Separation of Water-Acetone Mixture Using Suitable Entrainer (Simulation)

by

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CERTIFICATION OF APPROVAL

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Approved by,

(Professor Thanabalan Murugesan)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

June 2010

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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KHAIRUNNISA BINTI ABDUL RAPAH

ABSTRACT

Acetone and Water mixture formed azeotrope and inflections point depending on the operating temperature and pressure. Hence, this mixture cannot be separated by using simple distillation. In this work, a systematic study of the separation of acetone water with the addition of entrainer by extractive distillation is performed. Acetone-Water extractive binary column distillation system is simulated in PETRONAS iCON Software. The simulations supported data and findings were taken from literature review and experimental studies of the same systems. The objective of the project is to investigate the effect of reflux ratio, feed ratio, and number of stages on the product purities. The challenge in this project is to find the most effective entrainer as well as to obtain the optimum separation parameter in order to have a feasible separation process. Three different types of entrainers have been tested in the simulator as to determine the most effective entrainer for the separation of Acetone-Water mixture.

ACKNOWLEDGEMENT

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(KHAIRUNNISA BINTI ABDUL RAPAH)

TABLE OF CONTENT

CHAPTER 1 INTRODUCTION

CHAPTER 2 LITERATURE REVIEW

CHAPTER 3 METHODOLOGY

CHAPTER 4 RESULTS AND DISCUSSION

4.4.1 Effects of Reflux Ratio

4.4.2 Effects of feed ratio

4.4.2 Effects of number of stages

LIST OF FIGURES

LIST OF TABLE

CHAPTER 1

PROJECT BACKGROUND

1.1 BACKGROUND OF STUDY

In the chemical industry, separation of multi-component liquid mixtures into one or more high purity products is one of the most crucial tasks. There are several methods used to separate this mixture, such as distillation, liquid-liquid extraction, crystallization, evaporation, etc. Among these, distillation is far the most widespread and has a long history in chemical technology. However, until recently, there has been no systematic approach to design of distillation separation for non ideal and complex mixture where azeotropes and inflections point may occur.

The five methods for separating azeotropic mixtures are: (i) Extractive distillation and homogeneous azeotropic distillation; (ii) Heterogeneous azeotropic distillation, or more commonly, azeotropic distillation; (iii) Distillation using ionic salts; (iv) Pressure swing distillation; and (v) Reactive Distilation (Ruthven D.M., 1997)

This study discusses the procedure and theory for separating binary mixture of water acetone mixture by extractive distillation technique which ease the separation process. For this case study, extractive distillation method is chosen since it primarily modifies liquid-phase behavior to alter the relative volatility of the components of the mixture. This study also involves a computer simulation to enable performance comparison among a few possible solvents as to achieve acetone purity of 99 percent.

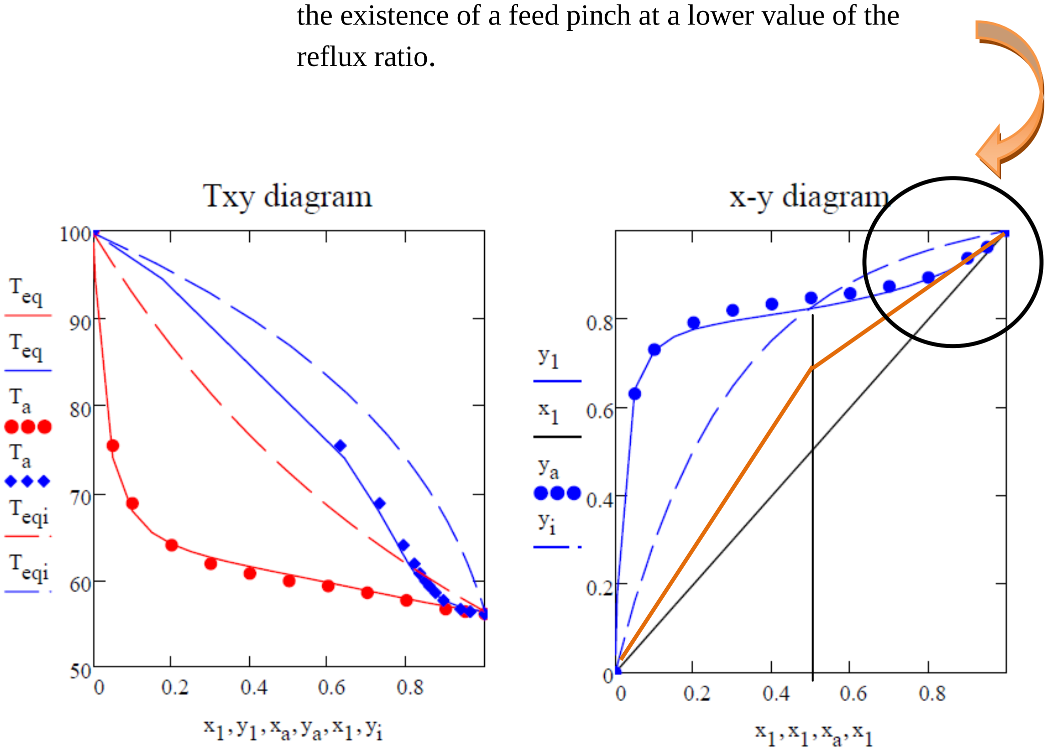
1.2 PROBLEM STATEMENT

Water and acetone mixture is a non ideal mixture, which display quite unusual phase behavior. For a non ideal mixture, it violates and deviates from the ideality of prefect gas law which known as Raoult's Law. In mathematically, Roult's Law can be expressed as:

$$\alpha_{AB} = \frac{p^0{}_A}{p^0{}_B}$$

At certain temperature and pressure, the mixture of water and acetone can form azeotrope depending on the ratio of acetone to water. Once azeotrope is formed, the acetone and water will vaporize together and ruin the separation process. However, at atmospheric pressure, acetone and water mixture does not form azeotropic but the mixture has inflections point. The separation can be done by using simple distillation column but in a finite number of stages at a slightly higher reflux ratio. In order to overcome the constraints imposed by azeotrope and inflections point, entrainer can be used to help to enhance the separation. However, a suitable entainer needs to be chosen as to produce pure acetone that meets certain specification.

The current practice in the design of distillation separations for non ideal mixture is to guess a design and improve it by successive simulations. Basically, there is no systematic method to estimate the reflux ratio and the number of theoretical stages in the separation column. For ideal mixture that has constant relative volatility, shortcuts methods such as Frenske-Underwood-Gilliland method have been devised to establish the number of minimum stages and minimum reflux which establish limits on column design and operation. (Okullo, 1999).



The tangent pinch controls the minimum reflux, despite the existence of a feed pinch at a lower value of the reflux ratio.

Figure 1-1: Binary VLE disgrams for Acetone and Water at 1 atm pressure. Dashed lines represent ideal model, solid line represent nonideal model, points represent experimental data. (Adapted from Mathcad-acetone water vle.2.xmcd, Retrieved May 06, 201from http://chemeng.nmsu.edu/ChE307/notes/water_acetone%20vle%20models.pdf)

For that reason, this research is important as to simulate the understanding on the entrainer selection for separation of homogeneous mixture such as water and acetone that formed azeotrope. The results from the study will provide basic design information in applications associated with extractive distillation.

1.3 LIMITATION OF STUDY

The major limitation of this study is to validate the simulation result obtained from the iCON Simulation with the reliable source of experimental data. The experimental data for Acetone-Water mixture is not readily available in the open literature.

According to Coulson and Richardson (2005)

> If the purity if the acetone product required is less than 95 per cent, inaccuracies in the vapor liquid equilibrium plot will have little effect on the estimate of the number of stages required, as the relative volatility is very high. If a high purity is wanted (x = 99 percent), then reliable data are needed in this region as the equilibrium line approaches the operating line (a pinch point occurs). Of the reference cited, non gives values in the region above 95 percent, and only two give values above 90 percent; more experimental values are needed to design with confidence. There is a possibility that system forms an azeotrope in this region.

Moreover, this study is focusing in simulating the effects of entrainer in the PETRONAS iCON Simulation. Hence, no laboratory work was done to evaluate the feasibility of the entrainer chosen.

1.4 OBJECTIVE AND SCOPE OF STUDY

The main objectives of this project are:

- To study the entrainer selection for non ideal mixture that would result in azeotrope and inflections point.
- To simulate the effects of entrainer as to find the best separation parameters, in terms of reflux ratio (energy requirement), number of stages, and product purities of 99% Acetone by using software tool, PETRONAS iCON Software.
- To select the best entrainer to separate water-acetone mixture.

This study is comprised into 4 major parts which are listed as below:

- Understanding the topic from the related literature review; e.g books, journal and website as to get as much information and idea about the project.
- Understanding the approach of basic data and models for separation system and principle based on the distillation
- Develop and test the model simulation in software tool in difference approach and optimization of design
- Interpret and analyze all the result from the simulation

CHAPTER 2

LITERATURE REVIEW

The literature review for this research study has been taken from few reliable sources such as journals, books, articles and theses that are much related to the topic. The reviews consist of the four major parts which are listed as below:

i) Fundamental of distillation
ii) Azeotropes and inflections point
iii) Solvent screening and selection
iv) Extractive Distillation

2.1 FUNDAMENTALS OF DISTILLATION

The fundamentals of distillation need to be understood first as to have a better understanding about this separation method. In figure 2-1, it shows the distillation operation using a total condenser and partial reboiler. The feed contains binary mixture with different boiling point and volatility enters the column at a feed stage, f. The pure component having higher volatility will easily evaporate and become as the overhead product. Meanwhile, the lower volatility component which is in liquid phase will be collect at the bottom product.

Based on Seader (2006), the operation consists of a column containing the equivalent of N theoretical stages; a total condenser in which the overhead vapor leaving the top stage is totally condensed to give a liquid distillate product and liquid reflux that is returned on the top stage; a partial reboiler in which liquid from the bottom products and vapor boilup that is returned to the bottom stage, and an intermediate feed stage.

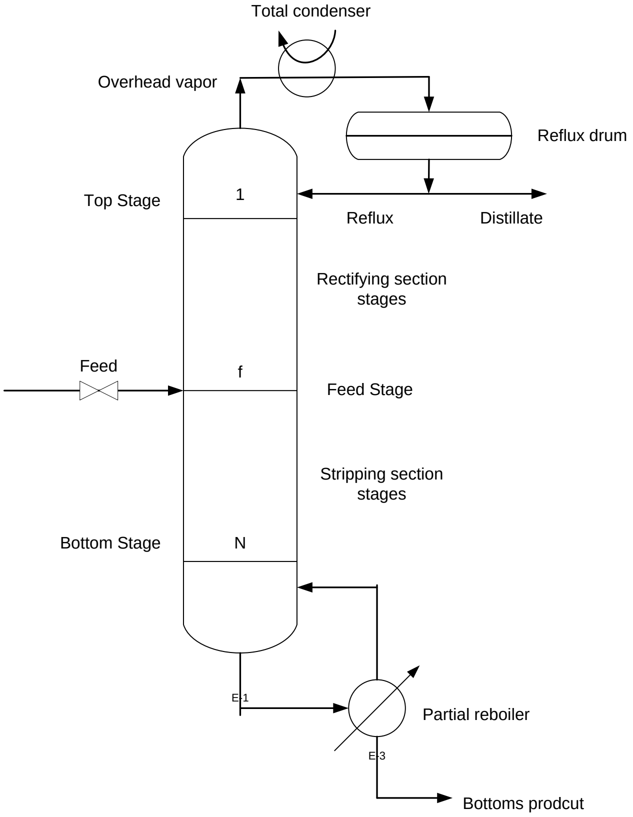


Figure 2-1 Distillation operations using total condenser and partial reboiler

Based on Doherty and Malone (2001), the reboiler is considered to be one stage, since vapor and liquid phase are both present. A partial condenser is treated like –wise.

2.2 AZEOTROPES AND INFLECTIONS POINT

According to Langston *et.al* (2005)

> Azeotropes are complex, non-ideal mixtures that occur when the components of the mixture have low relative volatilities. The components of these mixtures are very difficult and hence expensive to separate. They can be separated effectively by means of extractive distillation whereby the addition of a solvent is made to a distillation column. The solvent acts to increase the relative volatility of the mixture by increasing the activities of the components, as given in the non-ideal binary component mixture relationship:
>
> $$\alpha_{AB} = \frac{\gamma_A p^0{}_A}{\gamma_B p^0{}_B} \tag{1}$$
>
> where: γ_A and γ_A and are the activity coefficients of components A and B and $p^0{}_A$ and $p^0{}_B$ are the vapour pressure of components A and B. As the relative volatility is raised; the light key can be controlled from the top of the distillation column and the mixture of heavy key and solvent retrieved from the column product for subsequent separation.

Based on Smith (2005), the problem with the azeotropic behavior is that, for highly nonideal mixture, at a specific composition, a constant boiling mixture can form that has the same composition for the vapor and liquid at an intermediate composition for the vapor and liquid at an intermediate composition away from the required product purity. This depends on the vapor-liquid equilibrium physical properties. Distillation can thus be used to separate a composition approaching azeotropic composition, but the azeotropic composition cannot be approached closely in a finite number of distillation stages, and the composition cannot be crossed, even with an infinite number of stages.

In general an azeotropic state is defined as a state in which mass transfer occurs between phases while the composition of each phase remains constant, but not necessarily equal (see Prigogine and Defay,1967; Rowlinson, 1969). The usage of entrainer or known as mass separation agent, is to make the separation possible where the entrainer will interacts strongly with one of the azeotrope-forming components that the other. Entrainer will break the azeotrope by altering the relative volatility behavior between the heavy and light key components.

Minimum reflux (reboil) occurs when the operating line for the rectifying section (stripping) section touches the equilibrium curve. It is quite common for nonideal mixtures to exhibit inflections in their isobaric T-x-y phase diagrams, which in turn generate inflections in the corresponding equilibrium x-y diagrams. In such cases, it is possible for one of the operating lines to become tangent to the equilibrium curve, thereby causing a pitch in only one section of the column, away from the feed. A typical construction is shown in Figure 2-2. (Doherty and Malone, 2001)

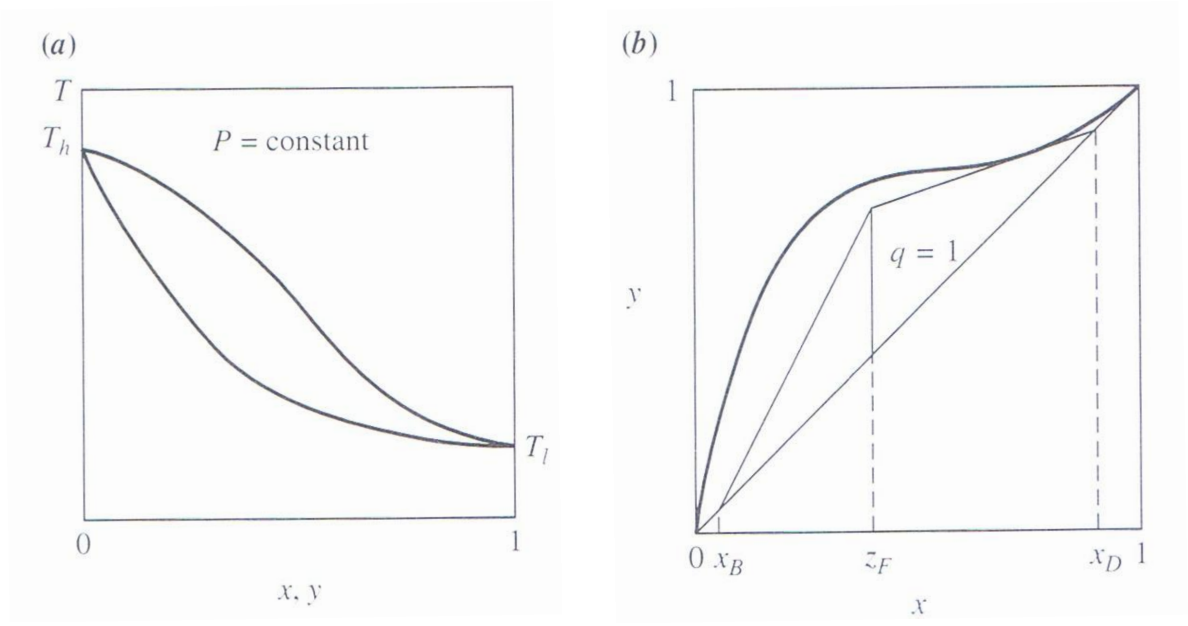


Figure 2-2: Schematic diagrams showing a tangent. a) T-x-y phase diagram. (b) Corresponding McCabe-Thiele diagram taken from Doherty and Malone (2001, pp 95).

2.3 SOLVENT SCREENING AND SELECTION

Yee *et al.* says that in order to develop an economical extractive distillation sequence in selecting a good solvent. Approaches to the selection of an extractive distillation solvent are discussed by Berg, Ewell *et al*. ‘ and Tassions. In general, selection criteria include the following:

1. Should enhance significantly and natural relative volatility of the key component.
2. Should not require an excessive ratio of solvent to nonsolvent.
3. Should remain soluble in the feed components and should not lead to the formation of two phases.
4. Should be easily separable from the bottom product.
5. Should be inexpensive and readily available.
6. Should be stable at the temperature of the distillation and solvent separation.
7. Should be nonreactive with the components in the feed mixture.
8. Should have a low latent heat.
9. Should be noncorrosive and nontoxic.

The selection of entrainer needs to be feasible as to ensure the separation of the mixture will occur. A good entrainer will lead to higher product purities. Meanwhile, in order to design a cost effective distillation column, the reflux ratio and number of stages of distillation column must be kept at minimum. (Okullo, 1999).

Since the solvent is the heart of extractive distillation, more attention should be paid on the selection of potential solvents. The affinity of hydrocarbon to polar solvent depends directly on their degree of un-saturation. A highly unsaturated hydrocarbon is more soluble in a polar solvent, and the solvent decreases the volatility of the hydrocarbon. Based on Perry’s Handbook, several features are essential:

1. The solvent must be chosen to affect the liquid-phase behavior of the key components differently; otherwise no enhancement in separability will occur.

2. The solvent must be higher boiling than the key components of the separation and must be relatively nonvolatile in the extractive column, in order to remain largely in the liquid phase.
3. The solvent should not form additional azeotropes with the components in the mixture to be separated.
4. The extractive column must be a double-feed column, with the solvent feed above the primary feed; the column must have an extractive section.

According to Wankat (2007)

> Selection of the solvent is extremely important. Usually, a solvent is selected that is more similar to the heavy key. Then the volatility of the heavy key will be reduced. Solvent selection can be aided by considering the polarities of the compounds to the separated. A short list of classes of compounds arranged in order of increasing polarity is given in Table 2-1. If two compounds of different polarity are to be separated, a solvent can be selected to attract either the less polar or the more polar of the two.

Table 2-1: Increasing polarities of classes of compound

Hydrocarbon
Ethers
Aldehydes
Ketones
Esters
Alcohols
Glycols
Water

2.4 EXTRACTIVE DISTILLATION

Extractive distillation is a technique to enhance separation of mixtures that cannot undergo ordinary distillation due to certain circumstances. An entrainer in a large amount of a relatively high-boiling point is being introduced as the feed into the column. Generally, it acts to modify the relative volatility of the key component so that it becomes more favorable. Entrainer is introduced near the top of the column, so that it present in liquid phase on all the trays below.

In general, the component with higher boiling point will become the overhead product as a pure distillate, and the component which has a lower boiling point is present in the bottom product. For water acetone binary mixture, the entrainer will attract the water and leaves behind acetone as the overhead product. Meanwhile, water will leaves with the entrainer via the bottom streams. The entrainer and water (non product) can undergo further separation in a second distillation column to separate between those two components. The entrainer can be reuse by recycling back to the first distillation column. Figure 2-3 shows the example of extractive distillation flow sheet taken from Smith (2005, pp. 248)

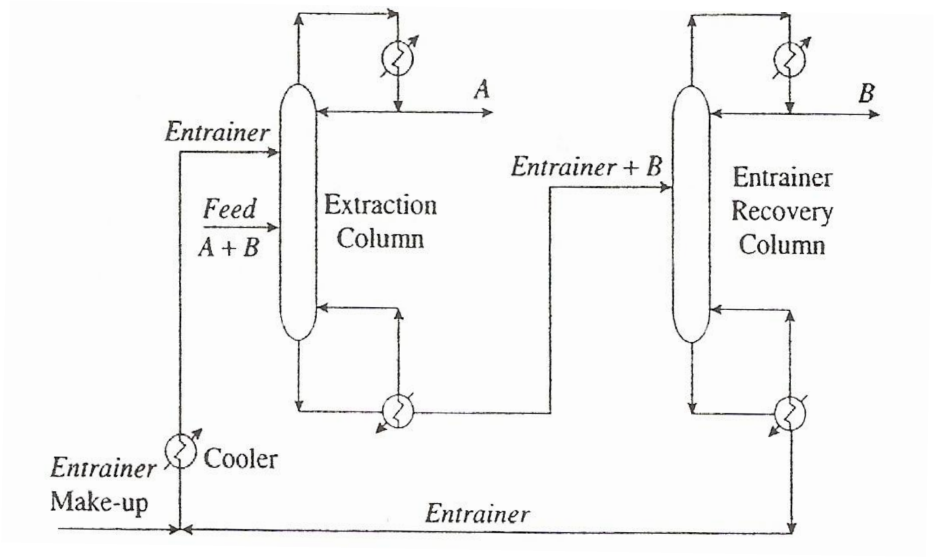


Figure 2-3: Extractive distillation flow sheet

According to Smallwood (2002)

> Extractive Distillation can be divided into five sections as shown in Figure 2-4. Of these, two (B and C) can be considered as 'active' in that entrainer is present in these along with components 1 and 2. The remaining three sections, A,D and E, are performing 'cleaning-up' operations, Consideration of the functions of all these sections will reveal the criteria for choosing a suitable entrainer.

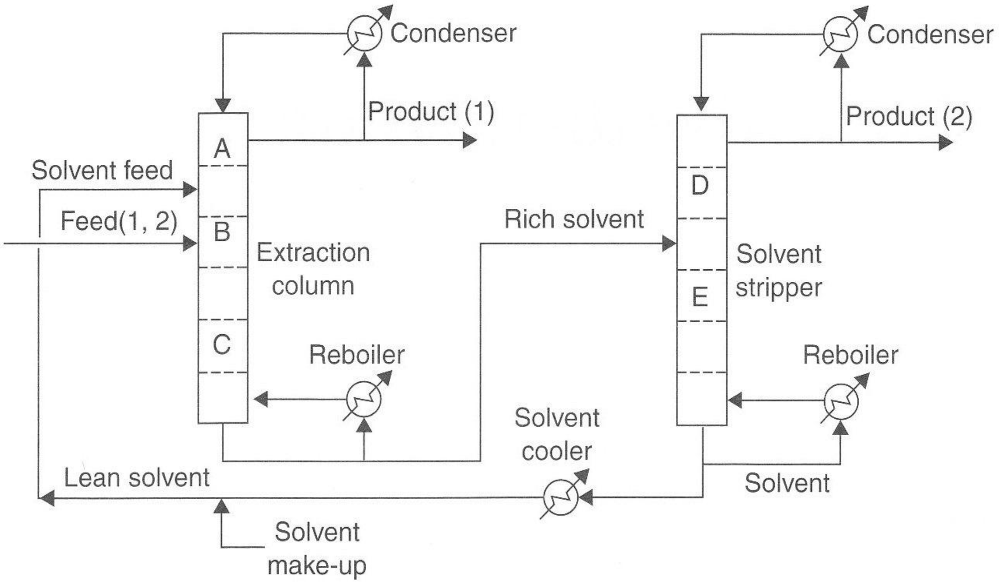


Figure 2-4: Sections in Extractive Distillation Column. Source: (Swallwood, 2002)

The function and characteristic of each section are describes in Table 2-2.

Table 2-2: The function and characteristic of each section in Extractive Distillation Source: (Swallwood, 2002)

Section	Function and Characteristic
A	• At the section, entrainer is being removed from the top product. • This process is easy since entrainer is normally very much volatile than the tops • This column section is doing a conventional duty and large liquid loads in Section B and Section C are not present in Section A. • There is possibility that entrainer may be lost into the tops from Section and it is costly chemical. • The reflux returned to this section should be minimized as, when it reaches Section B, it will be mixed with at least 4 mol of entrainer.
B	• The relatively large amount of entrainer being injected at the top of this section should be cooled to a temperature close to the boiling point of component 1. • This is probably to require the entrainer, which leaves the bottom of Section E at its boiling point, to be cooled further. • The liquid load in Section B is usually high in comparison with that in a conventional column and care must be taken not to overload the downcomers if they are not designed for an extractive distillation service.
C	• If the feed does not contain equal molar concentration of components 1 and 2, it will follow that at the top of Section C or that bottom of Section C the mole fraction of the entrainer will be appreciable higher than the average.
D	• The combination of using reduced pressure to keep the boiling point low while condensing the very much more volatile product 2 and handling large amounts of liquid creates more problems for equipment not designed for the duty.
E	• It is important to strip all the component 2 from the entrainer because little fractional will take place in Section A and the work done o Section B and C are useless if the returned entrainer is not pure.

CHAPTER 3

METHODOLOGY

3.1 RESEARCH METHODOLOGY

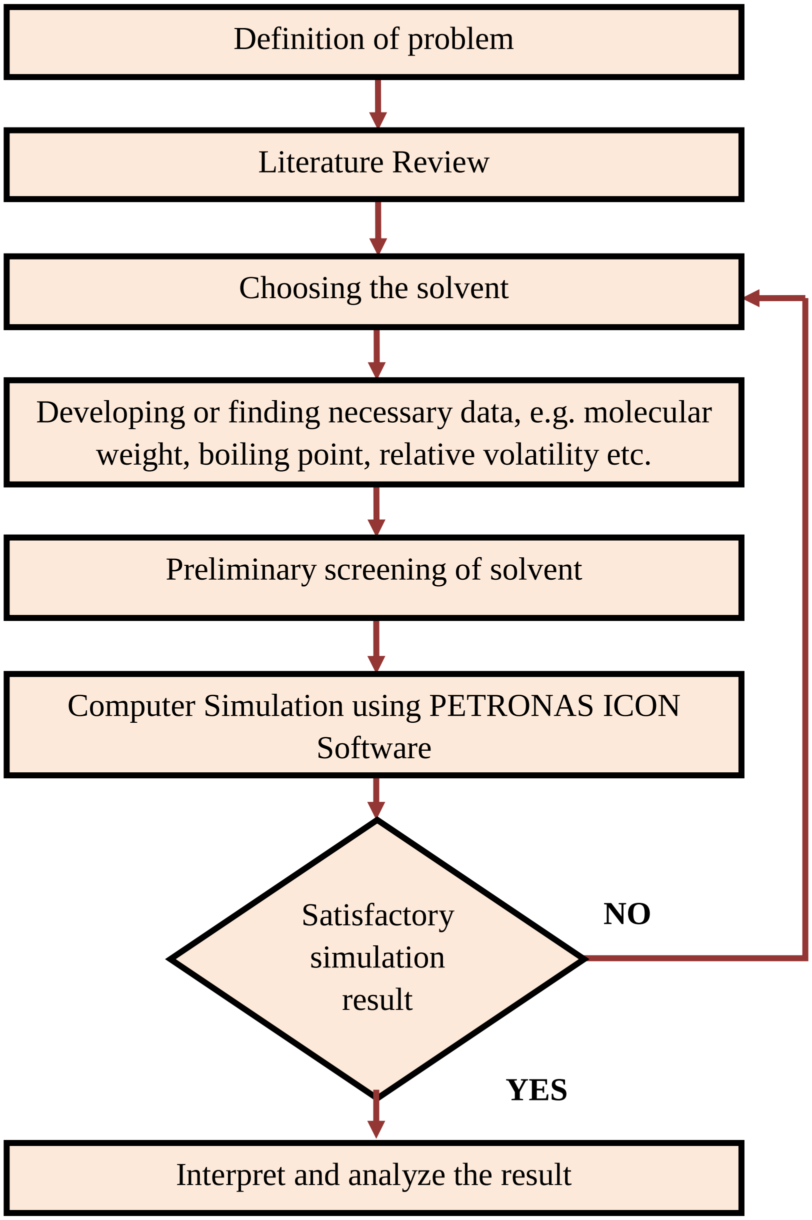


Figure 3-1: Summary of the project methodology upon completion

From figure 3-1, first step in this research project is defining the problem. This is important to get some ideas and overview picture of the project all about. This can be done by reading some journals, articles, books and literature review. The simulations supported data and findings were taken from literature review and experimental studies of the same systems. By doing solvent screening, the entrainer selection for this system can be narrow down based on certain criteria. Moreover, the specification of each parameter needs to be defined. After all the information is being gathered, the next step is to simulate the design in iCON Simulation. Familiarization of using this software will be the successful key to produce the good simulation in order to get a feasible result.

When the simulation satisfied the process, the next step is to do some operability study. Some parameter studies on the effect on changing design parameters such as reflux ratio, amount of entrainer, number of stages to the tower operation is studied. From this result, further manipulation of the process parameters or column design specifications can be manipulated to get better production of acetone. All the findings will be analyzed to compare the performance among the entrainers.

3.2 PROJECT ACTIVITIES

The design is modeled in PETRONAS iCON Software to enable performance comparison among a few possible solvents as to achieve acetone purity of 99%. Firstly, the author needs to find the water and acetone characteristic for instance molecular formula, molecular weight, boiling point, relative volatility etc. All the physical properties of the pure components are shown in the Table 3-1.

Table 3-1: The physical properties of Water and Acetone

Component	Synonym	Molecular Formula	Molecular Weight (g/mol)	Boiling Point (^{O}C) at 1atm
Water	-	H_20	18.01	100
Acetone	Propanone, Dimethyl ketone	C_3H_60H	58.08	56.5

Source: The values were adapted from Perry's Chemical Handbook.

These parameters are used to determine the heavy and light key component for the model design. All these parameters are important as to ensure the outcome of this study is accurate and relevant. Based on the boiling point of the pure component, acetone become as the light component meanwhile water will become as the heavy component. Moreover, this study requires the Vapor Liquid Equilibrium (VLE) data of the mixtures in order to begin the simulation. Some of the information is adapted from the Vapor Liquid Equilibrium Data Collection of the DECHEMA Chemistry Data Series.

An assumption is made where the operating pressure of this model need to be set at atmospheric pressure, 1 atm. The pressure is held constant throughout the study which leads to isobaric condition. At pressure 1 atm, the mixture of water and acetone does not form any azeotrope but does exhibits an inflections point. A comparison between VLE diagrams at different pressure for acetone and water system are shown in APPENDIX A.

According to Doherty and Malone (2001)

> There are two common features of non ideality binary phase diagrams that particularly troublesome for distillation column design. The first is the appearance of inflections in the isobaric T-x-y diagram, which in turn generate inflections in the corresponding y-x diagram. The second difficulty is associated with extrema in the phase diagram that give rise to homogeneous binary azeotropes. At such points, the equilibrium liquid and vapor compositions are equal and the y-x curve crosses the 45^{O} line with positive slope.
>
> However, the y-x data can be corrected by the empirical expression

$$y = \frac{ax}{1+(a-1)x} + bx(1-x) \tag{2}$$

This equation can be used to correlate the binary nonideal x-y data. The table 3-2 shows the constants in the empirical Vapor Liquid Equilibrium model (Eq. 2) for selected binary mixtures.

Table 3-2: Constants in the empirical VLE model (Eq. 2) for Acetone and Water Mixture

Mixtures with inflections but no azeotropes					
Light component	Heavy component	(bp, ^{O}C)		a	b
Acetone	Water	56.1	100.0	32.0	-0.58

Source: The experimental y-x data were taken from the DECHEMA Vapor-Liquid Equilibrium Data Collection. The pressure is 1 atm unless noted otherwise and the boiling point are given at the same pressure as the VLE Data.

Figure 3-2 shows the T-x-y and y-x diagrams for the binary mixture of acetone and water at operating pressure 1 atm. These figures indicate that the binary mixture exhibits inflections where there is deviation display in the T-x-y diagram.

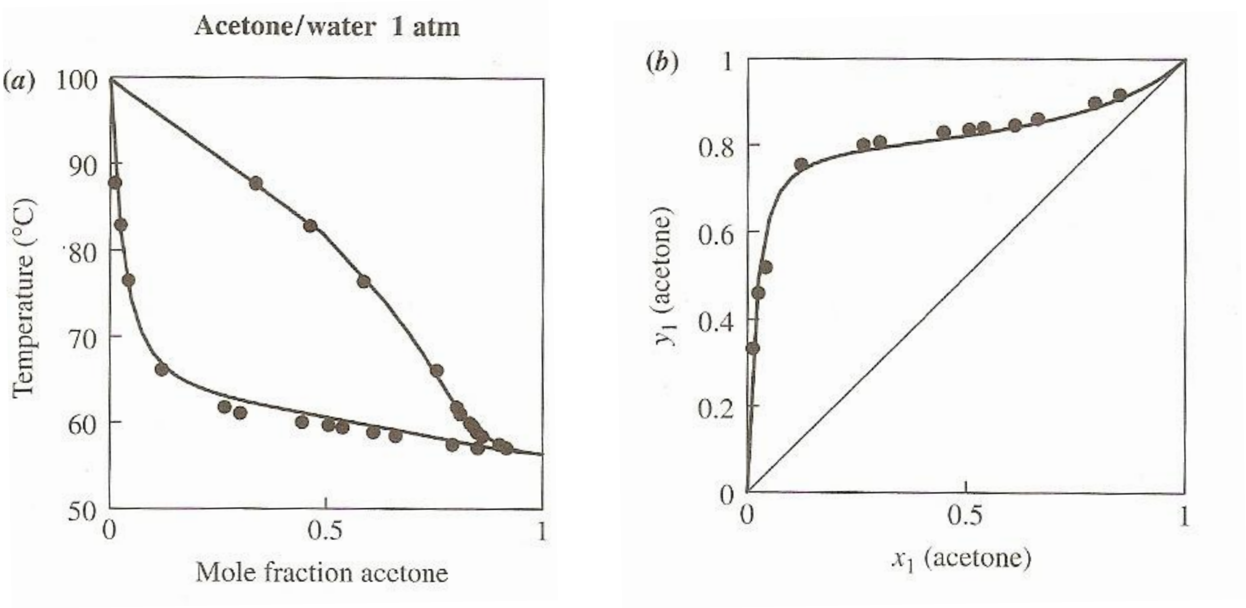


Figure 3-2: Binary VLE diagrams for Acetone (1) and Water (2) at 1 atm pressure. (a) Temperature-composition diagram. (b) y_1-x_1 diagram. The points are experimental data; colid lines are calculated from the Wilson Equation. All data and model parameters are taken from Gmehling and Onken (1977,pp..237).

3.3 KEY MILESTONE

In this project, there are several milestones that had been set up to asses the project status and to properly planned the next activities to ensure the project can be completed in the frametime given. Below are the key milestones for the second semester of 2-Semester Final Year Project:

Table 3-3: Milestone for the Second Semester of 2-Semester Final Year Project

No	Detail/Week	WEEK	1	2	3	4	5	6	7	8	9	10	11	12	13	14
		DATES	25-Jan	1-Feb	8-Feb	15-Feb	22-Feb	23-Feb	1-Mar	8-Mar	15-Mar	22-Mar	29-Mar	5-Apr	12-Apr	19-Apr
1	Project Work Continue i) Simulation in ICON (Without entrainer) ii)Simulation in ICON (1st entrainer)		🟥	🟥	🟥										Oral Presentation	Submission of Project Dissertation (Hard Bound)Legend Used
2	Submission of Progress Report 1					●										
3	Project Work Continue i) Simulation in ICON (2nd entrainer) ii)Comparison Analysis					🟥	🟥	🟥	🟥							
4	Submission of Progress Report 2										●					
5	Seminar (Compulsory)											🟥	🟥	🟥		
6	Project work continue										🟥	🟥	🟥	🟥		
7	Poster Exhibition											●				
8	Submission of Project Dissertation (Soft Bound)												●			
9	Documentation												🟥	🟥		

● Suggested Milestone

🟥 Process

CHAPTER 4

RESULT AND DISCUSSION

This section is comprises of several subsection based on the flow of project. The subsections are:

- Designing Simple Distillation for Water-Acetone Mixture
- Entrainer Selection for Water-Acetone Mixture
- Designing Extractive Distillation Column
- Entrainer Performance Comparison
- Validation of Simulation Results

4.1 DESIGNING SIMPLE DISTILLATION FOR WATER ACETONE MIXTURE

Firstly, a simple distillation column for binary mixture was constructed before starting an extractive distillation column design. The reason is because to investigate the highest purity of acetone that can be achieved by using simple distillation column. The figure below shows the simple distillation column for acetone production. The main operation parameter of the distillation unit is shown in Table 4-1. The result from iCON simulation was being extracted to Excel to be analyzed. The accuracy of the equilibrium data required calculating the number of stages needed for the separation of mixture and water by distillation is taken from Coulson and Richardson (2005). (see Appendix B)

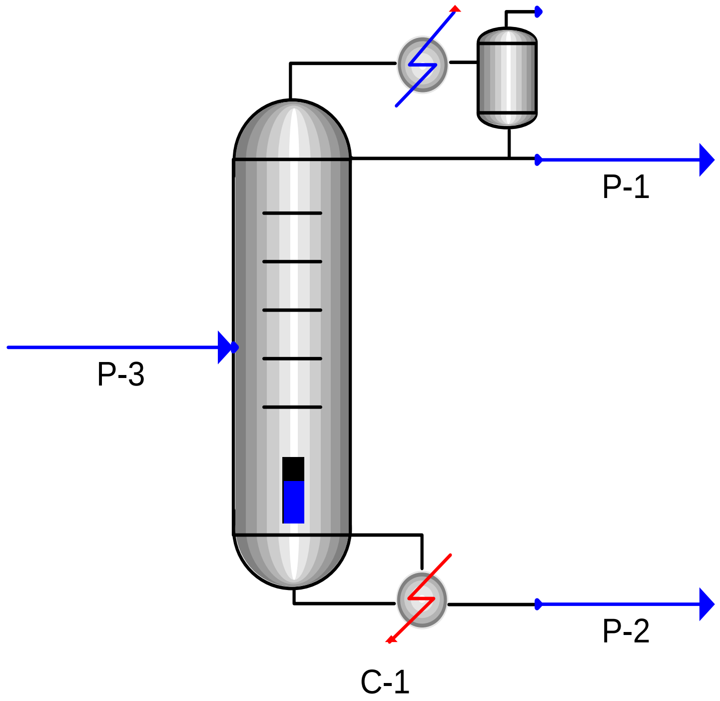


Figure 4-1: Separation of Water Acetone Mixture using Simple Distillation Column

Table 4-1: Distillation Unit Summary

Unit Tag	Description	Operating Parameter
C-1	Simple Distillation Column	• Operating pressure = Top (1atm) = Bottom (2atm) • Number of tray = 17 • Feed Tray = 2 • Reflux Ratio = 1.5
P-3	Feed Stream	• Total Molar Flowrate = 100 kgmole/hr • Composition i) Acetone = 0.5mole ii) Water = 0.5 mole
P-1	Top Product Stream	• Composition i) Acetone = 0.832 mole ii) Water = 0.168 mole
P-2	Bottom Product Stream	• Composition i) Acetone = 0.193 mole ii) Water = 0.807 mole

By referring to the results in Table B-1 (see APPENDIX C) and Figure 4-2, it shows that once the reflux ratio is increasing, the number of stages will be reduced. Based on theory, when the reflux ratio increased from the minimum value, the number of plates will be reducing, the column diameter increases, and the reboiler steam and condenser cooling-water requirements increase. Reflux ratio also gives significant effect to distillate flow. If the reflux ratio is increased, the distillate flow will drop unless the reboil ratio is also increased to reserve the energy balance in the column. This is because when the reflux ratio increased, the liquid flow (reflux) will increases and reduces the gas flow (distillate). Smith (2005) reported that usually the optimum number of reflux ratio is often 1.1. However, most designers are reluctant to design columns closer to minimum reflux than 1.1 except in special circumstances, since a small error in design data or a small change in operating might lead to an infeasible design.

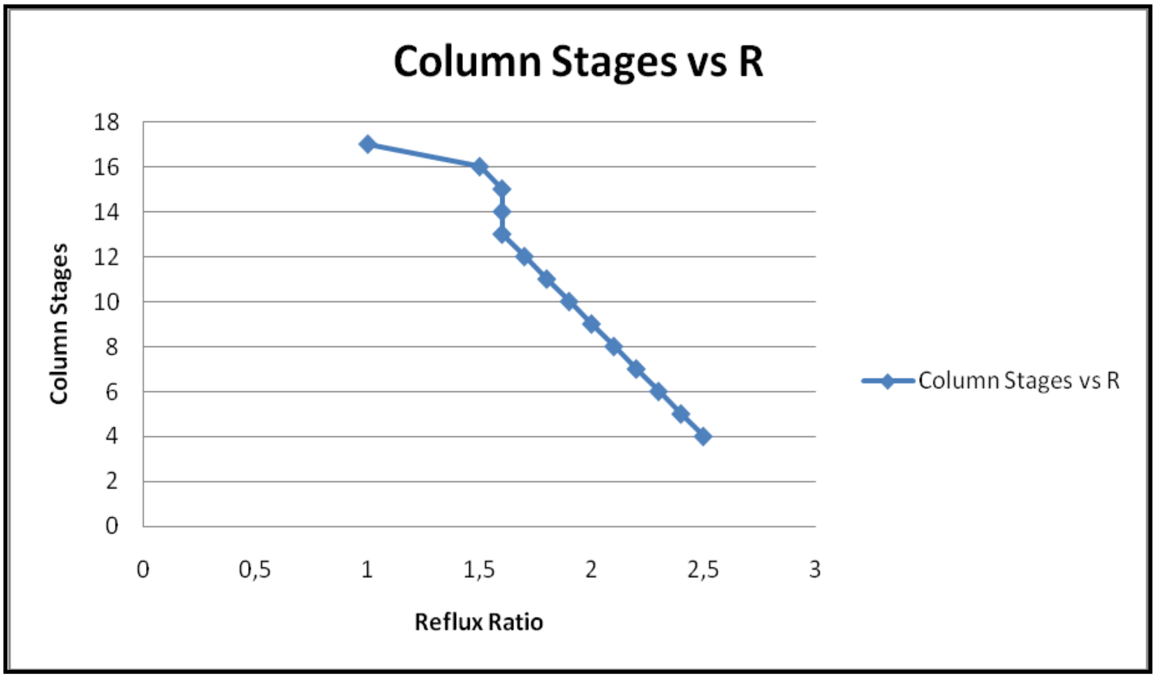


Figure 4-2: Graph of Column Stages versus Reflux Ratio

Based on previous research, there was a significant effect of increasing or reducing the reflux ratio. The reflux ratio need to be optimum since there is a capital-energy trade-off, as illustrated in Figure 4-3 taken from Smith (2005).

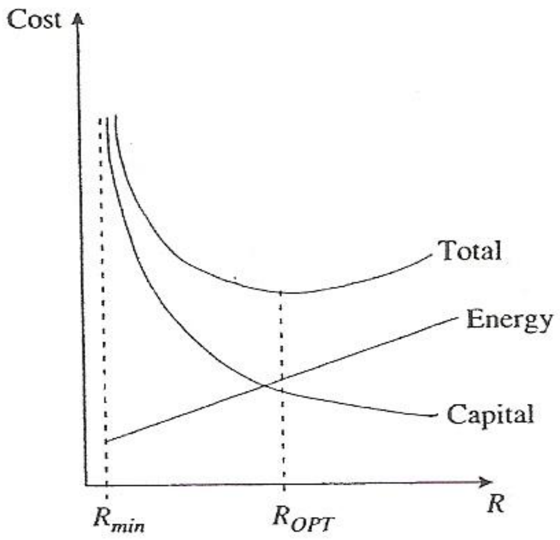


Figure 4-3: The capital energy trade-off standalone distillation column by Smith (2005, pp.175)

The changes in column stages do not give any effect to flow rate of acetone at the top product as shown in Figure 4-4.

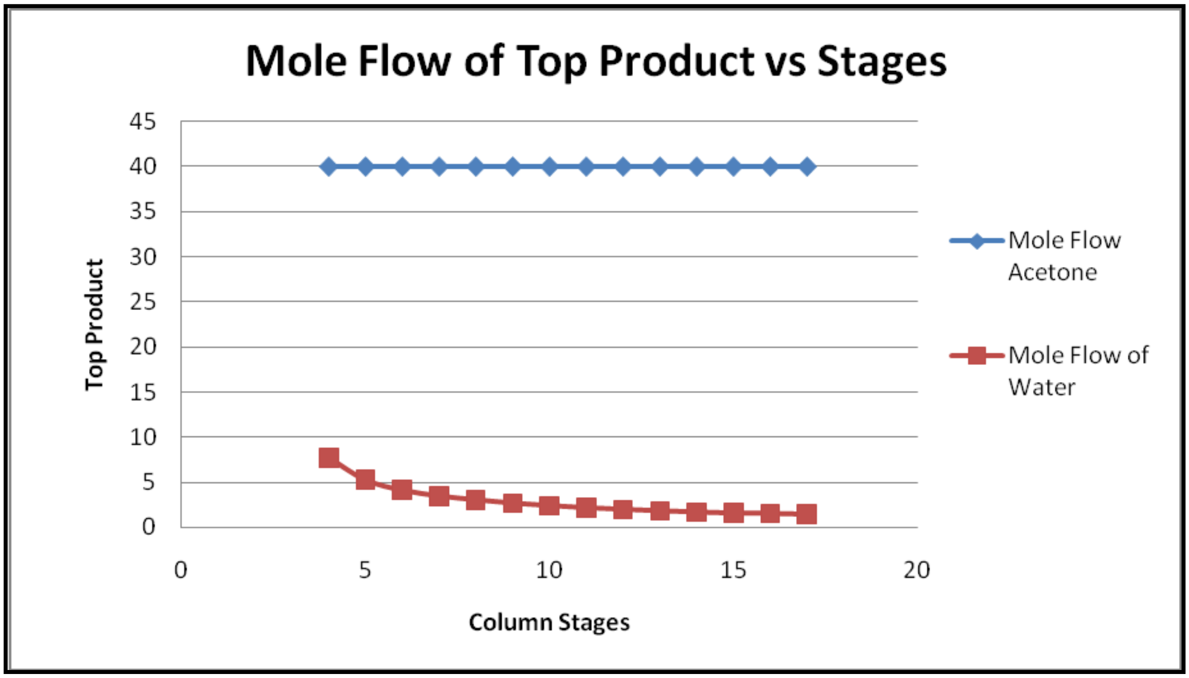


Figure 4-4: Graph of Flow Top Product versus Column Stages

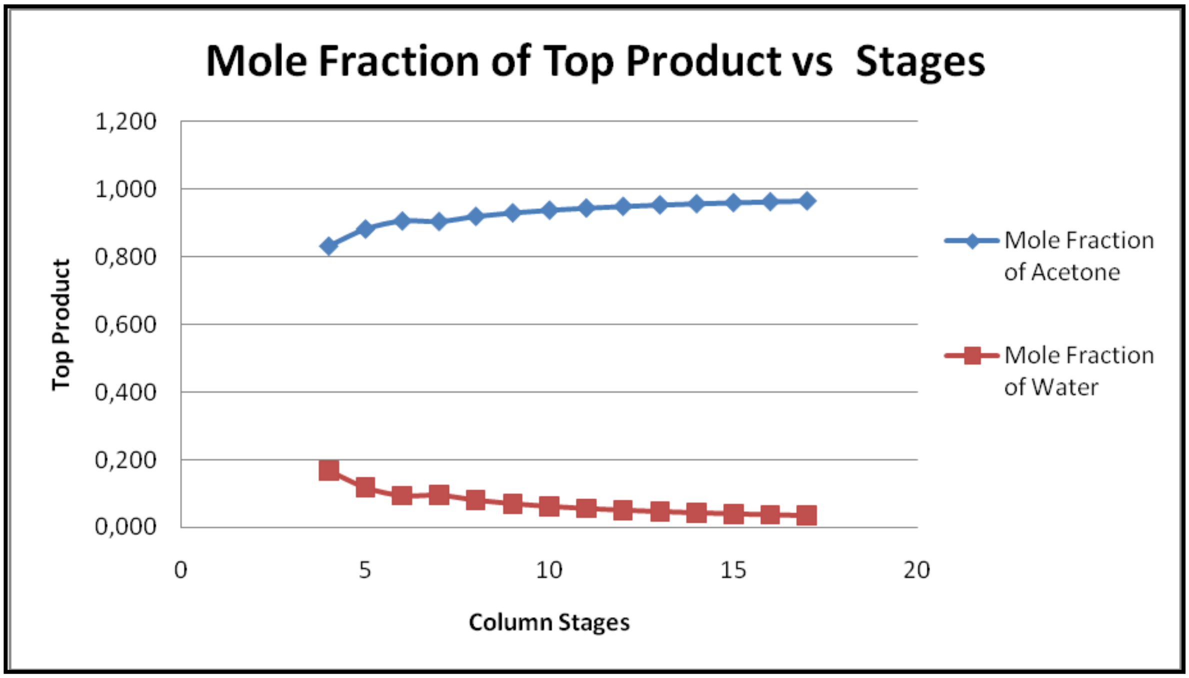


Figure 4-5: Graph of Composition Top Product versus Column Stages

Meanwhile, the purity of Acetone at the top product is gradually increased until it reaches up to 0.966 moles as shown in Figure 4-5. However, at this point, the numbers of stages become large which are 17 stages with reflux ratio, 2.5. In order to obtain purity specification of 99% mole acetone, larger number of stages and greater reflux ratio are required. Hence, it is not economical to use a simple distillation column since the operational cost and capital cost will increase markedly. Moreover, as been mentioned in the chapter 1 under the limitation of the study, there was no experimental values data for the region above 95 percent purity of Acetone as to support this study.

4.2 ENTRAINER SELECTION FOR WATER ACETONE BINARY MIXTURE

For extractive distillation, there is an almost infinite number of entrainer can be chosen. The screening of entrainers that are indicated by theory as being suitable does not require a lot of laboratory work. Experimental verification is best undertaken only after a list of promising candidate solvents has been generated and demonstrated via preliminary process modeling.

Few candidate entrainers that had been put to the iCON, included Diethlyene Glycol Dimethyl Ether, Dipropylene Glycol Methyl Ether and Dipropylene Glycol Dimethyl Ether. Diethylene Glycol Dimethyl Ether (Diglyme) has been chosen as the first solvent to be tried out in the simulator. The second and third entrainers have the same homologous group as Diglyme which is Ethers. All of these candidate entrainers have higher normal boiling point about $30^{O}C$-$40^{O}C$ than the boiling point of the key components. This is to ensure that the solvent is relatively nonvolatile and remains largely in the liquid phase. Based on Perry's Handbook, candidate solvents should be chosen from high boiling homologous series of both light and heavy key components. As being recommended by Perry's Handbook, polarities characteristics can be considered as well in order to select suitable entrainer. Candidate solvent can be selected from chemical groups that tend to show higher polarity than one key component or lower polarity than the other key. The general trend in polarity based on the functional group of a molecule is given in Table 2-1. From the table, it shows that hydrocarbons and ethers have lower polarities compared to ketone and water. Hence, candidate entrainers from homologous group ethers were chosen for this system. Entrainer from homologous group hydrocarbon was not been selected because most if it have lower boiling point than the key components. The properties of candidate solvents for Water-Acetone Mixture are shown in Table 4-2.

Table 4-2: Properties of Candidate Solvents for Water-Acetone System

Properties	**Solvent**		
	Diethylene Glycol Dimethyl Ether (DIGLYME)	Dipropylene Glycol Methyl Ether (DPGME)	Dipropylene Glycol Dimethyl Ether (DPDME)
Synonyms	Ethane; 1-1'-oxybis [2-methoxy- ;diethylene glycol dimethyl ether; diglyme; bis (2-methoxyethyl) ether.	Dipropylene glycol methyl ether; Dipropylene glycol monomethyl ether; Methoxypropoxypropanol; DGME;DPGME	1-methoxy-3-(3-methoxypropoxy);propane; Dipropylene glycol dimethyl ether; DPDME; DPGDME
CAS No.	111-96-6	34590-94-8	111109-77-4
Molecular Weight	134.18	148.2	162.23
Chemical Formula	$(CH_3OCH_2CH_2)_2O$	CH3-(OC3H6)2-OH	$CH_3OC_3H_6OC_3H_6OCH_3$
Boiling point	$162^{O}C$	$193.53\ ^{O}C$	$170.88\ ^{O}C$
Azeotrope with water and acetone	None	None	None
Solubility in water	Total	Total	Total

4.3 DESIGNING EXTRACTIVE DISTILLATION COLUMN

The first step in designing a column in any simulation is to choose a suitable simulation package. This physical property is used to describe accurately the phase equilibrium of the chemical component system. Based on Luyben W.L. (2006), if operating data from a laboratory, pilot plant, or plant column are available, they can be used to determine what physical property method fits the column data.

For nonideal system, Margules, Wilson or UNIQUAC models are more suitable to predict the VLE behavior of the system. From these three models, the UNIQUAC was used to predict the activity coefficients and ideal gas model to fugacity coefficient. The binary interaction parameters using UNIQUAC model for Water-Acetone were obtained from the iCON simulation. Furthermore, the binary vapour-liquid and liquid-liquid equilibrium data gathered from previous research and experimental result are used to estimate the binary parameters of the UNIFAC method of predicted binary UNIQUAC parameters. This is due to no interaction parameters present for the binary of Water-Diglyme and Acetone-Diglyme. Both sets of model parameters are used to model the vapor-liquid equilibrium of ternary mixture containing Water-Acetone and Diethylene Glycol Dimethyl Ether (Diglyme). Table 4-3 shows the binary interaction vapor liquid equilibrium data for Water-Acetone-Diglyme by Okullo (1999).

Table 4-3: The Binary Interaction Parameters for the UNIQUAC model and estimates UNIFAC for system 1.

j \ i	**Acetone**	**Water**	**Diglyme**
Acetone	0	-52.3022	218.3864*
Water	601.6118	0	-398.2705*
Diglyme	-114.8491*	-389.2705*	0

Source: The UNIFAC estimates binary data denotes by * were taken from the Eduljee, H.E. Ran Ind.Eng.Chem,Eng.Data Series 3,44(1958).

However, the binary interaction data for Water-Diglyme and Acetone-Diglyme from iCON software gave different readings compared to the values given in above table. This is might due to the different source of model parameters.

Similarly, the UNIQUAC ideal model was also used to simulate the ternary systems of Acetone-Water-DPGME and Acetone-Water-DPDME. The information for both of these ternary systems was available in the iCON.

Table 4-4: The Binary Interaction Parameters for the UNIQUAC model and estimates UNIFAC for System 2

j i	**Water**	**Acetone**	**DPGME**
Water	0	46.0406	-649.3252
Acetone	-340.9525	0	58.7200
DPGME	291.0823	-109.0318	0

Table 4-5: The Binary Interaction Parameters for the UNIQUAC model and estimates UNIFAC for System 3

j i	**Water**	**Acetone**	**DPDME**
Water	0	-340.9525	95.7615
Acetone	46.0406	0	-370.2922
DPDME	-158.7138	131.5933	0

For designing a distillation column, two pressures are design variables to be optimized, as well as the number of trays in each column and feed-tray locations. The larger the difference in the two pressures, further apart the azeotropic compositions, less recycle is required and the lower of the energy consumption. However, the lower the pressure in the low-pressure column, the larger the diameter and the coolant required in the condenser. The higher the pressure in the high-pressure column will lead to higher pressure of the steam that must be used in the reboiler and other problems with high temperature at reboiler. Hence, a few iteration need to be done at distillation column as to get the optimum separation parameters, in terms of reflux ratio, number of stages, and product purities.

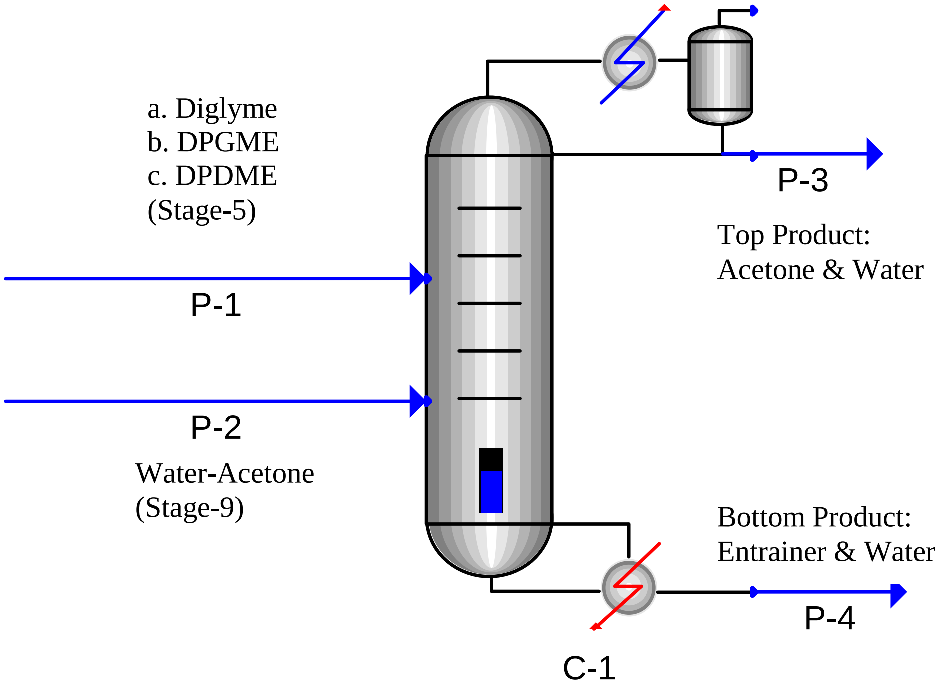


Figure 4-6: Extractive Distillation Unit for Acetone Production

The distillation column having 17 stages and the feed is introduced at bottom stage (stage 9). The previous study showed that the extraction column could be reasonably within HYSIS by 16 ideal stages. All simulations were carried out at a column top pressure of 1 atm and bottom pressure of 2 atm. The composition of feed is 0.5 mole water and 0.5 mole acetone where as the entrainer is fed at 1 mole. For the composition of entrainer, it is normal to operate at range of 0.8 to 0.9 mole fraction of entrainer which then can raise the relative volatility to a value at which separation is easy. The three systems considered in this study were simulated with same basic data, shown in Table 4-6.

Table 4-6: Extractive Distillation Unit Summary

Unit Tag	Description	Operating Parameter
C-1	Extractive Distillation Column	• Operating pressure = Top (1atm) Bottom (2atm) • Number of stages = 17 • Feed tray (Stream P-8) = 4 • Solvent feed tray (Stream P-5) = 9 • Reflux Ratio, R = 1.5
P-1	Feed Stream	• Total Molar Flowrate = 100 kgmole/hr • Composition i) Acetone = 0.5 mole ii) Water = 0.5 mole
P-2	Solvent Stream	• Total Molar Flowrate = 15 kgmole/hr • Composition Entrainer = 1.0 mole

According to Steltenpohl. *et.al*

> Extractive solvent is effective only in the liquid phase and, being the least volatile component of all; it is present primarily in the liquid phase flowing from the column top downwards. Counter-current flow of feed and entrainer within the distillation column was assumed on order to improve the contact of entrainer with separated mixture. Therefore, the inlet tray for entrainer was situated at the top stage, allowing good contact of the extractive solvent with the separated mixture. However, the entrainer stage should not be fed at the top of the column ranges from stage 1 to stage 4, because there will be some amount of entrainer release in the distillate.

4.4 ENTRAINER PERFORMANCE COMPARISON

The simulation model is used to study the effect of various design and operating parameters to the purity of the acetone produced. The design factor investigated included reflux ratio, feed ratio and the number of theoretical stages. All the simulation results can be referred at Appendix C.

4.4.1 Effect of Reflux Ratio

Reflux ratio does give affect to the purity of the top product. As reflux ratio keep increasing, the top product is more purified as well. However, in order to have a cost effective distillation column, a minimum number of reflux of ratio must be maintained. This is because a higher number of reflux ratio will lead to greater energy consumption of reboiler and condenser. Other parameters such as the number of trays, feed ratio and so forth were kept constant. Below graphs show the effect of reflux ratio to the composition and mole flow of top product.

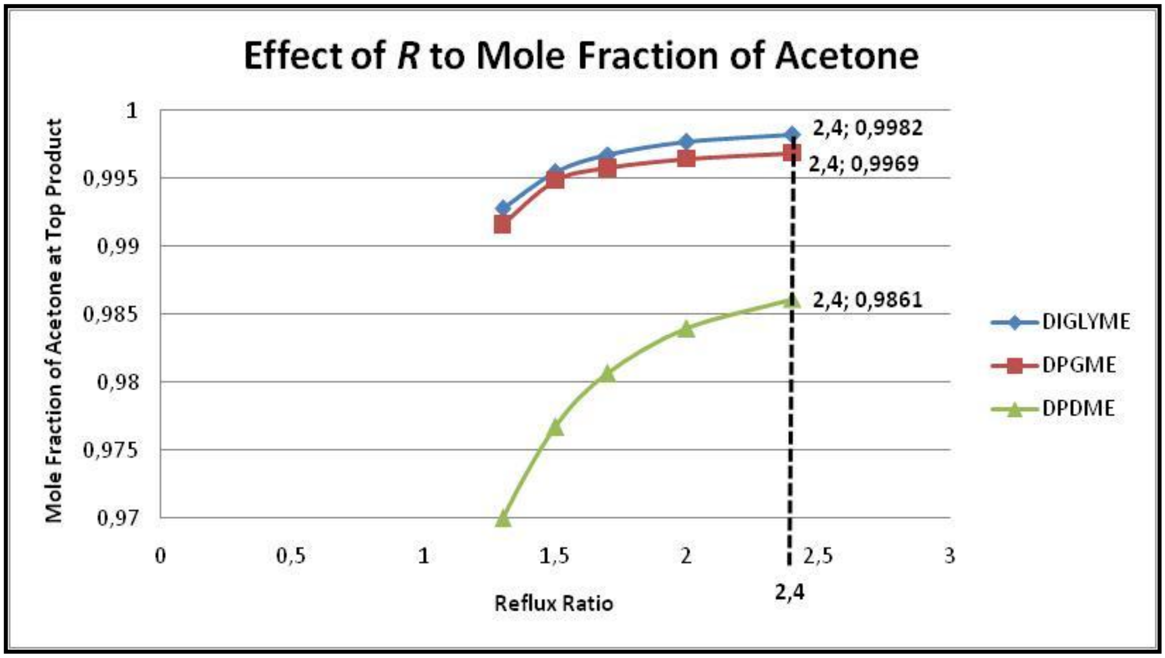


Figure 4-7: The effects of Reflux Ratio to the Composition of Acetone at Top Product

From figure 4-7, it shows that at reflux ratio 1.5, the highest purity that can be achieved is 0.995 using Diglyme and DPGME. The result of using diglyme and DPGME did not give large difference. However, the composition of acetone by using DPDME only reached up to 0.976. Hence, diglyme and DPGME can be considered as the suitable entrainer for this system since the purity could achieve 0.99 with low reflux ratio in the same condition. Reflux ratio will affect the reboiler charge. If can decrease the reboiler consumption if etiher diglyme or DPGME is used as entrainer.

Table 4-7: The effects of Reflux Ratio to the Mole Flow of Acetone at Top Product

Solvent	Mole Flow Acetone (kgmole/hr)	Percentage separation efficiency (%)
Diglyme (Diethylene Glycol Dimethyl Ether)	26.03	52.06
DPGME (Dipropylene Glycol Methyl Ether)	33.32	66.64
DPDME (Dipropylene Glycol Dimethyl Ether)	37.05	74.1

The effect of reflux ratio to the mole flow of acetone at top product was investigated as well. From the result shown in Table 4-7, DPDME gave the highest amount of acetone as the top product compared to Diglyme and DPGME. The second highest mole flow of acetone was achieved by using DPGME which is 33.32 kgmole/hr. On the other hand, Diglyme gave the lowest amount of acetone at the top product. In this case, the most potential entrainer would be DPGME. Moreover, further purification by increasing the number of reflux ratio is not necessary. The optimum number of reflux ratio was set 1.5 throughout the study. This value allowed optimum contact of the vapour and liquid phases preserving good separation efficiency of the column.

4.4.2 Effect of feed ratio

In order to illustrate the advantage of solvent, the effect of amount of entrainer to the purity of top product and bottom product on the separation was then investigated. To do this, the reflux ratio was maintained at 1.5, whilst the amount of entrainer was varied from 10 kgmole to 40 kgmole.

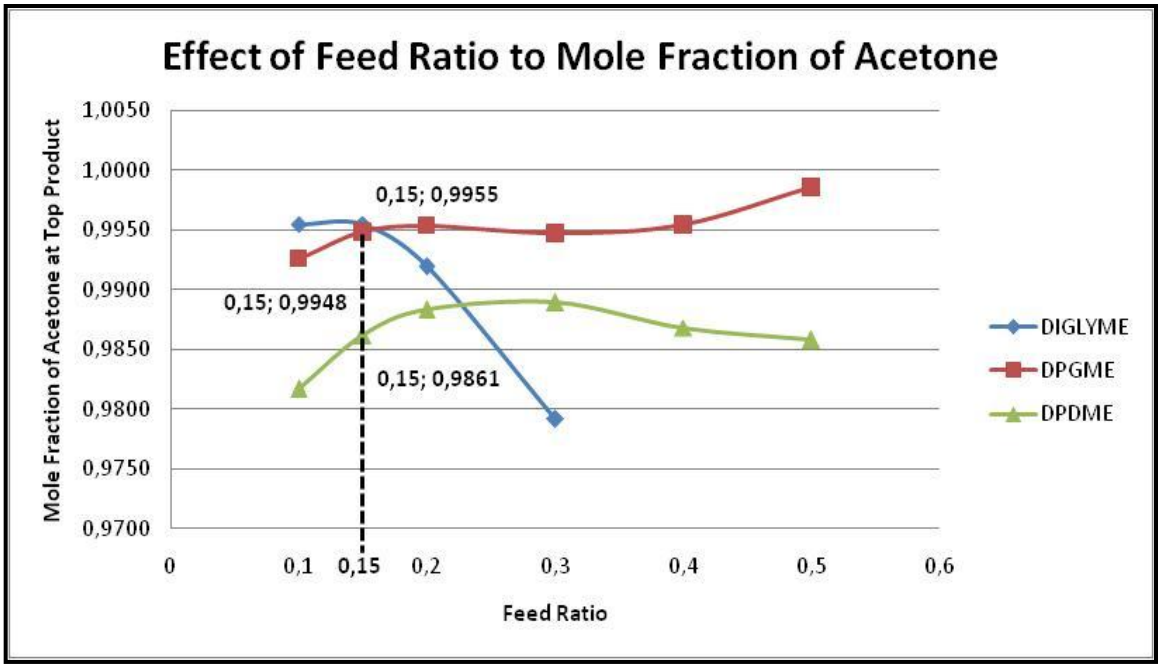


Figure 4-8: The effects of Feed Ratio to the Composition of Acetone at Top Product

Figure 4-8 shows the concentration of acetone in distillate decreased with an increase in solvent for all entrainers except for DPGME. When the feed ratio is equal to 0.15, the mole fractions of acetone in first system and second system are almost the same which are 0.995. Meanwhile, the mole fraction of DPDME could only be achieved around 0.986. This concluded that Diglyme and DPGME can be used as entrainer instead of DPDME because both of these entrainers could decrease the consumption of solvent largely. Apparently, the purity of water in the bottoms product decreases as there is more entrainer in the system.

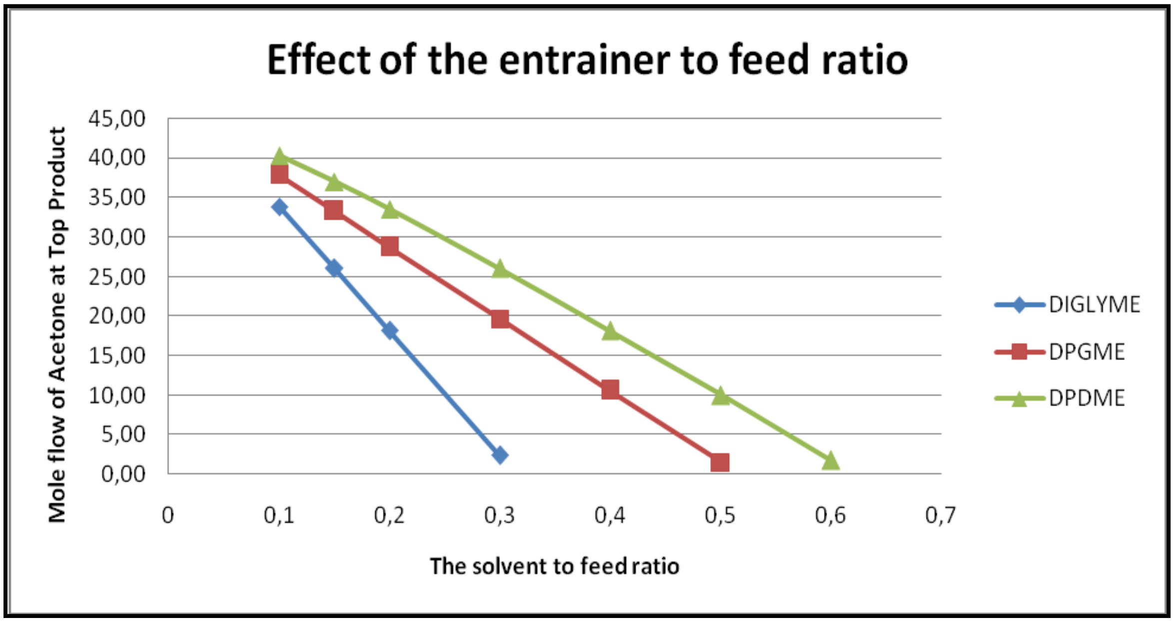


Figure 4-9: The effects of Feed Ratio to the Mole Flow of Acetone at Top Product

The figure shows that the changes in feed ratio give a significant effect to the mole flow of acetone at top product. Compared with DPGME, there is an optimum amount of diglyme that can be used in this system which ranges between 15 kgmole/hr to 20 kgmole/hr. Even though by using DPDME gives the highest mole flow, but as mentioned earlier, the composition of top product produced is very low and did not meet the target composition.

4.4.3 Effect of number of stages

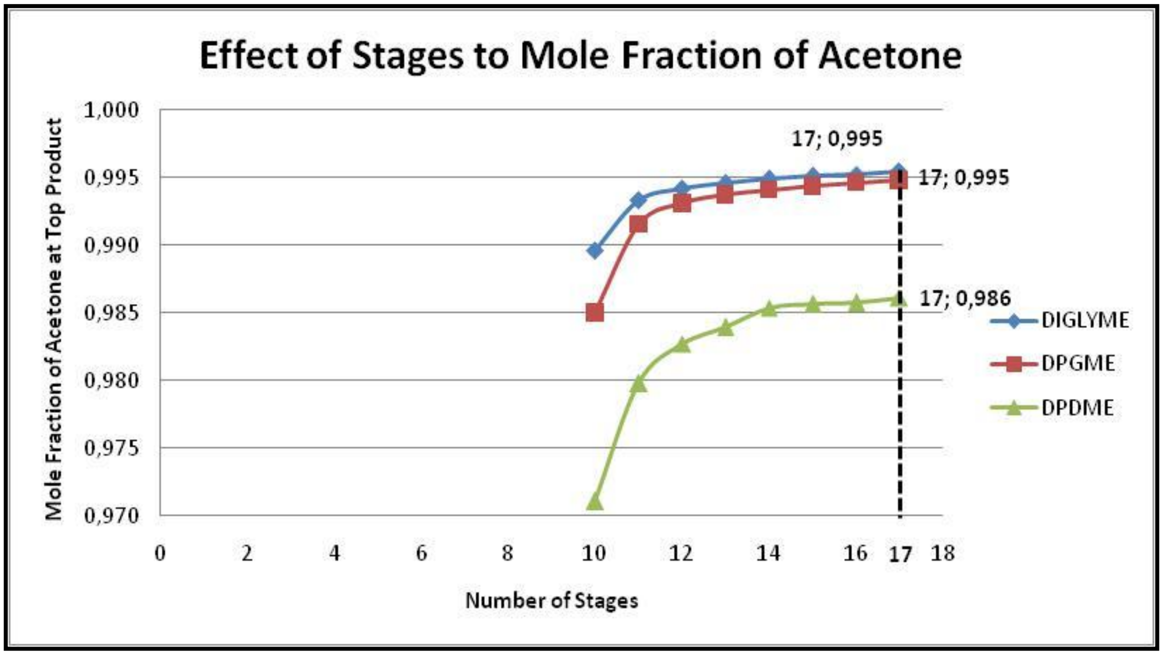


Figure 4-10: The effects of Stages to the Composition of Acetone at Top Product

Based on Knapp and Doherty (1994), by increasing the theoretical stages, it will improve the performance of the column by increasing the purity of at least one the distillation product. Theoretically, by increasing the number of stages, there will be a greater surface contact between the entrainer and the mixture. At this condition, intensive-enough contact of vapour and liquid phases was achieved, allowing reaching prescribed distillate purity even if relatively small amount of entrainer was used. As a result, the separation between acetone and water will become more efficient. In figure 4-10, when the stages increased from stage 10 to 17, the mole fraction of the top product gradually improved. However, the product purity can only reached up to 0.986 moles by using DPDME and definitely, this do not meet the product specification. Hence, it is obvious that diglyme and DPGME are more suitable to be chosen as the entrainer compared to DPDME. In order to evaluate quantitatively the column separation efficiency, the amount of the separated acetone in distillate was compared to its amount in the feed. As to get a better quality product, we would like to recover acetone as the distillate rather than from the bottom stream. Simulation result showing that DPGME will produce the desire production rate of more than 33.32 kgmole/hr with the solvent flow rate of 15 kgmole/hr. The optimum results of separation of Water and Acetone by using DPGME can be referred in APPENDIX D.

Table 4-8: The Mole Flow of Acetone at Distillate by Utilizing Different Solvents

Solvent	Mole Flow Acetone (kgmole/hr)	Percentage separation efficiency (%)
Diglyme (Diethylene Glycol Dimethyl Ether)	26.03	52.06
DPGME (Dipropylene Glycol Methyl Ether)	33.32	66.64
DPDME (Dipropylene Glycol Dimethyl Ether)	37.05	74.1

4.5 Validation of Simulation Results

For the validation of simulation results obtained from the iCON Simulator, it is quite difficult to compare it with any experimental data since there was no detailed research for the same system available in the open literature. For general comparison, a journal from Okulla (1999) was taken as the reference as to compare the trend of the results produced by the iCON Simulator. The overall results were reflected with the result from the journal referred it is logical and reasonable. For example, the composition of feed was the highest at feed stage and decreased along the remaining trays. Meanwhile, the product composition was highest at distillates or bottom column with respectively to their volatility. The other example is that acetone was recovered highest at distillate compared to the bottom. This is due to the relative volatility and boiling point temperature of acetone is much lower than other components. Therefore, it recovered more at the distillate. The results from the research done by Xu *et.al* (2006) also gave the same trend with this study even the components that have been tasted are different.

Moreover, Xu et.al (2006) has mentioned that the feasibility of their process via simulation and by experiment in packing column was confirmed.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATION

In conclusion, Dipropylene Glycol Methyl Ether (DPGME) was chosen as the suitable entrainer for the acetone and water mixture by extractive distillation. The feasibility of the process via simulation was confirmed. At this stage, the author has completed all the objectives which are to study the entrainer selection for non ideal mixture that would result in azeotrope and inflections point. The second objective is to study the distillation column sensitivities to feed ratio, number of stages and reflux ratio. Last objective is to simulate the effects of entrainer as to find the suitable solvent to separate acetone and water mixture. By using DPGME, the concentration of the acetone product achieves 99% purity with column stages 17, reflux ratio 1.5 and low feed ratio (0.15), which illustrates the good character of the solvent. DPGME was used as the entrainer instead of diglyme and DPDME, because DPGME consumption can be decreased.

There is some technical recommendation which is to use the latest version of iCON. The software needs to be updated from time to time. This might give a better result or otherwise the result will be incorrect and unreasonable. Other than that, the simulation can also be performed in more established and reliable software. Commercial software like Aspen Plus and HYSIS has a wide application and these are the popular choices for researchers in simulation study. In the mean time, Aspen Plus has been used to construct residue curve maps which facilitate this study. Detailed experiment data about the optimum separation parameters in the same system is needed to obtain a thorough evaluation. Experimental verification is best undertaken only after a list of promising candidate solvents has been generated and demonstrated via preliminary process modeling. For future works, it is also recommended to carry out a batch experiment in a small laboratory column to evaluate the feasibility of the entrainer chosen from this preliminary study. Due to the time constraint, the economic evaluation for the system has not been performed. However, the scope of the research project was to focus on finding the suitable entrainer and optimum separation parameters as to produce 99% purity of Acetone. Hence, an economic evaluation of the process can be done for the expansion and continuation of this research project as to evaluate the economic effect of varying the separation parameters of the column.

Much knowledge is gained in the learning process especially about iCON. Even though, if iCON is considered as a very powerful simulation and it is commonly used in process plant, still not type of the package are implemented because the packages included depends on the process run. There are some lessons learned during the undertaking of the project which are:

- It is important to be familiar with the software used. Even if the simulation process might face some trouble, there might be other solution in overcoming the problem.
- Find as many information as possible concerning the process and design before starting on the simulation process. This will prevent any delay in solving problem during simulation due to lack of information.

Last but not least, hopefully this skills gained in this research project will be very useful and be a guidance to be applied in the future.

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APPENDICES

APPENDIX A

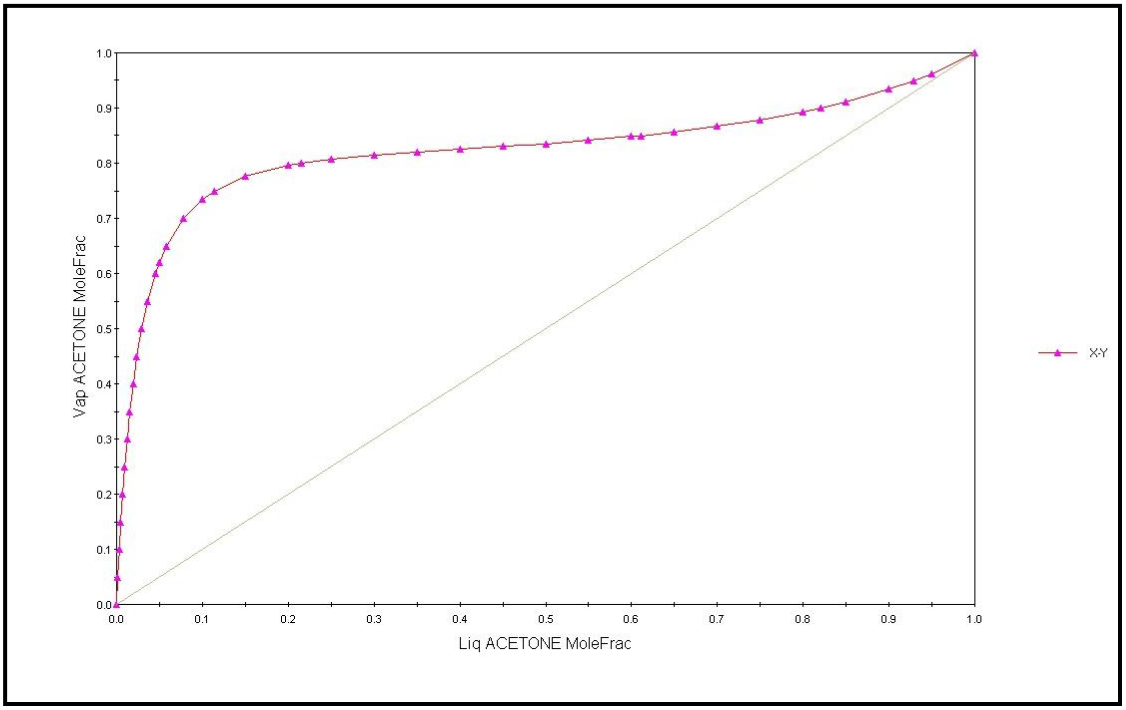


Figure A-1: VLE Diagram of Water Acetone Mixture at Pressure 1 atm

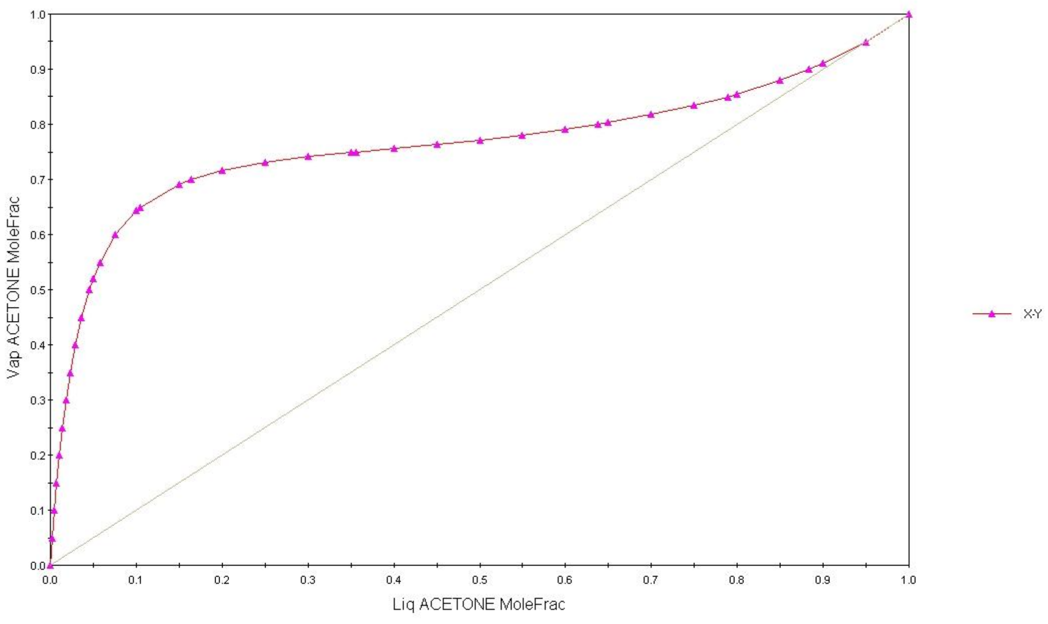


Figure A-2: VLE Diagram of Water Acetone Mixture at Pressure 3 atm

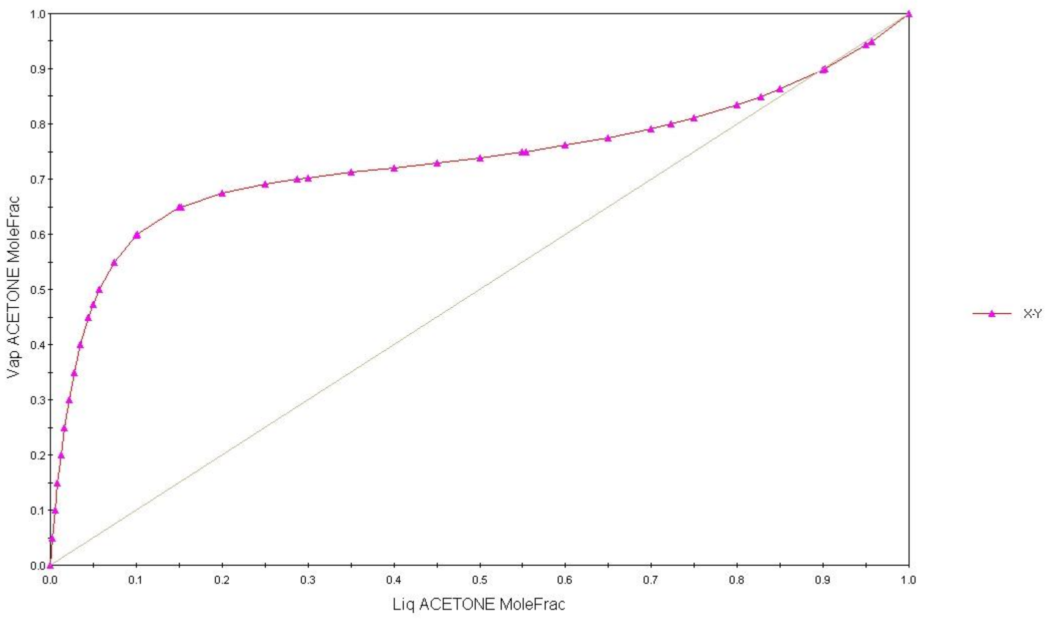
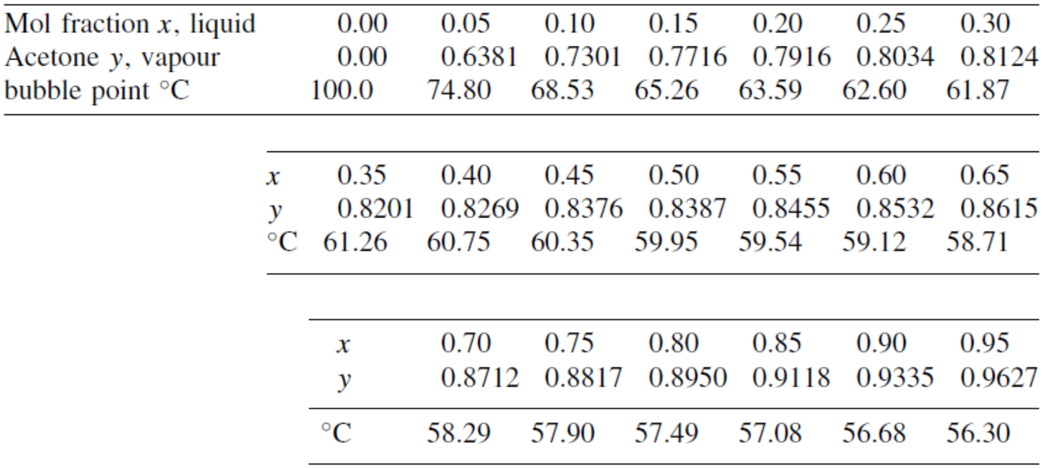


Figure A-3: VLE Diagram of Water Acetone Mixture at Pressure 5 atm

APPENDIX B

Acetone is to be recovered from an aqueous waste stream by continuous distillation. The feed will contain 10 per cent w/w acetone. Acetone of at least 98 per cent purity is wanted, and the aqueous effluent must not contain more than 50 ppm acetone. There is no point in operating this column at other than atmospheric pressure.

The data of Kojima *et al*. will be used.



Mol fraction x, liquid	0.00	0.05	0.10	0.15	0.20	0.25	0.30
Acetone y, vapour	0.00	0.6381	0.7301	0.7716	0.7916	0.8034	0.8124
bubble point °C	100.0	74.80	68.53	65.26	63.59	62.60	61.87

x	0.35	0.40	0.45	0.50	0.55	0.60	0.65
y	0.8201	0.8269	0.8376	0.8387	0.8455	0.8532	0.8615
°C	61.26	60.75	60.35	59.95	59.54	59.12	58.71

x	0.70	0.75	0.80	0.85	0.90	0.95
y	0.8712	0.8817	0.8950	0.9118	0.9335	0.9627
°C	58.29	57.90	57.49	57.08	56.68	56.30

The equilibrium curve can be drawn with sufficient accuracy to determine the stages above the feed by plotting the concentrations at increments of 0.1. The diagram would normally be plotted at about twice the size of Figure B-1.

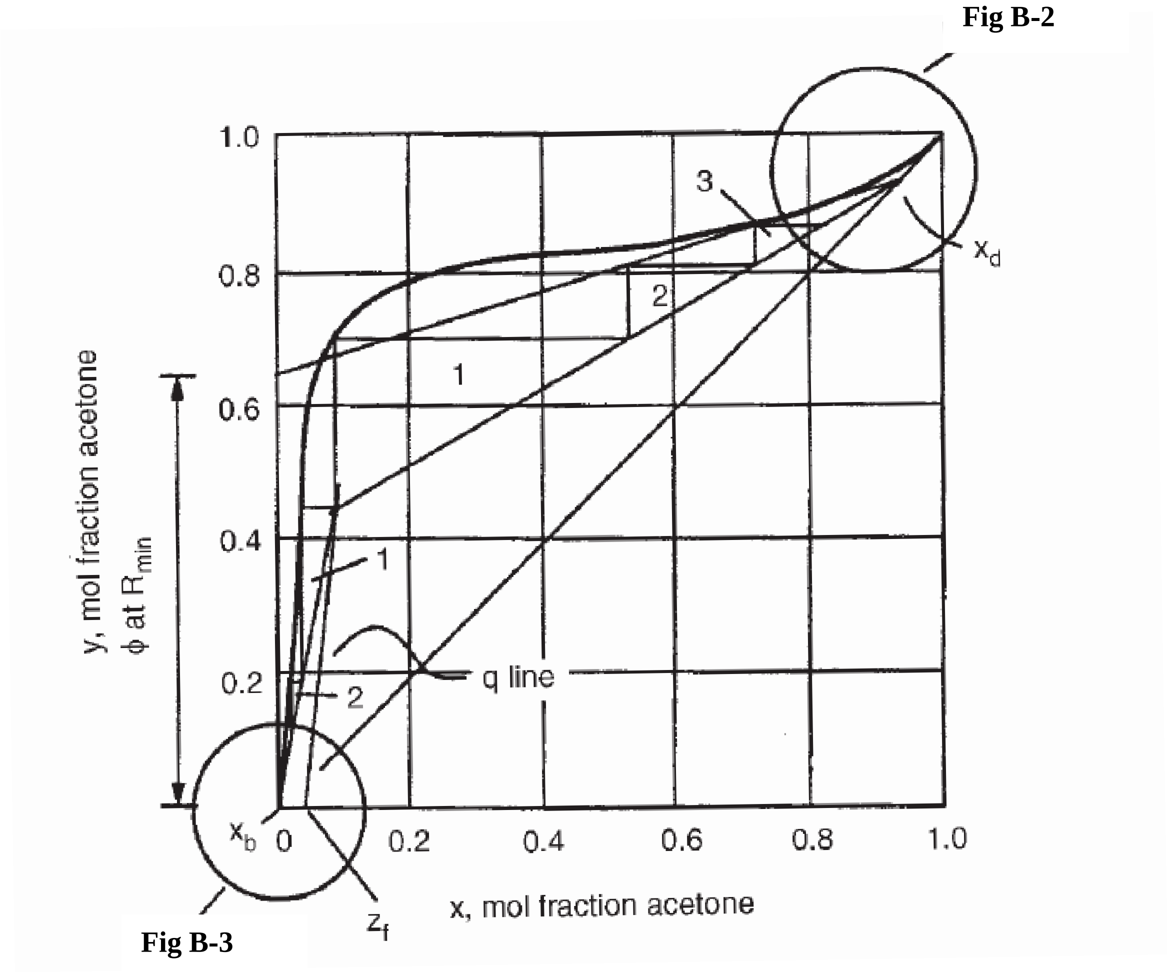


Figure B-1: McCabe-Thiele plot, adapted from Coulson and Richarson. (2005, pp. 508)

Molecular weights, acetone = 58, water = 18

$$\text{Mol fractions acetone feed} = \frac{\dfrac{10}{58}}{\dfrac{10}{58} + \dfrac{90}{18}} = 0.033$$

$$\text{top product} = \frac{\dfrac{98}{58}}{\dfrac{98}{58} + \dfrac{2}{18}} = 0.94$$

$$\text{bottom product} = 50 \times 10^{-6} \times \frac{18}{58} = 15.5 \times 10^{-6}$$

Mean specific heats, water 75.3, acetone 128 J/mol °C

Latent heat of feed = 28,410 x 0.033 + (1 - 0.033) 41,360 = 40,933 J/mol

Specific heat of feed = (0.033 x 128) + (1 - 0.033) 75.3 = 77.0 J/mol °C

Heat to vaporize 1 mol of feed = (83 - 20) 77.0 + 40,933 = 45,784 J

$$q = \frac{45{,}784}{40{,}933} = 1.12$$

$$\text{Slope of } q \text{ line} = \frac{1.12}{1.12 - 1} = 9.32$$

For this problem the condition of minimum reflux occurs where the top operating line just touches the equilibrium curve at the point where the q line cuts the curve.

From the Figure B-1,

ø for the operating line at minimum reflux = 0.65

From equation $\phi = \frac{x_d}{1 + R}$

R_{min} = 0.94/0.65 - 1 = 0.45

Take R = R_{min} x 3

As the flows above the feed point will be small, a high reflux ratio is justified; the

condenser duty will be small.

$$\text{At } R = 3 \times 0.45 = 1.35, \quad \phi = \frac{0.94}{1 + 1.35} = 0.4$$

For this problem it is convenient to step the stages off starting at the intersection of the operating lines. This gives three stages above the feed up to y = 0.8. The top section is drawn to a larger scale, Figure B-2, to determine the stages above y = 0.8: three to four stages required; total stages above the feed 7.

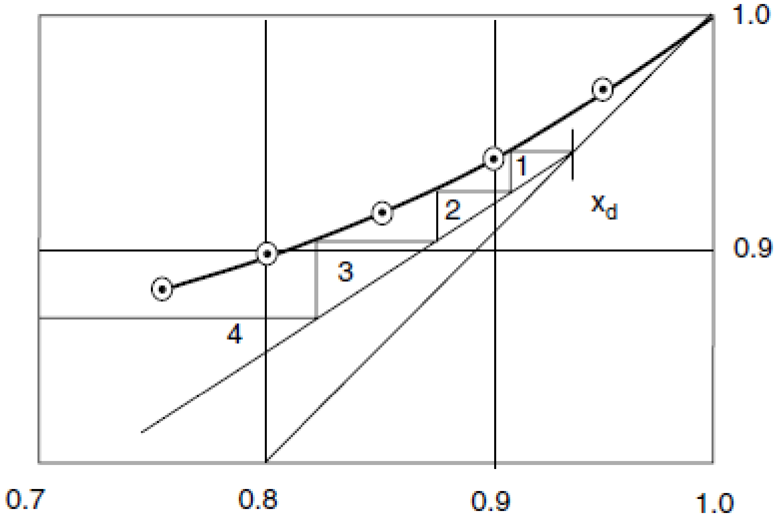


Figure B-2: Top section enlarged

Below the feed, one stage is required down to x = 0.04. A log-log plot is used to determine the stages below this concentration. Data for log-log plot: operating line slope, from Figure B-1 = 0.45/0.09 = 5.0

operating line equation, $y = 4.63(x - x_b) + x_b$

$= 5.0x - 62.0 \times 10^{-6}$

equilibrium line slope, from v- l- e data = 0.6381/0.05 = 12.8

	$x =$	4×10^{-2}	10^{-3}	10^{-4}	4×10^{-5}	2×10^{-5}
Equilibrium line	$y =$	0.51	1.3×10^{-2}	1.3×10^{-3}	5.1×10^{-4}	2.6×10^{-4}
Operating line	$y =$	0.20	4.9×10^{-3}	4.4×10^{-4}	1.4×10^{-4}	3.8×10^{-5}

From Figure B-3, number of stages required for this section = 8

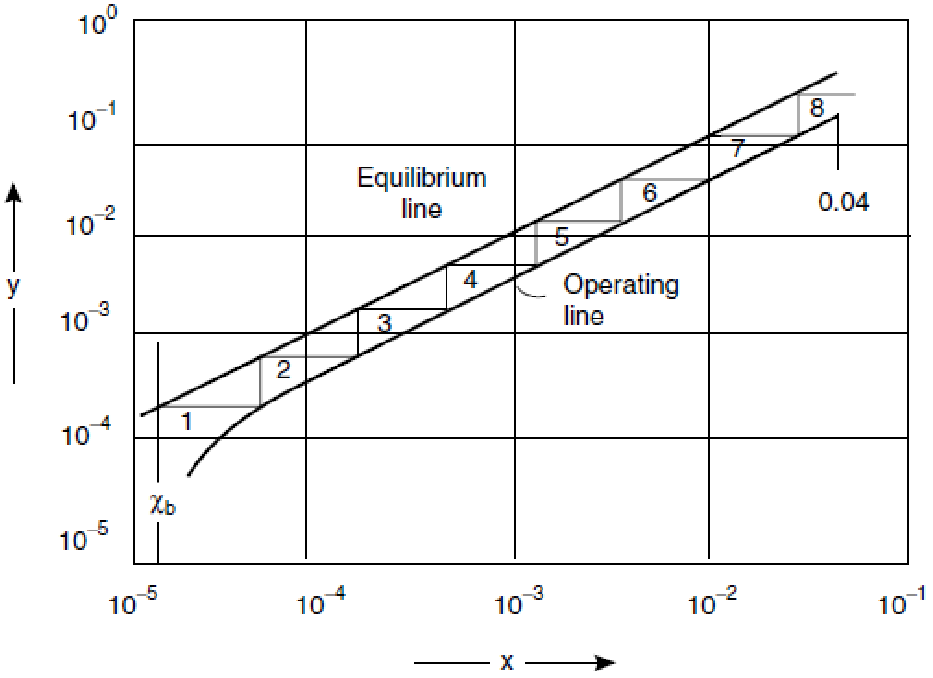


Figure B-3: Log-log plot of McCabe-Thiele diagram

Total number of stages below feed = 9

Total stages = 7 + 9 = 16

APPENDIX C

Table C-1: Results of Simple Distillation Column extracted from PETRONAS iCON Simulation

Column Stages	Feed Position	Top Product (CONDENSER L)		Top Product Flow(CONDENSER L)		RR
		xAC	xH2O	AC	H2O	
4	2	0.832	0.168	40	7.73	2.5
5	3	0.883	0.117	40	5.25	2.4
6	4	0.907	0.093	40	4.12	2.3
7	5	0.905	0.095	40	3.47	2.2
8	6	0.920	0.080	40	3.04	2.1
9	7	0.931	0.069	40	2.67	2
10	8	0.939	0.061	40	2.39	1.9
11	9	0.945	0.055	40	2.16	1.8
12	10	0.950	0.050	40	1.97	1.7
13	11	0.954	0.046	40	1.81	1.6
14	12	0.958	0.042	40	1.67	1.6
15	13	0.961	0.039	40	1.55	1.6
16	14	0.964	0.036	40	1.51	1.5
17	15	0.966	0.034	40	1.41	1

Table C-2: Results of Manipulating Reflux Ratio in PETRONAS iCON Simulation

Reflux Ratio	Mole Fraction of Acetone at Top Product			Moleflow of Acetone at Top Product (kgmole/hr)		
	DG	DPGME	DPDME	DG	DPGME	DPDME
1.2	NOT CONVERGED		0.9649	26.04	33.32	37.08
1.3	0.9928	0.9916	0.9700	26.03	33.32	37.07
1.5	0.9955	0.9949	0.9768	26.03	33.32	37.05
1.7	0.9968	0.9958	0.9807	26.03	33.32	37.04
2	0.9977	0.9965	0.9840	26.03	33.31	37.04
2.4	0.9982	0.9969	0.9861	26.03	33.31	37.03

Table C-3: Results of Manipulating Feed Ratio in PETRONAS iCON Simulation

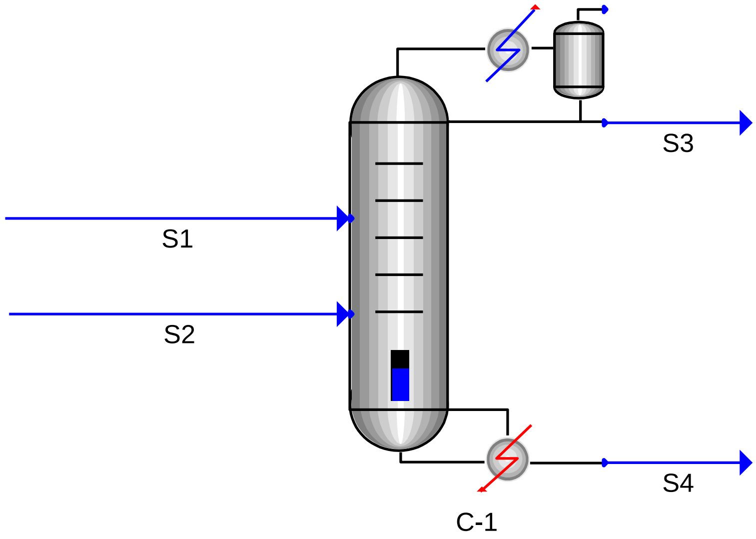
Amount of Entrainer	Amount of Feed	Feed Ratio	Mole Fraction of Acetone at Top Product			Moleflow of Acetone at Top Product (kgmole/hr)		
kgmole/hr			DG	DPGME	DPDME	DG	DPGME	DPDME
10	100	0.1	0.9955	0.9926	0.9817	33.84	37.85	40.36
15	100	0.15	0.9955	0.9948	0.9861	26.03	33.32	37.03
20	100	0.2	0.9919	0.9953	0.9883	18.18	28.77	33.53
30	100	0.3	0.9792	0.9947	0.9889	2.40	19.66	26.05
40	100	0.4	NOT CONVERGED	0.9954	0.9868	NOT CONVERGED	10.57	18.14
50	100	0.5		0.9986	0.9858		1.52	10.00

Table C-4: Results of Manipulating Number of Stages in PETRONAS iCON Simulation

Stages	Mole Fraction of Acetone at Top Product			Moleflow of Acetone at Top Product (kgmole/hr)		
	DG	DPGME	DPDME	DG	DPGME	DPDME
10	0.990	0.985	0.971	26.04	33.34	37.06
11	0.993	0.992	0.980	26.03	33.32	37.05
12	0.994	0.993	0.983	26.03	33.32	37.04
13	0.995	0.994	0.984	26.03	33.32	37.04
14	0.995	0.994	0.985	26.03	33.32	37.03
15	0.995	0.994	0.986	26.03	33.32	37.03
16	0.995	0.995	0.986	26.03	33.32	37.03
17	0.995	0.995	0.986	26.03	33.32	37.03

APPENDIX D

SIMULATION RESULTS OF THE SEPARATION OF WATER ACETONE MIXTURE USING DIPROPYLENE GLYCOL METHYL ETHER (DPGME) IN PETRONAS iCON SIMULATION.

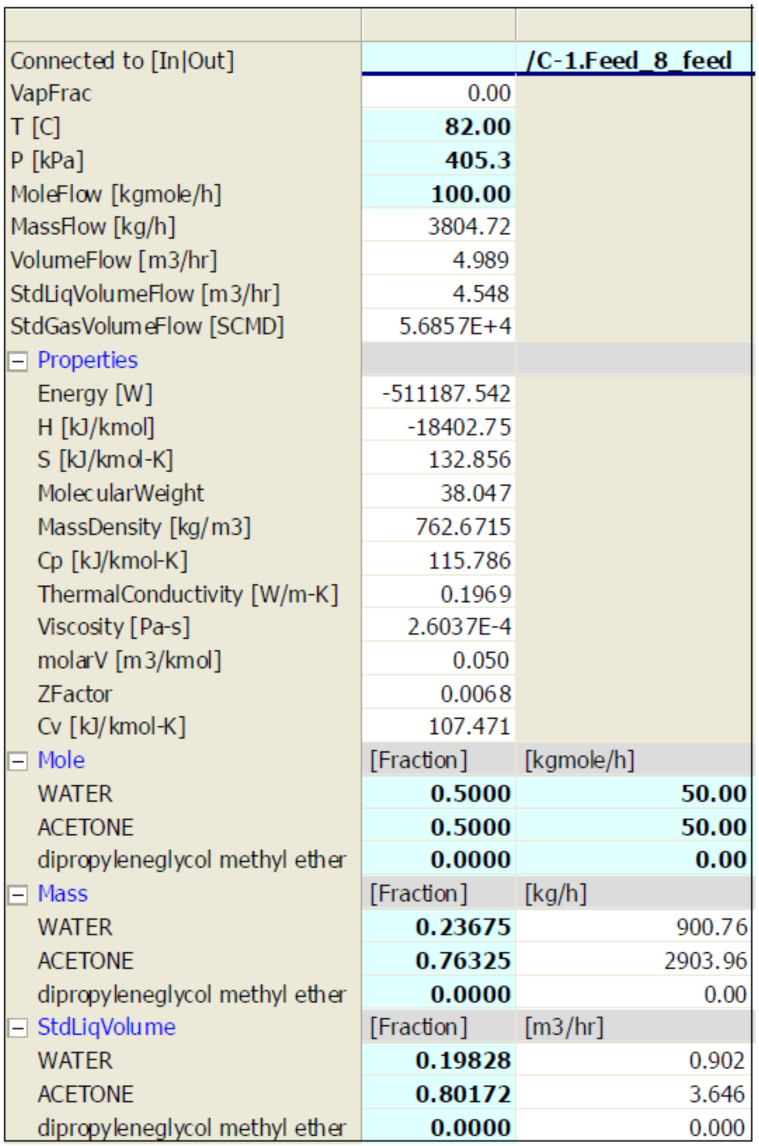


Name	S1	S2	S3	S4
VapFrac	0	0	0.00001	0
T [C]	82	100	56.2	105
P [kPa]	405.3	405.3	101.325	202.65
MoleFlow [kgmole/h]	100	50	1.52	148.48
MassFlow [kg/h]	3804.72	7410.01	88.08	11126.65
MoleFraction [Fraction]				
WATER	0.5	0	0	0.34
ACETONE	0.5	0	1	0.33
dipropyleneglycol methyl ether	0	1	0	0.34
MassFraction [Fraction]				
WATER	0.2367	0	1.28E-04	0.081
ACETONE	0.7633	0	0.9999	0.2531
dipropyleneglycol methyl ether	0	1	6.75E-06	0.666

/S1
Stream.Stream_Material
Name / Status

Summary

Material

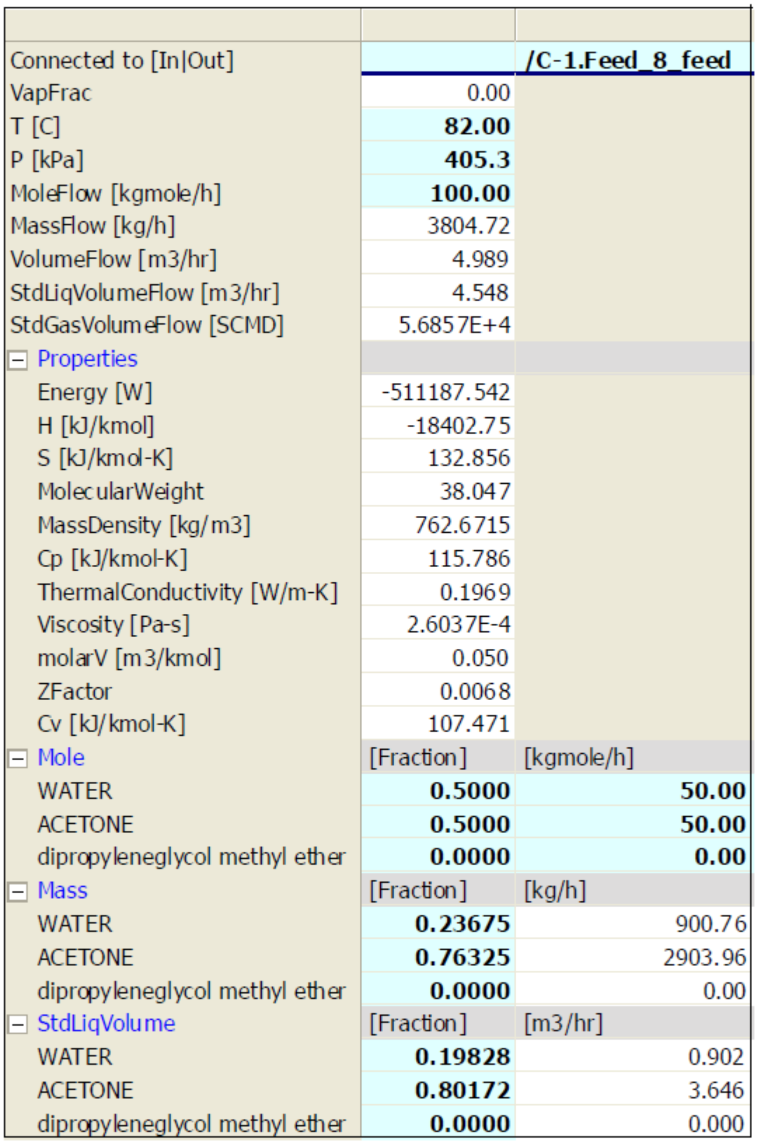


Connected to [In|Out]		**/C-1.Feed_8_feed**
VapFrac	0.00	
T [C]	**82.00**	
P [kPa]	**405.3**	
MoleFlow [kgmole/h]	**100.00**	
MassFlow [kg/h]	3804.72	
VolumeFlow [m3/hr]	4.989	
StdLiqVolumeFlow [m3/hr]	4.548	
StdGasVolumeFlow [SCMD]	5.6857E+4	
⊟ Properties		
Energy [W]	-511187.542	
H [kJ/kmol]	-18402.75	
S [kJ/kmol-K]	132.856	
MolecularWeight	38.047	
MassDensity [kg/m3]	762.6715	
Cp [kJ/kmol-K]	115.786	
ThermalConductivity [W/m-K]	0.1969	
Viscosity [Pa-s]	2.6037E-4	
molarV [m3/kmol]	0.050	
ZFactor	0.0068	
Cv [kJ/kmol-K]	107.471	
⊟ Mole	[Fraction]	[kgmole/h]
WATER	**0.5000**	**50.00**
ACETONE	**0.5000**	**50.00**
dipropyleneglycol methyl ether	**0.0000**	**0.00**
⊟ Mass	[Fraction]	[kg/h]
WATER	**0.23675**	900.76
ACETONE	**0.76325**	2903.96
dipropyleneglycol methyl ether	**0.0000**	0.00
⊟ StdLiqVolume	[Fraction]	[m3/hr]
WATER	**0.19828**	0.902
ACETONE	**0.80172**	3.646
dipropyleneglycol methyl ether	**0.0000**	0.000

/S2
Stream.Stream_Material
Name / Status

Summary

Material

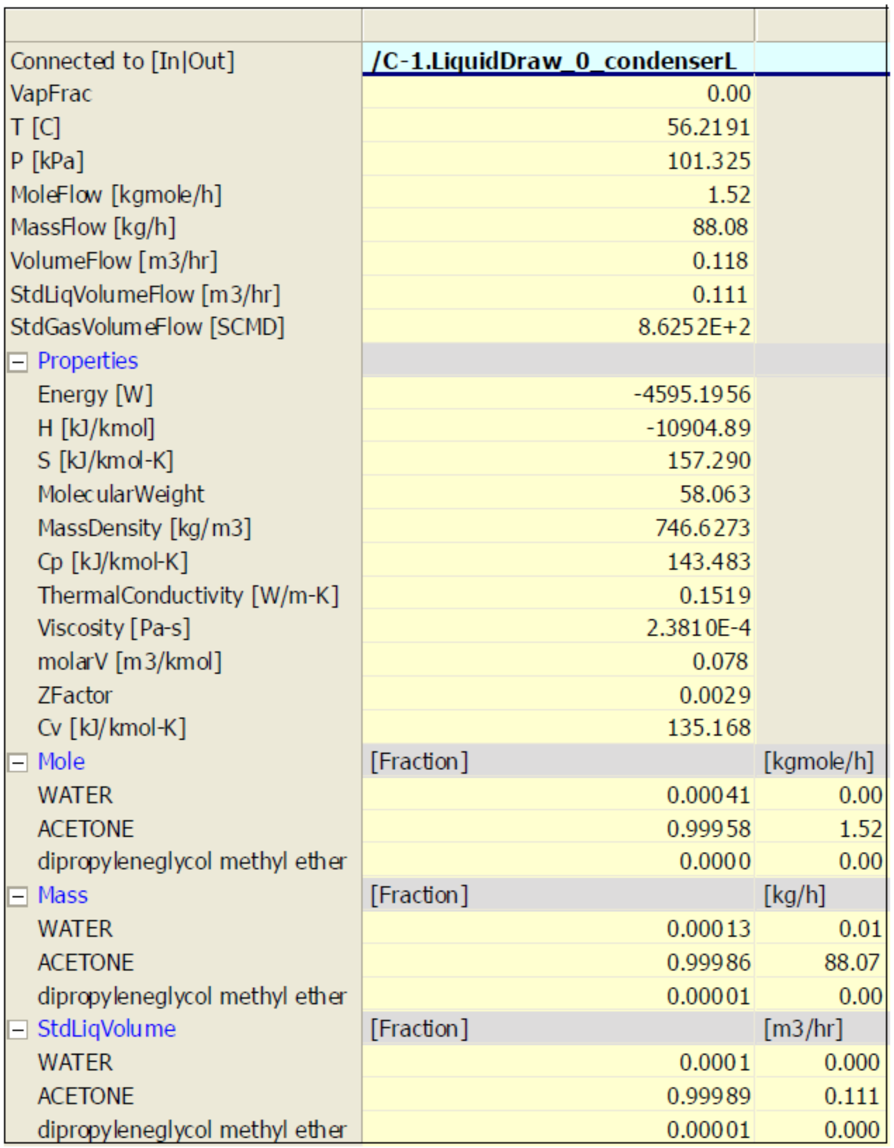


Connected to [In|Out]		/C-1.Feed_8_feed
VapFrac	0.00	
T [C]	**82.00**	
P [kPa]	**405.3**	
MoleFlow [kgmole/h]	**100.00**	
MassFlow [kg/h]	3804.72	
VolumeFlow [m3/hr]	4.989	
StdLiqVolumeFlow [m3/hr]	4.548	
StdGasVolumeFlow [SCMD]	5.6857E+4	
⊟ Properties		
Energy [W]	-511187.542	
H [kJ/kmol]	-18402.75	
S [kJ/kmol-K]	132.856	
MolecularWeight	38.047	
MassDensity [kg/m3]	762.6715	
Cp [kJ/kmol-K]	115.786	
ThermalConductivity [W/m-K]	0.1969	
Viscosity [Pa-s]	2.6037E-4	
molarV [m3/kmol]	0.050	
ZFactor	0.0068	
Cv [kJ/kmol-K]	107.471	
⊟ Mole	[Fraction]	[kgmole/h]
WATER	**0.5000**	**50.00**
ACETONE	**0.5000**	**50.00**
dipropyleneglycol methyl ether	**0.0000**	**0.00**
⊟ Mass	[Fraction]	[kg/h]
WATER	**0.23675**	900.76
ACETONE	**0.76325**	2903.96
dipropyleneglycol methyl ether	**0.0000**	0.00
⊟ StdLiqVolume	[Fraction]	[m3/hr]
WATER	**0.19828**	0.902
ACETONE	**0.80172**	3.646
dipropyleneglycol methyl ether	**0.0000**	0.000

/S3
Stream.Stream_Material
Name / Status

Summary

Material

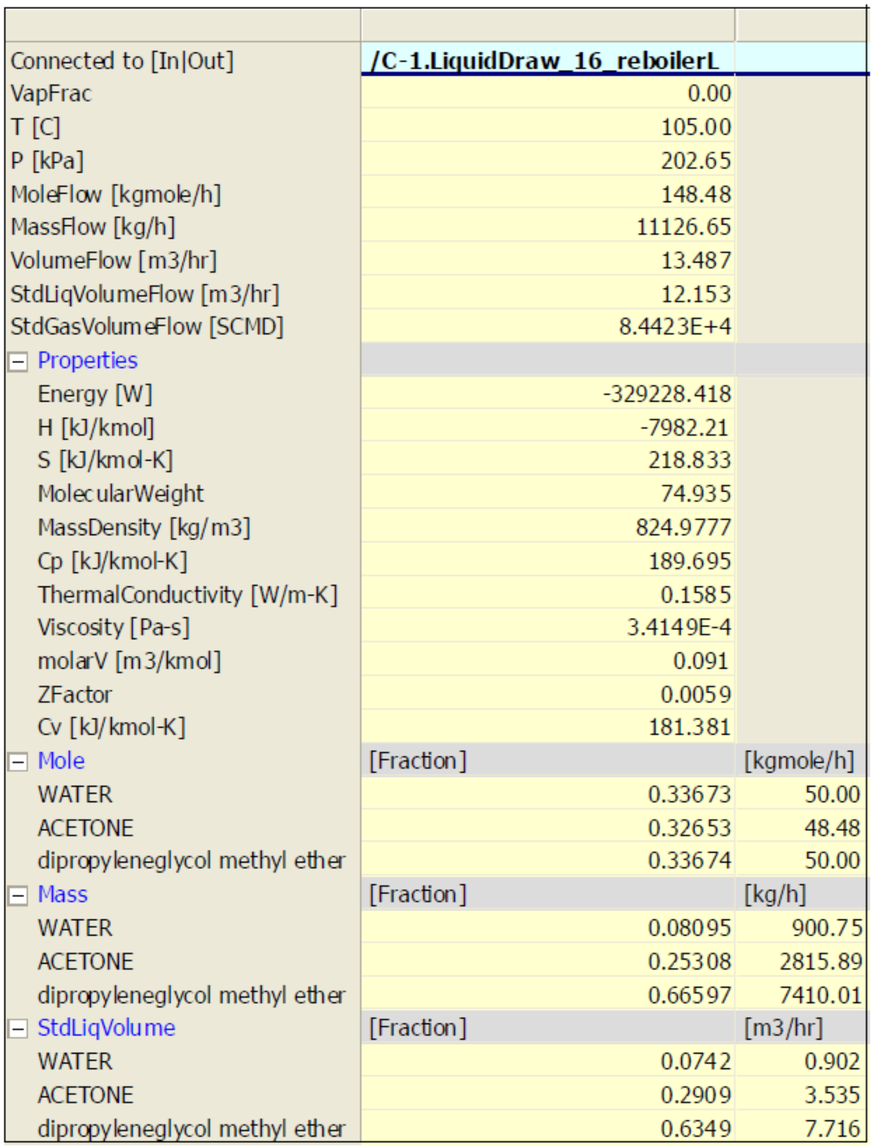


Connected to [In|Out]	/C-1.LiquidDraw_0_condenserL	
VapFrac	0.00	
T [C]	56.2191	
P [kPa]	101.325	
MoleFlow [kgmole/h]	1.52	
MassFlow [kg/h]	88.08	
VolumeFlow [m3/hr]	0.118	
StdLiqVolumeFlow [m3/hr]	0.111	
StdGasVolumeFlow [SCMD]	8.6252E+2	
Properties		
Energy [W]	-4595.1956	
H [kJ/kmol]	-10904.89	
S [kJ/kmol-K]	157.290	
MolecularWeight	58.063	
MassDensity [kg/m3]	746.6273	
Cp [kJ/kmol-K]	143.483	
ThermalConductivity [W/m-K]	0.1519	
Viscosity [Pa-s]	2.3810E-4	
molarV [m3/kmol]	0.078	
ZFactor	0.0029	
Cv [kJ/kmol-K]	135.168	
Mole	[Fraction]	[kgmole/h]
WATER	0.00041	0.00
ACETONE	0.99958	1.52
dipropyleneglycol methyl ether	0.0000	0.00
Mass	[Fraction]	[kg/h]
WATER	0.00013	0.01
ACETONE	0.99986	88.07
dipropyleneglycol methyl ether	0.00001	0.00
StdLiqVolume	[Fraction]	[m3/hr]
WATER	0.0001	0.000
ACETONE	0.99989	0.111
dipropyleneglycol methyl ether	0.00001	0.000

/S4
Stream.Stream_Material
Name / Status

Summary

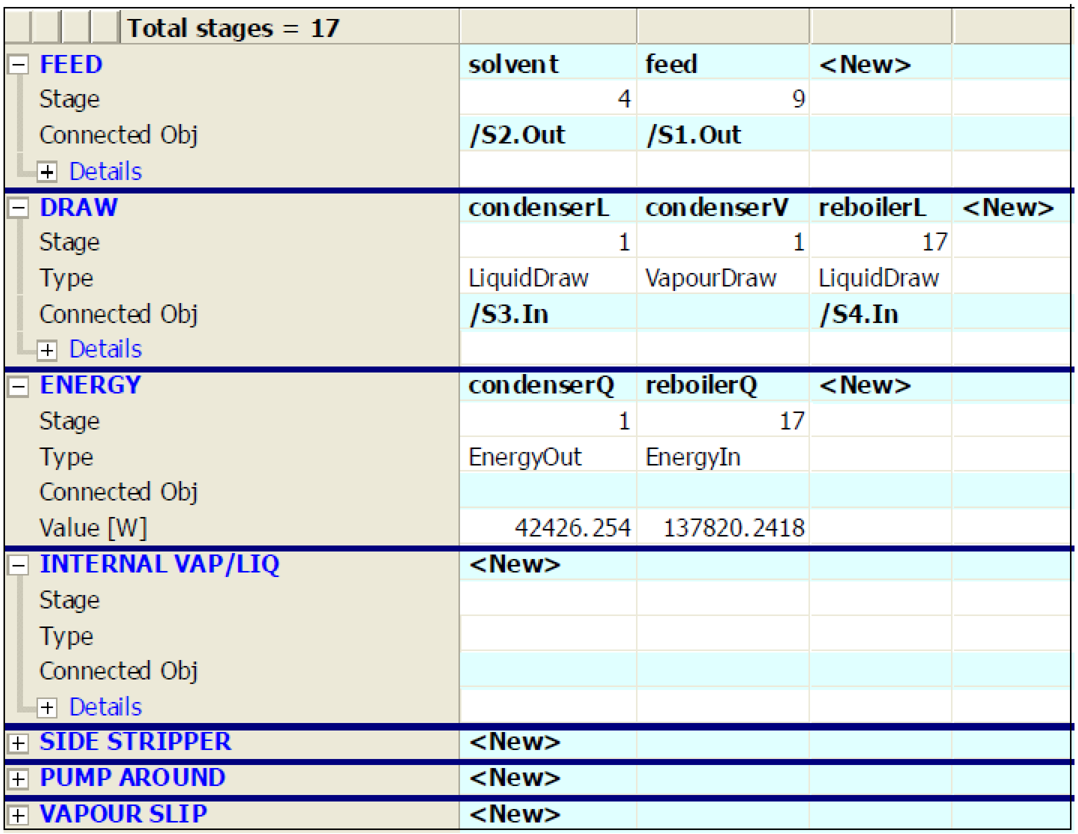
Material



Connected to [In|Out]	**/C-1.LiquidDraw_16_reboilerL**	
VapFrac	0.00	
T [C]	105.00	
P [kPa]	202.65	
MoleFlow [kgmole/h]	148.48	
MassFlow [kg/h]	11126.65	
VolumeFlow [m3/hr]	13.487	
StdLiqVolumeFlow [m3/hr]	12.153	
StdGasVolumeFlow [SCMD]	8.4423E+4	
⊟ Properties		
Energy [W]	-329228.418	
H [kJ/kmol]	-7982.21	
S [kJ/kmol-K]	218.833	
MolecularWeight	74.935	
MassDensity [kg/m3]	824.9777	
Cp [kJ/kmol-K]	189.695	
ThermalConductivity [W/m-K]	0.1585	
Viscosity [Pa-s]	3.4149E-4	
molarV [m3/kmol]	0.091	
ZFactor	0.0059	
Cv [kJ/kmol-K]	181.381	
⊟ Mole	[Fraction]	[kgmole/h]
WATER	0.33673	50.00
ACETONE	0.32653	48.48
dipropyleneglycol methyl ether	0.33674	50.00
⊟ Mass	[Fraction]	[kg/h]
WATER	0.08095	900.75
ACETONE	0.25308	2815.89
dipropyleneglycol methyl ether	0.66597	7410.01
⊟ StdLiqVolume	[Fraction]	[m3/hr]
WATER	0.0742	0.902
ACETONE	0.2909	3.535
dipropyleneglycol methyl ether	0.6349	7.716

/C-1 (DistillationColumn): 17 Stages , Degree of Freedom = 0
Condenser: Partial
Reboiler: Kettle

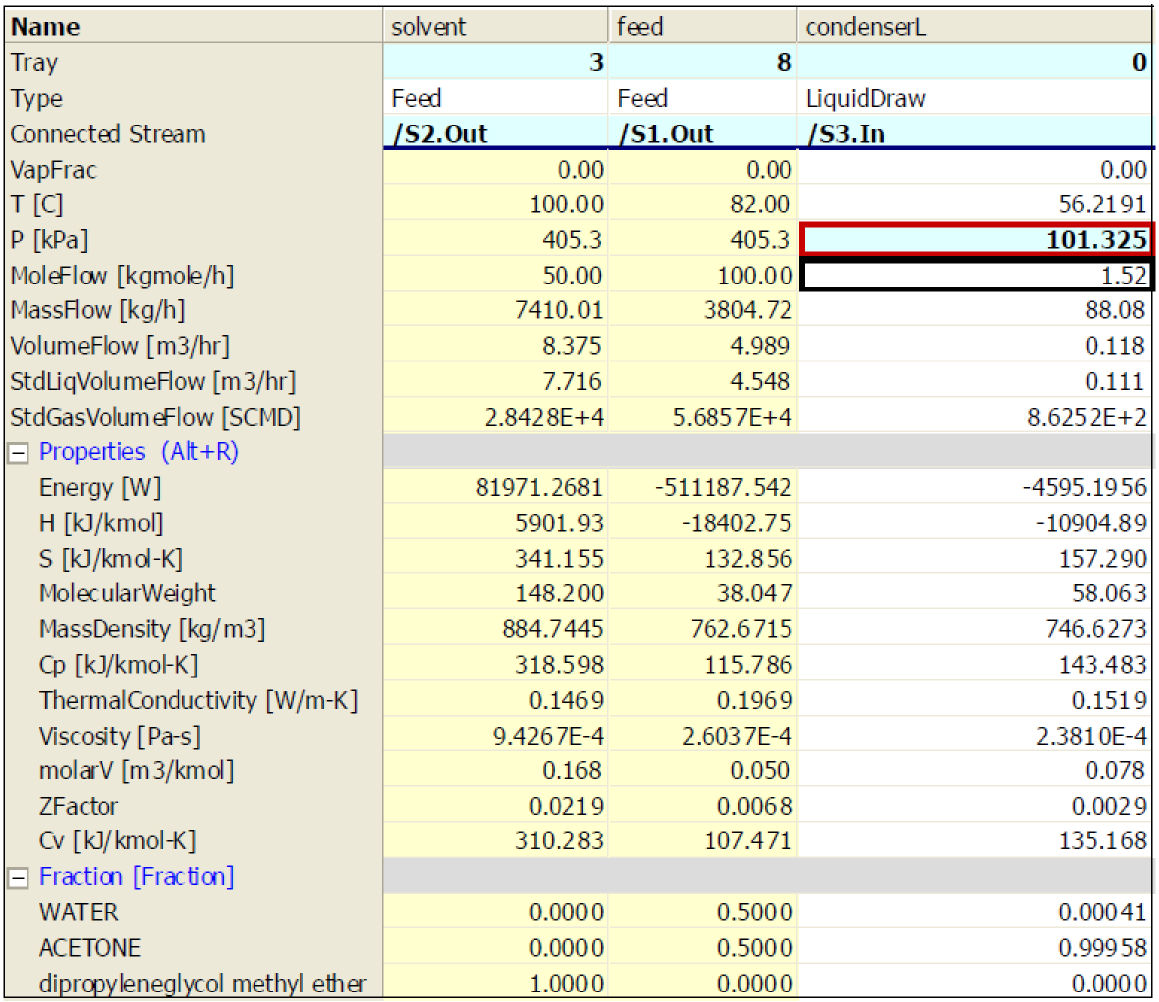
Configuration



Total stages = 17				
FEED	**solvent**	**feed**	**<New>**	
Stage	4	9		
Connected Obj	**/S2.Out**	**/S1.Out**		
Details				
DRAW	**condenserL**	**condenserV**	**reboilerL**	**<New>**
Stage	1	1	17	
Type	LiquidDraw	VapourDraw	LiquidDraw	
Connected Obj	**/S3.In**		**/S4.In**	
Details				
ENERGY	**condenserQ**	**reboilerQ**	**<New>**	
Stage	1	17		
Type	EnergyOut	EnergyIn		
Connected Obj				
Value [W]	42426.254	137820.2418		
INTERNAL VAP/LIQ	**<New>**			
Stage				
Type				
Connected Obj				
Details				
SIDE STRIPPER	**<New>**			
PUMP AROUND	**<New>**			
VAPOUR SLIP	**<New>**			

Number of Ideal Stages: 17
Degrees of freedom : 0
Condenser: Partial
Status: Converged

Feed / Product



Name	solvent	feed	condenserL
Tray	**3**	**8**	**0**
Type	Feed	Feed	LiquidDraw
Connected Stream	**/S2.Out**	**/S1.Out**	**/S3.In**
VapFrac	0.00	0.00	0.00
T [C]	100.00	82.00	56.2191
P [kPa]	405.3	405.3	**101.325**
MoleFlow [kgmole/h]	50.00	100.00	1.52
MassFlow [kg/h]	7410.01	3804.72	88.08
VolumeFlow [m3/hr]	8.375	4.989	0.118
StdLiqVolumeFlow [m3/hr]	7.716	4.548	0.111
StdGasVolumeFlow [SCMD]	2.8428E+4	5.6857E+4	8.6252E+2
⊟ Properties (Alt+R)			
Energy [W]	81971.2681	-511187.542	-4595.1956
H [kJ/kmol]	5901.93	-18402.75	-10904.89
S [kJ/kmol-K]	341.155	132.856	157.290
MolecularWeight	148.200	38.047	58.063
MassDensity [kg/m3]	884.7445	762.6715	746.6273
Cp [kJ/kmol-K]	318.598	115.786	143.483
ThermalConductivity [W/m-K]	0.1469	0.1969	0.1519
Viscosity [Pa-s]	9.4267E-4	2.6037E-4	2.3810E-4
molarV [m3/kmol]	0.168	0.050	0.078
ZFactor	0.0219	0.0068	0.0029
Cv [kJ/kmol-K]	310.283	107.471	135.168
⊟ Fraction [Fraction]			
WATER	0.0000	0.5000	0.00041
ACETONE	0.0000	0.5000	0.99958
dipropyleneglycol methyl ether	1.0000	0.0000	0.0000

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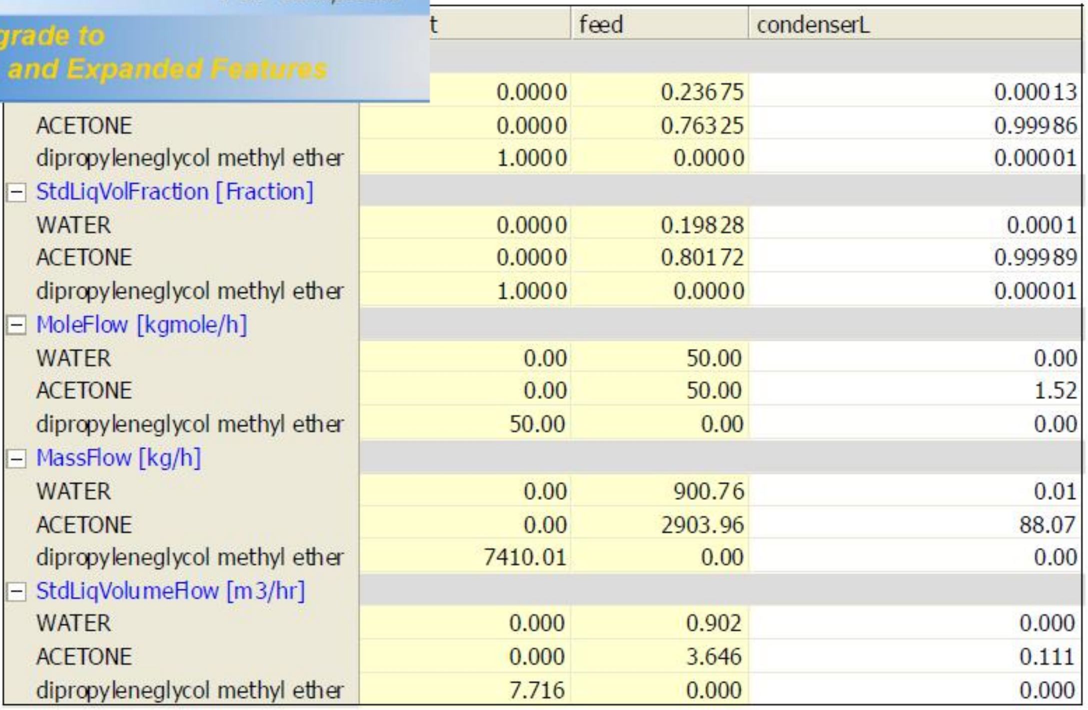

	t	feed	condenserL
	0.0000	0.23675	0.00013
ACETONE	0.0000	0.76325	0.99986
dipropyleneglycol methyl ether	1.0000	0.0000	0.00001
⊟ StdLiqVolFraction [Fraction]			
WATER	0.0000	0.19828	0.0001
ACETONE	0.0000	0.80172	0.99989
dipropyleneglycol methyl ether	1.0000	0.0000	0.00001
⊟ MoleFlow [kgmole/h]			
WATER	0.00	50.00	0.00
ACETONE	0.00	50.00	1.52
dipropyleneglycol methyl ether	50.00	0.00	0.00
⊟ MassFlow [kg/h]			
WATER	0.00	900.76	0.01
ACETONE	0.00	2903.96	88.07
dipropyleneglycol methyl ether	7410.01	0.00	0.00
⊟ StdLiqVolumeFlow [m3/hr]			
WATER	0.000	0.902	0.000
ACETONE	0.000	3.646	0.111
dipropyleneglycol methyl ether	7.716	0.000	0.000

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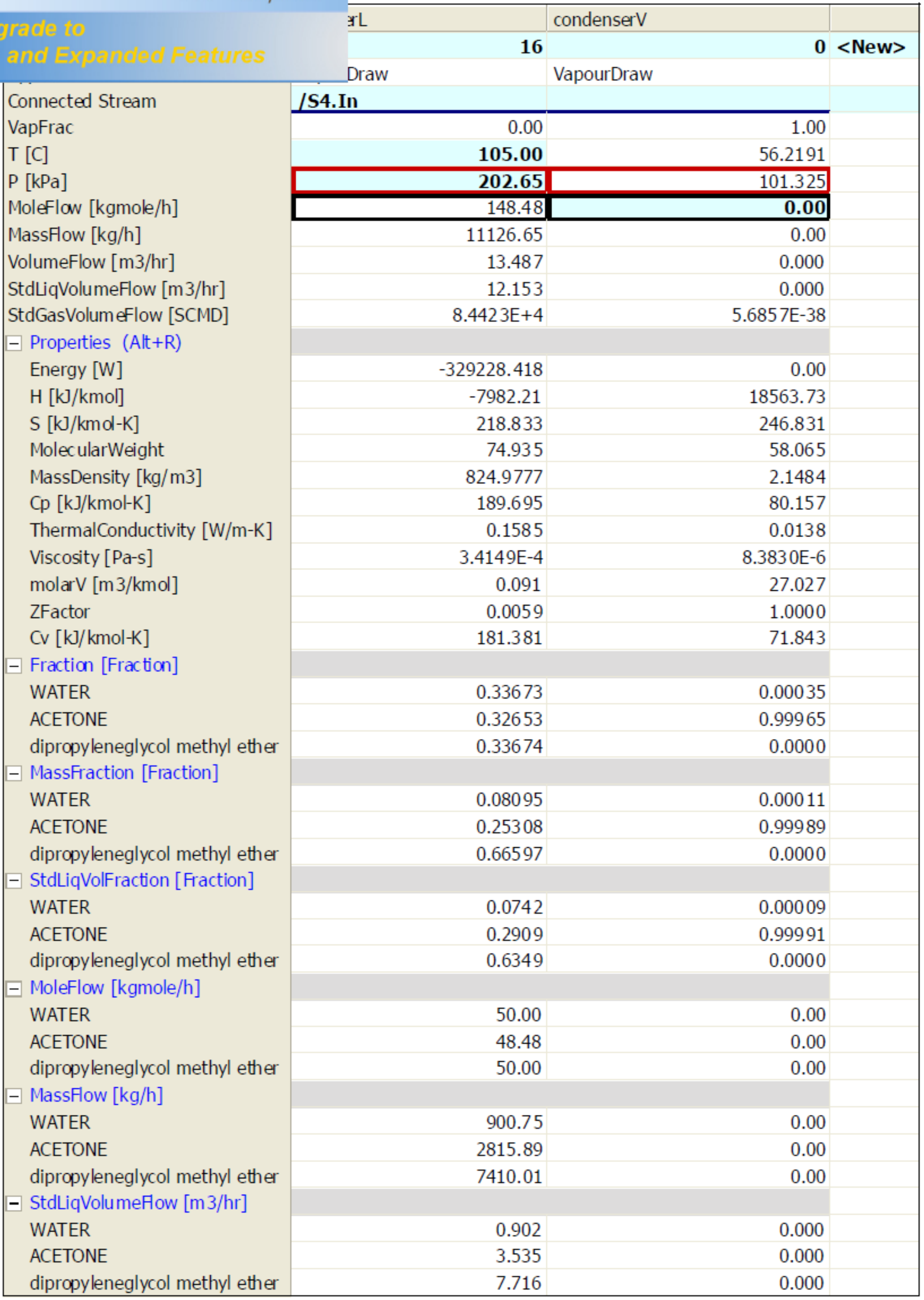

	erL	condenserV	
	16	**0**	**<New>**
	Draw	VapourDraw	
Connected Stream	**/S4.In**		
VapFrac	0.00	1.00	
T [C]	**105.00**	56.2191	
P [kPa]	**202.65**	101.325	
MoleFlow [kgmole/h]	148.48	**0.00**	
MassFlow [kg/h]	11126.65	0.00	
VolumeFlow [m3/hr]	13.487	0.000	
StdLiqVolumeFlow [m3/hr]	12.153	0.000	
StdGasVolumeFlow [SCMD]	8.4423E+4	5.6857E-38	
⊟ Properties (Alt+R)			
Energy [W]	-329228.418	0.00	
H [kJ/kmol]	-7982.21	18563.73	
S [kJ/kmol-K]	218.833	246.831	
MolecularWeight	74.935	58.065	
MassDensity [kg/m3]	824.9777	2.1484	
Cp [kJ/kmol-K]	189.695	80.157	
ThermalConductivity [W/m-K]	0.1585	0.0138	
Viscosity [Pa-s]	3.4149E-4	8.3830E-6	
molarV [m3/kmol]	0.091	27.027	
ZFactor	0.0059	1.0000	
Cv [kJ/kmol-K]	181.381	71.843	
⊟ Fraction [Fraction]			
WATER	0.33673	0.00035	
ACETONE	0.32653	0.99965	
dipropyleneglycol methyl ether	0.33674	0.0000	
⊟ MassFraction [Fraction]			
WATER	0.08095	0.00011	
ACETONE	0.25308	0.99989	
dipropyleneglycol methyl ether	0.66597	0.0000	
⊟ StdLiqVolFraction [Fraction]			
WATER	0.0742	0.00009	
ACETONE	0.2909	0.99991	
dipropyleneglycol methyl ether	0.6349	0.0000	
⊟ MoleFlow [kgmole/h]			
WATER	50.00	0.00	
ACETONE	48.48	0.00	
dipropyleneglycol methyl ether	50.00	0.00	
⊟ MassFlow [kg/h]			
WATER	900.75	0.00	
ACETONE	2815.89	0.00	
dipropyleneglycol methyl ether	7410.01	0.00	
⊟ StdLiqVolumeFlow [m3/hr]			
WATER	0.902	0.000	
ACETONE	3.535	0.000	
dipropyleneglycol methyl ether	7.716	0.000	