SALT-ADDED METHOD FOR BREAKING AZEOTROPE OF BINARY IPA-WATER SYSTEM: USING ASPEN PLUS

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SALT-ADDED METHOD FOR BREAKING AZEOTROPE OF BINARY IPA-WATER SYSTEM: USING ASPEN PLUS

SHAHIDATUL NADIAH BINTI MHD SAID

A thesis submitted in fulfillment of the
Requirements for the award of the degree of
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APRIL 2008

I declare that this thesis entitled “Salt-added Method for Breaking Azeotrope of Binary IPA and Water System: Using Aspen Plus” is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

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To the missing pieces of courage and hope.
May it soon find its way home.

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ABSTRACT

Distillation process is a method for separating various components of a liquid solution depending upon the distribution of these components between a vapour phase and a liquid phase. It is commonly used as a solvent recovery method, a technology in many areas of pharmaceutical and especially chemical industries. IPA is a rubbing alcohol used as cleaner and solvent in industries. It forms azeotrope with water that ordinary distillation can never separate both components directly. Mostly in industries, azeotropy and highly nonideal behavior during distillation complicates the recovery of solvents and the not recovered solvents usually end up as toxic waste. Apart from that, the interest of this project is to study the azeotrope breaking of binary IPA-water system with salt-added method to recover purity of IPA by using batch distillation in the Aspen Plus environment. Then, the concentration of salt added to break the azeotrope of IPA-water system in batch distillation process is investigated. After coming up with a simulation solution based on the optimum condition of chosen parameters, the result show that the azeotrope breaking of binary IPA-Water system with salt added method is not successful by using batch distillation via simulation of Aspen Plus. The azeotropic point of the binary IPA-Water system has only shifted but failed to break. Thus, it is recommended to do an experimental of the batch distillation in order to understand more of the salt-added method in breaking the azeotope system and then to implement the same method in simulation to achieve the objective.

ABSTRAK

Process penyulingan adalah satu cara untuk mengasingkan komponen-komponen larutan cecair yang pelbagai berdasarkan pengagihan komponen ini di antara fasa gas dan fasa cecair. Ia secara umumnya diguna sebagai cara untuk mandapatkan larutan yang tertentu, satu teknologi dalam pelbagai bidang farmasi dan lebih-lebih lagi dalam bidang industri kimia. IPA ialah sejenis alkohol yang digunakan sebagai pembersih dan pelarut dalam pelbagai industri. Ia membentuk azeotrope dengan air yang mana penyulingan biasa tidak mampu mengasingkan kedua-dua komponen secara terus. Kebanyakan di dalam industri, azeotrope dan ciri-ciri yang tidak ideal semasa penyulingan menyukarkan penghasilan larutan tersebut dan kebanyakannya penghasilkan bahan buangan bertoksik. Tujuan projek ini ialah untuk mengkaji pemecahan azeotrope di dalam sistem IPA-air dengan cara menambahkan garam untuk mengembalikan ketulenan IPA dengan menggunakan penyulingan berkelompok secara simulasi menggunakan Aspen Plus. Kemudian, untuk mengkaji pengkhususan terhadap penambahan garam untuk memecahkan azeotrope dalam sistem IPA-air dalam proses penyulingan berkelompok. Selepas menjalankan simulasi penghasilan yang berdasarkan parameter yang dipilih berdasarkan keadaannya pada tahap optimum, kajian dalam memecahkan azeotrope bagi sistem IPA-air dengan cara penambahan garam tidak berjaya dengan menggunakan penyulingan berkelompok secara simulasi dalam Aspen Plus. Titik azeotropik pada sistem berganda IPA-air hanya berubah dan gagal di pisahkan. Oleh itu, dicadangkan bahawa satu kajian melalui eksperimen penyulingan berkelompok dijalankan untuk meningkatkan pemahaman terhadap pemecahan sistem azeotrope dengan penambahan garam. Kajian yg sama juga dijalankan dengan menggunakan simulasi Aspen Plus untuk mencapai objektif projek.

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CHAPTER 1

INTRODUCTION

1.1 Project Background

Distillation process is a method for separating the various components of a liquid solution depending upon the distribution of these components between a vapour phase and a liquid phase (C.J.Geankoplis, 2003). In this project, we focus more on the usage of Batch Distillation. It is commonly used as a solvent recovery method, a technology in many areas of pharmaceutical and especially chemical industries (I.R-Donis, E.P-Fondevila, V.Gerbaung, X.Joulia, 2001).

In the world of Chemical Engineering, solvent recovery is important to reduce the number of hazardous waste and pollutions. In the industries, IPA (Isopropyl Alcohol) is known as rubbing alcohol used as a cleaner and solvent. It is miscible with water, thus forming azeotrope with water at certain temperature. An azeotrope cannot be separated by ordinary distillation since no enrichment of the vapour phase occurs at this point. Therefore, in most cases, azeotropic mixtures require special methods to facilitate their separation such as a mass separating agent like a membrane-material for pervaporation or an entrainer for extractive distillation. Extractive and heteroazeotropic distillation are the most common methods to break this azeotrope behaviour. In this project, the salt added method is used to break the azeotrope of IPA-Water system. Sodium Chloride (NaCl) is used in this process as the entrainer.

Aspen Plus is used to conduct the simulation of process involves in an existing plant. It is a tool that can help engineers to predict the behaviour of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. With reliable thermodynamic data, realistic operating conditions and the rigorous Aspen Plus equipment models, they can simulate actual plant behaviour.

1.2 Project Problem Statement

Solvent recovery is important in a fine- and specialty chemical industries. The recovery and reuse of organic solvent is generally practiced because of the increasing of solvent cost and potential solvent shortages. IPA is known as rubbing alcohol used as cleaner and solvent in industries. It forms azeotrope with water at 80.37°C that ordinary distillation can never separate both components directly. Mostly in industries, azeotropy during distillation complicates the recovery of solvents and the not recovered solvents usually end up as toxic waste. Other than that, disposal of waste is often results in violation of air-, water-, or land-pollution regulation (Eva-Katrine Hilmen, 2000).

The problem in this situation is the difficulty of the separation due to the azeotropic state of IPA-Water system and the way to comprehend the process without ever going to put up a bench scale or pilot plant. Even by improving a readily built plant, it will costs time and money and it is one of the challenges faced by Process Engineers these days. Experience alone is not always sufficient to answer the questions that continually arise and ‘trial and error’ efforts to provide meaningful insight is costly and potentially dangerous. Thus, this requires cost-effective tools that help identify and ‘correct’ the anticipated problems before they occur.

1.3 Project Objectives

1. To study the azeotrope breaking of binary IPA-water system with salt-added method to recover purity of IPA by using batch distillation in the Aspen Plus environment.
2. To investigate the concentration of salt added to break the azeotrope of IPA-water system in batch distillation process.

1.4 Project Scopes

In order to achieve the objective of the project, some boundary or scope need to be specified. This project covers the breaking of azeotrope of binary IPA-Water system, salt added method, batch distillation and Aspen Plus.

Firstly, the salt added used in this project is sodium chloride (NaCl). It is chosen for it’s highly availability and also it is the most common salt used in the industries, for example in manufacturing of pulp, textile and detergent products. The concentration of sodium chlorides use in this project will vary to get the optimum concentration.

Secondly is to run several simulations using Aspen Plus to get optimum results. So, certain parameters will take place in order to achieve the objective. The parameters consist of:

- concentration of salt added
- time constraints
- reflux ratio

CHAPTER 2

LITERATURE REVIEW

2.1 Batch Distillation

Separation process plays a big role in chemical engineering. In general, separation of homogeneous liquid mixtures requires the creation or addition of another phase within the system. The most common method is repeated vaporization and condensation – distillation (Eva-Katrine Hilmen, 2000). Distillation process is a method for separating the various components of a liquid solution depends upon the distribution of these components between a vapour phase and a liquid phase (C.J.Geankoplis, 2003). Alternatives to distillation are adsorption, membrane separation, crystallization, liquid-liquid extraction, chromatography and others (Smith, 1995).

In this project, the focus is on the area of batch distillation. Batch distillation is one of the solvent recovery methods, a technology in many areas of pharmaceutical and especially chemical industries (I.R-Donis et. al, 2001) but why batch distillation? Batch distillation is less energy efficient than continuous distillation and it offers possibility of separating multi-component mixtures into high purity products using single columns. So, it is less expensive compared to continuous distillations that required (n-1) columns. It is flexible and robust to variation in feed composition and specification. It is important for production of seasonal or low capacity chemicals. Batch distillation also can be used for liquids with contaminants such as solids, tars and resins. (Rousseau, 1987)

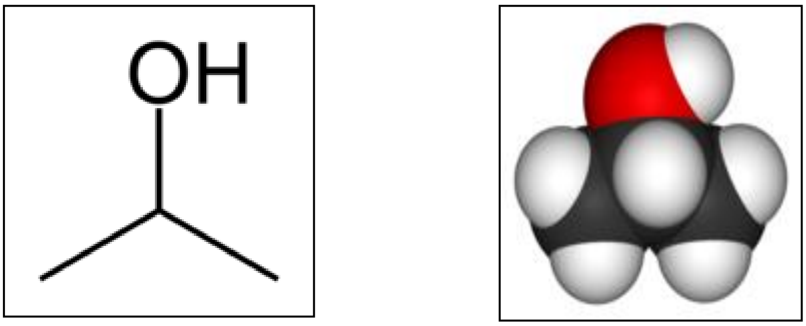
"Designing equipment for such [azeotropic] separations is a real challenge to the distillation engineer. Often, sufficient data are not available for complete calculation so that the process must be developed in the laboratory, or, at least, assumptions checked. Combinations of continuous and batch distillations, decanting, multistage extraction, and chemical treatment may often be combined in a successful process." Drew as quoted by Schweitzer (1997)

From the above statement from Schweitzer (1997), azeotrope behaviour has put many engineers up for challenges in designing distillation. To date, there has been many kind of distillation methods that fit for azeotropic separations such as the extractive distillation, combination of column and decanting distillation and also reactive distillation.

2.2 IPA-Water System

2.2.1 IPA

IPA is a short form for Isopropyl Alcohol. Known as rubbing alcohol, Isopropyl alcohol or Isopropanol is a secondary alcohol with chemical formula C_3H_8O. It is colourless and has a strong odour that resembles ethanol. IPA has high flammability with a very wide combustible range. Its vapour is heavier than air and it can explode through deflagration. It is commonly used as a cleaner agent and solvent in industry such as a cleaning agent for electronic devices (CDs, DVDs, cell phones, etc). It is also used in "dry-gas" fuel additives. If poisoned, it can cause symptoms such as dizziness, nausea and fatal whereas a long term on skin can cause defatting. IPA is totally miscible in water. For example as the fuel additives, it completely mixed with water in the supply fuel lines that keep away insoluble water especially during freezing season. IPA forms azeotrope with water at 87.4 mass% alcohols at temperature 80.37^{o}C. Since in this project we focus on breaking the azeotrope, it is known that IPA can be separated from aqueous solutions for example water by adding salt (NaCl, Na_2SO_4 or inorganic salts)



a) IPA – Skeletal view

b) IPA – 3D view

Figure 2.1 : IPA skeletal view and 3D view

Table 2.1 : Physical & Chemical Properties of IPA

Isopropyl alcohol	
General	
Systematic name	Propan-2-ol
Other names	2-propanol, isopropanol, Isopropyl alcohol
Molecular formula	C_3H_8O
Molar mass	60.10 g/mol
Appearance	Colourless liquid
Properties	
Density and phase	0.785 g/cm^3, liquid
Solubility in water	Fully miscible
Solubility in brine	Slightly soluble
In ethanol, ether In acetone, toluene	Fully miscible Soluble
Melting point	-89 °C (185 K)
Boiling point	82.3 °C (355 K)
Acidity (pK_a)	16.5 for H on hydroxyl
Viscosity	2.86 cP at 15 °C 1.77 cP at 30 °C
Dipole moment	1.66 D (gas)

2.2.2 Water

Water is mainly the most important substance in the world. It is a chemical substance consists of 2 of hydrogen atom and one oxygen atom. It is tasteless, odourless liquid at ambient temperature and pressure. Water appeared to be colourless or more to a very light blue hue. It is also known as the universal solvent.

Figure 2.2 : Water skeletal view and 3D view

Table 2.2 : Physical & Chemical Properties of Water

Water	
General	
Systematic name	Water
Other names	Aqua, dehydrogen monoxide, hydrogen hydroxide
Chemical formula	H_2O
Molar mass	18.0153 g/mol
Properties	
Density and phase	0.998 g/cm^3 (liquid at 20 °C) 0.92 g/cm^3 (solid)
Melting point	0 °C (273.15 K) (32 ºF)
Boiling point	100 °C (373.15 K) (212 ºF)
Specific heat capacity	4.184 J/(g•K) (liquid at 20 °C)

2.2.3 IPA-Water Binary System

At atmospheric condition, a binary mixture of 2-propanol (isopropyl alcohol, IPA)–water forms a homogeneous minimum-boiling azeotrope at 87.4–87.7 mass% and 80.3–80.4 ◦C. Some investigations have reported that IPA–water azeotrope can also be broken with other azeotropic distillations to form heterogeneous azeotropic systems by adding one of the following entrainers: isopropyl ether, benzene, methyl ethyl ketone, and isopropyl acetate. Sometimes, ethyl ether is used as entrainer at pressures substantially above atmospheric (R.D. Kirk, D.F. Othmer, Encyclopedia of Chemical Technology, vol. 16, second ed., John Wiley and Sons Inc., NY, 1968)

2.3 Vapour-Liquid Phase Equilibrium, Nonideality and Azeotropy

At low to moderate pressures and temperatures away from the critical point, the vapour-liquid phase equilibrium for a multicomponent mixture may be expressed as:

$$y_i\,P \quad = \quad x_i\,\gamma_i(T,x)\,P_i^{sat}(T), \qquad i = 1,2,...,n \tag{2.1}$$

where yi and xi are the vapor and liquid compositions of component i, respectively, P and T are the system pressure and temperature, i is the activity coefficient of component i in the liquid phase, and Psat i is the saturated vapor pressure of component i. The activity coefficient i is a measure of the nonideality of a mixture and changes both with temperature and composition. When i = 1, the mixture is said to be ideal and Equation (8.2) simplifies to Raoult’s law:

$$y_i\,P = x_i\,P_i^{sat}(T), \qquad i = 1,2,...,n \tag{2.2}$$

Nonideal mixtures exhibit positive ($i > 1$) or negative ($i < 1$) deviations from Raoult’s law. If these deviations become so large that the vapor pressure exhibits an extremal point at constant temperature, or, equivalently, an extremal point in the boiling temperature at constant pressure, the mixture is *azeotropic*. At azeotropic points, the liquid phase and its equilibrium vapor phase have the same composition $x = y$, and the condensation and boiling temperature curves are tangential with zero slope (see Figure 2.1a).

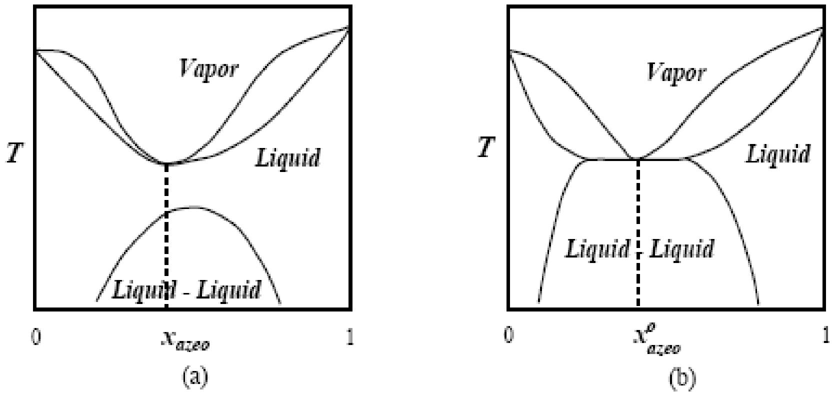


Figure 2.3 : Azeotropes may be homogeneous or heterogenous: (a) minimum-boiling homoazeotrope (b) heteroazeotrope.

If the positive deviations are sufficiently large ($i > 4$, typically), phase splitting may occur and form a heteroazeotrope where the vapor phase is in equilibrium with two liquid phases (see Figure 2.1b). In the heteroazeotropic point the overall liquid composition x_o azeo is equal to the vapor composition, and the vapor and liquid temperature surfaces are tangential with zero slopes, but the three coexisting phases have distinct compositions. In ternary and multicomponent systems *saddle* azeotropes may occur, which Swietoslawski (1963) call *positive-negative* azeotropes.

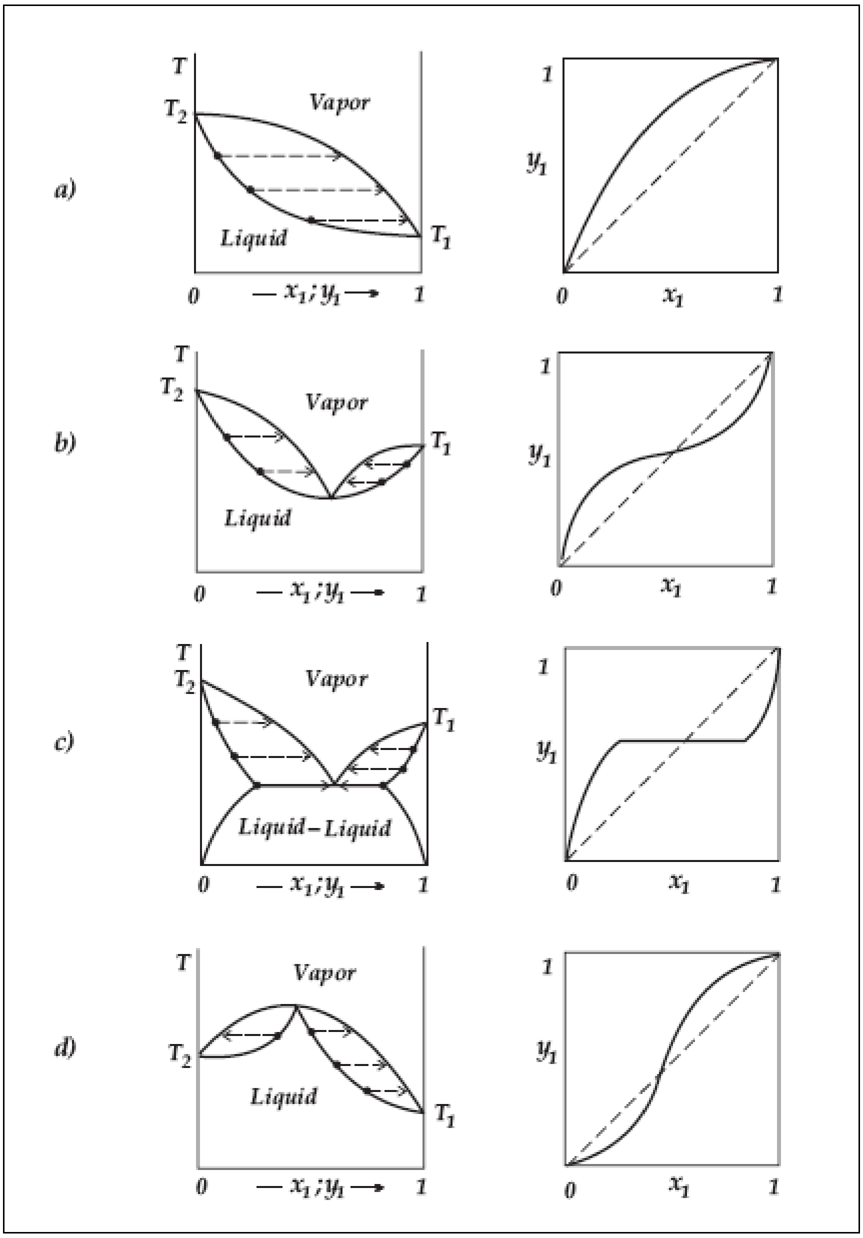


Figure 2.4: Graphical representations of the VLE for the most common types of binary mixtures at constant pressure: a) zeotropic; b) minimum-boiling homoazeotrope; c) minimum-boiling heteroazeotrope;d) maximum-boiling azeotrope. Left: boiling temperature T_{bp} and condensation temperature T_{dp} and the equilibrium mapping vectors in T = x; y space. Right: x - y relationship (equilibrium line)

2.3.1 Binary Vapor-Liquid Equilibrium Data

This is an example of binary vapor-liquid equilibrium data of Isopropanol and water within the pressure of 760mmHg.

Table 2.3 : Binary Vapor-Liquid Equilibrium Data

Vapor-liquid Equilibrium for Isopropanol/Water[2] *P* = 760 mm Hg		
BP Temp. °C	**% by mole isopropanol**	
	liquid	**Vapor**
82.2	100.00	100.00
81.48	95.35	93.25
80.70	87.25	83.40
80.37	80.90	77.45
80.23	76.50	73.70
80.11	69.55	69.15
80.16	66.05	67.15
80.15	64.60	66.45
80.31	55.90	62.55
80.38	51.45	60.75
80.67	44.60	59.20
80.90	38.35	57.00
81.28	29.80	55.10
81.29	29.75	55.40
81.23	28.35	55.30
81.62	24.50	53.90
81.75	19.35	53.20
81.58	18.95	53.75
81.99	16.65	52.15
82.32	12.15	51.20
82.70	10.00	50.15
84.57	5.70	45.65
88.05	3.65	36.55
93.40	1.60	21.15
95.17	1.15	16.30
100.0	0.00	0.00

2.3.2 Vapor-Liquid Equilibrium Graph

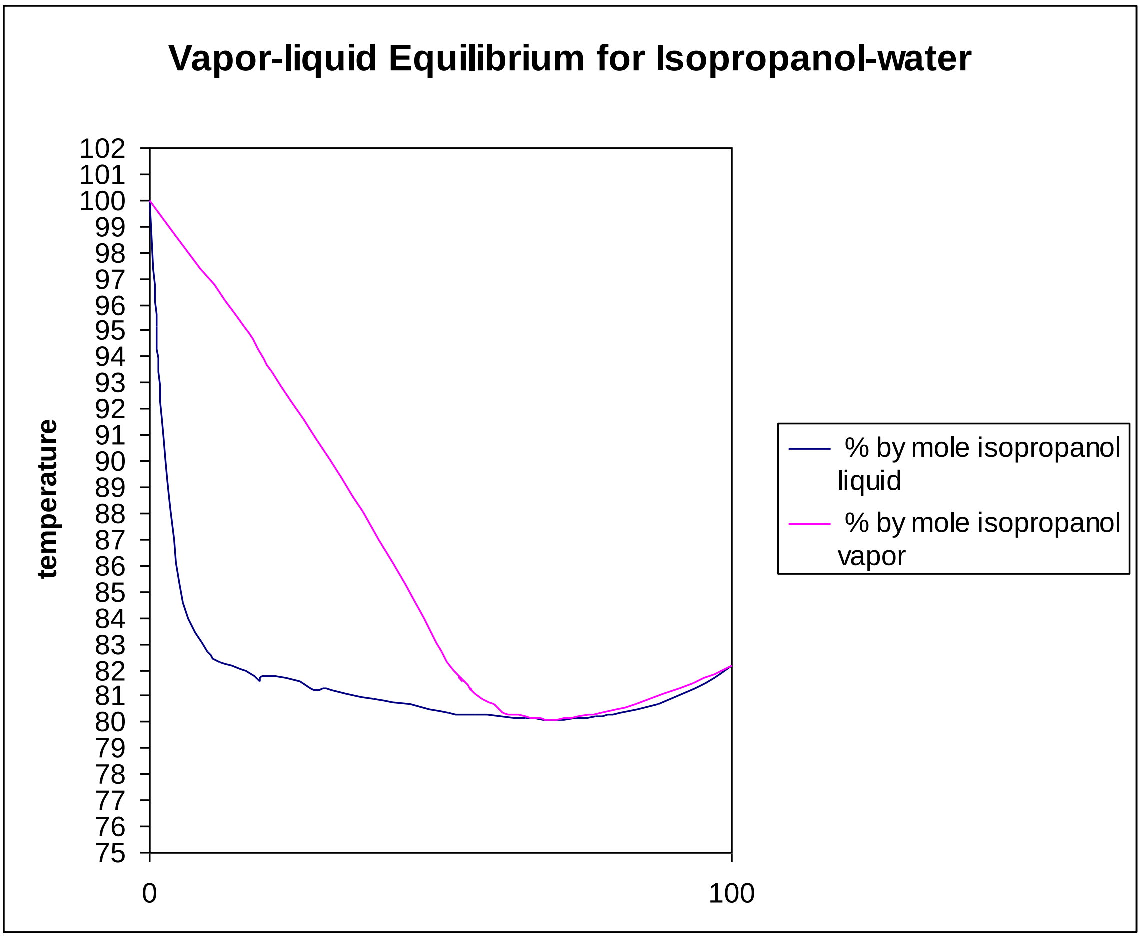


Figure 2.5 : Vapor-Liquid Equilibrium Graph

The graph above is plotted using Microsoft Excel. The graph shows that the IPA and Water have the minimum azeotrope boiling point.

2.4 Azeotrope and Entrainer

"An understanding of azeotropes is desirable for two reasons. First, they often occur in distillation and make a given separation impossible by ordinary distillation. Secondly, they may be utilized to separate mixtures not ordinarily separable by straight distillation." Ewell *et al.* (1944)

The term azeotrope means "nonboiling by any means" (Greek: a - non, zeo - boil, tropos - way/mean), and denotes a mixture of two or more components where the equilibrium vapor and liquid compositions are equal at a given pressure and temperature (Eva-Katrine Hilmen,2000). It was Wade and Merriman who had first introduce the term azeotrope in 1911 to designate mixtures that have a minimum or maximum boiling point at constant pressure (Doherty & Malone, 2001) or, equivalently, in the vapour pressure under isothermal conditions (Swietoslawski, 1963; Malesinkski, 1965). They define the azeotropy state as a stationary point in the equilibrium T-x,y or P-x,y. The mixture whose composition corresponds to an extremal point is called an azeotrope. If at the equilibrium temperature the liquid mixture is homogeneous, the azeotrope is a homoazeotrope. If the vapor phase coexists with two liquid phases, it is a heteroazeotrope. Systems which do not form azeotropes are called zeotropic (Swietoslawski, 1963).

The formation of azeotrope is due to the differences in the intermolecular forces of attraction among the mixture components. There are 3 groups that particularly deviate from the ideality that simply explains the binary mixtures (Eva-Katrine Hilmen,2000). They are :

1. *Positive deviation from Raoult's law:* The components "dislike" each other. The attraction between identical molecules (A-A and B-B) is stronger than between different molecules (A-B). This may cause the formation of a minimum-boiling azeotrope and heterogeneity.

2. *Negative deviation from Raoult's law:* The components "like" each other. The attraction between different molecules (A-B) is the strongest. This may cause the formation of a maximum-boiling azeotrope.

3. *Ideal mixture obeys Raoult's law:* The components have similar physiochemical properties. The intermolecular forces between identical and different molecules (A-A, B-B and A-B) are equal.

The tendency a mixture to form an azeotrope depends on 2 factors (Horsely, 1973; King, 1980):

1. the differences in the pure component boiling point
2. the degree of nonideality

Due to azeotrope and resulting phase behaviour, there are profound effects on the feasibility and technology for distillation-based operation.

2.4.1 Entrainer-addition Distillation Methods

A Physiochemical change of the VLE behaviour of an azeotropic mixture by the addition of an extraneous liquid component offers a number of possibilities. We name the mixture to be separated as the *original mixture*, and the added component that facilitates the separation the *entrainer*. For the purpose of ease of visualization, we limit our considerations to binary homoazeotropic original mixtures and one-component entrainers. The same separation techniques apply to multicomponent mixtures where the key components form characteristic mixtures falling into the categories discussed, and the entrainer may be a mixture of components.

We distinguish between three different conventional entrainer-addition based distillation methods depending on the properties and role of the entrainer and the organization (scheme) of the process (Eva-Katrine Hilmen,2000):

1. ***Homogeneous azeotropic distillation*** (ordinary distillation of homoazeotropic mixtures): The entrainer is completely miscible with the components of the original mixture. It may form homoazeotropes with the original mixture components. The distillation is carried out in a conventional single-feed column.

2. ***Heteroazeotropic distillation*** (decanter-distillation hybrids that involve heteroazeotropes): The entrainer forms a heteroazeotrope with at least one of the original mixture components. The distillation is carried out in a combined column and decanter system.

3. ***Extractive distillation***: The entrainer has a boiling-point that is substantially higher than the original mixture components and is selective to one of the components. The distillation is carried out in a two-feed column where the entrainer is introduced above the original mixture feed point. The main part of the entrainer is removed as bottom product.

4. **Reactive distillation***:* The entrainer reacts preferentially and reversibly with one of the original mixture components. The reaction product is distilled out from the non-reacting component and the reaction is reversed to recover the initial component. The distillation and reaction is usually carried out in one column (catalytic distillation).

5. **Chemical drying (chemical action and distillation)***:* The volatility of one of the original mixture components is reduced by chemical means. An example is dehydration by hydrate formation. Solid sodium hydroxide may be used as an entrainer to remove water from tetra hydro furan (THF). The entrainer and water forms a 35-50 % sodium hydroxide solution containing very little THF (Schweitzer, 1997).

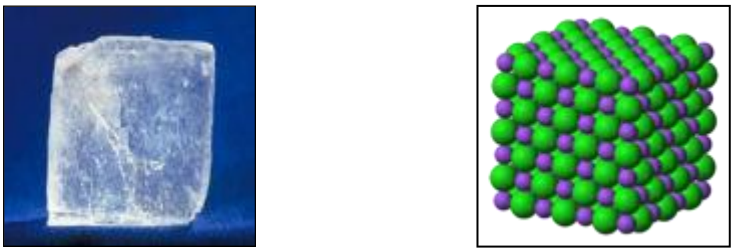
6. **Distillation in the presence of salts:** The entrainer (salt) dissociates in the mixture and alters the relative volatilities sufficiently so that the separation becomes possible. A salt added to an azeotropic liquid mixture will reduce the vapor pressure of the component in which it is more soluble. Thus extractive distillation can be applied using a salt solution as the entrainer. An example is the dehydration of ethanol using potassium acetate solution (Furter, 1968).

2.4.2 Sodium Chloride (NaCl) as Entrainer

2.4.2.1 Sodium Chloride

Sodium chloride is commonly known as the common salt, table salt or halite. It is a chemical compound with formula NaCl. It is responsible of the salinity of the ocean and also the extracellular fluid of multicellular organism. Sodium chloride can be produced by a) the evaporation of sea water b) brine such as brine wells and salt lakes and c) mining rock salt (halite). Approximately 0.3933 gram of sodium and 0.6067 gram of chlorine is found in 1 gram of NaCl. The usage of salt varies from the manufacturing of pup & paper to setting dyes in textiles & fabrics till the products of soaps & detergents. It is commonly used as flavour enhances, producing chlorine in synthetic uses (PVC & pesticides) and also the road salts (De-icing salt).

2.4.2.2 Physical & Chemical Properties



a) Picture of Sodium Chloride b) Sodium Chloride – 3D

Figure 2.6 : Sodium Chloride picture and 3D view

Table 2.4 : Physical & Chemical Properties of Sodium Chloride

Sodium chloride	
General	
Systematic name	Sodium chloride
Other names	Common salt, halite, table salt
Chemical formula	$NaCl$
Molar mass	58.442 g/mol
Appearance	white and crystallized
Properties	
Density and phase	2.16 g/cm^3, solid
Solubility in water	35.9 g/100 ml (25 °C)
Melting point	801 °C (1074 K)
Boiling point	1465 °C (1738 K)

2.5 Simulator: Aspen Plus

Aspen Plus is a component of the Aspen Engineering Suite™ (AES), an integrated set of products designed specifically to promote best engineering practices and to optimize and automate the entire innovation and engineering workflow process throughout your plant and across your enterprise. Automatically integrate process models with your engineering knowledge databases, investment analyses, production optimization and numerous other business processes. Aspen Plus contains data, physical properties, and unit operation models, built-in defaults, reports and other features and capabilities developed for specific industrial applications, such as electrolyte simulation.

Aspen Plus solves the critical engineering and operating problems that arise throughout the lifecycle of a chemical process, such as designing a new process, troubleshooting a process unit or optimizing operations of a full process like an Acrylic Acid plant. The process simulation capabilities of Aspen Plus enables engineers to predict the behaviour of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. With reliable thermodynamic data, realistic operating conditions and the rigorous Aspen Plus equipment models, they can simulate actual plant behaviour. Appendix A: Figure A1 shows the Flowsheet connectivity of BatchFrac.

2.5.1 Aspen Plus Flowsheet

The Aspen Plus Flowsheet is a section where there are a group of blocks and streams within the flowsheet. It is use for enhancing clarity; simplify viewing of the simulation and to print large flowsheet. Besides that it simplifies assignments of physicals property specification or stream classes. Refer to Appendix A : Figure A2 for Aspen Plus Flow Sheet with Steam Table.

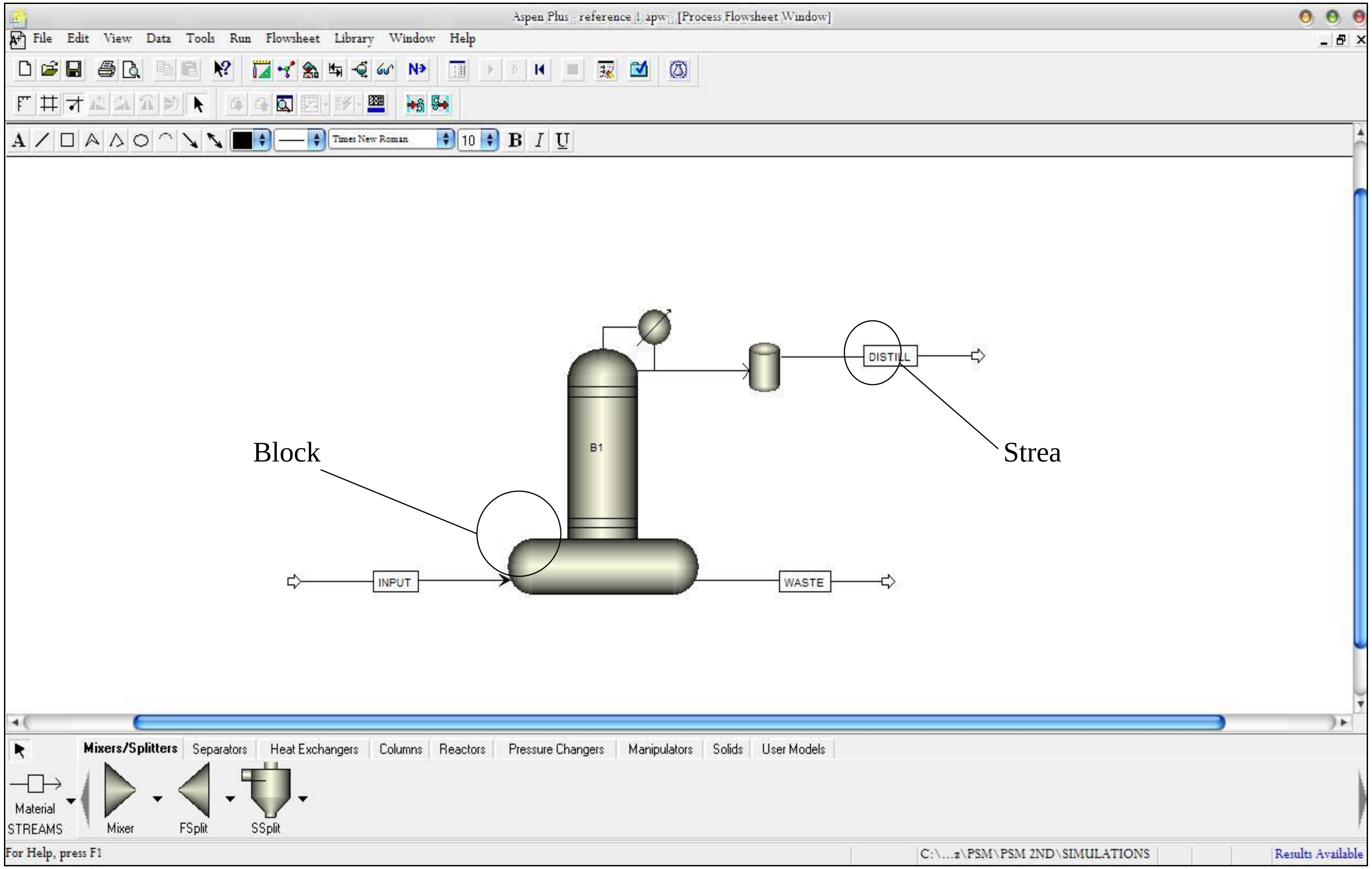


Figure 2.7 : Aspen Plus Flowsheet

2.5.2 Aspen Plus Databanks

In Aspen Plus, there are several databanks storing components with its physical property parameters. Thus, the selection of databanks has to be correct in order to select the correct components use in the simulation.

Table 2.5 : Contents and Use of the Aspen Plus Databanks

Databank	Contents	Use
PURE11	Pure component parameters for mostly organic components	Primary component databank in Aspen Plus
AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Simulations containing electrolytes
SOLIDS	Pure component parameters for strong electrolytes, salts, and other solids	Simulations containing electrolytes and solids
INORGANIC	Pure component parameters for inorganic and organic components	Solids, electrolytes, and metallurgy applications
PURE856	Version of main pure component databank delivered with Aspen Plus Release 8.5-6	For upward compatibility with previous releases of Aspen Plus
PURE93	Version of main pure component databank delivered with Aspen Plus Release 9.3	For upward compatibility with previous releases of Aspen Plus
PURE10	Version of main pure component databank delivered with Aspen Plus Version 10	For upward compatibility with previous releases of Aspen Plus
AQU92	Version of AQUEOUS delivered with Aspen Plus Release 9.2	For upward compatibility with previous releases of Aspen Plus
ASPENPCD	Version of main pure components databank delivered with Aspen Plus Release 8.5-6	For upward compatibility with previous releases of Aspen Plus
COMBUST	Pure component parameters for combustion products, free radicals	For high temperature, gas phase calculations
ETHYLENE	Pure component parameters for components typically found in ethylene processes for the SRK property method	Ethylene processes

2.5.3 Aspen Plus Method Properties

A simulation cannot run without the correct property methods. A property method is the collection of methods that Aspen Plus uses to compute the thermodynamic and transport properties needed in the simulation. The selections of the correct property methods can be done using the Method Property Guide given by Aspen Plus. From the given guidelines, this project uses NRTL methods to run the simulation.

Refer Appendix A : Table A1 for Method Property Guide of Aspen Plus

2.5.4 Aspen Plus BatchFrac

The type of aspen plus block used in this is BatchFrac™. It is the unit operation model for batch distillation. it is a rigorous model for simulating multistage batch distillation columns. From aspen plus help, BatchFrac uses a robust and efficient algorithm to solve the unsteady-state heat and material balance equations that describe the behaviour of batch distillation processes. Rigorous heat balances, material balances, and phase equilibrium relationships are applied at each stage.

BatchFrac assumes:

- Equilibrium stages are used.
- There is constant liquid hold-up and no vapor hold-up.
- Column hydraulics is not modelled.

CHAPTER 3

METHODOLOGY

3.1 Project Methodology

This project uses Aspen Plus to conduct a batch distillation process to break the azeotrope of IPA-water system with an addition of salt as the entrainer. The method used is according to the model library used in Aspen Plus.

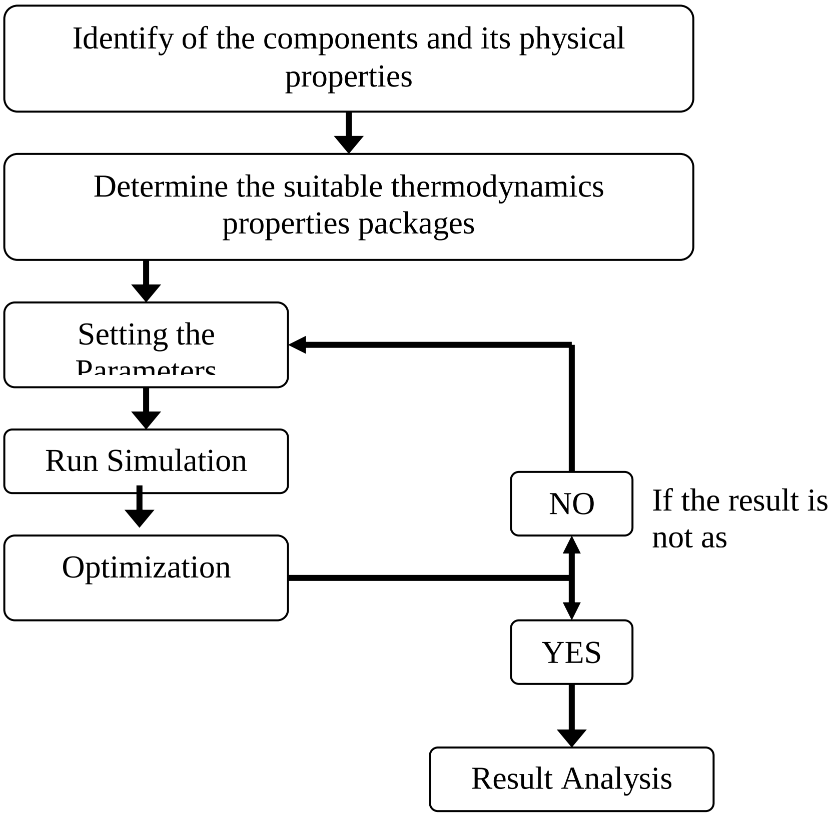


Figure 3.1 – Project Methodology

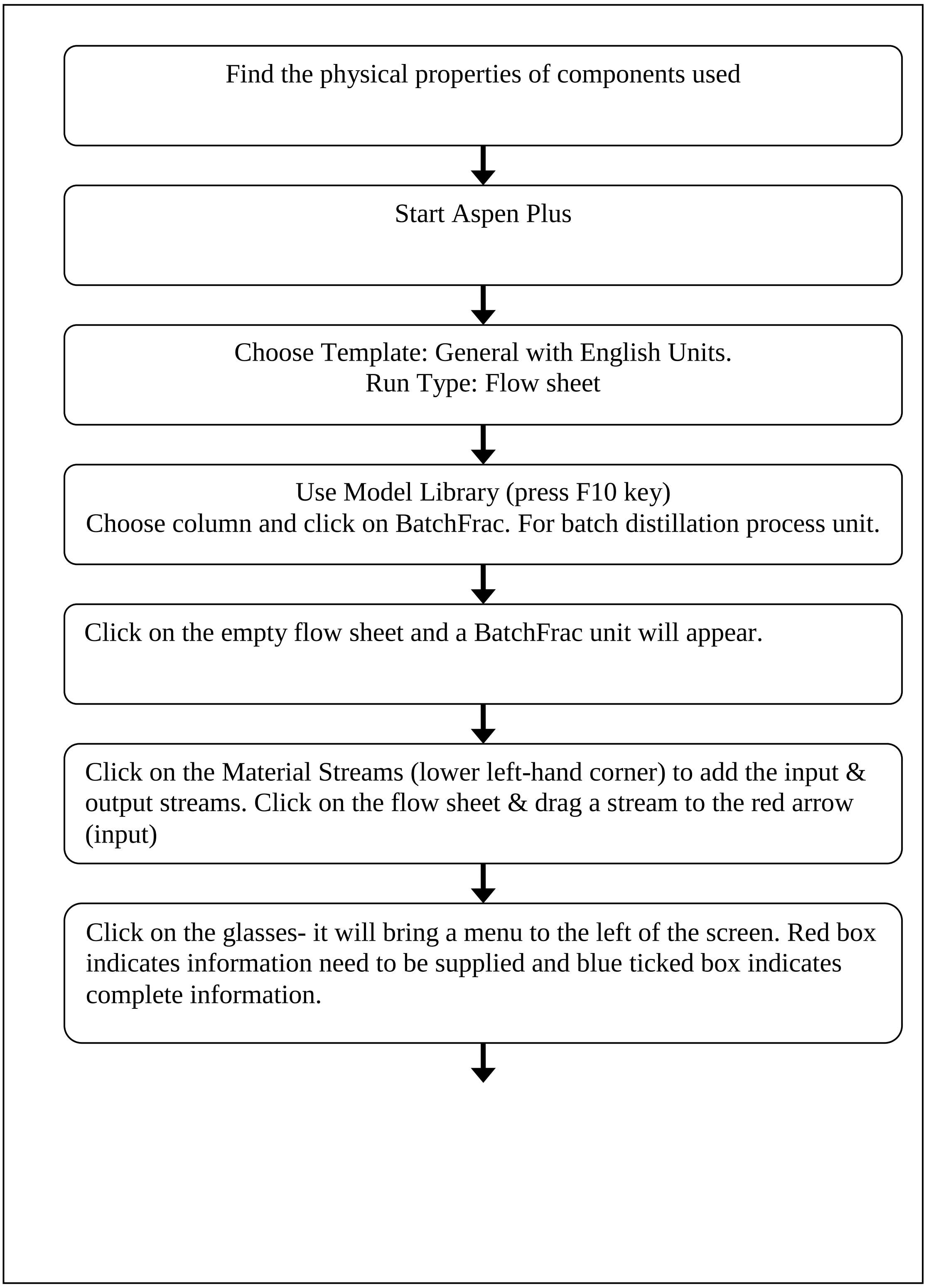
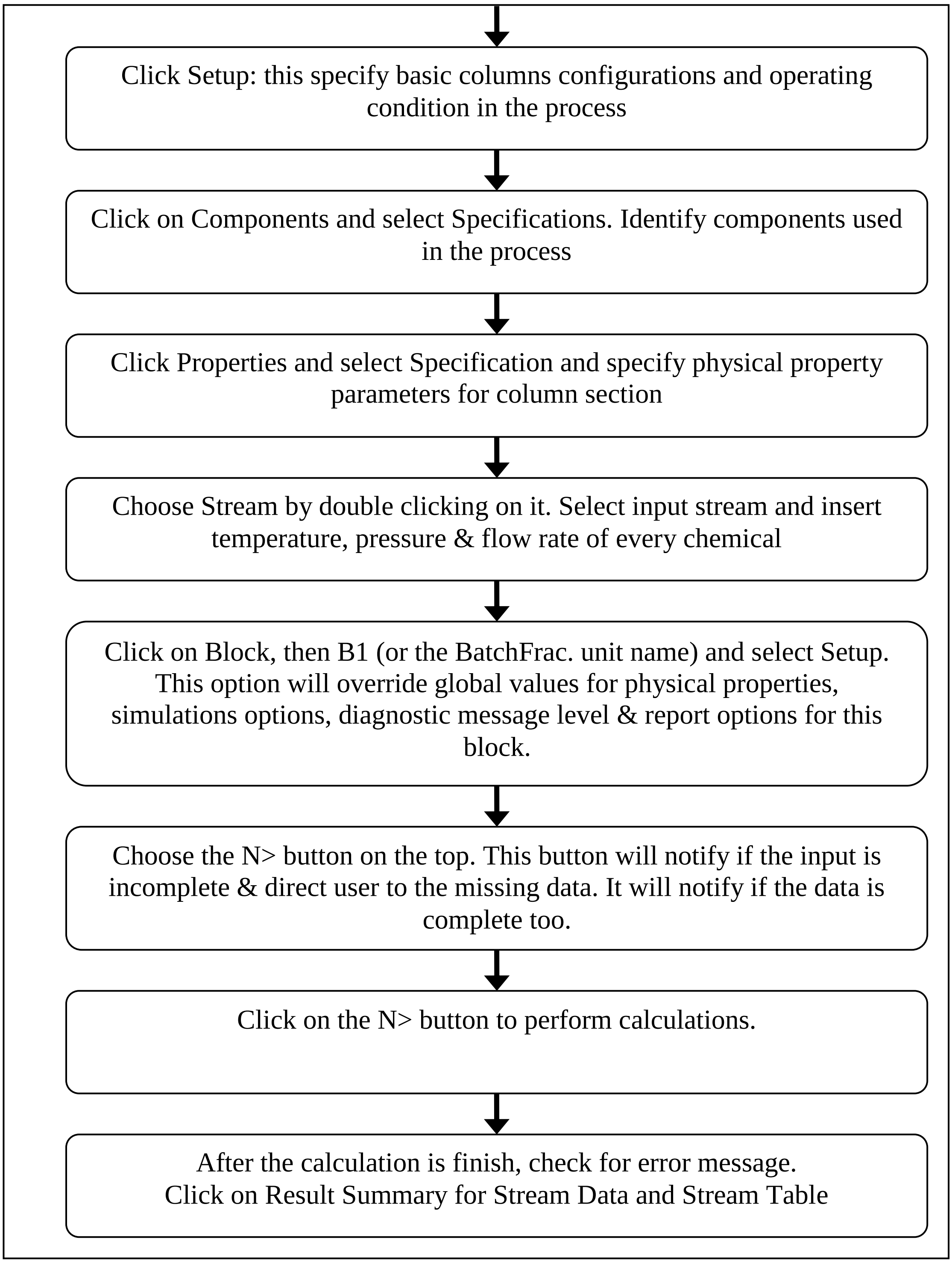


Figure 3.2 – Aspen Plus Methodology



Click Setup: this specify basic columns configurations and operating condition in the process

Click on Components and select Specifications. Identify components used in the process

Click Properties and select Specification and specify physical property parameters for column section

Choose Stream by double clicking on it. Select input stream and insert temperature, pressure & flow rate of every chemical

Click on Block, then B1 (or the BatchFrac. unit name) and select Setup. This option will override global values for physical properties, simulations options, diagnostic message level & report options for this block.

Choose the N> button on the top. This button will notify if the input is incomplete & direct user to the missing data. It will notify if the data is complete too.

Click on the N> button to perform calculations.

After the calculation is finish, check for error message.
Click on Result Summary for Stream Data and Stream Table

Figure 3.2 – Aspen Plus Methodology- Continue

3.2 Determining Mass, Volume and Concentration of IPA, Water, Sodium Chloride

According to the minimum boiling azeotrope temperature point of IPA and water, there is almost 66 mole% to 70 mole% IPA. 1 kmole or 1000 mole is subjected to this project for the concentration of IPA and water solution with 70% of its content is IPA and the rest is water. With concentration of IPA and water available, the determination of mass and volume of IPA and water can be calculated.

Basis	= 1000 mole	= 1 kmole
Feed time	= 1 hour	
Flow rate	= 1000 mole/hr	= 1 kmole/hr

Fraction of IPA and water solution

IPA = 70 mole%

Water = 30 mole%

Azeotrope minimum boiling point temperature = 80.37°C

Mol fraction = 68.54% IPA/Water

Table 3.1 : Concentration, Mass and Volume of IPA and Water

		Components		Concentration		Mass		Volume	
	unit	IPA	Water	IPA	Water	IPA	Water	IPA	Water
Basis	mole	1000		700	300				
Fraction	mole%	0.7	0.3						
M.W	g/mole	60.1	18.02			42070g	5406g		
Density	g/cm^3	0.7851	1.000					53589 cm^3	5406 cm^3
						42.070	5.406	53.589	5.406
Total				**1000 mole**		**47.4760 kg**		**58.995L ≈ 59L**	

The salt distribution is according to table 4.2. It is known that the solubility of salt in water is 35.9 g/100 ml water at 25 °C.

Table 3.2: Concentration, Mass and Volume for Salt

Mole of NaCl (mole)	Molecular weight (g/mole)	Mass (g)	Mass (kg)	Density (g/cm3)	Volume (cm3)	Volume (L)
50	58.4400	2922	2.9220	2.1650	1349.6536	1.3497
100		5844	5.8440		2699.3072	2.6993
150		8766	8.7660		4048.9607	4.0490
200		11688	11.6880		5398.6143	5.3986
250		14610	14.6100		6748.2679	6.7483
300		17532	17.5320		8097.9215	8.0979

The fraction for each component is also calculated according to the needed total flow rate in the input stream.

Table 3.3 : Components mole fraction

Total mole	mole			fraction		
	salt added	IPA	Water	IPA	Water	Salt
1000	0	700	300	0.7000	0.3000	0.0000
1050	50	700	300	0.6667	0.2857	0.0476
1100	100	700	300	0.6364	0.2727	0.0909
1150	150	700	300	0.6087	0.2609	0.1304
1200	200	700	300	0.5833	0.2500	0.1667
1250	250	700	300	0.5600	0.2400	0.2000
1300	300	700	300	0.5385	0.2308	0.2308

3.3 Aspen Plus: Parameters of BatchFrac and Default Simulation

In the Aspen Plus Simulator, before any simulation to be run, the parameters of the process have to be keyed-in. the best parameters used is selected according to the process and also from journals. The Aspen Plus Simulator Help-desk also provide the guidelines for the parameter needed for BatchFrac process.

Table 3.4 : Parameters in Aspen Plus

Properties Method	NRTL
Stream	
Input Pressure	101.3 kPa
Input Temperature	25oC
Blocks	
Number of Stages	12
Initial Feed Charge	1 hour
Condenser Pressure	101.3 kPa
Condenser Holdup	10 mole
Stage Holdup	1 mole
Operation Specifications	
Distillate Rate	0.7 kmole/hr
Default Reflux Ratio	1

CHAPTER 4

RESULT & DISCUSSION

4.1 IPA and Water Analysis

Most of the data of Isopropanol and Water gained from journals and research. To make sure that all the references are correct and usable for this project, an analysis is done by using Aspen Plus. After entering the components used in the Aspen Plus Components Specifications, the analysis tool is used to analyze the component property and the binary property of IPA and water. A y-x graph of IPA mole fraction is plotted. This shows that IPA in water solutions forms azeotrpe at 68.45 mole% at atmosphere pressure (Appendix B : Figure B1). Then, a T-xy graph of IPA and water binary system is plotted. Figure 4.1 shows that the mixture of IPA and water solution is a positive azeotrope with minimum boiling point of 80.37^{o}C. The mole fraction at azeotrope point is 68.45 mole% IPA/Water. This confirms that the references are usable and the data of Aspen Plus is correct. The full result analysis can be referred in Appendix B

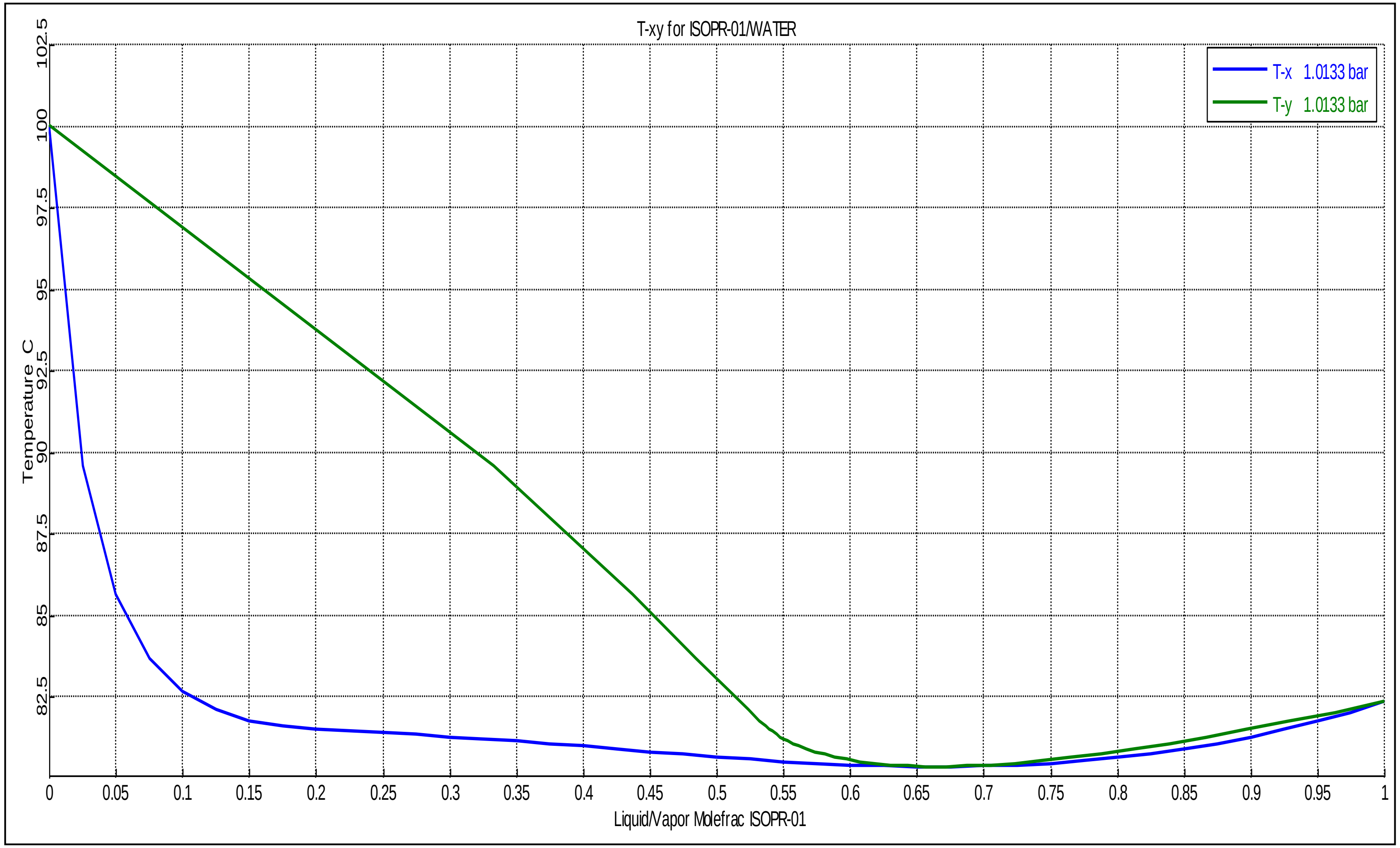


Figure 4.1 : T-xy graph of IPA and Water Binary System

4.2 Simulation A: Salt Concentration

There are 6 simulation involve with different concentration of sodium chloride. The salt concentration varies from 50 moles to 1000 moles. The mass of the salt can be referred to table 4.1. The initial condition of the simulation is in 101.3 kPA for pressure at 25 degree Celsius. The simulation time is for 1 hour with a total of reflux ratio. Detailed results of the simulation are in appendix. The result is simplified in the table below.

Table 4.1 : Simulation Results with Different Salt Concentration

simulations	Components Concentration (kmole)			IPA Fraction	% IPA increase
	Salt	IPA	Water		
default	0	0.4770	0.2230	0.6814	0%
1	50	0.4820	0.2180	0.6886	1%
2	100	0.4870	0.2130	0.6957	1%
3	150	0.4910	0.2090	0.7014	2%
4	200	0.4940	0.2060	0.7057	2%
5	250	0.4970	0.2030	0.7100	3%
6	300	0.4990	0.2010	0.7129	3%

From the result above, the simulation without salt added is fixed to be the default simulation. The IPA fraction is taken from the distillate stream. In this simulation operation, the distillate stream is fixed to have 0.7 kmole/hr and the IPA fraction is observed. In default simulation, the IPA mole fraction is 0.6814 or 68% mole of IPA distilled which we will get as the azeotrope point appears to be at 66 mole% to 70 mole% IPA.

Sodium Chloride is used to solubilized with water and the IPA solution can be distilled and decreasing the amount of water in the distillate stream. IPA is not soluble in salt and thus, hypothetically the distillate stream will be filled with IPA and less of water. The salt and water will be the remaining component in the distillation. A graph of IPA mole fraction versus Salt concentration is plotted.

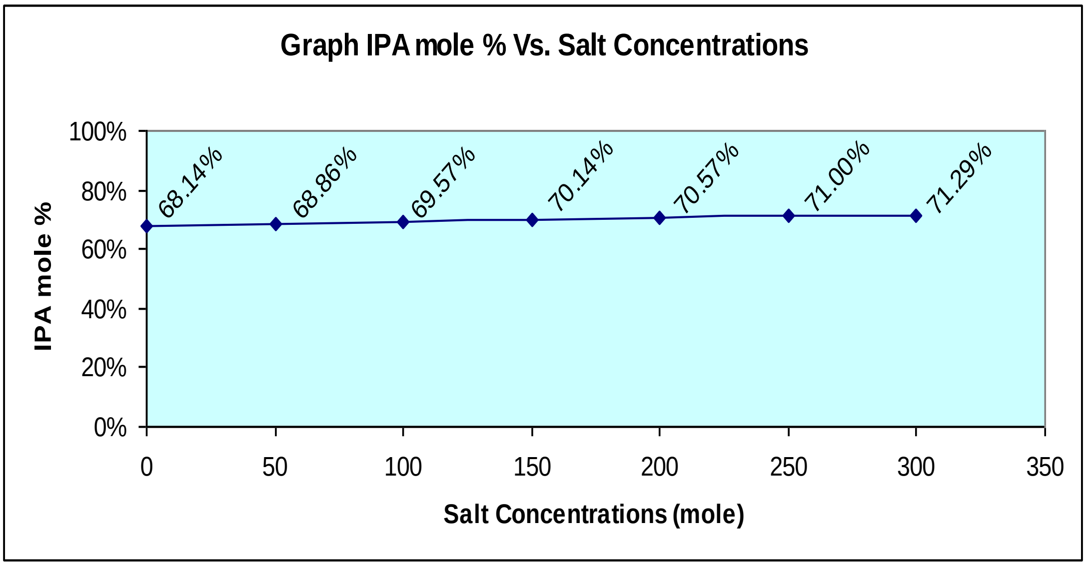


Figure 4.2 : Graph of IPA Composition vs. Salt Concentration

From the graph above, it showed that the compositions of IPA continuously increase with the increasing of salt concentrations. The increasing of IPA composition is in the average of 2% only. It is concluded from the result that only a slight increase of IPA is distilled in the distillate stream. Even with salt added within a large mount, the IPA composition cannot be obtained 100%.

Since with salt added into the system, the composition of IPA increased. This proved that the addition of salt has made a difference in the equilibrium of IPA and water. The addition has caused the shifted of azeotrope point. Thus, by adding salt, it has helped to move the azeotrope point of IPA and water solution but not enough to break of the azeotrope. It is also concluded that the best salt concentration is the concentration with the highest IPA composition. Thus, the 300 mole of Sodium Chloride is selected.

4.3 Simulation B: Time Constraints

Time constraint is the range of time for the batch distillation to operate. Range of time is important in distillation process as it shows the amount of product distillate with certain time. The best distillation operation is the one with the less time consuming but producing product with the highest purity.

Time constraint parameter ranges from 0.5 hours, 0.75 hours, 1 hours (default time), 1.25 hours, 1.5 hours, 1.75 hours and 2 hours. The simulation is operated with the addition of 300 mole of sodium chloride with fixed reflux ratio equals to 1. The result of the simulation done is simplified in table 4.2. In this simulation, the effect of salt added with the operation time is also observed in order to investigate the breaking of azeotropic point of IPA and water solution.

Table 4.2: Simulation Result with Different Time Constraints

Time constraint (hours)	IPA Mole Flow rate Distillate (kmole/hr)	IPA Composition
0.5	0.2480	0.7086
0.75	0.3730	0.7105
1.00	0.4990	0.7129
1.25	0.6240	0.7131
1.50	0.6950	0.7092
1.75	0.6950	0.7092
2.00	0.6950	0.7092

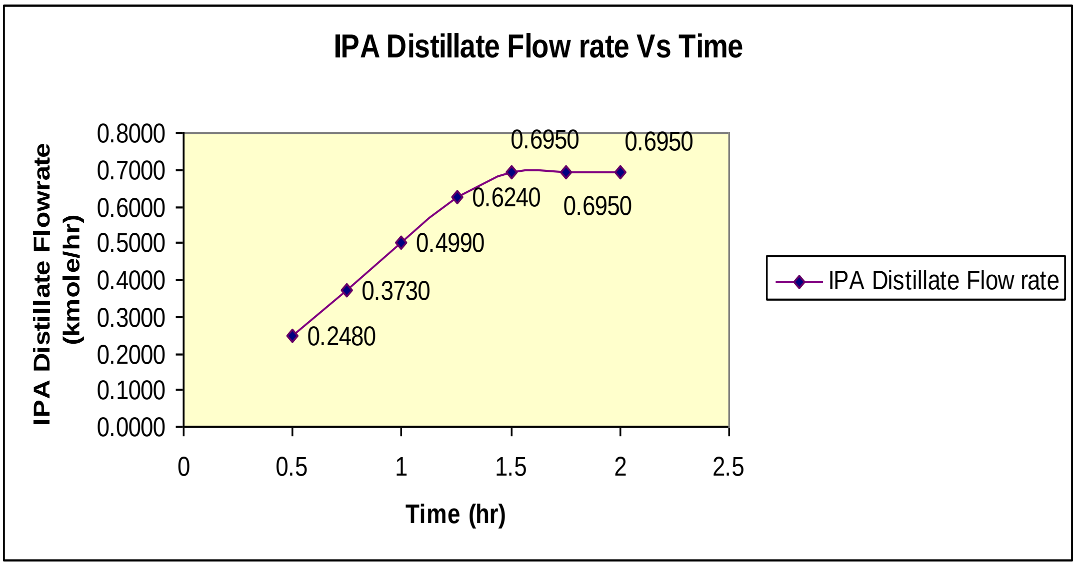


Figure 4.3 : Graph of IPA Distillate Flow rate vs Time Constraints

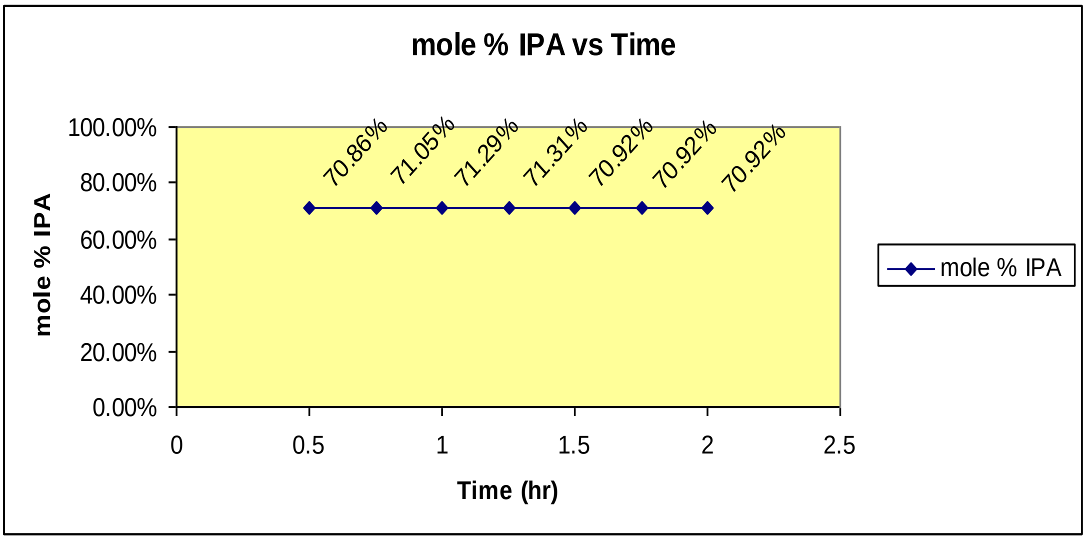


Figure 4.4 : Graph of Mole % IPA vs Time Constraints

From the table 4.2, the IPA mole flow rate is increasing with time. The composition of IPA has a slight increase until 1.25 hours but decreases when it reaches 1.50 hours. The highest composition of IPA is 71.31mole % at 1.25 hours. A graph of IPA mole flow rate versus time constraint is plotted. The graph showed that the flow rate of IPA stop increasing when it reaches 1.50 hours.

From both graphs, the time constraint has effect the flow rate of the distillate product. The composition of IPA in the distillate stream shows only a little differences. With a longer period of time, the composition slightly decreases. From figure 4.4, the best time is 1.25 with the highest composition of IPA which is 71.31%. Since the solution is added with 300 mole of Sodium Chloride, the composition of IPA also increase slightly from the composition of IPA in default time 1 hour. This is because, the longer time permits the absorption of more water in salt and increasing the concentration of IPA distilled. But IPA composition did not reach more than 90% and it still contains water, thus the azeotrope of IPA and water did not break, but only shifted slightly with the increasing of time.

4.4 Simulation C: Reflux Ratio

Reflux ratio is in distillation is define as the amount of the refluxed liquid in mole over the amount of liquid product distilled (distillate). Refluxed liquid is the remaining liquid from the condenser which is returned back (refluxed) as a liquid to the top tray of the distillation. Theoretically from McCabe-Thiele Method, higher reflux ratio will produce minimum distillate flow rate but with higher purity of the light component from the solution.

Reflux ratio is chosen as one of the parameters in this project to see whether it has effect on the breaking of IPA and water azeotrope in batch distillation along with the addition of salt. Reflux ratios chosen ranged from 0.1, 0.5, 1.0, 5.0, 10, 15 and 20. Simulation done is fixed for 1 hour of operation with 300 mole of Sodium Chloride added into the solution. The result of simulation for 1 hour operation with reflux ratios is listed in table 4.3. Simulation result can be referred in appendix.

Table 4.3 : Simulation Results with Different Reflux Ratios

simulations	reflux ratios	IPA Mole Distillate (kmole)	IPA Compostion
1	0.1	0.5120	0.7314
2	0.5	0.5060	0.7229
3	1.0	0.4990	0.7129
4	5.0	0.4710	0.6729
5	10.0	0.4680	0.6686
6	15.0	0.4680	0.6686
7	20.0	0.4680	0.6686

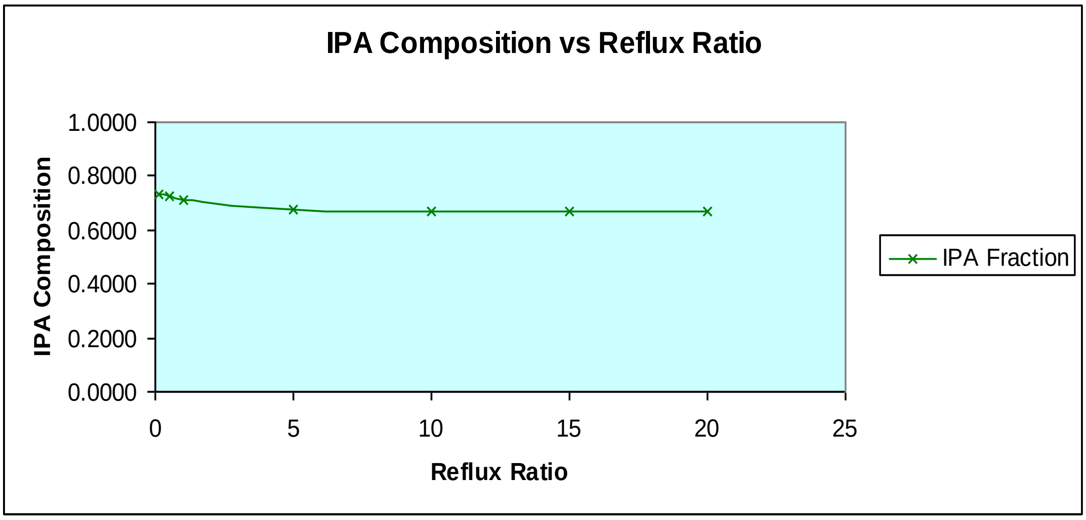


Figure 4.5 : Graph of IPA Composition vs Reflux Ratio

From the result in table 4.3, the IPA concentration from the distillate stream has slightly decreased with the increase of reflux ratio. The IPA composition also has a slightly decrease. Graph of IPA composition versus reflux ratio is plotted to see the trend of the reflux ratios effects on IPA composition in distillate stream. Figure 4.4 shows, even with high reflux ratio; there is no significant change in the IPA composition.

As discussed earlier, the theory is that reflux ratio can help in increasing the composition of IPA recovered in the distillate stream. As the simulation as been done, the reflux ratios shows no differences in the IPA composition. It is concluded that reflux ratio did not contribute in breaking the azeotropic point of IPA and water.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

This project objective is to study the azeotrope breaking of binary IPA-water system with salt-added method by using batch distillation. The batch distillation process is done by Aspen Plus Simulator. The concentration of salt added is also observed in order to break the azeotropic point. The parameters used in this project consist of salt concentration, time constraint of the process and also reflux ratio.. The salt added used is Sodium Chloride for its cheap price and also availability in the market.

From simulation A, sodium chloride is added until the concentration amount is the same with the amount of water which is 300 moles. The results show that with the increasing of salt, the will be a slight increase in the IPA composition in the distillate product. This shows that with the increase of IPA composition, the azeotrope point of IPA and water has shifted. IPA composition has not reached more than 90%, thus the azeotrope breaking by salt-added method is not achieved as expected.

From simulation B, the time constraints of the batch distillation process is increased to see the effects in the composition of IPA. Salt-added used is 300 mole. The results showed that the IPA flow rate in the distillate stream increased by the hours until 1.50 hours where it stops increasing. The IPA composition of each hour has a slight increase. The best time constraint is 1.25 hours with 71.31

% of IPA distilled. With a longer time period, the azetropic point of IPA and Water has shifted but failed to break.

The last parameter is the reflux ratio used in batch distillation process. Results has determined that even with large reflux ratio, there has no significant changes in the IPA composition. As a conclusion, the reflux ratio did not help in the breaking of azeotrope of IPA and water binary system.

Overall, the salt-added method to break the azeotrope of IPA and water binary system has not achieved in the batch distillation via simulation of Aspen Plus. The salt added also showed that it has only manage to shift the azeotropic point bt the slight increase of IPA composition distilled but failed to break the azeotrope.

5.2 Recommendation

This project can be continued to investigate the salt-added method in breaking the azeotrope of IPA and water binary system by experiment. The simulation can be done using the same parameters and comparing both result of experiment and simulation will determine the validity of each result. The simulator must also have adequate information of the azeotropic system. This is important because the simulation processed differently than experiment and without enough information, the process will not be the same as the experimental process.

Other than that, this project can also be done by using different kind of distillation process such as extractive or reactive distillation. The reaction in the solution with salt must be considered as there may be effects on the composition of IPA recovered in the distillate product.

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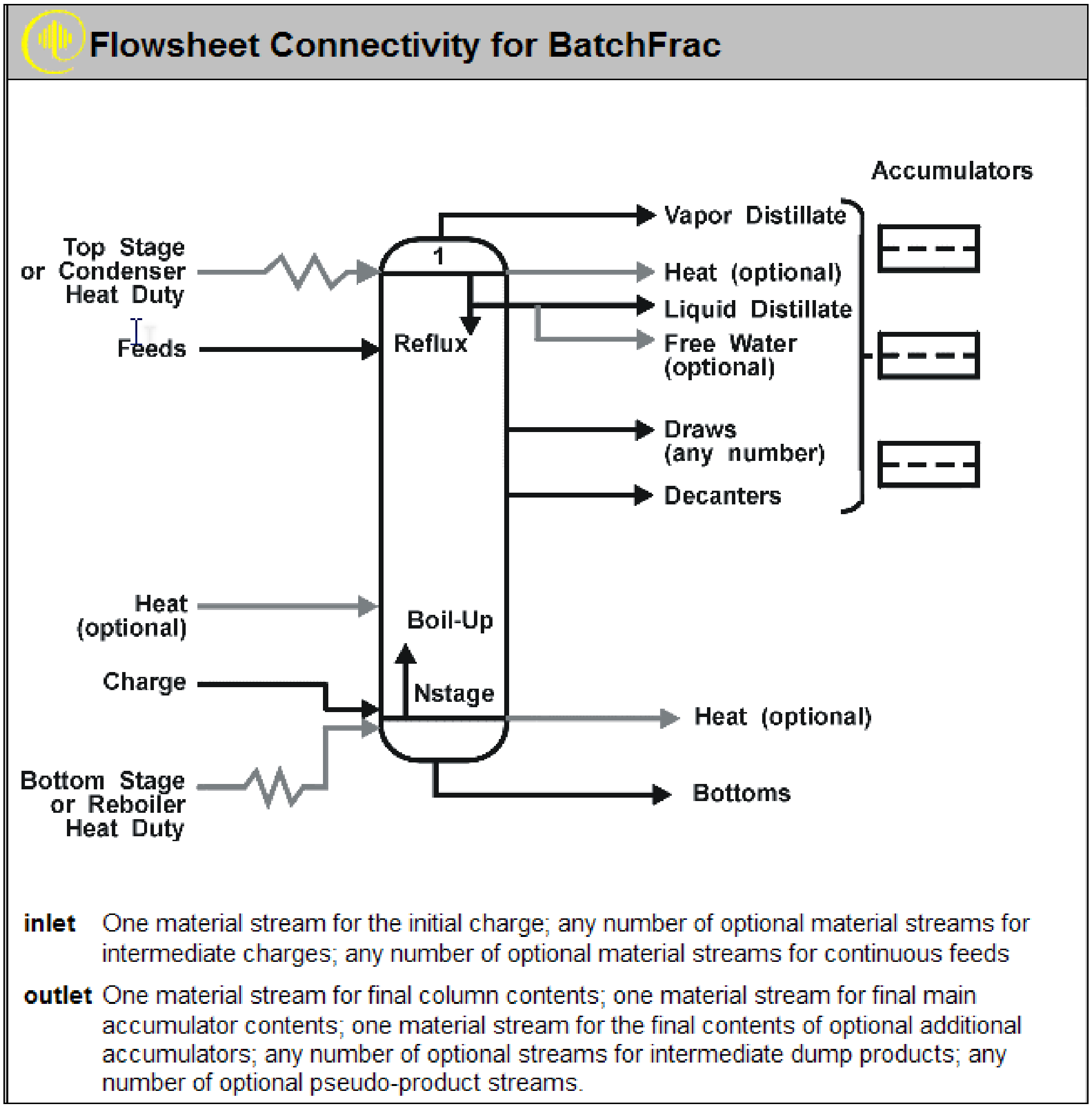
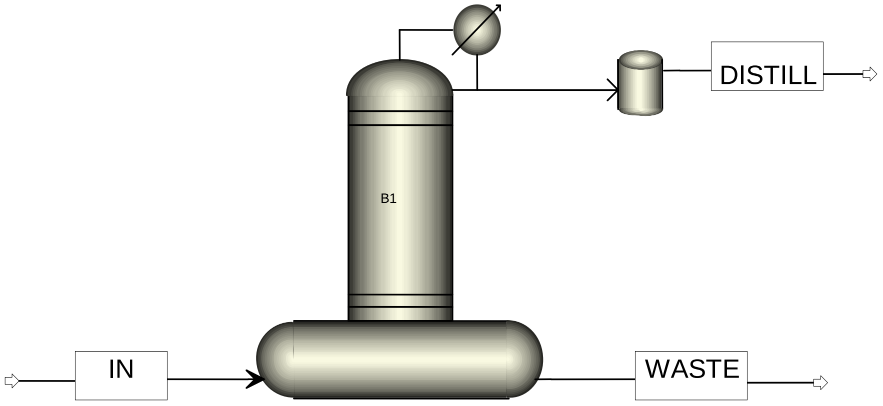
APPENDIX A



Flowsheet Connectivity for BatchFrac

inlet	One material stream for the initial charge; any number of optional material streams for intermediate charges; any number of optional material streams for continuous feeds
outlet	One material stream for final column contents; one material stream for final main accumulator contents; one material stream for the final contents of optional additional accumulators; any number of optional streams for intermediate dump products; any number of optional pseudo-product streams.

Figure A1 : Flowsheet Connectivity for BatchFrac

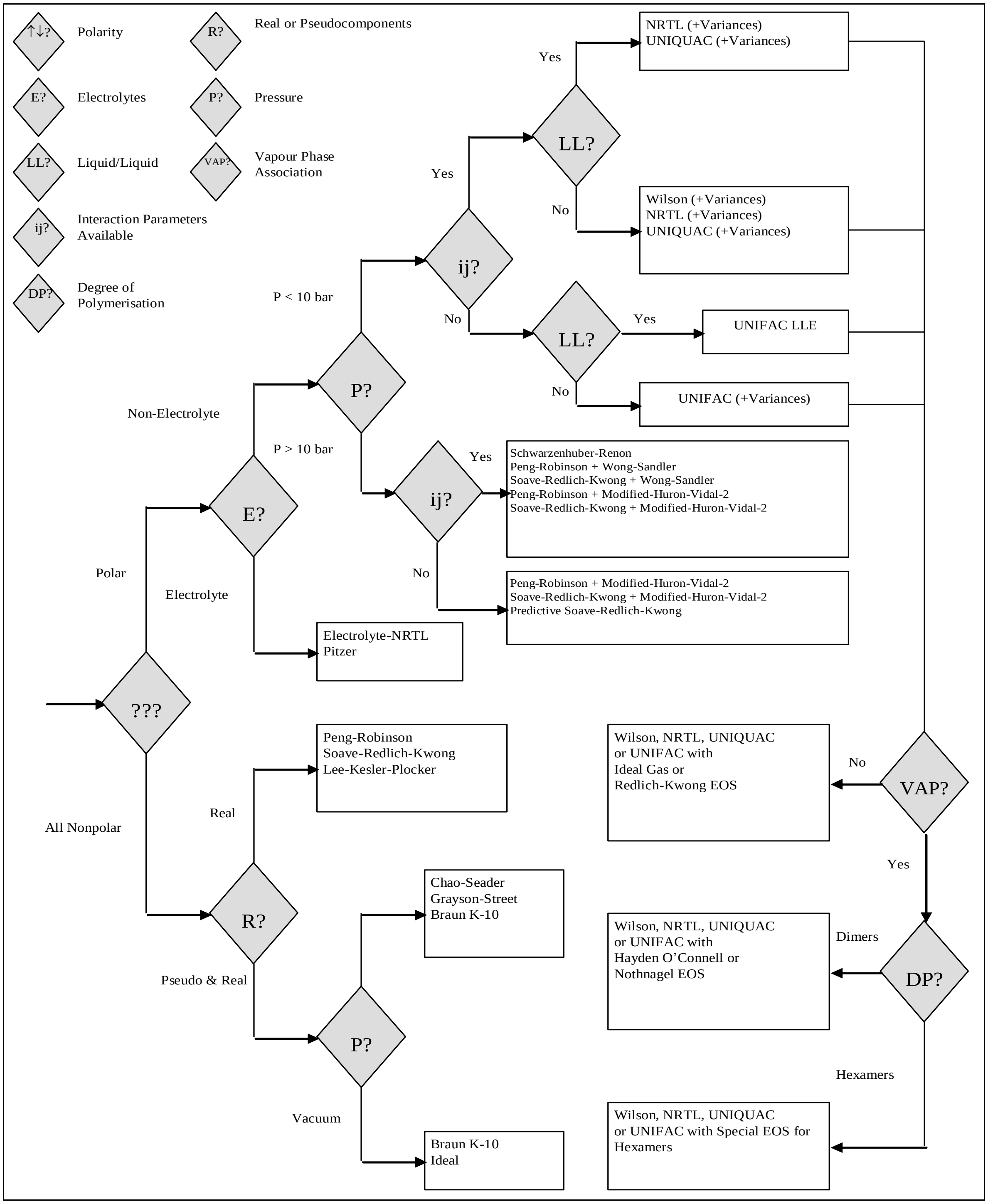


batch distillation

Stream ID		IN	DISTILL	WASTE
Temperature	C	25.0	80.4	88.3
Pressure	bar	1.013	1.013	1.013
Vapor Frac		0.000	0.000	< 0.001
Mole Flow	kmol/hr	1.100	0.700	0.400
Mass Flow	kg/hr	53.316	33.108	20.208
Volume Flow	cum/hr	0.056	0.044	0.019
Enthalpy	MMkcal/hr	-0.082	-0.050	-0.030
Mole Flow	kmol/hr			
ISOPR-01		0.700	0.487	0.213
WATER		0.300	0.213	0.087
SODIU-01		0.100	trace	0.100

Figure A2 : BatchFrac Flowsheet with Steam Table

Table A1 : Property Methods Guidelines



APPENDIX B

Table B (a): Binary Analysis Results of Isoprpanol and Water

PRESURE	MOLEFRAC ISOPR-01	TOTAL TEMP	TOTAL KVL ISOPR-01	TOTAL KVL WATER	LIQUID GAMMA ISOPR-01	LIQUID GAMMA WATER	VAPOR MOLEFRAC ISOPR-01	VAPOR MOLEFRAC WATER	LIQUID MOLEFRAC ISOPR-01	LIQUID MOLEFRAC WATER
bar		C								
1.01325	0	100.0177	28.00484	0.9999959	14.51903	1	0	1	0	1
1.01325	0.025	89.59939	13.33431	0.6837349	10.08414	1.003571	0.3333593	0.6666407	0.025	0.975
1.01325	0.05	85.63417	8.744094	0.5924658	7.690402	1.013148	0.4371319	0.5628681	0.05	0.95
1.01325	0.075	83.69353	6.465004	0.5569165	6.131393	1.027753	0.4848378	0.5151622	0.075	0.925
1.01325	0.1	82.66218	5.099599	0.5444959	5.03636	1.046759	0.5099449	0.4900551	0.1	0.9
1.01325	0.125	82.09705	4.191729	0.544035	4.233182	1.069688	0.5239637	0.4760363	0.125	0.875
1.01325	0.15	81.78422	3.546723	0.5505686	3.626461	1.096149	0.5320128	0.4679872	0.15	0.85
1.01325	0.175	81.60921	3.067048	0.5615219	3.157858	1.125814	0.5367418	0.4632582	0.175	0.825
1.01325	0.2	81.50729	2.698253	0.575421	2.789414	1.1584	0.5396614	0.4603386	0.2	0.8
1.01325	0.225	81.44101	2.407457	0.591366	2.495359	1.193665	0.5416902	0.4583098	0.225	0.775
1.01325	0.25	81.38877	2.17359	0.6087846	2.257637	1.231401	0.5434108	0.4565892	0.25	0.75
1.01325	0.275	81.33847	1.982509	0.6273049	2.063291	1.271424	0.5452037	0.4547963	0.275	0.725
1.01325	0.3	81.28386	1.82436	0.6466831	1.902828	1.313574	0.5473218	0.4526782	0.3	0.7
1.01325	0.325	81.22226	1.692069	0.666762	1.76918	1.357712	0.5499359	0.4500642	0.325	0.675
1.01325	0.35	81.15319	1.580428	0.6874429	1.657003	1.403711	0.5531624	0.4468376	0.35	0.65
1.01325	0.375	81.07748	1.485521	0.7086689	1.562204	1.45146	0.5570823	0.4429177	0.375	0.625
1.01325	0.4	80.99674	1.404355	0.7304129	1.481609	1.500858	0.5617526	0.4382474	0.4	0.6
1.01325	0.425	80.91296	1.334602	0.7526695	1.412733	1.55181	0.5672153	0.4327847	0.425	0.575
1.01325	0.45	80.82831	1.274432	0.7754494	1.353607	1.60423	0.5735029	0.4264971	0.45	0.55

Table B (b): Binary Analysis Results of Isoprpanol and Water (Continue)

PRESURE	MOLEFRAC ISOPR-01	TOTAL TEMP	TOTAL KVL ISOPR-01	TOTAL KVL WATER	LIQUID GAMMA ISOPR-01	LIQUID GAMMA WATER	VAPOR MOLEFRAC ISOPR-01	VAPOR MOLEFRAC WATER	LIQUID MOLEFRAC ISOPR-01	LIQUID MOLEFRAC WATER
bar		C								
1.01325	0.475	80.74503	1.222391	0.7987758	1.302658	1.658036	0.5806427	0.4193573	0.475	0.525
1.01325	0.525	80.59118	1.138233	0.8472057	1.220456	1.769495	0.5975771	0.4024229	0.525	0.475
1.01325	0.55	80.52131	1.104249	0.8722745	1.187332	1.826994	0.6074687	0.3925313	0.55	0.45
1.01325	0.575	80.46511	1.075052	0.8982077	1.15854	1.88558	0.6182532	0.3817468	0.575	0.425
1.01325	0.6	80.42005	1.049927	0.924912	1.133507	1.945172	0.6300269	0.3699731	0.6	0.4
1.01325	0.625	80.38777	1.028441	0.9524485	1.111747	2.005694	0.6428246	0.3571754	0.625	0.375
1.01325	0.65	80.36985	1.010238	0.9808827	1.092853	2.067066	0.6566855	0.3433145	0.65	0.35
1.01325	0.675	80.36775	0.9950182	1.010284	1.07648	2.129206	0.6716541	0.3283459	0.675	0.325
1.01325	0.7	80.38286	0.9825352	1.040726	1.062332	2.192027	0.6877806	0.3122194	0.7	0.3
1.01325	0.725	80.4165	0.9725841	1.072288	1.050157	2.255439	0.7051215	0.2948785	0.725	0.275
1.01325	0.75	80.46993	0.9649966	1.10505	1.039738	2.319347	0.7237398	0.2762602	0.75	0.25
1.01325	0.775	80.54438	0.9596352	1.139101	1.030885	2.383647	0.743706	0.256294	0.775	0.225
1.01325	0.8	80.64101	0.9563892	1.174531	1.023435	2.448234	0.7650982	0.2349018	0.8	0.2
1.01325	0.825	80.76098	0.9551713	1.211438	1.017243	2.512993	0.7880029	0.2119971	0.825	0.175
1.01325	0.85	80.9054	0.9559153	1.249923	1.012182	2.577801	0.8125156	0.1874844	0.85	0.15
1.01325	0.875	81.07537	0.9585731	1.290094	1.008139	2.64253	0.8387414	0.1612586	0.875	0.125
1.01325	0.9	81.27196	0.9631133	1.332062	1.005014	2.707041	0.8667956	0.1332044	0.9	0.1
1.01325	0.925	81.49624	0.96952	1.375945	1.002716	2.771189	0.8968045	0.1031955	0.925	0.075
1.01325	0.95	81.74923	0.9777907	1.421867	1.001162	2.834818	0.9289059	0.0710941	0.95	0.05
1.01325	0.975	82.03195	0.987936	1.469956	1.00028	2.897765	0.96325	0.0367499	0.975	0.025
1.01325	1	82.34594	1	1.520375	1	2.959853	1	0	1	0

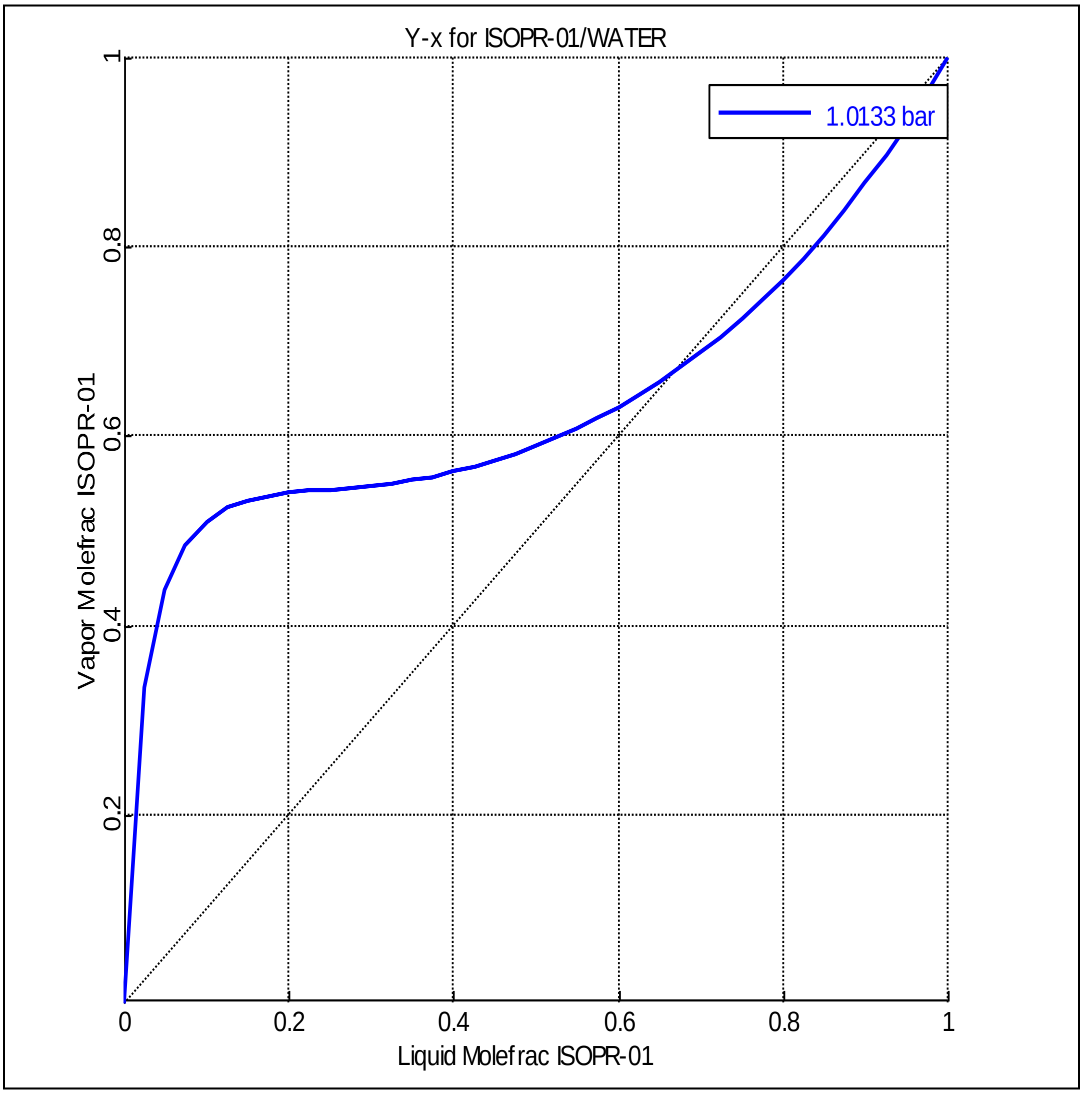


Figure B1 : y-x graph for Isopropanol Mole Fraction

Appendix C

Simulation A: Salt Concentration

No Salt

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	80.4000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.0000	0.7000	0.3000
Mass Flow kg/hr	47.4720	32.6760	14.7960
Volume Flow cum/hr	0.0580	0.0440	0.0200
Enthalpy MMkcal/hr	-0.0740	-0.0500	-0.0220
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4770	0.2230
WATER	0.3000	0.2230	0.0770
SODIU-01	0.0000	0.0000	0.0000

50 mole NaCl

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	84.5000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.0500	0.7000	0.3500
Mass Flow kg/hr	50.3940	32.9140	17.4800
Volume Flow cum/hr	0.0560	0.0440	0.0190
Enthalpy MMkcal/hr	-0.0780	-0.0500	-0.0260
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4820	0.2180
WATER	0.3000	0.2180	0.0820
SODIU-01	0.0500	0.0000	0.0500

100 mole NaCl

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	88.3000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.1000	0.7000	0.4000
Mass Flow kg/hr	53.3160	33.1080	20.2080
Volume Flow cum/hr	0.0560	0.0440	0.0190
Enthalpy MMkcal/hr	-0.0820	-0.0500	-0.0300
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4870	0.2130
WATER	0.3000	0.2130	0.0870
SODIU-01	0.1000	0.0000	0.1000

150 mole NaCl

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	91.8000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.1500	0.7000	0.4500
Mass Flow kg/hr	56.2380	33.2680	22.9700
Volume Flow cum/hr	0.0560	0.0440	0.0200
Enthalpy MMkcal/hr	-0.0860	-0.0500	-0.0340
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4910	0.2090
WATER	0.3000	0.2090	0.0910
SODIU-01	0.1500	0.0000	0.1500

200 mole NaCl

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	95.1000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.2000	0.7000	0.5000
Mass Flow kg/hr	59.1600	33.4020	25.7580
Volume Flow cum/hr	0.0570	0.0450	0.0220
Enthalpy MMkcal/hr	-0.0900	-0.0500	-0.0380
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4940	0.2060
WATER	0.3000	0.2060	0.0940
SODIU-01	0.2000	0.0000	0.2000

250 mole NaCl

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	98.1000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.2500	0.7000	0.5500
Mass Flow kg/hr	62.0820	33.5140	28.5690
Volume Flow cum/hr	0.0580	0.0450	0.0230
Enthalpy MMkcal/hr	-0.0950	-0.0500	-0.0420
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4970	0.2030
WATER	0.3000	0.2030	0.0970
SODIU-01	0.2500	0.0000	0.2500

300 mole NaCl

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	101.0000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	33.6100	31.3950
Volume Flow cum/hr	0.0600	0.0450	0.0250
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4990	0.2010
WATER	0.3000	0.2010	0.0990
SODIU-01	0.3000	0.0000	0.3000

Simulation B : Time Contraints

Time : 0.5 hours

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	91.0000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.3500	0.9500
Mass Flow kg/hr	65.0040	16.7220	48.2820
Volume Flow cum/hr	0.0600	0.0220	0.0430
Enthalpy MMkcal/hr	-0.0990	-0.0250	-0.0710
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.2480	0.4520
WATER	0.3000	0.1020	0.1980
SODIU-01	0.3000	0.0000	0.3000

Time : 0.75 hours

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	94.4000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.5250	0.7750
Mass Flow kg/hr	65.0040	25.1530	39.8520
Volume Flow cum/hr	0.0600	0.0340	0.0340
Enthalpy MMkcal/hr	-0.0990	-0.0380	-0.0590
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.3730	0.3270
WATER	0.3000	0.1520	0.1480
SODIU-01	0.3000	0.0000	0.3000

Time : 1.00 hours

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	101.0000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	33.6100	31.3950
Volume Flow cum/hr	0.0600	0.0450	0.0250
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4990	0.2010
WATER	0.3000	0.2010	0.0990
SODIU-01	0.3000	0.0000	0.3000

Time : 1.25 hours

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	119.9000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.8750	0.4250
Mass Flow kg/hr	65.0040	42.0290	22.9750
Volume Flow cum/hr	0.0600	0.0560	0.0170
Enthalpy MMkcal/hr	-0.0990	-0.0630	-0.0340
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.6240	0.0760
WATER	0.3000	0.2510	0.0490
SODIU-01	0.3000	0.0000	0.3000

Time : 1.50 hours

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	1077.4000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0640
Mole Flow kmol/hr	1.3000	0.9800	0.3200
Mass Flow kg/hr	65.0040	46.8980	18.1060
Volume Flow cum/hr	0.0600	0.0630	2.2950
Enthalpy MMkcal/hr	-0.0990	-0.0700	-0.0230
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.6950	0.0050
WATER	0.3000	0.2850	0.0150
SODIU-01	0.3000	0.0000	0.3000

Simulation C :Reflux Ratio

Reflux ratio : 0.1

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	101.2000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	34.1550	30.8500
Volume Flow cum/hr	0.0600	0.0460	0.0240
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.5120	0.1880
WATER	0.3000	0.1880	0.1120
SODIU-01	0.3000	0.0000	0.3000

Reflux ratio : 0.5

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	101.1000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	33.9200	31.0850
Volume Flow cum/hr	0.0600	0.0450	0.0240
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.5060	0.1940
WATER	0.3000	0.1940	0.1060
SODIU-01	0.3000	0.0000	0.3000

Reflux ratio : 1.0

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	101.0000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	33.6100	31.3950
Volume Flow cum/hr	0.0600	0.0450	0.0250
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4990	0.2010
WATER	0.3000	0.2010	0.0990
SODIU-01	0.3000	0.0000	0.3000

Reflux ratio : 5.0

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	100.8000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	32.4390	32.5650
Volume Flow cum/hr	0.0600	0.0430	0.0260
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4710	0.2290
WATER	0.3000	0.2290	0.0710
SODIU-01	0.3000	0.0000	0.3000

Reflux ratio : 10.0

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	100.7000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	32.3250	32.6800
Volume Flow cum/hr	0.0600	0.0430	0.0260
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4680	0.2320
WATER	0.3000	0.2320	0.0680
SODIU-01	0.3000	0.0000	0.3000

Reflux ratio : 15.0 and 20.0

	IN	DISTILL	WASTE
Temperature C	25.0000	80.4000	100.7000
Pressure bar	1.0130	1.0130	1.0130
Vapor Frac	0.0000	0.0000	0.0000
Mole Flow kmol/hr	1.3000	0.7000	0.6000
Mass Flow kg/hr	65.0040	32.3020	32.7020
Volume Flow cum/hr	0.0600	0.0430	0.0260
Enthalpy MMkcal/hr	-0.0990	-0.0500	-0.0460
Mole Flow kmol/hr			
ISOPR-01	0.7000	0.4680	0.2320
WATER	0.3000	0.2320	0.0680
SODIU-01	0.3000	0.0000	0.3000