out the simulation on the production of n-butyl acrylate. One of the assumptions was that the vapor and liquid are in equilibrium when leaving each stage with negligible heat of mixing of liquid and vapor mixtures. Besides that, it is assumed that the column was operating under adiabatic conditions and the vapor holdup was assumed negligible. Lastly, it was assumed that the reactions only occur in the liquid phase, with this, each stage in reaction section can be considered as a perfectly mixed stirred-tank reactor (CSTR) (Taylor and Krishna, 2000).

3.5 Equilibrium stage model

3.5.1 Equilibrium stage model equation

Reactive distillation has been seen as a series of distillation rather than an independent process up till today. Most of its development has been the work of researches which have a good knowledge in the thermal separation field and this can be seen on the way modelling of the reactive distillation process was approached.

The simpler and well known model for the simulating a regular distillation column is the equilibrium stage model. Bhatia *et al.* (2007) and Bhatt and Patel (2012) have implemented equilibrium stage model for the production of isopropyl palmitate and butyl acetate respectively in their past research papers. This model assumed that the column can be divided into stages (transversal cuts of the column for packed columns), where mass transfer operation took place. It also assumed that the liquid and vapor leaving the stage are in thermodynamic equilibrium with each other. Liquid phase reaction is also being considered in a reactive distillation column. Figure 3.2 shows a simple schematic of an equilibrium stage model.

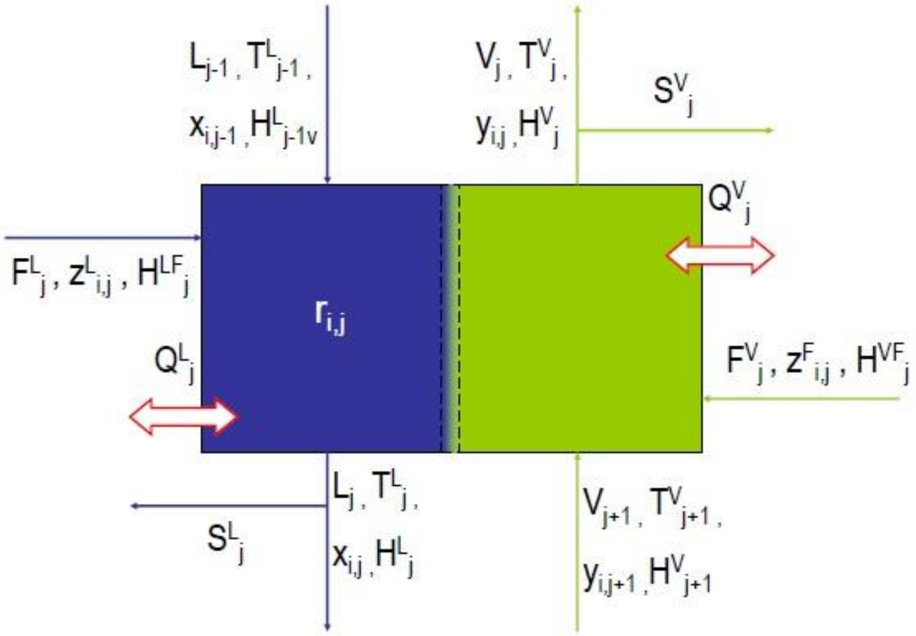


Figure 3.2: Equilibrium stage model. Adapted from Taylor and Krishna (2003) (Blue: Liquid, Green: Vapor).

The equation which would model the equilibrium stages is known as the MESH equations. The M stand for the material balance which is the total material balance of the system in the form of:

$$\frac{dU_j}{dt} = V_{j+1} + L_{j-1} + F_j - (1+r_j^V)V_j - (1+r_j^L)L_j + \sum_{m=1}^{r}\sum_{i=1}^{c} v_{i\,.m}\, R_{m\,.j}\,\varepsilon_j \tag{3.2}$$

The component material balance (neglecting vapor hold-up) is:

$$\frac{dU_j\, x_{i,j}}{dx} = V_{j+1}y_{i,j+1} + L_{j-1}x_{i,j-1} + F_j z_{i,j} - (1 + r_j^V)V_j y_{i,j} - (1 + r_j^L)L_j x_{i,j} + \sum_{m=1}^{r} v_{i,m}\, R_{m,j}\,\varepsilon_j \tag{3.3}$$

where U_j is the hold up on stage j, L represents the liquid phase molar flow rate (mol/s), F represents the feed flow rate (mol/s), z represents the mole fraction of the component in the feed, i represents the component index, j represents the segment index and $v_{i,m}$ represents the stoichiometric coefficient of component i in reaction m. In the material balance equations given above r_j is the ratio of side stream flow to inter stage flow. Next, the E equations represent the phase equilibrium relations

$$y_{i.j} = K_{i.j}x_{i.j} \tag{3.4}$$

The S equations states the summation equations

$$\sum_{i=1}^{c} x_{i.j} = 1, \sum_{i=1}^{c} y_{i.j} \tag{3.5}$$

Lastly, the enthalpy balance is given as:

$$\frac{dUj\,Hj}{dt} = V_{j+1}H_{j+1}^{V} + L_{j-1}H_{j-1}^{L} + F_jH_j^{F} - (1+r_j^{V})V_jH_j^{V} - (1+r_j^{L})L_jH_j^{L} - Q_j \tag{3.6}$$

with the superscripted *H*'s are the enthalpies of the appropriate phase.

3.6 Thermodynamic aspect

Design of separation processes, chemical and biochemical product design usually requires thermodynamic data, especially phase equilibria. About 40% of the cost in many processes is related to the separation units includes the importance of thermodynamics (Kontogeorgis and Folas, 2010, p.3). As of today, several commercial simulators have a large spectrum of thermodynamic model to select from and the ‘decision or selection trees’ method was applied by all of the companies in selecting the suitable models to represent their specific productions. Figure 3.3 summarizes the algorithm in choosing the appropriate thermodynamic models.

There consists of four factors that should be highlighted when choosing the property methods. They consist of the nature of the properties of interest, composition of mixture, pressure and temperature range of the system and the availability of parameters (Carlson, 1996). Nature of the properties of interest focuses on the vapor-liquid equilibrium (VLE) which plays an important role in the chemical engineering process for distillation, evaporation or stripping. As for solvent extraction and extractive distillation, liquid-liquid equilibrium (LLE) is very important. Another critical consideration was pure-component and mixture enthalpy as it will determine the outcome for the reactive distillation. Besides that, the composition of the mixture focus on what are the composition present in the mixture as it affect the phase equilibria greatly.

The pressure and temperature range clearly affect the property method. Methods such as Raoult’s law, Hendry’s law or the use of activity coefficient are being considered when it comes to the phase equilibia calculations. Lastly, for the availability of parameters, data from experimental work, literature data, estimating parameters or choosing a least rigorous method is being considered when there is insufficient data for pure- and binary component parameters.

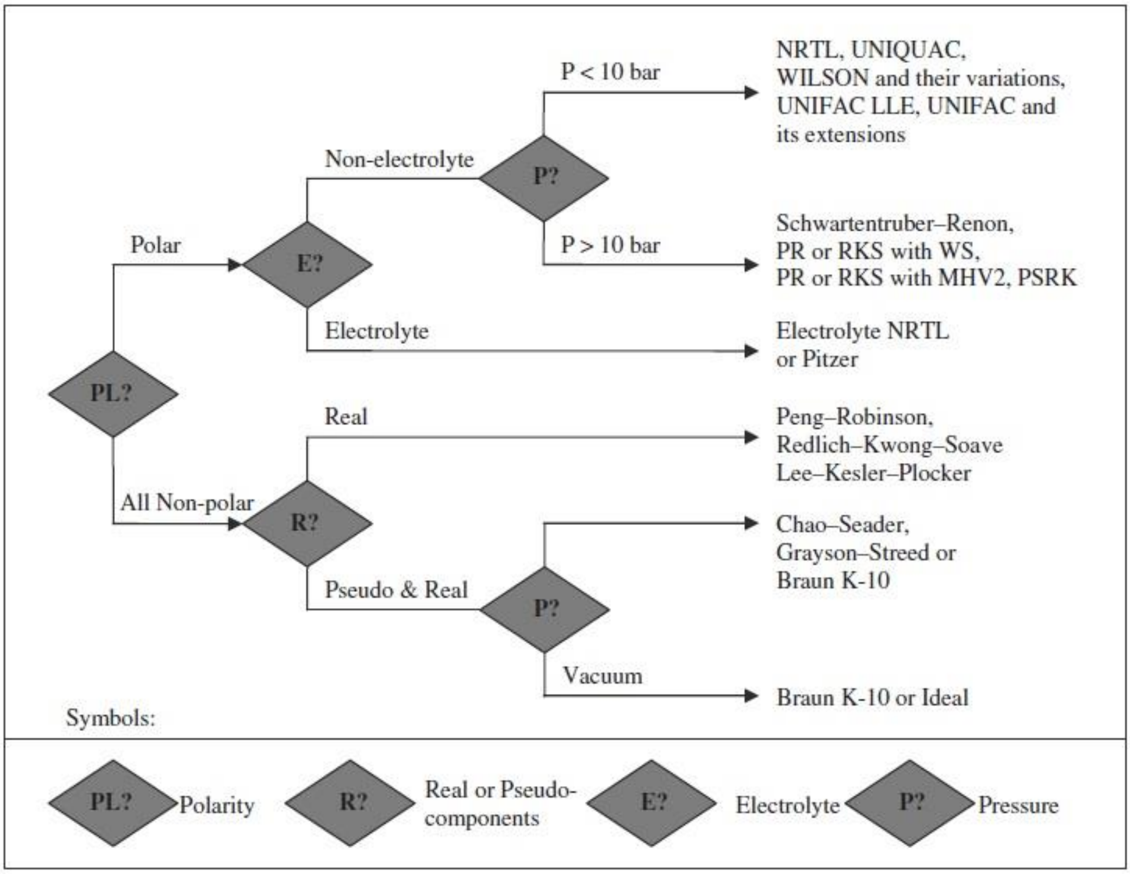


Figure 3.3: Selection of appropriate thermodynamic models base on the type of compounds involves (Carlson, 1996).

In this study, the liquid phase non-idealities is characterized by the activity coefficient (γ) calculated from the UNIQUAC model while it was assumed to be ideal in the gas phase. Past researches which have presented the UNIQUAC model to calculate the activity coefficient are by:

- Kim and Han (2012) for the esterification process between acetic acid and methanol.
- Steinigeweg and Gmehling (2002) for the esterification process between acetic acid and n-butanol.

- Niesbach *et al.* (2012) and Niesbach *et al.* (2013) for the esterification process between acrylic acid and n-butanol.

3.7 Reaction kinetics

Homogeneous or heterogeneous model can be applied to the reaction system depending on the type of catalyst which is present in the system. In this present study, the heterogeneous model is being chosen due to the present of solid acidic ion-exchange resin for the production of n-butyl acrylate. In general, the rate of a heterogeneous reaction is affected by external/internal diffusion, adsorption/desorption, surface reaction and the non-ideality of the reacting mixtures. Past researches have reported several kinetic models to describe the kinetic behaviour of heterogeneous esterification process. Sanz *et al.* (2002) have reported an Eley-Rideal (ER) model and a Langmuir-Hinshelwood-Hougen-Watson (LHHW) for the esterification between lactic acid and methanol. Meanwhile, Ali and Merchant (2006) have reported pseudo-homogeneous (PH), Eley-Rideal (ER) and Langmuir-Hinshelwood (LH) for the esterification between acetic acid and 2-propanol.

In this study, the reaction kinetics of n-butyl acrylate synthesis from acrylic acid and n-butanol and Amberlyst-46 as the acid ion exchange resin catalyst was based on the simple pseudohomogeneous (PH) model. It was developed based on an activity-based Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach (Hougen and Watson, 1943; Hougen and Watson, 1947). The reaction rate was described as follows (Hougen and Watson, 1943; Hougen and Watson, 1947):

$$r_i = \frac{dni}{dx} = v_i m_{cat,dry} c_{act} \frac{k_o \exp\left(\frac{-Ea}{RT(K)}\right)\left(a_{AA}a_{BuOH} - \frac{1}{Keq}a_{BA}a_{water}\right)}{(1+ K_1 a_{AA} + K_2 a_{BuOH} + K_3 a_{BA} + K_4 a_{water})2} \tag{3.7}$$

$$K_{eq}(\mathrm{T}) = \exp\left(\frac{-1888.66}{T(K)} + 8.17\right) \tag{3.8}$$

with k_o is at 3.41 x 10^{10}mol/(eq(H^+) s), E_a equals to 81260 J/mol and finally K_1, K_2 and K_3 is at a value of 0.244, 0.748 and 2.105 respectively.

The PH model was chosen to represent the reaction kinetics for the esterification of acrylic acid and n-butanol. The PH model was developed based on concentration instead of activity coefficient. This is due to the limitation of inserting LHHW model and activity coefficient into Aspen Plus V7.0 whereby the only available reaction kinetics model in Aspen Plus V7.0 was defined on the basic of concentration or mole fraction basic. In order to develop a PH model based on LHHW, several calculations were made in order to express the PH model in terms of concentration for every species. Excel spreadsheet developed by Elliot and Lira (2000) was used in order to determine the gamma of the activity coefficient whereby it was then plotted against composition in order to determine the relationship between gamma and composition. Next, the results obtained were written into Polymath 6.10 in order to determine the concentration of every species. Thus, the PH model based on concentration can be express as follows:

$$r_i = \frac{dn_i}{dt} - k({C_{AA}}^2 C_{BuOH} - \frac{1}{K_{eq}} {C_{BA}}^2 C_W) \tag{3.9}$$

All the calculations were done by varying the temperature from 350K – 380K. Even though the PH model has a major drawback whereby it neglects the sorption effects (Steinigeweg and Gmehling, 2003), it was chosen for this research due to the limitation of inserting LHHW model and activity coefficient into Aspen Plus V7.0. The results obtained from excel which were written into Polymath 6.10 for temperature varied from 350K – 380K are shown in Appendix A.

Four adjustable parameters (k_1, k_{-1}, $E_{A,1}$, $E_{A,-1}$) whereby k_1 and k_{-1} are the pre-exponential factor for forward and backward reactions and $E_{A,1}$ and $E_{A,-1}$ are the activation energies for the forward and backward reactions. The results are summarized in Table 3.1 below whereas Figure 3.4 and Figure 3.5 illustrates the Arrhenius diagram of the rate constants for the forward, k_1 and backward reaction, k_{-1} of the esterification reaction.

Table 3.1: Kinetics Parameters for the Pseudohomogeneous Kinetic Model

Reaction	i	k_i (mol kg^{-1} s^{-1})	$E_{A,I}$ (J mol^{-1})	R^2
Forward	1	1.889×10^{12}	84,220.82	1
Backward	-1	4.427×10^{9}	79,776.987	1

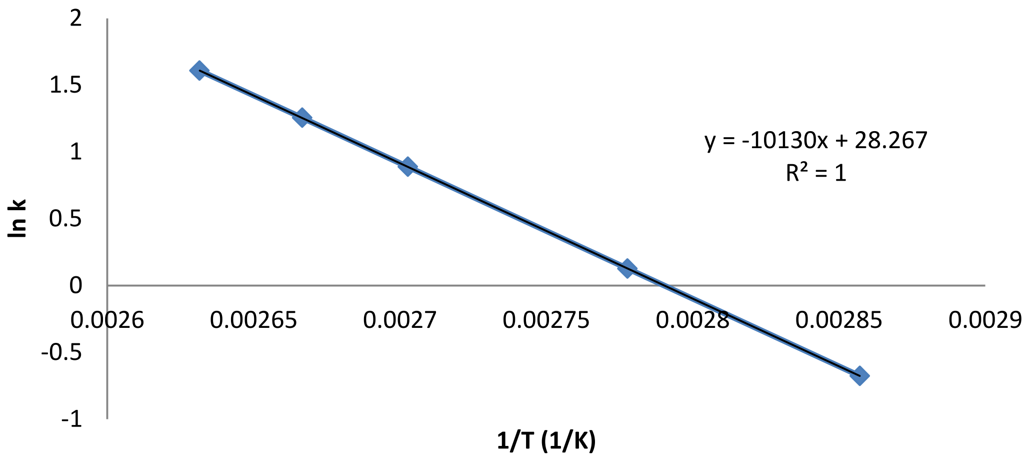


Figure 3.4: Arrhenius diagram of the rate constant for forward reaction

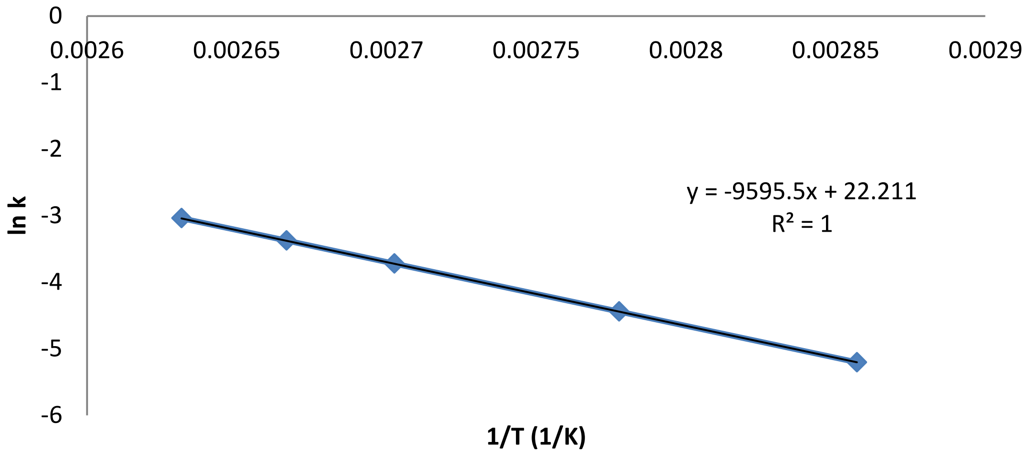


Figure 3.5: Arrhenius diagram of the rate constant for backward reaction

3.8 RADFRAC module

In this study, a commercial simulator, RADFRAC in Aspen Plus V7.0 was used to simulate the reactive distillation process. It is based upon a rigorous equilibrium stage model for solving the mass and energy balances, vapor-liquid equilibrium, summation equation and enthalpy equation (MESH). Vapor liquid equilibrium was assumed at every stage through equilibrium model. Height equivalent to theoretical plate (HETP) was taken into consideration so as the efficiency of the trays can be further improved. Table 3.2 describes the HETP values of the packing used.

Table 3.2: HETP values of the packing used in reactive distillation (Niesbach *et al.*, 2012).

Packing used	**HETP value**
Sulzer BX	0.14 m
Sulzer Katapak SP-11	0.5 m

Physical and chemical properties for all species were taken from Aspen Plus component database. Figure 3.6 shows the basic RADFRAC simulation procedures for the reactive simulation process. Further details regarding the steps involved were described below:

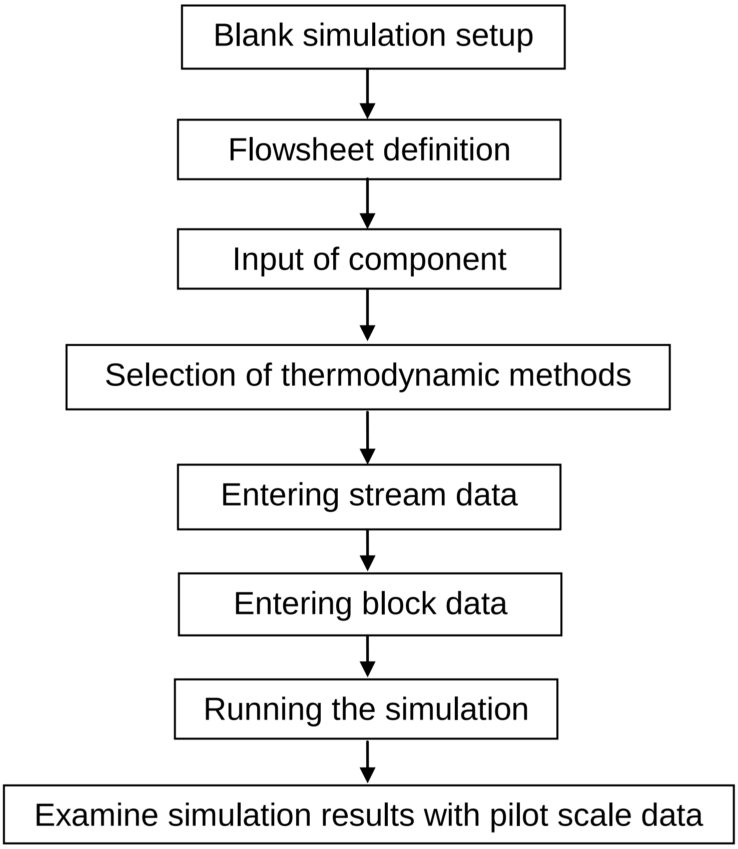


Figure 3.6: Basic RADFRAC simulation steps to be taken for the simulation of the reactive distillation process.

i. Flowsheet definition
   1. The RADFRAC block was selected from the Aspen Plus model library. (Figure 3.7)
   2. The block was further define by connecting the input and output streams. (Figure 3.7)

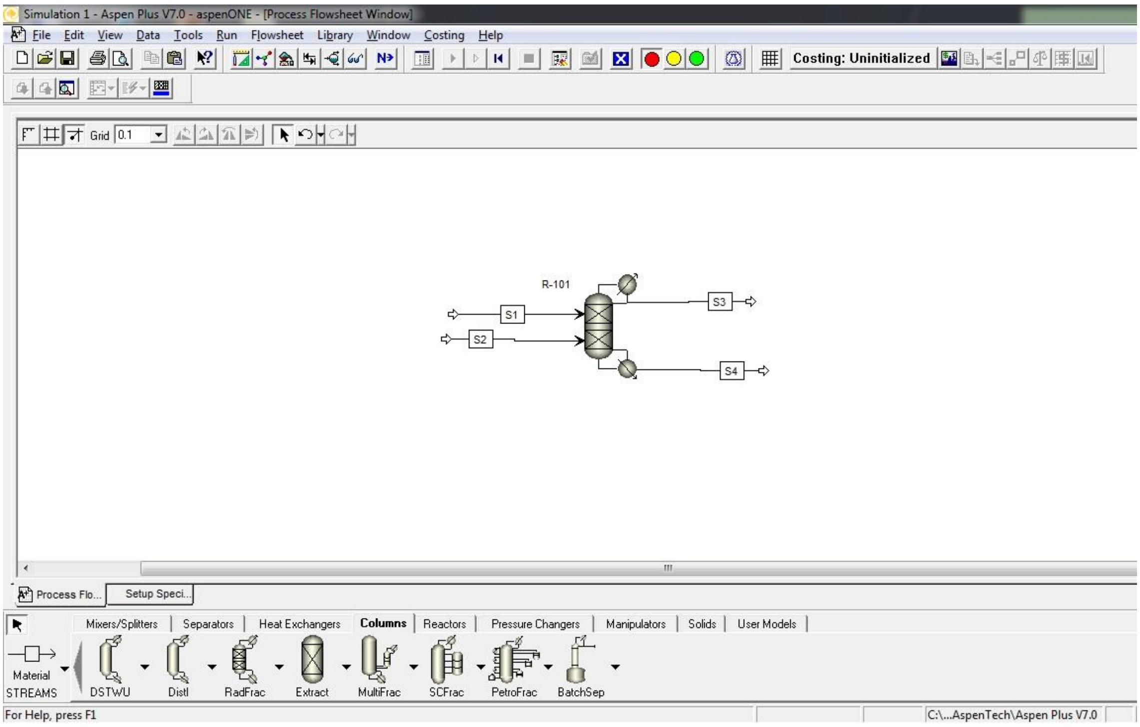


Figure 3.7: Defining the flowsheet for reactive distillation process.

ii. Component input

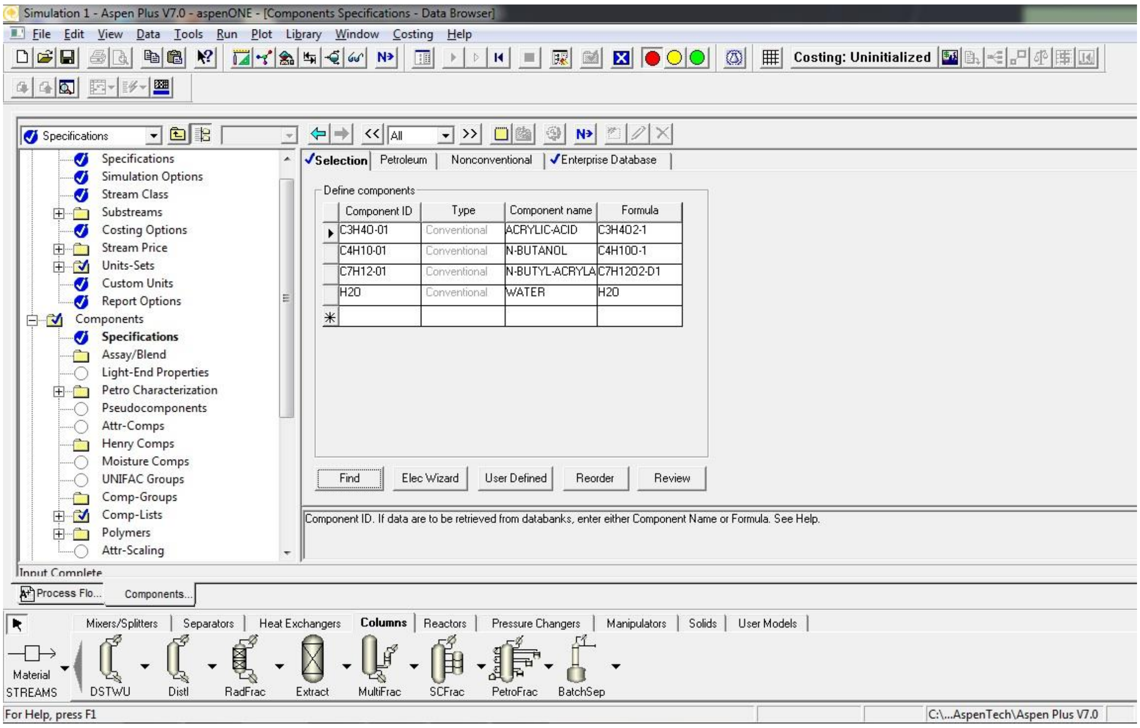
1. The components present for this simulation were Acrylic Acid (AA), n-Butanol (BuOH), n-Butyl Acrylate (BA) and water (H_2O) (Figure 3.8).
2. All the components involved were available in the Aspen Plus software databank. Thus, there was no estimation carried out (Figure 3.8).

iii. Selection of thermodynamic method

1. The property method was selected from Properties specification global sheet (Figure 3.9).
2. UNIQUAC model was chosen for this study. Any absent UNIQUAC activity model interaction parameters in Aspen Plus library were estimated from UNIFAC (Figure 3.9).

iv. Entering stream data

1. The state variable and component flow specification for the Acrylic Acid feed stream were entered to Stream 1 specification sheet (Figure 3.10).
2. The same procedure was applied for the n-Butanol feed stream (Figure 3.11).

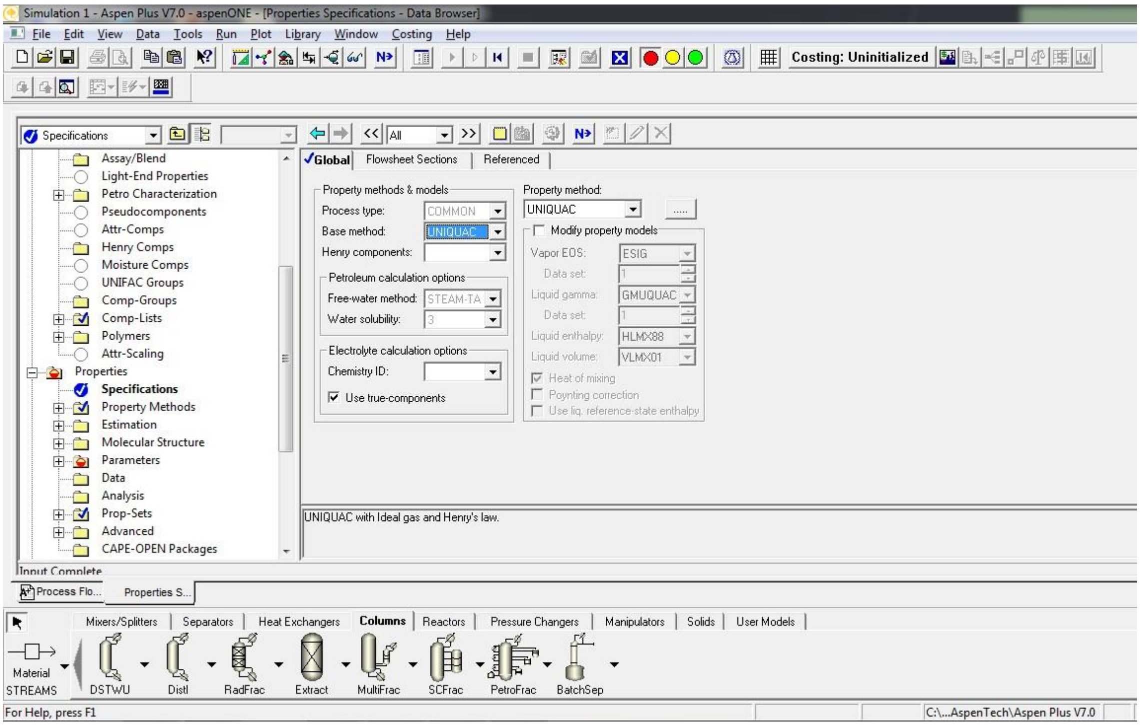


Define components

Component ID	Type	Component name	Formula
C3H4O-01	Conventional	ACRYLIC-ACID	C3H4O2-1
C4H10-01	Conventional	N-BUTANOL	C4H10O-1
C7H12-01	Conventional	N-BUTYL-ACRYLA	C7H12O2-D1
H2O	Conventional	WATER	H2O

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

Figure 3.8: Entering of the component present to the component selection sheet.



Property methods & models
Process type: COMMON
Base method: UNIQUAC
Henry components:

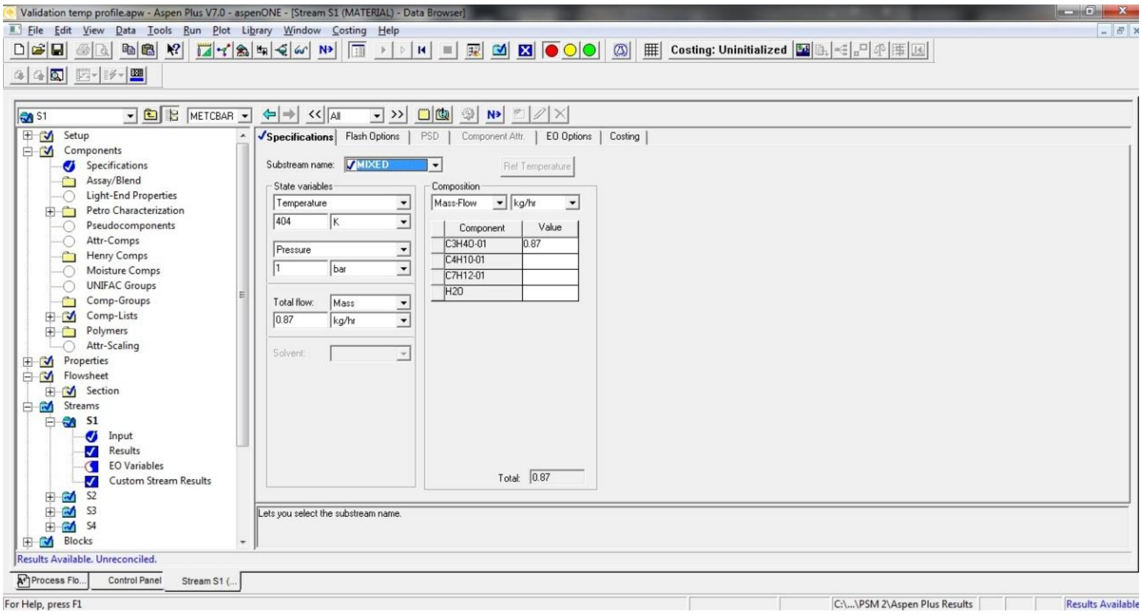
Petroleum calculation options
Free-water method: STEAM-TA
Water solubility: 3

Electrolyte calculation options
Chemistry ID:
☑ Use true-components

Property method: UNIQUAC
☐ Modify property models
Vapor EOS: ESIG
Data set: 1
Liquid gamma: GMUQUAC
Data set: 1
Liquid enthalpy: HLMX88
Liquid volume: VLMX01
☑ Heat of mixing
☐ Poynting correction
☐ Use liq. reference-state enthalpy

UNIQUAC with Ideal gas and Henry's law.

Figure 3.9: Input of thermodynamic model into the properties specification sheet.



Substream name: MIXED

State variables
Temperature: 404 K
Pressure: 1 bar
Total flow: Mass 0.87 kg/hr

Composition: Mass-Flow kg/hr

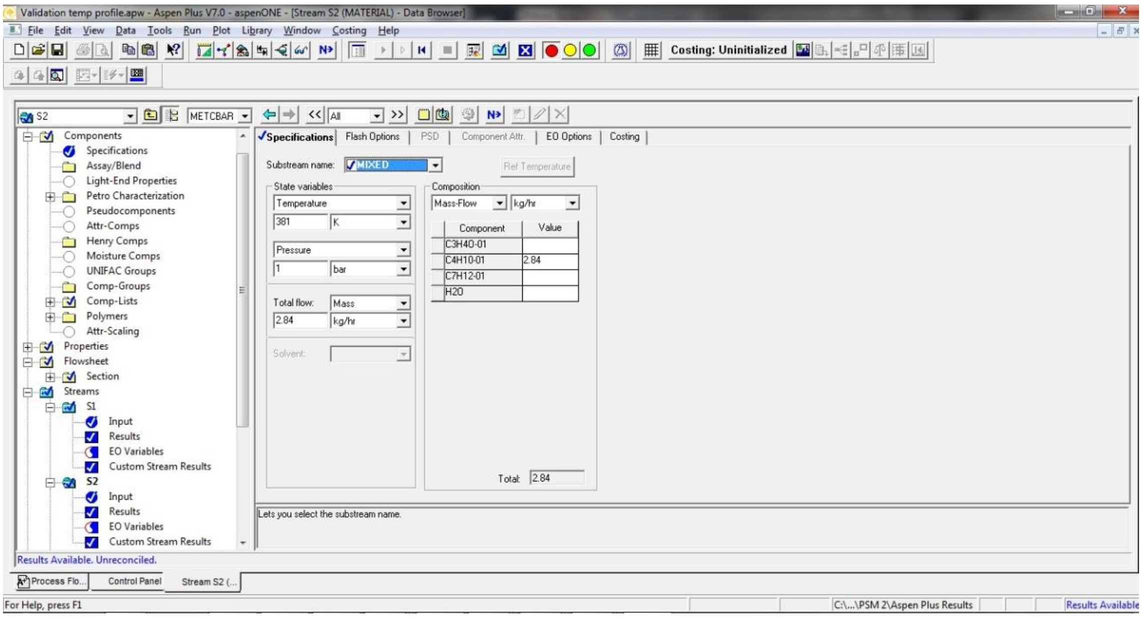
Component	Value
C3H4O-01	0.87
C4H10-01	
C7H12-01	
H2O	

Total: 0.87

Lets you select the substream name.

Results Available. Unreconciled.

Figure 3.10: Input of Acrylic Acid feed stream data into Stream 1 specification sheet.



Substream name: MIXED

State variables
Temperature: 381 K
Pressure: 1 bar
Total flow: Mass 2.84 kg/hr

Composition: Mass-Flow kg/hr

Component	Value
C3H4O-01	
C4H10-01	2.84
C7H12-01	
H2O	

Total: 2.84

Lets you select the substream name.

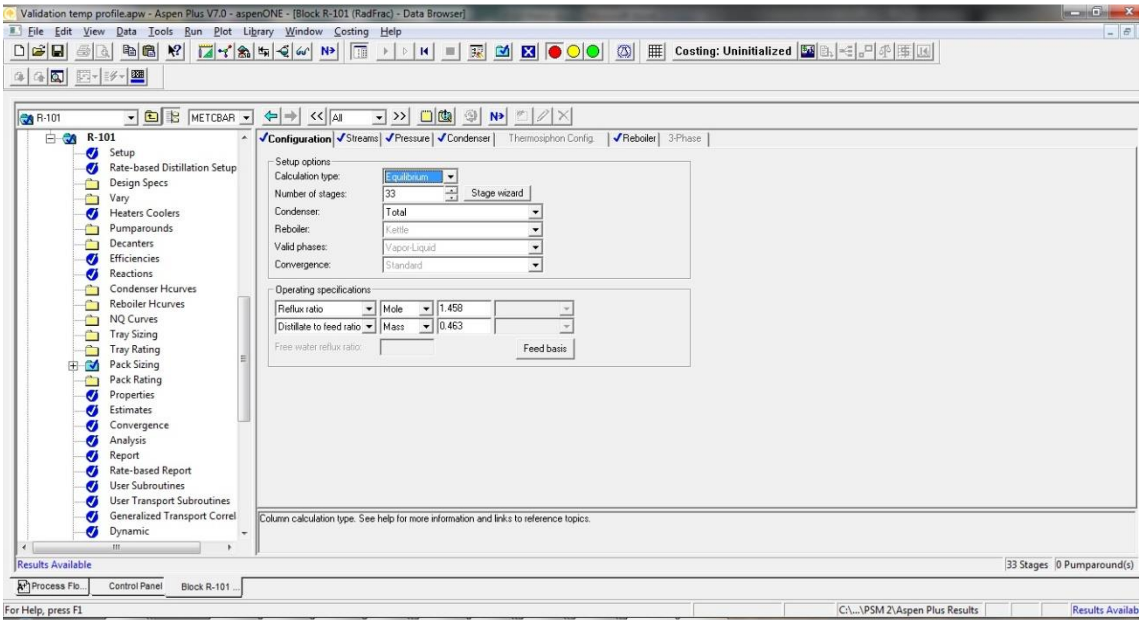
Results Available. Unreconciled.

Figure 3.11: Input of n-Butanol feed stream data into Stream 2 specification sheet.

v. Entering block data

1. The number of stages, the condenser type and the two operating specifications, which is the reflux ratio and distillate rate (kg/hr) were entered into the Block R-101 configuration sheet (Figure 3.12). The feed stages of Acrylic Acid and n-Butanol were also entered into the Block R-101 configuration sheet (Figure 3.13).

2. The top stage pressure of 0.352 bar was entered into the Block R-101 pressure sheet (Figure 3.14). The packing types and specification were also entered into the Block R-101 configuration sheet. For the rectifying and stripping section, the packing used was Sulzer BX while for the reaction section, Sulzer Katapak SP-11 is not available in the Aspen Plus library which was substituted with Mellapak 170Y (Figure 3.15 – 3.17).
3. The stoichiometry of the reaction was entered to the Reaction R-101 stoichiometry sheet (Figure 3.18). The reaction kinetics was entered into the Reaction R-101 kinetic sheet for the forward and backward reactions (Figure 3.19 and Figure 3.20). The activity coefficient (γ) was assumed as unity due to the unavailability of FORTRAN subroutine which caused the rate law to be express in terms of concentration and not activity based as stated in the literature.



Setup options

Calculation type: Equilibrium

Number of stages: 33

Condenser: Total

Reboiler: Kettle

Valid phases: Vapor-Liquid

Convergence: Standard

Operating specifications

Reflux ratio | Mole | 1.458

Distillate to feed ratio | Mass | 0.463

Free water reflux ratio:

Column calculation type. See help for more information and links to reference topics.

Results Available

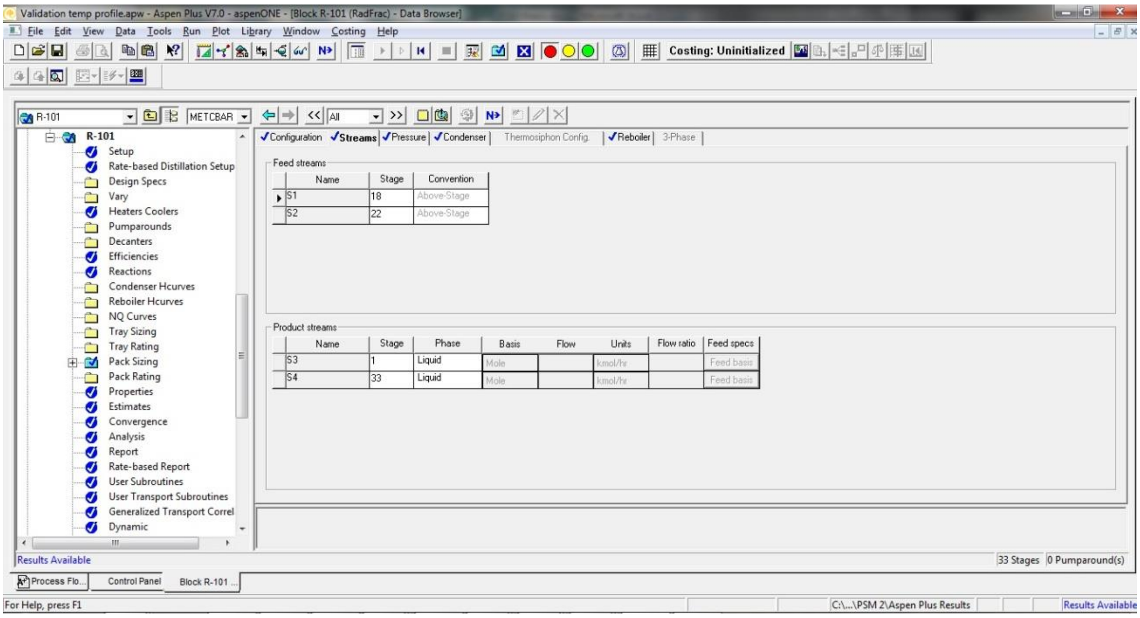
33 Stages

0 Pumparound(s)

C:\...\PSM 2\Aspen Plus Results

Results Availab

Figure 3.12: Input of operating specification to Block R-101 configuration sheet.



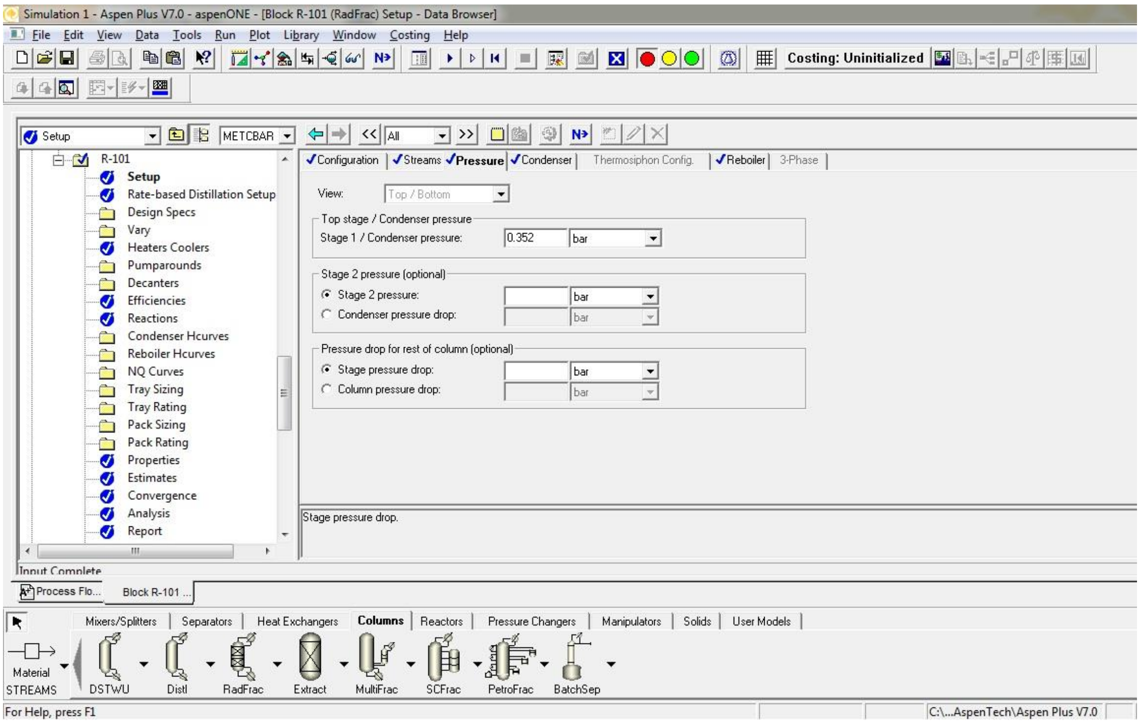
Feed streams

Name	Stage	Convention
S1	18	Above-Stage
S2	22	Above-Stage

Product streams

Name	Stage	Phase	Basis	Flow	Units	Flow ratio	Feed specs
S3	1	Liquid	Mole		kmol/hr		Feed basis
S4	33	Liquid	Mole		kmol/hr		Feed basis

Figure 3.13: Feed stages of AA and n-Butanol entered into Block R-101 configuration sheet.



View: Top / Bottom

Top stage / Condenser pressure

Stage 1 / Condenser pressure: 0.352 bar

Stage 2 pressure (optional)

● Stage 2 pressure: bar

○ Condenser pressure drop: bar

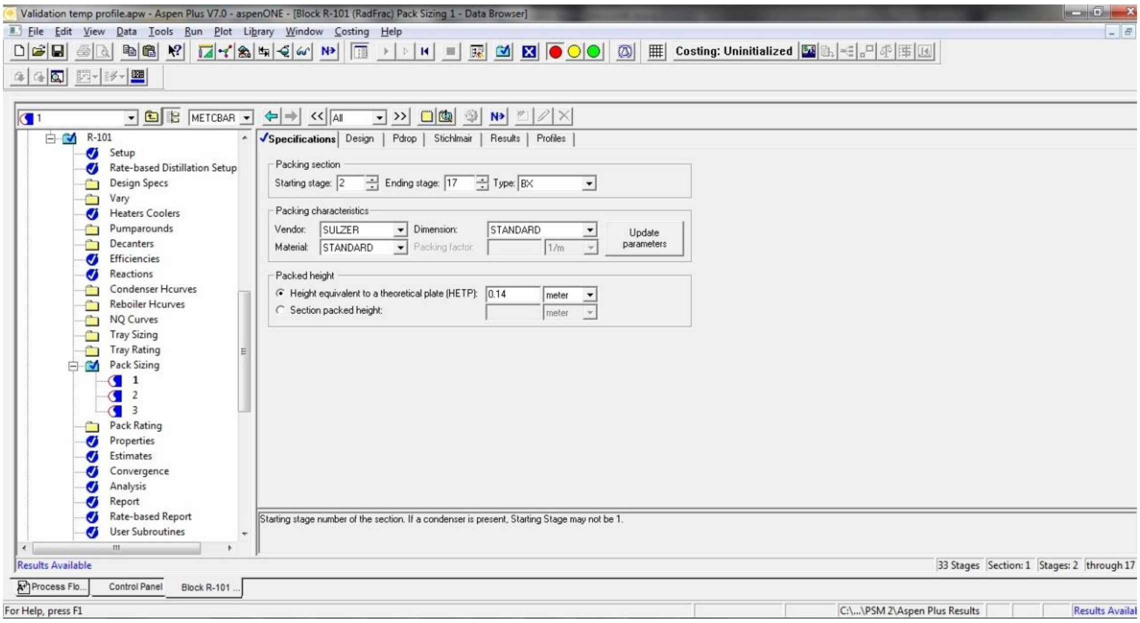
Pressure drop for rest of column (optional)

● Stage pressure drop: bar

○ Column pressure drop: bar

Stage pressure drop.

Figure 3.14: Block R-101 pressure sheet for input of condenser pressure.



Packing section

Starting stage: 2 Ending stage: 17 Type: BX

Packing characteristics

Vendor: SULZER Dimension: STANDARD

Material: STANDARD Packing factor: 1/m

Packed height

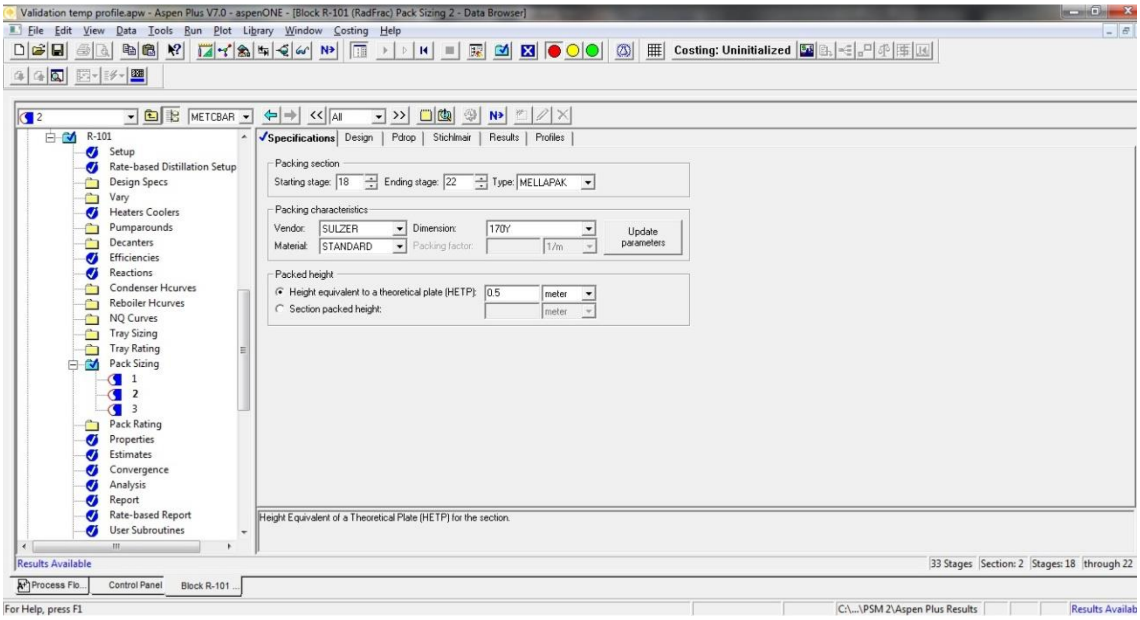
● Height equivalent to a theoretical plate (HETP): 0.14 meter

○ Section packed height: meter

Starting stage number of the section. If a condenser is present, Starting Stage may not be 1.

33 Stages Section: 1 Stages: 2 through 17

Figure 3.15: Specification for pack sizing in the rectifying section.



Packing section

Starting stage: 18 Ending stage: 22 Type: MELLAPAK

Packing characteristics

Vendor: SULZER Dimension: 170Y

Material: STANDARD Packing factor: 1/m

Packed height

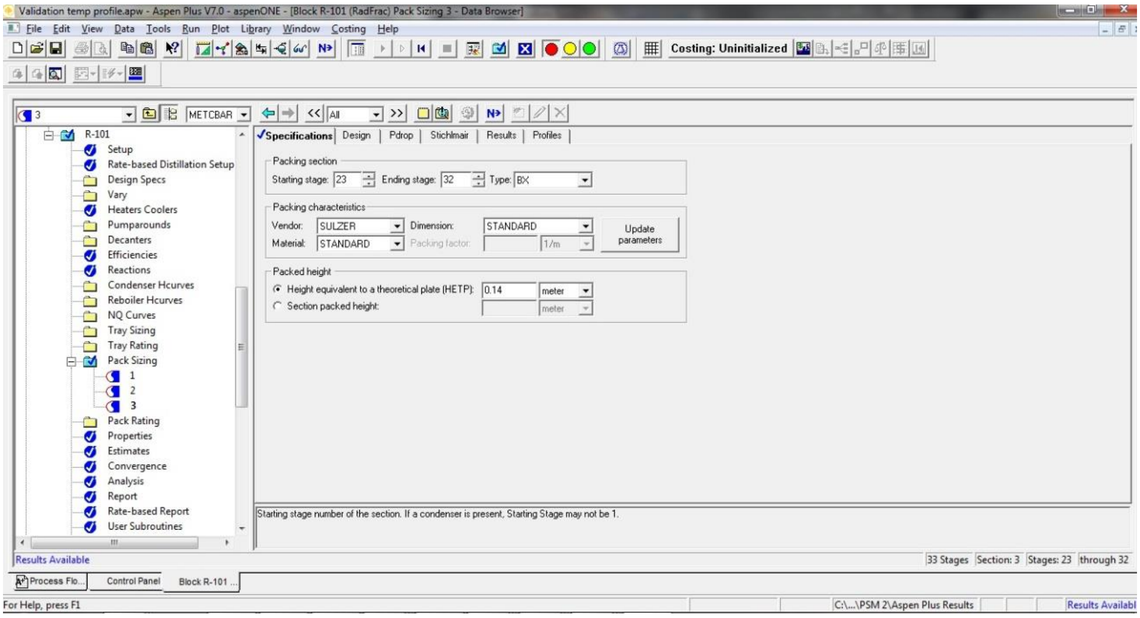
● Height equivalent to a theoretical plate (HETP): 0.5 meter

○ Section packed height: meter

Height Equivalent of a Theoretical Plate (HETP) for the section.

33 Stages Section: 2 Stages: 18 through 22

Figure 3.16: Specification for pack sizing in the reaction section.



Packing section

Starting stage: 23 Ending stage: 32 Type: BX

Packing characteristics

Vendor: SULZER Dimension: STANDARD

Material: STANDARD

Packed height

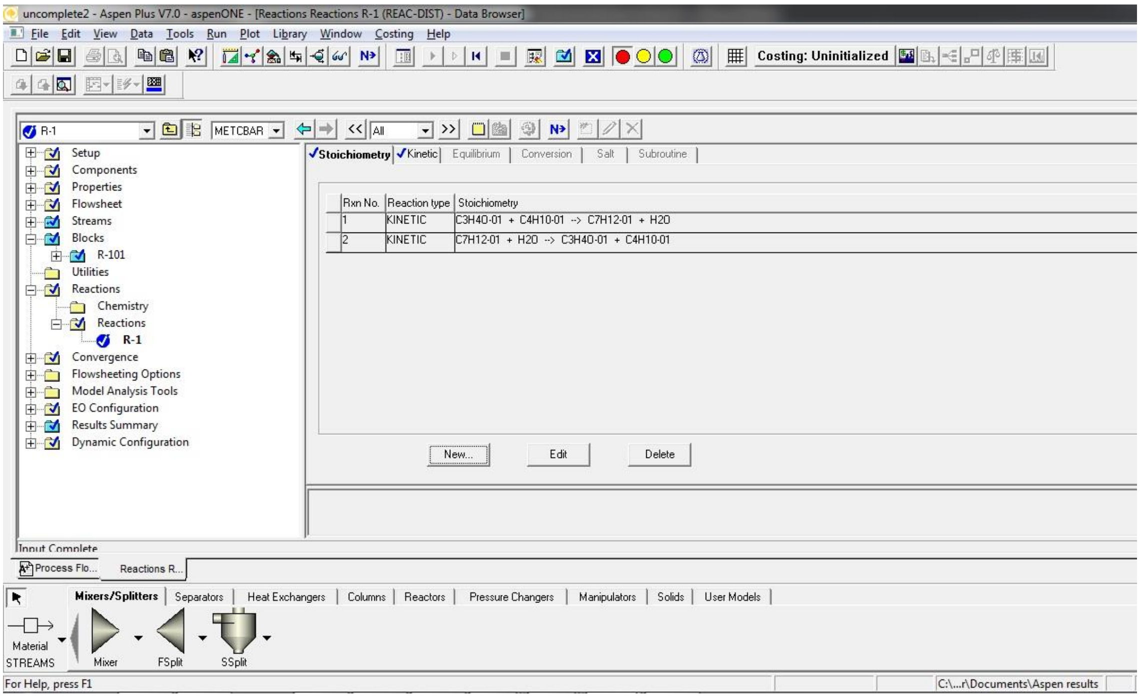
● Height equivalent to a theoretical plate (HETP): 0.14 meter

○ Section packed height:

Starting stage number of the section. If a condenser is present, Starting Stage may not be 1.

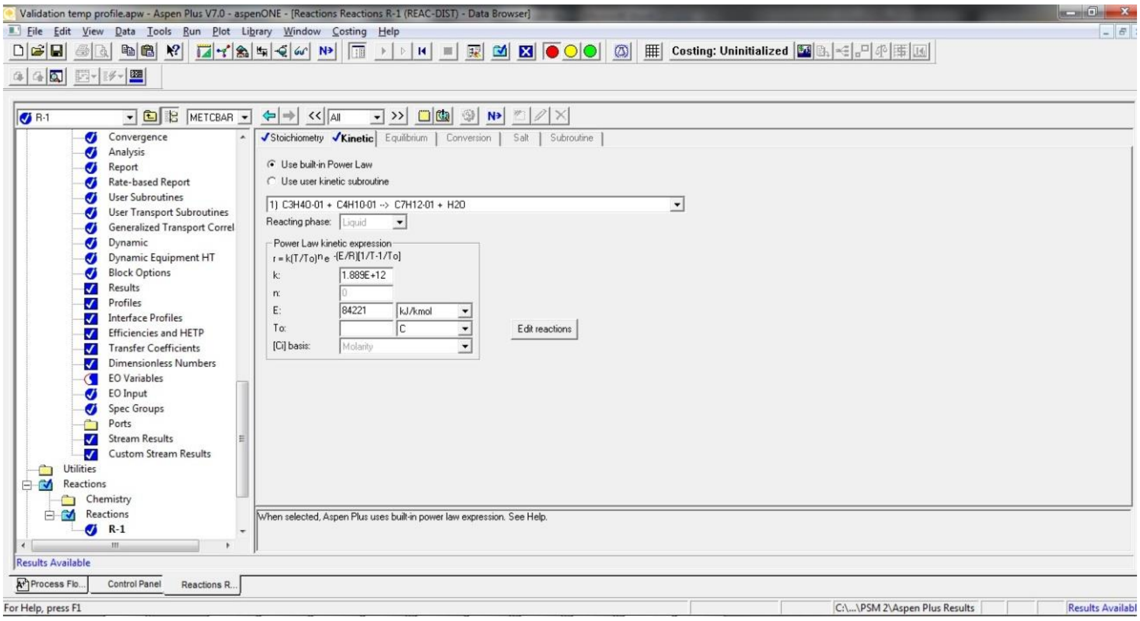
33 Stages Section: 3 Stages: 23 through 32

Figure 3.17: Specification for pack sizing in stripping section.



Rxn No.	Reaction type	Stoichiometry
1	KINETIC	C3H4O-01 + C4H10-01 --> C7H12-01 + H2O
2	KINETIC	C7H12-01 + H2O --> C3H4O-01 + C4H10-01

Figure 3.18: Input of stoichiometry of reaction into Block R-101 stoichiometry sheet.



Validation temp profile.apw - Aspen Plus V7.0 - aspenONE - [Reactions Reactions R-1 (REAC-DIST) - Data Browser]

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

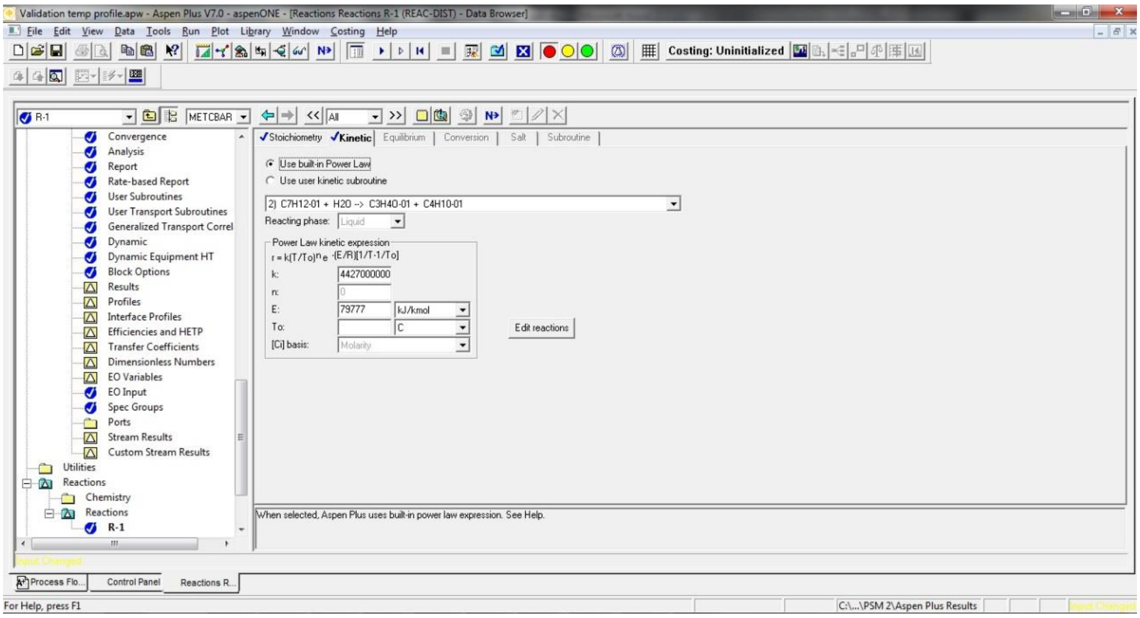
1) C3H4O-01 + C4H10-01 --> C7H12-01 + H2O

Reacting phase: Liquid

Power Law kinetic expression
$r = k(T/To)^n e^{-(E/R)[1/T-1/To]}$
k: 1.889E+12
n: 0
E: 84221 kJ/kmol
To: C
[Ci] basis: Molarity

When selected, Aspen Plus uses built-in power law expression. See Help.

Figure 3.19: Input of kinetic specification to the Block R-101 kinetic sheet for forward reaction.



Validation temp profile.apw - Aspen Plus V7.0 - aspenONE - [Reactions Reactions R-1 (REAC-DIST) - Data Browser]

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

2) C7H12-01 + H2O --> C3H4O-01 + C4H10-01

Reacting phase: Liquid

Power Law kinetic expression
$r = k(T/To)^n e^{-(E/R)[1/T-1/To]}$
k: 4427000000
n: 0
E: 79777 kJ/kmol
To: C
[Ci] basis: Molarity

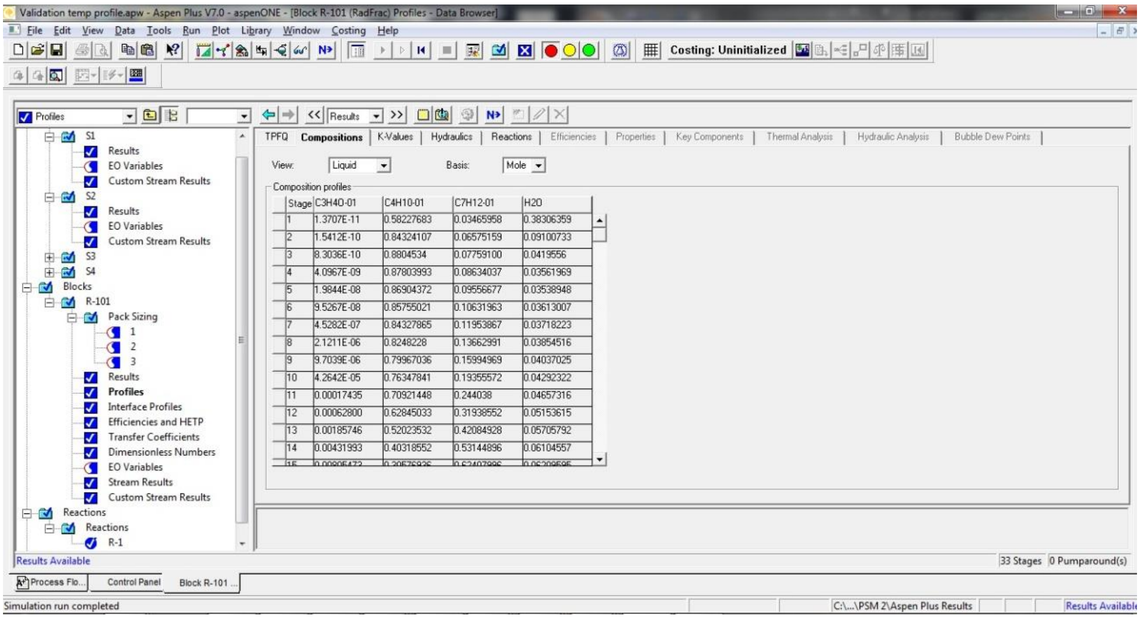
When selected, Aspen Plus uses built-in power law expression. See Help.

Figure 3.20: Input of kinetic specification to the Block R-101 kinetic sheet for backward reaction

vi. Running the simulation

1. The results shown in Figure 3.21 and 3.22 were obtained after running the simulation. Figure 3.23 shows the temperature profiles. The temperature profile was validated with temperature profile from experimental studies.

Several operating parameters such as Acrylic Acid concentration, catalyst loading, reflux ratio, reboiler duty and column configuration were studied by changing the parameters in the respective input specification sheet. In order to obtain a new set of results, the simulation was rerun with the changed input.

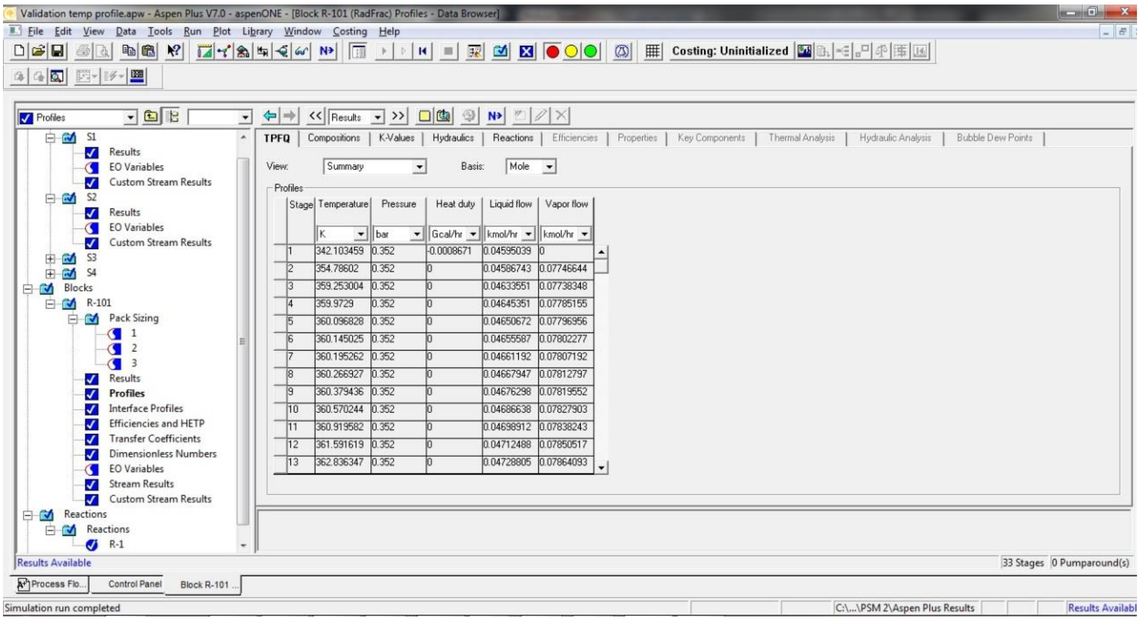


View: Liquid   Basis: Mole

Composition profiles

Stage	C3H4O-01	C4H10-01	C7H12-01	H2O
1	1.3707E-11	0.58227683	0.03465958	0.38306359
2	1.5412E-10	0.84324107	0.06575159	0.09100733
3	8.3036E-10	0.8804534	0.07759100	0.0419556
4	4.0967E-09	0.87803993	0.08634037	0.03561969
5	1.9844E-08	0.86904372	0.09556677	0.03538948
6	9.5267E-08	0.85755021	0.10631963	0.03613007
7	4.5282E-07	0.84327865	0.11953867	0.03718223
8	2.1211E-06	0.8248228	0.13662991	0.03854516
9	9.7039E-06	0.79967036	0.15994969	0.04037025
10	4.2642E-05	0.76347841	0.19355572	0.04292322
11	0.00017435	0.70921448	0.244038	0.04657316
12	0.00062800	0.62845033	0.31938552	0.05153615
13	0.00185746	0.52023532	0.42084928	0.05705792
14	0.00431993	0.40318552	0.53144896	0.06104557

Figure 3.21: Simulation results of liquid composition.



View: Summary   Basis: Mole

Profiles

Stage	Temperature K	Pressure bar	Heat duty Gcal/hr	Liquid flow kmol/hr	Vapor flow kmol/hr
1	342.103459	0.352	-0.0008671	0.04595039	0
2	354.78602	0.352	0	0.04586743	0.07746644
3	359.253004	0.352	0	0.04633551	0.07738348
4	359.9729	0.352	0	0.04645351	0.07785155
5	360.096828	0.352	0	0.04650672	0.07796956
6	360.145025	0.352	0	0.04655587	0.07802277
7	360.195262	0.352	0	0.04661192	0.07807192
8	360.266927	0.352	0	0.04667947	0.07812797
9	360.379436	0.352	0	0.04676298	0.07819552
10	360.570244	0.352	0	0.04686638	0.07827903
11	360.919582	0.352	0	0.04698912	0.07838243
12	361.591619	0.352	0	0.04712488	0.07850517
13	362.836347	0.352	0	0.04728805	0.07864093

Figure 3.22: Simulation results of temperature, pressure, heat duty, liquid flow and vapor flow.

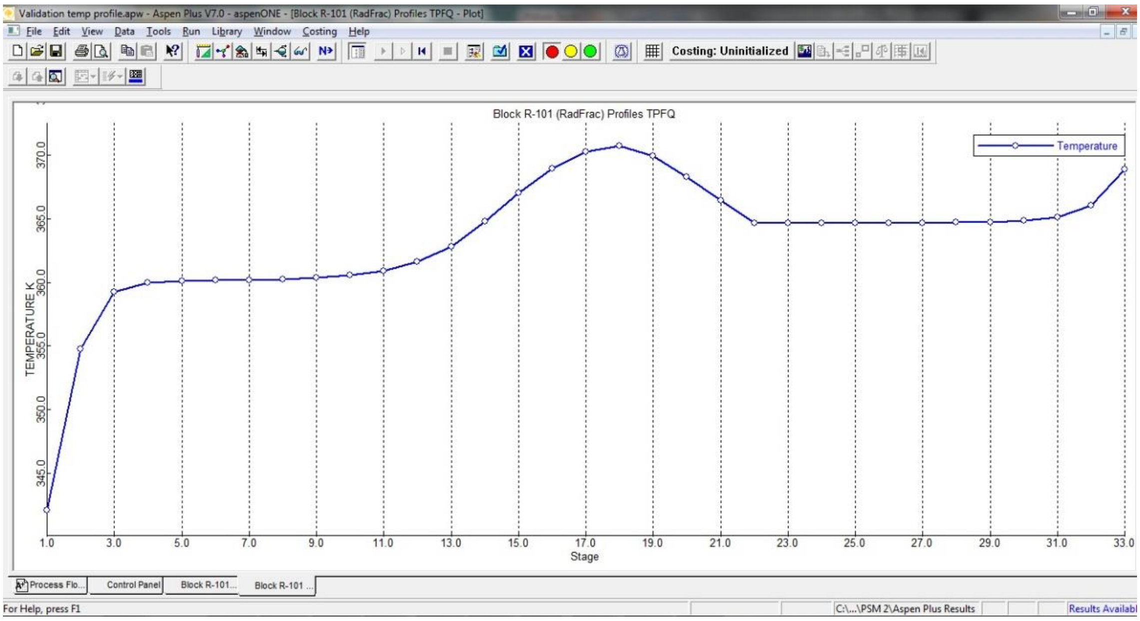


Figure 3.23: Temperature profile plotted in RADFRAC

3.9 Summary

A detailed procedure in carrying out RADFRAC simulation in Aspen Plus V7.0 for reactive process was stated above. This procedure will be a great reference for the future study on the simulation study for the recovery of acrylic acid through esterification in RDC.

4 RESULTS AND DISCUSSION

4.1 Overview

This chapter presents simulation results of RDC for the production of n-butyl acrylate though esterification process between dilute acrylic acid and n-butanol. Validation of the model proposed in this study was done by comparing the simulation results with experimental data from Niesbach *et al.* (2012). Sensitivity analysis on the effect of various operating parameter conditions such as AA concentration, catalyst loading, reboiler duty, reflux ratio, number of trays in reactive and separation sections were carried out using the validated model. Through the sensitivity analysis, the best operating parameter conditions were identified through the sensitivity analysis.

4.2 Model validation

The modelling of the RDC was based on the pilot scale data proposed by Niesbach *et al.* (2012). The stages are numbered from the top to the bottom whereby sage 1 is the condenser and stage N is the reboiler. The height equivalent to a theoretical plate (HETP) for Sulzer-BX packing was 0.14 m while the HETP for Katapak-SP 11 was 0.5 m. The reactive distillation column has a packed height of 5.7 m where 2.2 m for rectifying section (Sulzer-BX), 2.2 m for reactive section (Sulzer Katapak S-11) and 1.3 m for stripping section (Sulzer-BX). The RDC was then simulated as 31 equilibrium stages with 16 rectifying stages, 5 reactive stages, 10 stripping stages, a total condenser and a reboiler which makes up 33 stages in total. The specifications of the RDC are shown in Table 4.1 below:

Table 4.1: Specification of Pilot scale RDC. Adopted from Niesbach *et al.* (2012).

Column diameter	50 mm
Position of acrylic acid feed (Above the reaction section)	3.5 m
Position of n-butanol feed (Below the reaction section)	1.3 m
Inhibitor solution feed	Above condenser
Height of rectifying section	2.2 m

Height of reactive section	2.2 m
Mass of dry catalyst per meter reactive packing	0.205 kg m^{-1}
Condenser type	Total
Reboiler type	Naturally circulating evaporator
Operating top pressure range	0.3-0.4 bar

To validate the equilibrium stage model introduced in chapter 3, simulation results of the RDC for the production of n-butyl acrylate was compared with experimental data obtained by Niesbach *et al.* (2012). Experimental E7 data was chosen to validate the model. This is because Niesbach *et al.* (2012) discovered that the operating condition of E7 gives the best results compare to the other runs of the experiment. Table 4.2 summarized the operating condition of experiment E7 and Figure 4.1 shows the temperature profile which was obtained from the simulation study.

Table 4.2: Operating condition of experiment E7

Operating parameters	**Values**
Acrylic acid feed flow rate (kg/hr)	0.87
n-Butanol feed flow rate (kg/hr)	2.8362
Acrylic acid feed stage	18th
n-Butanol feed stage	22nd
Acrylic acid feed temperature (K)	404
n-Butanol feed temperature (K)	381
Top pressure (bar)	0.352
Reflux ratio	1.458
Distillate-to-feed ratio (kg/hr) / (kg/hr)	0.463

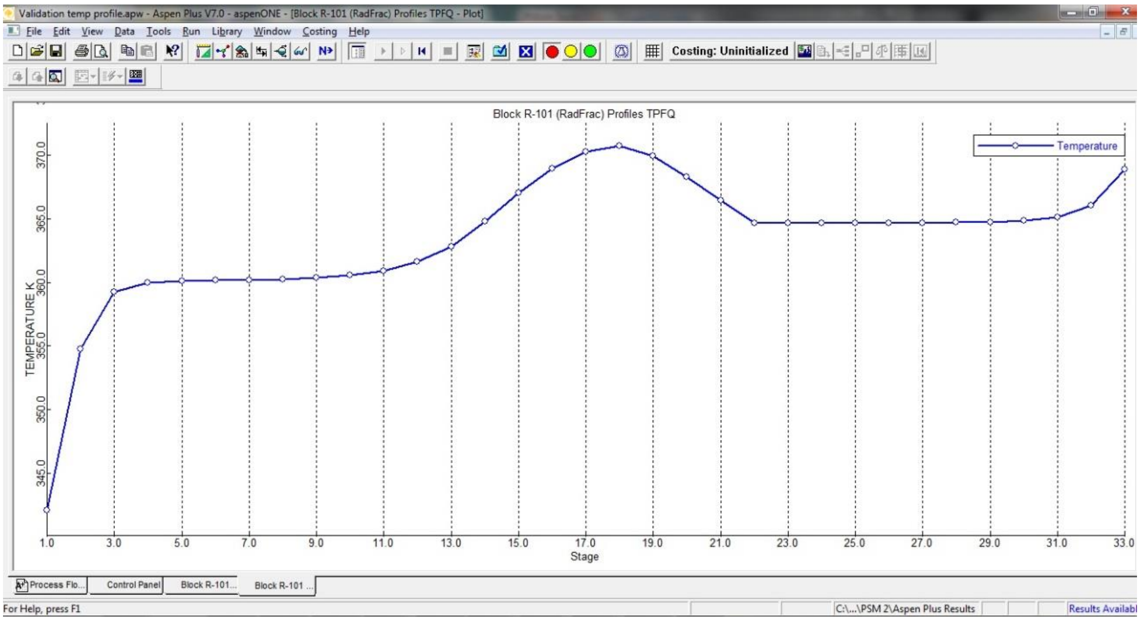


Figure 4.1: Temperature profile of n-butyl acrylate production.

Figure 4.1 above shows the temperature profile of the production of n-butyl at every stage in the column. The temperature reading was higher at the 18th stage which was the acrylic acid feed position compare to the temperature reading at the 22th stage which was the n-butanol feed position. This was due to the boiling point of acrylic acid is higher compare to n-butanol which are 414 K and 391 K respectively. The acrylic acid and n-butanol was fed into the column at temperature of 10K below of their boiling points.

In this present study, the model validation was done based on the temperature profile obtained from the simulation study which was compared with the temperature profile obtained from experimental results provided by Niesbach *et al.* (2012). Table 4.3 summarized the data obtained from these points and the errors are also shown in the table.

Table 4.3: Comparison of simulation and experimental results for temperature profile.

Tray of column	**Experimental Results**	**Simulation Results**	**Error (%)**
1	356 K	342 K	3.9
5	362 K	360 K	0.6

Tray of column	**Experimental Results**	**Simulation Results**	**Error (%)**
18	371 K	371 K	0.0
22	365 K	365 K	0.0
33	373 K	369 K	1.1

Based on the data tabulated above, it can be seen that the temperature profile of the simulation data is agreeable with the experimental temperature profile over the whole column height. The error is the largest at the 1st stage of the column with a 3.9 % error whereas stages 18th and 22nd which are the AA and BuOH feed stage respectively show 0 % error.

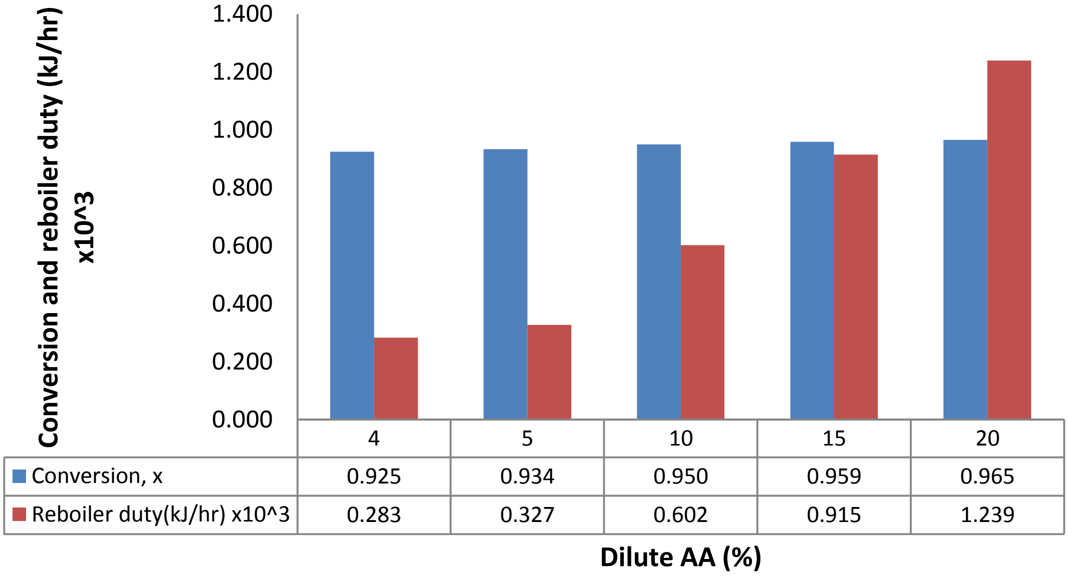
On the other hand, the simulation results obtained by Niesbach *et al.* (2012), showed an excellent agreement with the experimental results with the largest error was just 1.12 %. This is due to the fact that RATEFRAC was considered by Niesbach *et al.* (2012) in their simulation study whereas for this present study, RADFRAC was being applied. Thus, a relatively larger error obtained may be due to RADFRAC which does not consider the actual transport rates which include the mass and energy transfer of each stage (Taylor and Krishna, 2000). Nevertheless, the error is still within the acceptable range.

4.3 Process analysis

In this section, the validated model was used to investigate the effect of varying various process parameters on the resulting composition profile. This analysis illustrates the influence of the operating parameters on the conversion of AA to its product (BA) and also to identify a suitable operating condition to recover most of the dilute acrylic acid in the wastewater stream. Within this analysis, the AA concentration, catalyst loading, bottom rate, reflux ratio, number of stages required in reactive section and number of stages required in separator section were varied.

4.3.1 Acrylic acid (AA) concentration

AA concentration refers to the AA concentration in the feed stream. The AA concentration was varied from 4-20 % w/w in this present study. This was based upon the past research carried out by Kumar *et al.* (2010) which reported that the typical concentration of AA found to contain in the wastewater stream range from 4-10 % w/w. The AA concentration was varied from 4-20 % w/w with an increment of 1 % w/w for 4-5 % w/w and an increment of 5 % w/w from 5-20 % w/w. Figure 4.2 illustrates the effects of varying the AA concentration on the reboiler duty and conversion of the reactant with the feed ratio, top pressure, reflux ratio and distillate-to feed ratio were fixed.



	4	5	10	15	20
🟦 Conversion, x	0.925	0.934	0.950	0.959	0.965
🟥 Reboiler duty(kJ/hr) x10^3	0.283	0.327	0.602	0.915	1.239

Figure 4.2: The effects on conversion and reboiler duty for different AA concentration

Based on Figure 4.2, it was noted that there was not any significant changes in the conversion of the reactant as the AA concentration was varied from 4-20 % w/w. However, the reboiler duty of the RDC increased significantly as the AA concentration was varied from 4-20 % w/w. From Figure 4.2, when the AA concentration is at 4 % w/w, the reboiler duty was approximately 283 kJ/hr with a conversion of 0.925. On the other hand, when the AA concentration increased to 10 % w/w in the feed stream, the reboiler duty increases significantly to 602 kJ/hr but the conversion just increases slightly to 0.950. A higher AA concentration would cause an increased in the reboiler duty since a higher duty is needed in order to boil up the raffinate back to the column to enhance the separation process. Since the conversion for the systems with different AA concentration are comparable and most of the waste containing AA is less than 10 % w/w, thus, 4 % w/w of AA concentration was chosen for the subsequent simulation study. Results summary for selection value of AA concentration is stated in Appendix B.

4.3.2 Catalyst loading

Screening was done on the catalyst loading in order to determine the appropriate amount of catalyst in order to achieve the optimum conversion. It is an important factor which needs to be considered for RDC design. Table 4.4 summarized the operating conditions for the sensitivity analysis for catalyst loading while Figure 4.3 shows the graph of conversion versus catalyst loading.

Table 4.4: Operating conditions for catalyst loading sensitivity analysis

Operating conditions	**Value**
AA concentration	4 % w/w
Catalyst loading	0.055 – 0.205 kg/m
Reboiler duty	283.133 kJ/hr
Reflux ratio	1.458
Number of reactive trays	5
Number of rectifying trays	16
Number of stripping trays	10

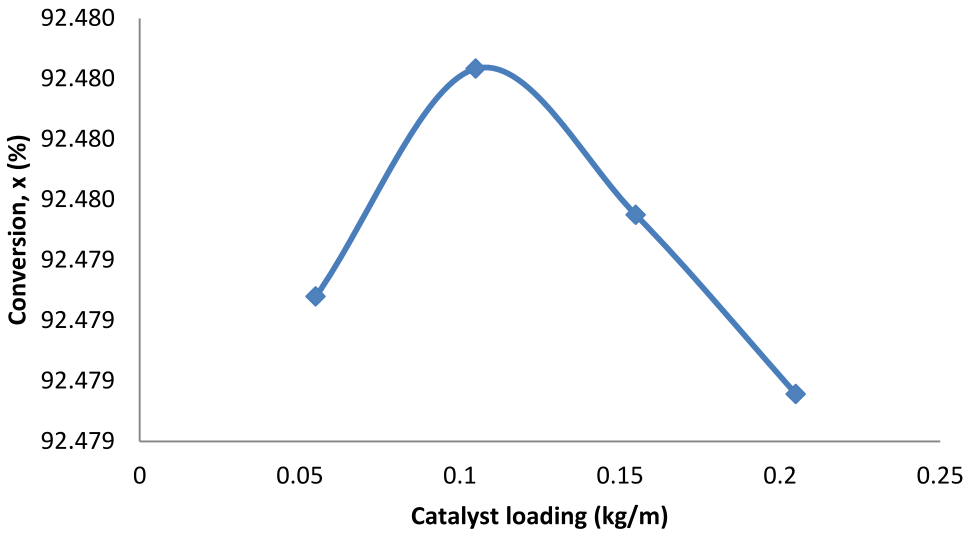


Figure 4.3: Conversion as a function of catalyst loading

From Figure 4.3, it can be seen that the conversion does not increase or decrease drastically as the catalyst loading increases from 0.05 to 0.205 kg/m with an increment of 0.005 kg/m. The maximum conversion for the dilute AA system of 92.480 % was obtained when the catalyst loading was at 0.105 kg/m whereas further increment in the catalyst loading will lead to the decrement of conversion of reactant. Excess catalyst has led to the ester decomposition (Subawalla and Fair, 1999). The catalyst loading lower than 0.105 kg/m is insufficient to yield the highest conversion. Therefore, a least amount of catalyst loading of 0.105 kg/m was used for further analysis. Result summary for each change in the catalyst loading is stated in the Appendix C.

4.3.3 Reboiler duty

Generally, reboilers are heat exchangers which were used to provide heat to the bottom of distillation columns. Reboiler aids in the separation process as it boils the liquid which was collected in the bottom stream to generate vapors which were then returned to the column. Table 4.5 shows the operating conditions for the sensitivity study on reboiler duty and Figure 4.4 illustrates the effects of varying the reboiler duty on the conversion of the reactant in the RDC.

Table 4.5: Operating conditions for reboiler duty sensitivity analysis

Operating conditions	**Value**
AA concentration	4 % w/w
Catalyst loading	0.105 kg/m
Reboiler duty	265 - 283.133 kJ/hr
Reflux ratio	1.458
Number of reactive trays	5
Number of rectifying trays	16
Number of stripping trays	10

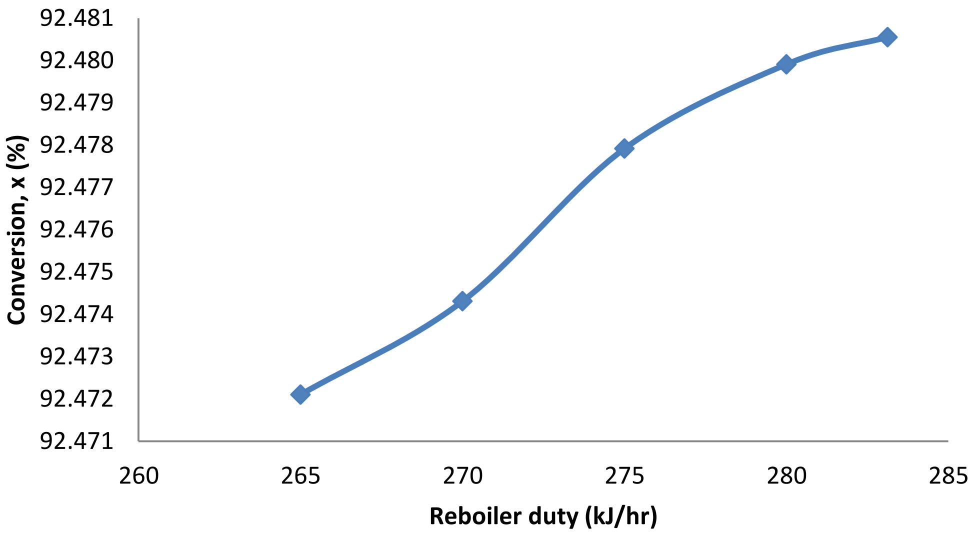


Figure 4.4: Conversion as a function of reboiler duty

Since the esterification of AA with n-butanol (BuOH) forms heterogeneous azeotropic mixture of AA-BuOH-BA at the bottom of the distillation column (Zeng *et al.*, 2006), then it is important to control the reboiler duty whereby it is an important aspect in obtaining the highest conversion and purity of the desired product (BA). Zeng *et al.* (2006) reported that higher purity of BA was achieved when the column was designed properly. Thus, by varying the reboiler duty in the RDC, it will ensure more BA to be recovered in the bottom stream as the separation process is enhanced.

From Figure 4.4, higher reboiler duty will results in higher conversion of AA. When the reboiler duty was 265 kJ/hr, the conversion was approximately 92.472 % and reached 92.481 % when the reboiler duty was 283.133 kJ/hr. Based on Figure 4.4, it can be seen that the conversion increased steadily as the reboiler duty increase. From Figure 4.5, it can be seen that a higher reboiler duty will promote a higher conversion of reactant with a decrease in temperature over the reactive section. Based on Le Chatelier's principles, since the esterification process between AA and BuOH is an exothermic and equilibrium-limited reaction, lower temperature is more desired as it will shift the equilibrium to the product side which will increase the conversion of AA to BA. For further sensitivity analysis, it can be concluded that higher reboiler duty results in an increase in reactant conversion. Results summary for changes in reboiler duty is stated in Appendix D.

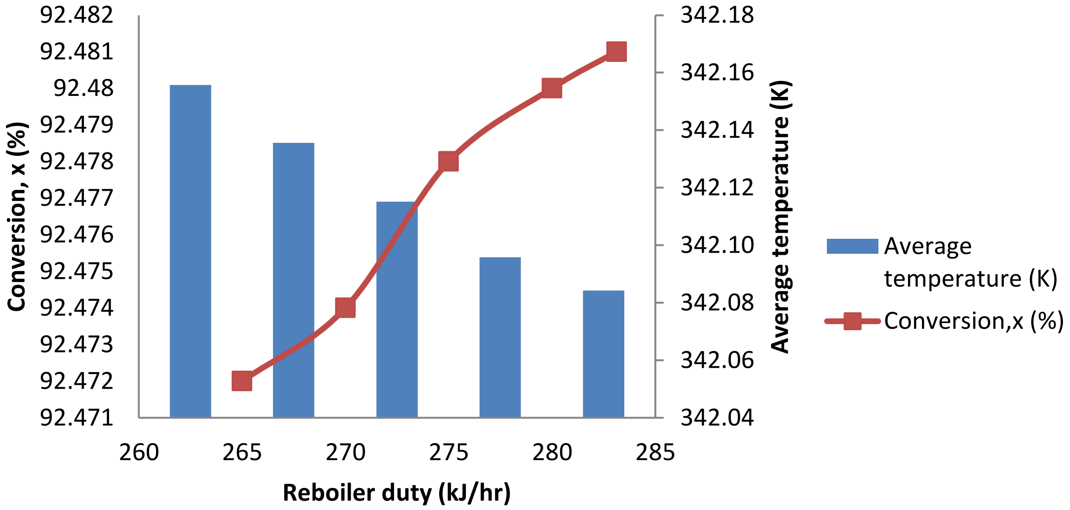


Figure 4.5: Average temperature in the reactive section and conversion as a function of reboiler duty

4.3.4 Reflux ratio

Reflux is the liquid condensed from the rising vapour which returns to the overhead. Reflux ratio is the ratio between the boil up rate and the take-off rate. It is also defined as the ratio between the amount of reflux that returns back into the column and the amount of reflux which was collected as distillate.

Reflux ratio drastically impacts the reactive zone residence time in equilibrium limited system. Incomplete conversion of reactant happens when excess reflux is present inside the column which would lead to operating hiccups and insufficient reaction holdup (Agreda *et al.*, 1990). Figure 4.6 shows the conversion as a function of reflux ratio while Table 4.6 summarized the operating conditions for the sensitivity study on reflux ratio.

Table 4.6: Operating condition for reflux ratio sensitivity analysis

Operating conditions	**Value**
AA concentration	4 % w/w
Catalyst loading	0.105 kg/m
Reboiler duty	283.133 kJ/hr
Reflux ratio	1.0 – 2.0
Number of reactive trays	5
Number of rectifying trays	16
Number of stripping trays	10

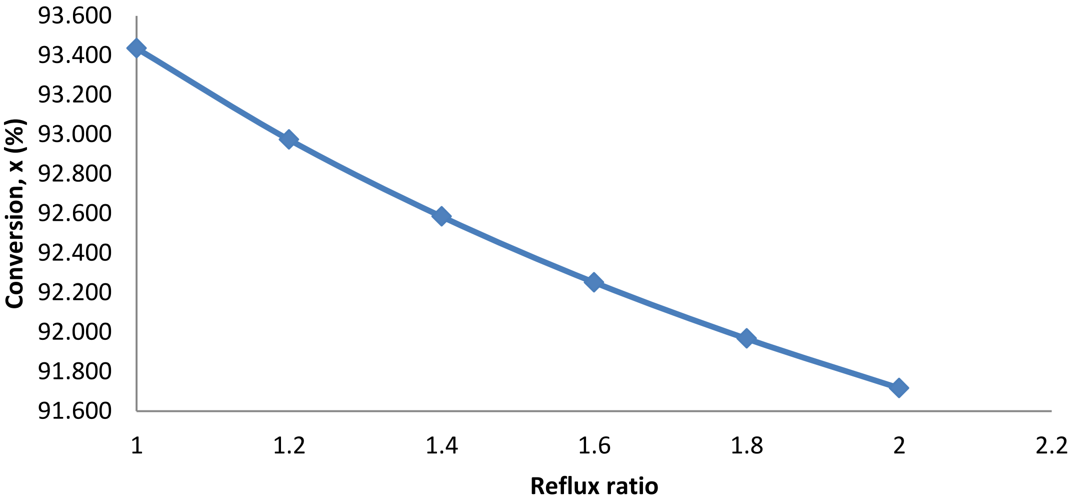


Figure 4.6: Conversion as a function of reflux ratio

From Figure 4.6, as the reflux ratio increase from 1.0 to 2.0 with an increment of 0.2, the conversion decreases significantly. When the reflux ratio was 1.0, the conversion was approximately 93.4 % and subsequently 1.2 (93.0 %), 1.4 (92.6 %), 1.6 (92.3 %), 1.8 (92.0 %) and 2.0 (91.7 %). Since there is a minimal difference in the boiling point between reactants and products of the esterification of AA and BuOH, the reflux ratio will greatly effects the conversion of AA. Table 4.7 below summarized the boiling point of each species in the esterification process. Increase in reflux ratio has led to low concentration of n-butyl acrylate and AA in the bottom and distillate stream respectively. In turn, the recycled distillate stream contains a high amount of BuOH which dilutes both AA and n-butyl acrylate. This in turn will cause the conversion to decreased due to the temperature and composition changes which results in slower reaction rate. Figure 4.7 illustrates the changes in liquid composition of AA, BuOH and BA as a function of reflux ratio and Figure 4.8 shows the changes in the temperature profile at the reactive section as a function of reflux ratio. Reflux ratio lesser than 1.0 cannot be analyzed as a value lower than 1.0 will cause the mass and energy balance in the RDC simulated by Aspen Plus cannot be balance due to convergence in the column cannot be achieved. Therefore, the sensitivity analysis on reflux ratio was carried out from 1.0 to 2.0. It can be concluded that lower reflux ratio is more favoured for this esterification process whereby it will be considered for further sensitivity studies. Result summary for changes in the reflux ratio is stated in Appendix E.

Table 4.7: Boiling point of each component

Component	**Boiling point (K)**
Acrylic Acid	414
n-Butanol	391
n-Butyl Acrylate	421
Water	373

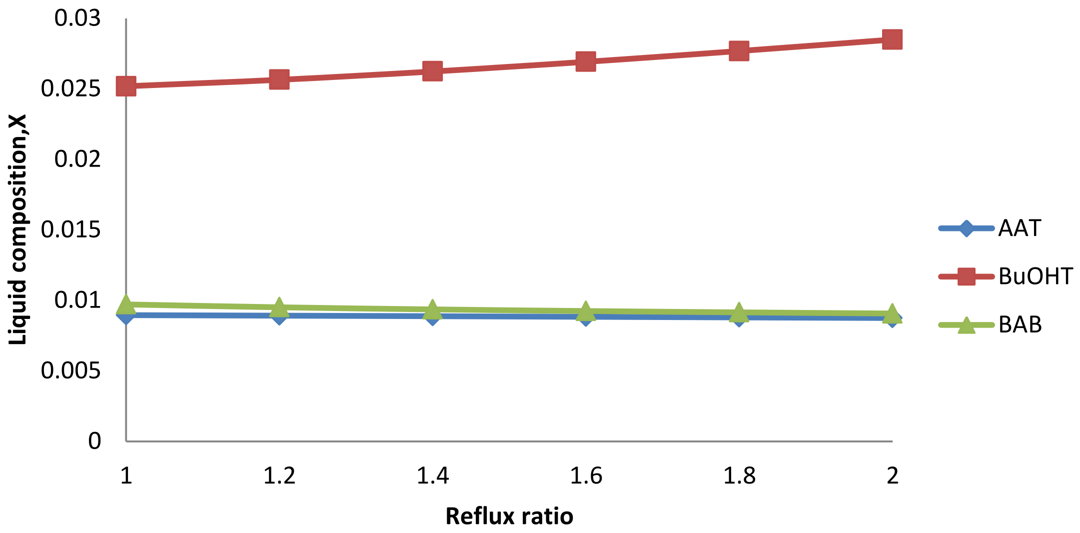


Figure 4.7: Liquid composition of AA, BuOH and BA as a function of reflux ratio

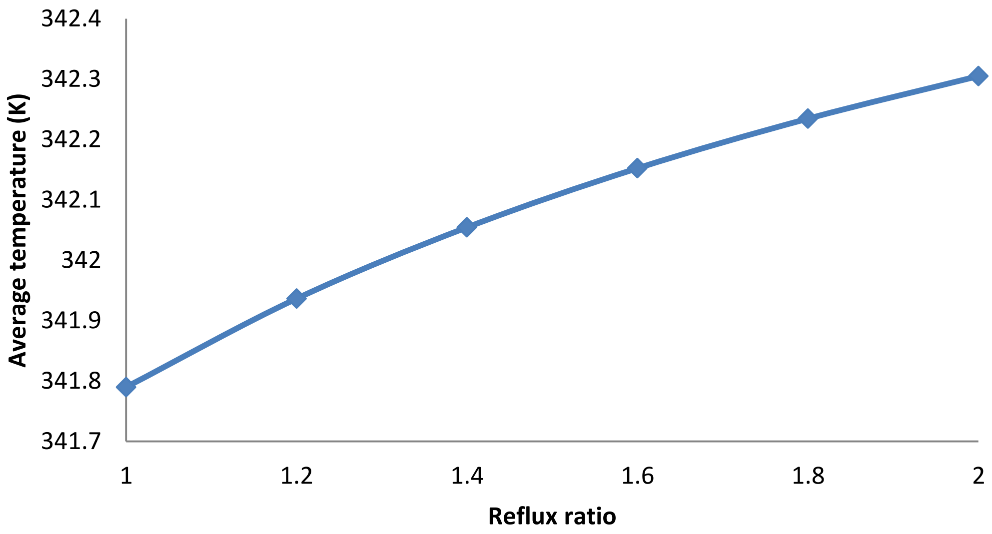


Figure 4.8: Temperature profile of reactive section as a function of reflux ratio

4.3.5 Number of trays required in reactive section

Increasing the reactive section trays requirement is not always the better choice due to the changes in the packing height could affect the column separation performance, thus changing the composition in the reactive section. Therefore, analysis study was carried out by varying the number of trays in the reactive section. Table 4.8 summarized the operating conditions while Figure 4.9 illustrates the conversion as a function of number of trays in the reactive section of the RDC.

Table 4.8: Operating conditions for the number of trays in reactive section sensitivity analysis

Operating conditions	**Value**
AA concentration	4 % w/w
Catalyst loading	0.105 kg/m
Reboiler duty	283.133 kJ/hr
Reflux ratio	1.0
Number of reactive trays	1-7
Number of rectifying trays	16
Number of stripping trays	10

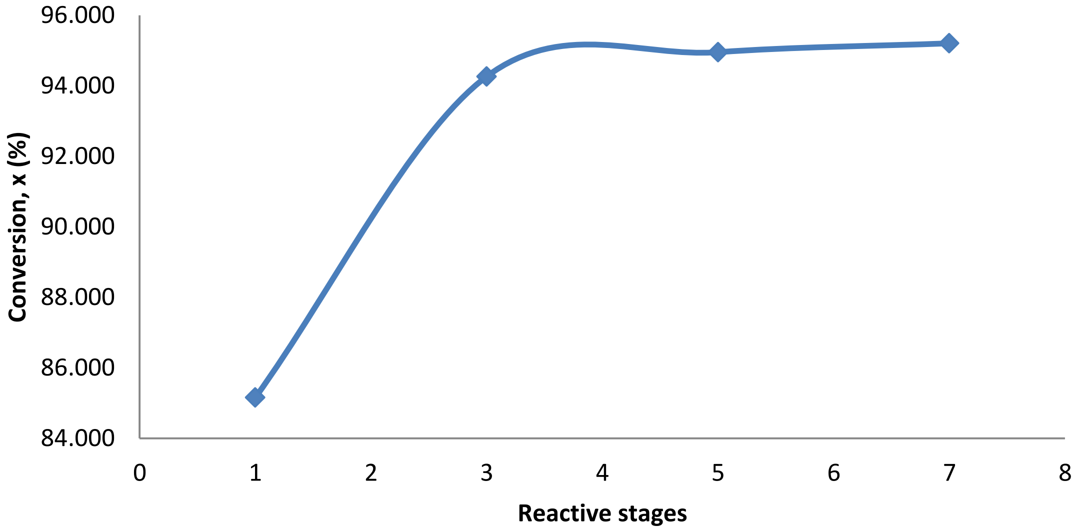


Figure 4.9: Conversion as a function of number of trays in reactive section

Based on Figure 4.9, it can be seen that conversion of 95.2 % is achieved when there are 7 trays in the reactive section whereas only 85.2 % of AA was converted when there was only 1 tray in the reactive section. Generally, from Figure 4.9, it can be seen that the number of trays in the reactive section played an important role in conversion of AA. This is because RDC plays a role as an efficient and effective separation unit that enhances the product productivity. As water acts as an intermediate boiler in the column, thus, it is important to maintain the separation efficiency in order to achieve a higher conversion by driving the equilibrium to the product side and thus, preventing any undesired side reactions between reactant and product. It is also to prevent detrimental sorption effect on the reaction kinetics since this process is equilibrium limited reaction (Steinigeweg and Gmehling, 2003). Furthermore, when the number of trays in the reactive section was further increased beyond 7, sensitivity analysis cannot be studied as the mass and energy balance in the RDC simulated by Aspen Plus cannot be balance due to convergence in the column cannot be achieved. Therefore, based on Figure 4.9, increasing the number of trays to 7 in the reactive section is more favourable compared to maintaining the original 5 trays in the reactive section as the conversion will increase as the number of trays increased to 7. Result summary for different number of trays in the reactive section on the composition is stated in the Appendix F.

4.3.6 Number of trays required in separation section

The separation section is made up of the rectifying and stripping section which are located above and below of the reactive section respectively. The rectifying section in this study plays a role in removing water from the reactive zone and to prevent loss of AA and BA from the reactive zone whereas for the stripping section, it is to prevent BA from remaining in the reactive section in order to shift the reaction to the product side and also to purify the product thus high purity of BA is achievable. Table 4.9 shows the operating conditions while Figure 4.10 and 4.11 shows the conversion as a function of number of trays required in the rectifying and stripping section respectively. Besides that, Figure 4.12 and 4.13 illustrates the liquid composition of AA and BA as a function of rectifying and stripping stages respectively.

Table 4.9: Operating conditions for number of trays of rectifying and stripping section sensitivity analysis

Operating conditions	**Value**
AA concentration	4 % w/w
Catalyst loading	0.105 kg/m
Reboiler duty	283.133 kJ/hr
Reflux ratio	1.0
Number of reactive trays	7

Operating conditions	Value
Number of rectifying trays	0 - 12
Number of stripping trays	0 - 4

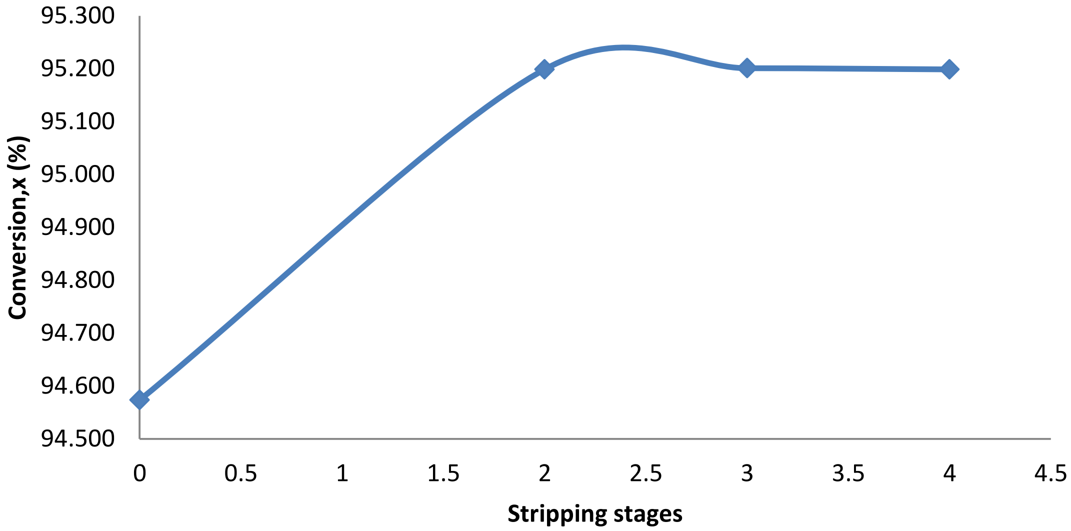


Figure 4.10: Conversion as a function of number of rectifying stages

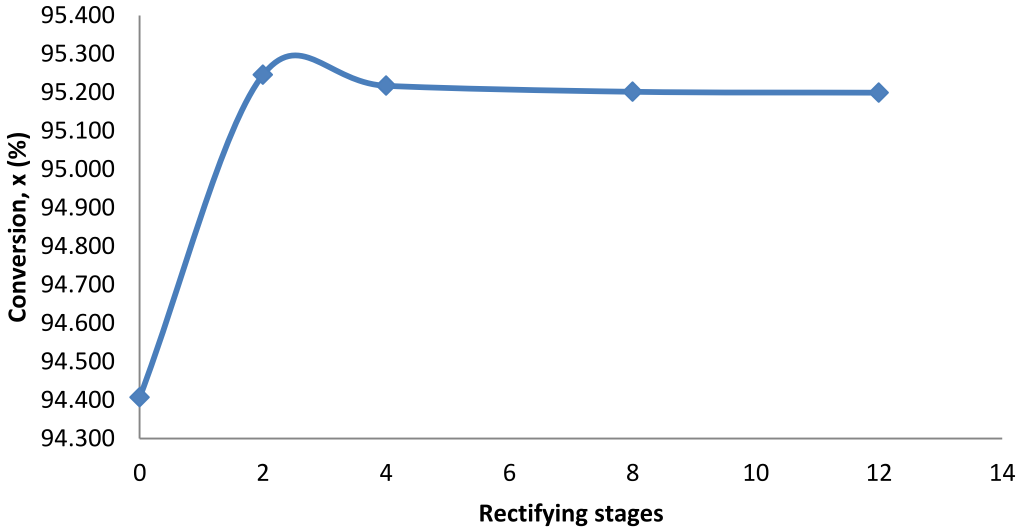


Figure 4.11: Conversion as a function of number of stripping stages

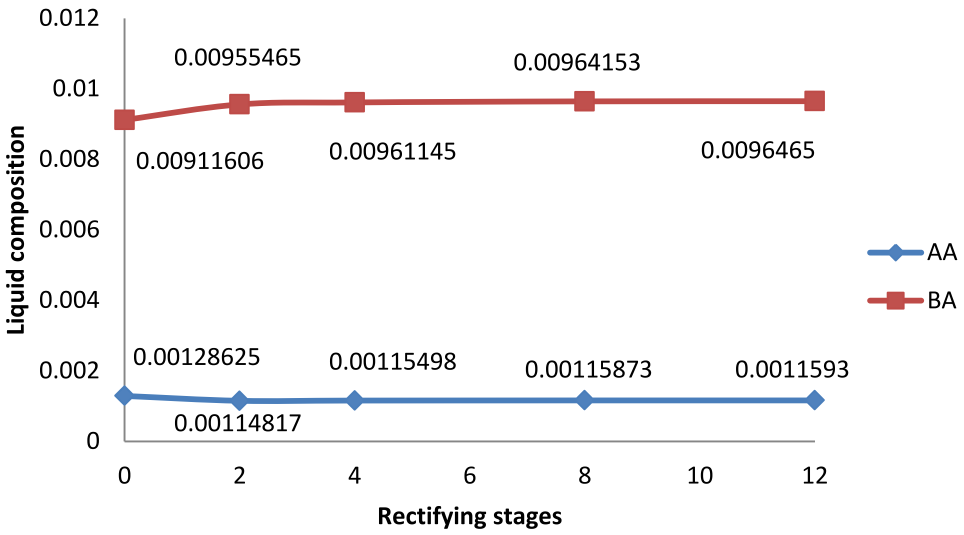


Figure 4.12: Liquid composition of AA and BA as a function of rectifying stages

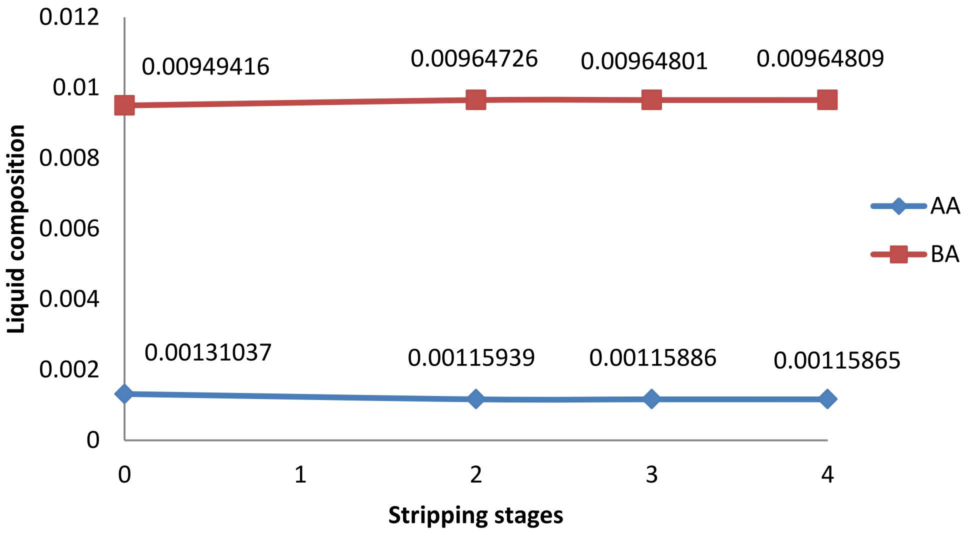


Figure 4.13: Liquid composition of AA and BA as a function of stripping stages

From Figure 4.10 and 4.11, it can be seen that both the rectifying and stripping section only required 2 stages respectively to achieve the optimum conversion. Besides that, from Figure 4.12 and 4.13, it can be seen that the liquid composition of AA decreased in order to form BA. The most significant changes in the liquid composition of both species could be seen when zero trays were introduced to 2 trays was introduced into the rectifying and stripping section respectively. From all the figures above, it can be seen that increasing the number of stages in the rectifying and stripping section will further enhance the separation process by removing water from the reactive section and purifies BA further in the bottom stream which in turn will increase the conversion.

Moreover, based on all figures above, increasing the number of stages in the rectifying and stripping section does not increased further the conversion of AA for the esterification process. Simulation studies shown that only 2 stages were needed in the rectifying and stripping section in order to achieved the optimum conversion. Result summary for variation on the number of stages in the rectifying and stripping section is stated in Appendix G and H.

4.4 The optimized process

After studying the various effect of operating parameter conditions, an optimized condition was identified by proposing a suitable configuration for the reactive distillation column. Figure 4.12 shows the mass balance and Table 4.10 shows the optimized condition for the esterification process of dilute AA in RDC.

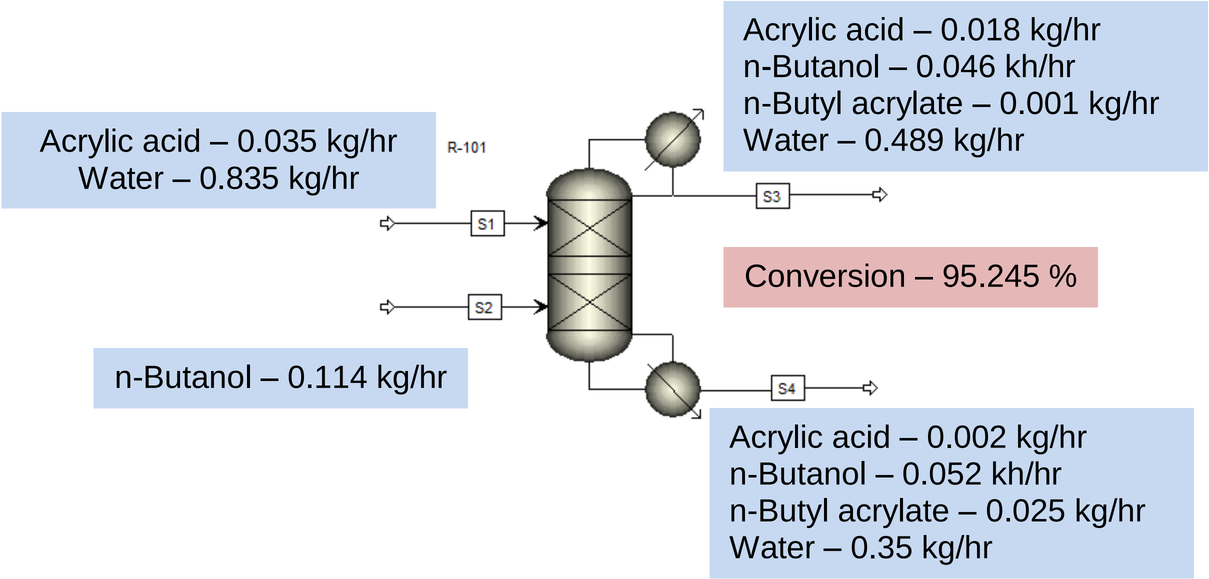


Figure 4.14: Mass balance for the esterification of dilute AA

Table 4.10: Optimized condition for esterification of dilute AA

Operating parameter conditions						
AA concentration	Catalyst loading	Reboiler duty	Reflux ratio	Number of reactive trays	Number of rectifying trays	Number of stripping trays
4 % w/w	0.105 kg/m	283.13 kJ/hr	1.0	7	2	2

4.5 Summary

By referring to the review done in the literature, a suitable model was proposed for the esterification of dilute AA in RDC. The proposed model was validated with experimental data from past research and it showed an agreeable result for the temperature profile between the simulation and experimental data. Finally, the validated modelwas used to study the effects of different operating parameter conditions for the esterification of dilute AA whereby an optimized condition was identified by the end of the study.

5 CONCLUSION AND RECOMMENDATION

5.1 Overview

This chapter discusses on the conclusion and recommendation that can be made from the results obtained from the simulation study. The conclusion was made in order to determine whether the main objective of this present study, which is to examine the efficiency of recovering AA from the wastewater containing AA and also to investigate the effects of different operating parameter conditions on the esterification of dilute AA with n-butanol in RDC, was accomplished. Besides, several recommendations were proposed in order to be referred to when further study is carry out in this esterification process in RDC.

5.2 Introduction

The environmental and economical issues regarding the recovery of dilute AA from the wastewater stream has gained a tremendous attention in the industry. Thus, a method for recovering AA was carried out in RDC through esterification process with BuOH in order to produce BA. This study was done through simulation studies in Aspen Plus V7.0. Before analysis studies were carried out in order to determine the best operating condition for the recovery of dilute AA in the wastewater stream, the model was chosen based on the appropriate RD model, kinetic model and thermodynamic model was validated with experimental data obtained from past research paper.

5.3 Conclusion for overall findings

From the simulation results collected, it can be concluded that the production of BA from dilute AA and BuOH through esterification process in RDC was feasible and concluding the achievement of the first objective of this study which is to examine the efficiency of recovering AA from the wastewater containing AA.

Finally, sensitivity analysis was conducted in order to determine the effect of different operating parameter conditions in recovering 4 % w/w AA from the wastewater stream. From the results, it can be concluded that the best operating conditions in recovering 4 % w/w from wastewater stream are with a catalyst loading of 0.105 kg/m, reboiler duty of 283.133 kJ/hr, reflux ratio of 1.0 and finally with 7 trays in the reactive section and 2 trays in the rectifying and stripping section respectively.

Furthermore, from the sensitivity analysis, it can be seen that reflux ratio and number of trays introduced into the reactive section affect greatly the overall reaction in the RDC. With these operating conditions, 95.245 % of AA managed to be converted into BA.

5.4 Recommendation

Several recommendations were proposed by the author in order to be considered in future work for the simulation of RDC for esterification process of dilute AA. The recommendations are as follows:

a. Other simulation engine such as PRO/II can be considered in order to study the esterification of dilute AA in RDC. PRO/II is a steady state process simulation for process design and operational analysis which does not differ far from Aspen Plus. Besides that, PRO/II allows the user to introduce a user defined subroutine easily whereby PRO/II comes with a built in program without the need of purchasing an external compiler unlike Aspen Plus. With this, the effect of introducing user defined subroutine in PRO/II for the esterification of dilute AA with n-butanol on the conversion and operating parameter conditions can be determined.
b. Other kinetic models such as Langmuir-Hinshelwood-Hougen-Watson (LHHW) which has been previously applied by Niesbach *et al.* (2012) in the esterification process of AA with BuOH can be considered in future study as to determine the effect of different kinetic model on the esterification process of dilute AA.
c. Lastly, non-equilibrium model (RATEFRAC) can be considered in future work for the production of n-butyl acrylate in RDC. This is to determine the effect imposed by RATEFRAC on the conversion and operating parameter conditions.

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APPENDIX A

```
# Stoichiometry
d(X) / d(t) = -rA / CA0
X(0) = 0
m=1       #kg/m dry catalyst mass
c=0.79         #concentration of active sites
rA = ((m*c)*(-k)*((aAA*aBuOH)-(aBA*aW/Ke))/((1+K1*aAA+K2*aBuOH+K3*aBA+K4*aW)^2))
CAA=CA0*(1-X)
CBuOH=CB0-CA0*X
CBA=CA0*X
CW=CA0*X
CA0=1.21       #kmol/L
CB0=3.94       #kmol/L
aAA=xAA*gAA
aBuOH=xBuOH*gBuOH
aBA=xBA*gBA
aW=xW*gW
CT=CAA+CBuOH+CBA+CW
xAA=CAA/CT
xBuOH=CBuOH/CT
t(0) = 0
t(f) = 24
xBA=CBA/CT
xW=CW/CT
gAA=(0.2782*(xAA)^2)+(0.0877*xAA)+0.4545
gBuOH=(-2.6139*(xBuOH)^2)+(3.8392*xBuOH)-0.4337
gBA=(0.9507*xBA)+0.2728
gW=(0.1132*(xW)^2)+(0.0024*xW)+0.0866
Ke=exp((-1888.66/T)+8.17)
T=350             #K
R=8.314
k=1.2276e14*exp(-81260/(R*T))
K1=0.244
K2=0.748
K3=2.105
K4=2.288
```

Figure A.1: Data analysis in Polymath for 350K

```
# Stoichiometry
d(X) / d(t) = -rA / CA0
X(0) = 0
m=1        #kg/m dry catalyst mass
c=0.79          #concentration of active sites
rA = ((m*c)*(-k)*((aAA*aBuOH)-(aBA*aW/Ke))/((1+K1*aAA+K2*aBuOH+K3*aBA+K4*aW)^2))
CAA=CA0*(1-X)
CBuOH=CB0-CA0*X
CBA=CA0*X
CW=CA0*X
CA0=1.21        #kmol/L
CB0=3.94        #kmol/L
aAA=xAA*gAA
aBuOH=xBuOH*gBuOH
aBA=xBA*gBA
aW=xW*gW
CT=CAA+CBuOH+CBA+CW
xAA=CAA/CT
xBuOH=CBuOH/CT
t(0) = 0
t(f) = 4
xBA=CBA/CT
xW=CW/CT
gAA=(0.2769*(xAA)^2)+(0.0885*xAA)+0.4699
gBuOH=(-2.5488*(xBuOH)^2)+(3.744*xBuOH)-0.3982
gBA=(0.9548*xBA)+0.2818
gW=(0.1215*(xW)^2)+(0.0016*xW)+0.0966
Ke=exp((-1888.66/T)+8.17)
T=360              #K
R=8.314
k=1.2276e14*exp(-81260/(R*T))
K1=0.244
K2=0.748
K3=2.105
K4=2.288
```

Figure A.2: Data analysis in Polymath for 360K

```
# Stoichiometry
d(X) / d(t) = -rA / CA0
X(0) = 0
m=1        #kg/m dry catalyst mass
c=0.79         #concentration of active sites
rA = ((m*c)*(-k)*((aAA*aBuOH)-(aBA*aW/Ke))/((1+K1*aAA+K2*aBuOH+K3*aBA+K4*aW)^2))
CAA=CA0*(1-X)
CBuOH=CB0-CA0*X
CBA=CA0*X
CW=CA0*X
CA0=1.21        #kmol/L
CB0=3.94        #kmol/L
aAA=xAA*gAA
aBuOH=xBuOH*gBuOH
aBA=xBA*gBA
aW=xW*gW
CT=CAA+CBuOH+CBA+CW
xAA=CAA/CT
xBuOH=CBuOH/CT
t(0) = 0
t(f) = 2
xBA=CBA/CT
xW=CW/CT
gAA=(0.2753*(xAA)^2)+(0.089*xAA)+0.4847
gBuOH=(-2.485*(xBuOH)^2)+(3.6507*xBuOH)-0.3635
gBA=(0.9577*xBA)+0.2905
gW=(0.1295*(xW)^2)+(0.0005*xW)+0.107
Ke=exp((-1888.66/T)+8.17)
T=370              #K
R=8.314
k=1.2276e14*exp(-81260/(R*T))
K1=0.244
K2=0.748
K3=2.105
K4=2.288
```

Figure A.3: Data analysis in Polymath for 370K

```
# Stoichiometry
d(X) / d(t) = -rA / CA0
X(0) = 0
m=1       #kg/m dry catalyst mass
c=0.79          #concentration of active sites
rA = ((m*c)*(-k)*((aAA*aBuOH)-(aBA*aW/Ke))/((1+K1*aAA+K2*aBuOH+K3*aBA+K4*aW)^2))
CAA=CA0*(1-X)
CBuOH=CB0-CA0*X
CBA=CA0*X
CW=CA0*X
CA0=1.21       #kmol/L
CB0=3.94       #kmol/L
aAA=xAA*gAA
aBuOH=xBuOH*gBuOH
aBA=xBA*gBA
aW=xW*gW
CT=CAA+CBuOH+CBA+CW
xAA=CAA/CT
xBuOH=CBuOH/CT
t(0) = 0
t(f) = 2
xBA=CBA/CT
xW=CW/CT
gAA=(0.2744*(xAA)^2)+(0.0892*xAA)+0.4919
gBuOH=(-2.4537*(xBuOH)^2)+(3.6049*xBuOH)-0.3464
gBA=(0.9586*xBA)+0.2948
gW=(0.1334*(xW)^2)-(0.0002*xW)+0.1124
Ke=exp((-1888.66/T)+8.17)
T=375              #K
R=8.314
k=1.2276e14*exp(-81260/(R*T))
K1=0.244
K2=0.748
K3=2.105
K4=2.288
```

Figure A.4: Data analysis in Polymath for 375K

```
# Stoichiometry
d(X) / d(t) = -rA / CA0
X(0) = 0
m=1       #kg/m dry catalyst mass
c=0.79          #concentration of active sites
rA = ((m*c)*(-k)*((aAA*aBuOH)-(aBA*aW/Ke))/((1+K1*aAA+K2*aBuOH+K3*aBA+K4*aW)^2))
CAA=CA0*(1-X)
CBuOH=CB0-CA0*X
CBA=CA0*X
CW=CA0*X
CA0=1.21       #kmol/L
CB0=3.94       #kmol/L
aAA=xAA*gAA
aBuOH=xBuOH*gBuOH
aBA=xBA*gBA
aW=xW*gW
CT=CAA+CBuOH+CBA+CW
xAA=CAA/CT
xBuOH=CBuOH/CT
t(0) = 0
t(f) = 1
xBA=CBA/CT
xW=CW/CT
gAA=(0.2734*(xAA)^2)+(0.0894*xAA)+0.4989
gBuOH=(-2.4228*(xBuOH)^2)+(3.5595*xBuOH)-0.3295
gBA=(0.9594*xBA)+0.299
gW=(0.1371*(xW)^2)-(0.0009*xW)+0.1179
Ke=exp((-1888.66/T)+8.17)
T=380              #K
R=8.314
k=1.2276e14*exp(-81260/(R*T))
K1=0.244
K2=0.748
K3=2.105
K4=2.288
```

Figure A.5: Data analysis in Polymath for 380K

APPENDIX B

Operating parameter conditions:

AA concentration: 4 % w/w
Catalyst loading: 0.205 kg/m
Reboiler duty: 283.13 kJ/hr
Reflux ratio: 1.458
Number of reactive trays: 5
Number of rectifying trays: 16
Number of stripping trays: 10

Table B.1: Result summary for AA concentration at 4 % w/w

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.46	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.41	68.46
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3397.43	-3304.6
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.17	-40.07
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.53	44.82
Mass Density	KG/CUM	0.55	722.54	931.15	924.09
Average Molecular Weight		18.57	74.12	20.01	20.62

Operating parameter conditions:

AA concentration: 5 % w/w
Reboiler duty: 283.13 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.205 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table B.2: Result summary of AA concentration at 5 % w/w

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.14	0.47	0.54
Volume Flow	CUM/HR	1.56	0	0	0
Temperature	C	130.85	107.85	68.21	68.16
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.18	-73.9	-68.06	-68.35
Mass Enthalpy	KCAL/KG	-3054.81	-997.03	-3350.48	-3185.72
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.31	-119.68	-39.59	-41.21
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.95	-1.92
Molar Density	KMOL/CUM	0.03	9.75	45.72	42.78
Mass Density	KG/CUM	0.56	722.54	928.73	917.76
Average Molecular Weight		18.72	74.12	20.31	21.45

Operating parameter conditions:

AA concentration: 10 % w/w	Catalyst loading: 0.205 kg/m
Reboiler duty: 283.13 kJ/hr	Reflux ratio: 1.458
Number of reactive trays: 5	Number of rectifying trays: 16
Number of stripping trays: 10	

Table B.3: Result summary of AA concentration at 10 % w/w

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.04	0	0.02	0.02
Mole Flow	KMOL/HR	0.04	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.28	0.53	0.62
Volume Flow	CUM/HR	1.5	0	0	0
Temperature	C	130.85	107.85	67.56	68.15
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.48	-73.9	-68.28	-69.55
Mass Enthalpy	KCAL/KG	-2951.21	-997.03	-3203.13	-2630.64
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.56	-119.68	-41.21	-47.55
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.93	-1.8
Molar Density	KMOL/CUM	0.03	9.75	43.13	33.72
Mass Density	KG/CUM	0.58	722.54	919.52	891.47
Average Molecular Weight		19.48	74.12	21.32	26.44

Operating parameter conditions:

AA concentration: 15 % w/w
Reboiler duty: 283.13 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.205 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table B.4: Result summary of AA concentration at 15 % w/w

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0.01	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.04	0	0.03	0.02
Mole Flow	KMOL/HR	0.04	0.01	0.03	0.02
Mass Flow	KG/HR	0.87	0.42	0.6	0.7
Volume Flow	CUM/HR	1.44	0	0	0
Temperature	C	130.85	107.85	67.28	68.54
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.81	-73.9	-68.4	-71.04
Mass Enthalpy	KCAL/KG	-2846.43	-997.03	-3123.88	-2164.32
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.85	-119.68	-42.23	-55.4
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.93	-1.69
Molar Density	KMOL/CUM	0.03	9.75	41.74	26.6
Mass Density	KG/CUM	0.6	722.54	913.92	873.09
Average Molecular Weight		20.31	74.12	21.9	32.82

Operating parameter conditions:

AA concentration: 20 % w/w
Catalyst loading: 0.205 kg/m
Reboiler duty: 283.13 kJ/hr
Reflux ratio: 1.458
Number of reactive trays: 5
Number of rectifying trays: 16
Number of stripping trays: 10

Table B.5: Result summary of AA concentration at 20 % w/w

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0.01	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.04	0	0.03	0.01
Mole Flow	KMOL/HR	0.04	0.01	0.03	0.02
Mass Flow	KG/HR	0.87	0.57	0.67	0.77
Volume Flow	CUM/HR	1.38	0	0	0
Temperature	C	130.85	107.85	67.12	69.13
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-58.16	-73.9	-68.48	-72.85
Mass Enthalpy	KCAL/KG	-2744.02	-997.03	-3068.53	-1782.64
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-9.18	-119.68	-42.98	-65.27
Mass Entropy	CAL/GM-K	-0.43	-1.61	-1.93	-1.6
Molar Density	KMOL/CUM	0.03	9.75	40.78	21.01
Mass Density	KG/CUM	0.63	722.54	909.94	858.67
Average Molecular Weight		21.19	74.12	22.32	40.86

APPENDIX C

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.13 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.055 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table C.1: Result summary of catalyst loading at 0.055 kg/m

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.46	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.41	68.46
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3397.45	-3304.59
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.17	-40.07
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.54	44.82
Mass Density	KG/CUM	0.55	722.54	931.15	924.09
Average Molecular Weight		18.57	74.12	20.01	20.62

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.13 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table C.2: Result summary of catalyst loading at 0.105 kg/m

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.46	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.41	68.46
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3397.42	-3304.61
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.17	-40.07
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.53	44.82
Mass Density	KG/CUM	0.55	722.54	931.14	924.09
Average Molecular Weight		18.57	74.12	20.01	20.62

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.13 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10
Catalyst loading: 0.155 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table C.3: Result summary of catalyst loading at 0.155 kg/m

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.46	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.41	68.46
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3397.42	-3304.62
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.17	-40.07
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.53	44.82
Mass Density	KG/CUM	0.55	722.54	931.14	924.09
Average Molecular Weight		18.57	74.12	20.01	20.62

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.13 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.205 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table C.4: Result summary of catalyst loading at 0.205 kg/m

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.46	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.41	68.46
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3397.43	-3304.6
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.17	-40.07
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.53	44.82
Mass Density	KG/CUM	0.55	722.54	931.15	924.09
Average Molecular Weight		18.57	74.12	20.01	20.62

APPENDIX D

Operating parameter conditions:

AA concentration: 4 % w/w	Catalyst loading: 0.105 kg/m
Reboiler duty: 265 kJ/hr	Reflux ratio: 1.458
Number of reactive trays: 5	Number of rectifying trays: 16
Number of stripping trays: 10	

Table D.1: Result summary of reboiler duty at 265 kJ/hr

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.45	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.61	68.29
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.95	-68.16
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3418.76	-3287.63
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.92	-40.29
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.92	44.52
Mass Density	KG/CUM	0.55	722.54	932.62	922.97
Average Molecular Weight		18.57	74.12	19.88	20.73

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 270 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10
Catalyst loading: 0.105 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table D.2: Result summary of reboiler duty at 270 kJ/hr

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.45	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.55	68.33
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.96	-68.16
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3412.87	-3292.24
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.99	-40.23
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.82	44.6
Mass Density	KG/CUM	0.55	722.54	932.22	923.28
Average Molecular Weight		18.57	74.12	19.91	20.7

Operating parameter conditions:

AA concentration: 4 % w/w	Catalyst loading: 0.105 kg/m
Reboiler duty: 275 kJ/hr	Reflux ratio: 1.458
Number of reactive trays: 5	Number of rectifying trays: 16
Number of stripping trays: 10	

Table D.3: Result summary of reboiler duty at 275 kJ/hr

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.45	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.5	68.38
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.97	-68.15
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3406.97	-3296.92
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.06	-40.17
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.71	44.68
Mass Density	KG/CUM	0.55	722.54	931.81	923.59
Average Molecular Weight		18.57	74.12	19.95	20.67

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 280 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table D.4: Result summary of reboiler duty at 280 kJ/hr

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.45	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.44	68.43
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3401.09	-3301.64
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.13	-40.11
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.6	44.76
Mass Density	KG/CUM	0.55	722.54	931.4	923.9
Average Molecular Weight		18.57	74.12	19.99	20.64

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10
Catalyst loading: 0.105 kg/m
Reflux ratio: 1.458
Number of rectifying trays: 16

Table D.5: Result summary of reboiler duty at 283.133 kJ/hr

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.46	0.53
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.41	68.46
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3397.44	-3304.6
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.17	-40.07
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.54	44.82
Mass Density	KG/CUM	0.55	722.54	931.15	924.09
Average Molecular Weight		18.57	74.12	20.01	20.62

APPENDIX E

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 16

Table E.1: Result summary of reflux ratio at 1.0

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.56	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.52	68.21
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.97	-68.19
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3406.88	-3269.59
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.05	-40.48
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.71	44.2
Mass Density	KG/CUM	0.55	722.54	931.85	921.88
Average Molecular Weight		18.57	74.12	19.95	20.86

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.2
Number of rectifying trays: 16

Table E.2: Result summary of reflux ratio at 1.2

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.51	0.48
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.47	68.33
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.97	-68.16
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3403.53	-3287.77
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.09	-40.27
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.65	44.52
Mass Density	KG/CUM	0.55	722.54	931.59	923.03
Average Molecular Weight		18.57	74.12	19.97	20.73

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.4
Number of rectifying trays: 16

Table E.3: Result summary of reflux ratio at 1.4

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.47	0.52
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.42	68.43
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.98	-68.14
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3398.94	-3301.29
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.15	-40.11
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.56	44.76
Mass Density	KG/CUM	0.55	722.54	931.26	923.88
Average Molecular Weight		18.57	74.12	20	20.64

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10
Catalyst loading: 0.105 kg/m
Reflux ratio: 1.6
Number of rectifying trays: 16

Table E.4: Result summary of reflux ratio at 1.6

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.03
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.43	0.55
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.36	68.51
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.99	-68.13
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3393.53	-3311.77
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.22	-39.99
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.46	44.94
Mass Density	KG/CUM	0.55	722.54	930.86	924.55
Average Molecular Weight		18.57	74.12	20.03	20.57

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.8
Number of rectifying trays: 16

Table E.5: Result summary of reflux ratio at 1.8

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.03
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.4	0.58
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.3	68.58
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-68	-68.11
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3387.47	-3320.18
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.29	-39.89
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.35	45.09
Mass Density	KG/CUM	0.55	722.54	930.42	925.09
Average Molecular Weight		18.57	74.12	20.07	20.51

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 2.0
Number of rectifying trays: 16

Table E.6: Result summary of reflux ratio at 2.0

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.03
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.37	0.61
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.24	68.64
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-68	-68.1
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3380.99	-3327.07
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.37	-39.81
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.95
Molar Density	KMOL/CUM	0.03	9.75	46.23	45.22
Mass Density	KG/CUM	0.55	722.54	929.95	925.52
Average Molecular Weight		18.57	74.12	20.11	20.47

APPENDIX F

Operating parameter conditions:

AA concentration: 4 % w/w	Catalyst loading: 0.105 kg/m
Reboiler duty: 283.133 kJ/hr	Reflux ratio: 1.0
Number of reactive trays: 1	Number of rectifying trays: 16
Number of stripping trays: 10	

Table F.1: Result summary of 1 reactive tray

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.59	0.4
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	67.27	72.83
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-68.25	-67.74
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3211.42	-3544.67
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-41.4	-37.18
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.95	-1.95
Molar Density	KMOL/CUM	0.03	9.75	43.21	49.13
Mass Density	KG/CUM	0.55	722.54	918.22	938.98
Average Molecular Weight		18.57	74.12	21.25	19.11

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 3
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 16

Table F.2: Result summary of 3 reactive trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.57	0.42
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.01	69.02
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-68.05	-68.07
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3347.88	-3346.97
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.74	-39.52
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	45.64	45.57
Mass Density	KG/CUM	0.55	722.54	927.75	926.95
Average Molecular Weight		18.57	74.12	20.33	20.34

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 5
Number of stripping trays: 10

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 16

Table F.3: Result summary of 5 reactive trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.56	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.52	68.21
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.97	-68.19
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3406.88	-3269.59
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-39.05	-40.48
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	46.71	44.2
Mass Density	KG/CUM	0.55	722.54	931.85	921.88
Average Molecular Weight		18.57	74.12	19.95	20.86

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 10
Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 16

Table F.4: Result summary of 7 reactive trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.95
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.23	-3237.74
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.75	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.17	43.64
Mass Density	KG/CUM	0.55	722.54	933.59	919.75
Average Molecular Weight		18.57	74.12	19.79	21.08

APPENDIX G

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 0

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 16

Table G.1: Result summary of 0 stripping trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.94
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.68	-3237.17
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.75	-40.89
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.18	43.63
Mass Density	KG/CUM	0.55	722.54	933.62	919.74
Average Molecular Weight		18.57	74.12	19.79	21.08

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 2
Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 16

Table G.2: Result summary of 2 stripping trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.95
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.18	-3237.8
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.75	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.17	43.64
Mass Density	KG/CUM	0.55	722.54	933.59	919.75
Average Molecular Weight		18.57	74.12	19.79	21.08

Operating parameter conditions:

AA concentration: 4 % w/w	Catalyst loading: 0.105 kg/m
Reboiler duty: 283.133 kJ/hr	Reflux ratio: 1.0
Number of reactive trays: 7	Number of rectifying trays: 16
Number of stripping trays: 3	

Table G.3: Result summary of 3 stripping trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.96
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.13	-3237.87
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.76	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.17	43.64
Mass Density	KG/CUM	0.55	722.54	933.58	919.76
Average Molecular Weight		18.57	74.12	19.79	21.08

Operating parameter conditions:

AA concentration: 4 % w/w	Catalyst loading: 0.105 kg/m
Reboiler duty: 283.133 kJ/hr	Reflux ratio: 1.0
Number of reactive trays: 7	Number of rectifying trays: 16
Number of stripping trays: 4	

Table G.4: Result summary of 4 stripping trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C_3H_4O-01	KMOL/HR	0	0	0	0
C_4H_{10}-01	KMOL/HR	0	0	0	0
C_7H_{12}-01	KMOL/HR	0	0	0	0
H_2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.95
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.21	-3237.76
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.75	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.17	43.64
Mass Density	KG/CUM	0.55	722.54	933.59	919.75
Average Molecular Weight		18.57	74.12	19.79	21.08

APPENDIX H

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 2

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 0

Table H.1: Result summary of 0 rectifying trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.53	0.45
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	69.01	67.82
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.91	-68.25
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3448.98	-3228.19
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.54	-41.04
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.48	43.46
Mass Density	KG/CUM	0.55	722.54	934.83	918.96
Average Molecular Weight		18.57	74.12	19.69	21.14

Operating parameter conditions:

AA concentration: 4 % w/w
Catalyst loading: 0.105 kg/m
Reboiler duty: 283.133 kJ/hr
Reflux ratio: 1.0
Number of reactive trays: 7
Number of rectifying trays: 2
Number of stripping trays: 2

Table H.2: Result summary of 2 rectifying trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.02	0.02
Mole Flow	KMOL/HR	0.05	0	0.02	0.03
Mass Flow	KG/HR	0.87	0.11	0.47	0.51
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	67.72	69.45
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-68.11	-68.01
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3305.69	-3385.36
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-40.26	-39.09
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.95	-1.95
Molar Density	KMOL/CUM	0.03	9.75	44.88	46.25
Mass Density	KG/CUM	0.55	722.54	924.76	929.25
Average Molecular Weight		18.57	74.12	20.61	20.09

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 2
Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 4

Table H.3: Result summary of 4 rectifying trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.56	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.95
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3431.62	-3238.49
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.76	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.16	43.65
Mass Density	KG/CUM	0.55	722.54	933.57	919.78
Average Molecular Weight		18.57	74.12	19.8	21.07

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 2

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 6

Table H.4: Result summary of 6 rectifying trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.8	67.87
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3433.17	-3236.49
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.74	-40.89
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.18	43.63
Mass Density	KG/CUM	0.55	722.54	933.59	919.99
Average Molecular Weight		18.57	74.12	19.79	21.09

Operating parameter conditions:

AA concentration: 4 % w/w
Reboiler duty: 283.133 kJ/hr
Number of reactive trays: 7
Number of stripping trays: 2

Catalyst loading: 0.105 kg/m
Reflux ratio: 1.0
Number of rectifying trays: 8

Table H.5: Result summary of 8 rectifying trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H_2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.95
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.14	-3237.84
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.75	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.17	43.64
Mass Density	KG/CUM	0.55	722.54	933.59	919.75
Average Molecular Weight		18.57	74.12	19.79	21.08

Operating parameter conditions:

AA concentration: 4 % w/w	Catalyst loading: 0.105 kg/m
Reboiler duty: 283.133 kJ/hr	Reflux ratio: 1.0
Number of reactive trays: 7	Number of rectifying trays: 12
Number of stripping trays: 2	

Table H.6: Result summary of 12 rectifying trays

		S1	S2	S3	S4
From				R-101	R-101
To		R-101	R-101		
Substream: MIXED					
Phase:		Vapor	Liquid	Liquid	Liquid
Component Mole Flow					
C3H4O-01	KMOL/HR	0	0	0	0
C4H10-01	KMOL/HR	0	0	0	0
C7H12-01	KMOL/HR	0	0	0	0
H2O	KMOL/HR	0.05	0	0.03	0.02
Mole Flow	KMOL/HR	0.05	0	0.03	0.02
Mass Flow	KG/HR	0.87	0.11	0.55	0.43
Volume Flow	CUM/HR	1.57	0	0	0
Temperature	C	130.85	107.85	68.78	67.95
Pressure	BAR	1	1	0.35	0.35
Vapor Fraction		1	0	0	0
Liquid Fraction		0	1	1	1
Solid Fraction		0	0	0	0
Molar Enthalpy	KCAL/MOL	-57.12	-73.9	-67.93	-68.24
Mass Enthalpy	KCAL/KG	-3075.53	-997.03	-3432.23	-3237.74
Enthalpy Flow	GCAL/HR	0	0	0	0
Molar Entropy	CAL/MOL-K	-8.26	-119.68	-38.75	-40.88
Mass Entropy	CAL/GM-K	-0.44	-1.61	-1.96	-1.94
Molar Density	KMOL/CUM	0.03	9.75	47.17	43.64
Mass Density	KG/CUM	0.55	722.54	933.59	919.75
Average Molecular Weight		18.57	74.12	19.79	21.08